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# 30<sup>TH</sup> YOUNG INVESTIGATORS' SEMINAR ON ANALYTICAL CHEMISTRY

## BOOK OF ABSTRACTS

Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia  
 June 30<sup>th</sup> - July 3<sup>rd</sup> 2025



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Chemistry (YISAC 2025)  
June 30<sup>th</sup> – July 3<sup>rd</sup>, Ljubljana, Slovenia*

## YISAC 2025 General Information

### Book of abstracts

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### Information

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### Location and date

The conference will be held in Lecture room 2, located on the 1st floor of the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

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## **Foreword by the Organizing committee**

The Yisac 2025 conference returns to Ljubljana, where the idea and concept of Yisac was "born" and presented first to the Slovenian-Austrian analytical community by Prof. Dr. Kurt Kalcher and Dr. Božidar Ogorevc. Both will be speaking to us in the next few lines and will be celebrating the 30<sup>th</sup> anniversary of Yisac with us. For the two organizers - the Faculty of Chemistry and Chemical Technology of the University of Ljubljana and the National Institute of Chemistry - this is a great honour and a special privilege. Above all, because the basic idea of Yisac is still unchanged and offers young researchers in the field of analytical chemistry one of the first opportunities to give lectures, get in touch with other students, professors and institutions and exchange their research ideas. Yisac is more than that, because it also allows students to discover other cultures and traditions that are characteristic for the country's organisation. And so, for three decades, Yisac has brought together several generations of students, professors, several countries in the region, some of us in the role of students, mentors and organizers. One of the »side effects« of Yisac is that fellow analysts have become friends, that Yisac has become an unforgettable experience for many and that a multitude of anecdotes, pictures and memories have been created. What can we add? An old Slovenian proverb says: "You don't change a winning horse," and so may Yisac live on for at least the next decades, uniting and enriching both the research and the human aspects. Finally, a special thanks to all the members of the Yisac 2025 organising committee and a remembrance of all our fellow professors who are sadly no longer with us.

Welcome to Ljubljana and best regards!

Yisac 2025 Organizing Committee



# *30<sup>th</sup> Young Investigators' Seminar on Analytical Chemistry (YISAC 2025)*

*June 30<sup>th</sup> – July 3<sup>rd</sup>, Ljubljana, Slovenia*

## **Foreword by Dr. Božidar Ogorevc**

It all began one sunny afternoon, during the visit of Prof. Kurt Kalcher to Ljubljana, in spring 1993 with a discussion between Prof. Kalcher and me about how to attract and stimulate young investigators (mostly postgraduates - PhD students and post-docs) and help them slide into scientific life, with an emphasis on presenting and discussing their research ideas and experimental results in front of the corresponding scientific community.

At that time, in fact, we all, at the National Institute of Chemistry (NIC) and the University of Ljubljana (ULJ) as well as at Karl-Franzens University Graz (KFUG), were already organizing student seminars, but because our analytical-chemistry departments were relatively small, these seminars were irregular and limited in scope. The idea of Kurt and I was therefore to combine such seminars in order to reach a critical mass of students and supervisors that would enable a broader range of presentations and more fruitful discussions.

And so, the very first YISAC meeting - the name I proposed as an acronym for *Young Investigators' Seminar on Analytical Chemistry*—was organized in February 1994 at the National Institute of Chemistry in Ljubljana. The total number of participants was 28, and the number of young investigators giving their oral presentations was 17 (eight from KFUG, six from NIC and three from ULJ).

At this point it is worth stating, in short, the essential rules of YISAC that have been more or less faithfully followed throughout all 30 years of its history until today. These are: (i) the seminar fees must not be charged, (ii) the presentations are all exclusively in oral form, (iii) the seminar length is two days, excluding arrivals and departures, (iv) the official language is English, (v) the participants are composed of young investigators as presenters and their supervisors (optional), (vi) the organizers should keep the seminar expenses (accommodation, etc.) as low as possible, (vii) a presentation slot time should be 15 min + 5 min for discussion, (viii) if the number of applications exceeds capacity of a meeting, the organizers should charge the scientific committee to reduce the number via abstract selection.

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All in all, the fact that the YISAC meeting series has run regularly for the past 32 years - paused only by a two-year gap during the COVID-19 pandemic - is compelling proof of the necessity and usefulness of such scientific events. This is also evident from the number of oral presentations, which after the early YISAC meetings steadily increased to reach the maximum possible of about 40 - 45 presentations per meeting. The growth is also evident from the increasing number of participating institutes and universities as well as the total number of all participants, reaching its peak at YISAC 2005 in Sarajevo with 93 total participants.

Finally, we now celebrate the 30th edition of YISAC, again in Ljubljana, led by a new generation of senior scientists from NIC and ULJ.

As a co-founder of the YISAC idea and meetings, I am very proud not only of the meeting's successful history but, above all, of the young investigators, organizers and supervisors who have enthusiastically participated and contributed their part to the scientific richness of the YISAC idea and life throughout the past years and, I hope, will continue to do so in the future!

Božidar Ogorevc

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## **Foreword by Prof. Dr. Kurt Kalcher**

This year we are celebrating the 30<sup>th</sup> anniversary of YISAC, or, just to be more precise, the 30<sup>th</sup> repetition of this event with a two years' break during the COVID 19 pandemic.

As a seminar without conference fees or reliable or fixed funding except sponsors (by the way, many thanks to all institutions which have so far contributed financially in order to make organization of the event significantly easier) its longevity seems remarkable. Apart from bringing young people together there are probably more fundamental reasons for this effect:

First, I think, there is a need for such scientific meeting with respect to preparing and educating advanced students to present their scientific data and opinions at an international level; regardless if staying as researcher at the university or joining a company in the future, it is essential to present projects, concepts, data, results and future aspects clearly and convincingly. Whereas the atmosphere at big international conferences is often cool and, occasionally maybe even frosty, YISAC offers a family-like, warm and soft climate.

Second, scientific events and meetings are ideal opportunities for students to increase the own horizon scientifically and pragmatically, to see and learn new ideas, critics, new interpretations of data and facts, new research concepts on the one hand, but also different types of how to present data and scientific results on the other.

If we look at the organizing and participating universities and research institutions over the 31 years, YISAC started as a bilateral seminar alternating between Ljubljana and Graz; soon we realized that there was enormous interest also from other universities with whom we had close research contact, in particular Pardubice, Venice, Krakow and Bratislava; as a consequence, the number of international participants was increasing from year to year. Eventually, Bosnia and Hercegovina, Croatia, Serbia, and Poland (Lodz) joined with participants as well as organizers of the event. At this point it is worth to mention that the CEEPUS project CZ-0212 (headed by Prof. Radovan Metelka, who is now also one managing head of YISAC) has been a very valuable structure to facilitate and support participation.

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Thus, I guess, YISAC is also a good probe and a perfect mirror for the scientific landscape of analytical chemistry in central and eastern Europe.

From my experience, I would also like to give a message to take home to all students: Don't be disappointed if your lecture is not perfect! You take profit only when you realize that some topics you could have done better in your presentations. We, the supervisors, love imperfect performances at YISAC, because this gives you an excellent opportunity to learn and improve! Another fact: the more often you participate in YISAC, the better you get!

Last but not least I would like to commemorate a few outstanding late colleagues whom we must respectfully thank for their valuable contributions: Prof. Jan Mocak from Bratislava, Prof. Karel Vytras from the University of Pardubice, and Prof. Valeria Guszvany from the University of Novi Sad. They are living on in our memory and heart as well as in their former students, who are nowadays the backbone of supervisors of the seminar.

Finally, I would like to thank the current organizers, the University of Ljubljana and the National Institute of Chemistry, for hosting the 30<sup>th</sup> YISAC jubilee this year!

Good success to all students for an exciting presentation of scientific projects and results!

And may YISAC still survive at least 30 more years or even longer!

Kurt Kalcher, co-founder of YISAC



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## YISAC 2025 Organizing Committee

*Faculty of Chemistry and Chemical Technology, University of  
Ljubljana, Ljubljana, Slovenia*

Mitja Kolar

Gregor Marolt

Helena Prosen

Maksimiljan Dekleva

Ema Gričar

Jernej Imperl

Aleksander Kravos

Tjaša Rijavec

*National Institute of Chemistry, Ljubljana, Slovenia*

Samo Hočevar

Božidar Ogorevc

Martin Šala

Nikola Tasić

Kristijan Vidović

Antea Hrepić

Mitja Koderman

Alnilan Maria Barros Lobato

# Scientific and social programme of YISAC 2025

**MONDAY, June 30<sup>th</sup>, 2025**

LOCATION: Lecture room 2, located on the 1<sup>st</sup> floor of the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

TIME

**19:00**

**Registration of participants  
Get-together party**

**TUESDAY, July 1<sup>st</sup>, 2025**

LOCATION: Lecture room 2, located on the 1<sup>st</sup> floor of the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

**9:00**

**Opening of YISAC 2025**

**9:30**

**GRZEGORZ KOWALSKI**

*Activation and modification of 3D-printed WE, RE and CE used for electroanalysis of paracetamol*

**9:45**

**ANDRZEJ KREMPIŃSKI**

*Electroanalytical studies of Brilliant Blue G at the electrified water-organogel interface*

**10:00**

**MARYIA-MAZHENA DZEMIDOVICH**

*Thin Organic Film Electrodes as a Promising Tool for The Investigation of The Anticancer Drug Docetaxel*

**10:15**

**SANDRA CHMIEL**

*Electroanalytical Determination of Penoxsulam on a Boron-Doped Diamond Electrode*

**10:30**

**MAKSIMILJAN DEKLEVA**

*Amino-acid Functionalized Mesoporous Silica Thin Film: A Promising Platform for Electrochemical Capture and Sensing of Polystyrene Nanoplastics*

**SESSION I**

**Electrochemical Methods**

*Moderators: Anilan Cristina Barros Lobato, Tijana Mutić*

# Scientific and social programme of YISAC 2025

10:45	Coffee break	
11:15	<b>AMINA PAŠOVIĆ</b> <i>Toward Smart Battery Diagnostics: Printed Sensors for Real-Time Monitoring of Transition Metal Dissolution</i>	<div>SESSION I</div> <div>Electrochemical Methods</div> <div>Moderators: Mohanraj Sadasivam, Aleksandar Mijajilović</div>
11:30	<b>ANJA SIHER</b> <i>Enhancement of cobalt hydroxide electrochemical performance through morphology control and composite formation</i>	
11:45	<b>BARBARA REPIČ</b> <i>Post-Deposition Treatment of Graphite-Based Working Electrode</i>	
12:00	<b>JOSIPA DUGEČ</b> <i>Mechanistic Insights into the Electrochemical (Ir)Reversibility of Gallic Acid at Carbon Nanotube Electrodes</i>	
12:15	<b>BARTŁOMIEJ HURNY</b> <i>Electroanalytical studies with electrode printed using direct ink writing</i>	
12:30	<b>SÁRA HERMOCHOVÁ</b> <i>Visualization of Latent Fingerprint with Poly(Neutral Red) and Study of its pH Dependence</i>	
12:45	Lunch break	
13:45	<b>BRANKA RUŽIČIĆ</b> <i>Antioxidant and antimicrobial properties of blackberry extract</i>	<div>SESSION II</div> <div>Chromatography</div> <div>Moderators: Tia Kralj, Špela Pok</div>
14:00	<b>NIKA MARIJA MURENC</b> <i>Deep Eutectic Solvents for Efficient and Sustainable Extraction of Bioactive Compounds from the Peels of Selected Slovenian apple varieties</i>	

# Scientific and social programme of YISAC 2025

<b>14:15</b>	<b>EMMA PAOLIN</b> <i>Application of a multidisciplinary approach combining sensory and TD-GC-MS-O analysis for the characterization of VOCs emitted by ancient Egyptian mummified bodies</i>	<b>SESSION II</b> <b>Chromatography</b> <i>Moderators: Tia Kralj, Špela Pok</i>
<b>14:30</b>	<b>ALEKSANDER KRAVOS</b> <i>How will water contaminants dissipate in marine environment? Sorption versus photodegradation</i>	
<b>14:45</b>	<b>Coffee break</b>	
<b>15:00</b>	<b>ANA ŠIJANEC</b> <i>Phospholipid Determination in Lecithin: A Standard-free Approach</i>	<b>SESSION II</b> <b>Chromatography</b> <i>Moderators: Tia Kralj, Špela Pok</i>
<b>15:15</b>	<b>KAJA GLIHA</b> <i>Use of deep eutectic solvents for the analysis of white mulberry (<i>Morus alba</i>) samples</i>	
<b>15:30</b>	<b>MATEVŽ POLAK</b> <i>Method development for the chromatographic separation and extraction of organic UV filters from seawater samples</i>	
<b>15:45</b>	<b>VENO JAŠA GRUJIĆ</b> <i>Pigment analysis in the alga <i>Haematococcus pluvialis</i></i>	
<b>16:00</b>	<b>Leisure time</b>	
<b>19:00</b>	<b>Supervisors' dinner</b> <b>Gostilna pri Žabarju</b> <b>Viška cesta 48, 1000 Ljubljana</b>	



# Scientific and social programme of YISAC 2025

**WEDNESDAY, July 2<sup>nd</sup>, 2025**

LOCATION: Lecture room 2, located on the 1<sup>st</sup> floor of the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

TIME		<b>SESSION III</b> <b>Electrochemical Sensors</b> <i>Moderators: Maksimilijan Dekleva, Josipa Dugeč</i>
<b>9:00</b>	<b>ALNILAN CRISTINA BARROS LOBATO</b> <i>Affinity-based Strategies for Electrochemical Detection of Viruses and Viroids</i>	
<b>9:15</b>	<b>GABRIELA SATORA</b> <i>Analytical characteristic of a biosensor based on Horseradish Peroxidase for electrochemical determination of estrogens</i>	
<b>9:30</b>	<b>TIJANA MUTIĆ</b> <i>Design and synthesis of neodymium-oxide for effective electrochemical detection of hazardous pesticide carbofuran</i>	
<b>9:45</b>	<b>MOHANRAJ SADASIVAM</b> <i>Label-free electrochemical immunosensor based on gelatin-CeO<sub>2</sub> nanocomposite for sensitive detection of insulin</i>	
<b>10:00</b>	<b>NINA TEŽAK</b> <i>Preparation and application of a molecularly imprinted polymer for indirect electrochemical sensing of acetamiprid</i>	
<b>10:15</b>	<b>EVA POSPÍŠILOVÁ</b> <i>Electrochemical Sensors for the Forensic Detection of New Psychoactive Substances</i>	
<b>10:30</b>	<b>ALEKSANDAR MIJAJLOVIĆ</b> <i>Lanthan's touch: designing La-Dy<sub>2</sub>O<sub>3</sub>/MWCNT sensor for electrochemical detection of metal in environmental and biological fluids samples</i>	
<b>10:45</b>	<b>MITJA KODERMAN</b> <i>Electrochemical Detection of PSA Biomarker Using a Ruthenium-Decorated Titanium Oxynitride Nanocomposite-Based Immunosensor</i>	

# Scientific and social programme of YISAC 2025

11:00	Coffee break	
11:30	<b>LAURA MILIŠIĆ</b> <i>Surface Characterization of ZnM<sup>3+</sup> Oxide Catalyst Supports by Physisorption and Chemisorption Methods</i>	<div>SESSION IV</div> <div>Optical and Surface Methods, Biochemistry</div> <div>Moderators: Ibrahim Elrefaey, Sára Hermochová</div>
11:45	<b>DOMINIK NOVÁK</b> <i>Using Multiparametric Surface Plasmon Resonance to determine the affinity of interaction between antigen and antibody</i>	
12:00	<b>ŠÁRKA BEDNÁŘOVÁ</b> <i>Immobilisation of Tyrosine Protein Kinase Src on Magnetic Microparticles for Myelin Basic Protein Phosphorylation</i>	
12:15	<b>MICHAELA BÁRTOVÁ</b> <i>Biomimetic Copper Complexes</i>	
12:30	<b>PETR RUDOLF</b> <i>Systematic development of LA-ICP-MS method for elemental analysis in organic-rich liquid samples</i>	
12:45	<b>KAROLÍNA KYNCLOVÁ</b> <i>Western Blot assay for Confirmation of Changes in CD44 Receptor Expression in Irradiated Lung-Derived Cells Treated with Hyaluronic Acid Nanoparticles</i>	
13:00	Lunch break	
14:00	<b>IBRAHIM ELREFAEY</b> <i>Investigating the Influence of Several Environmental Stressors on the Degradation of Non-weighted and Weighted Silk</i>	<div>SESSION V</div> <div>Environmental</div>
14:15	<b>ŠPELA POK</b> <i>Acidic emissions from PVC: A potential problem for museums and galleries</i>	

# Scientific and social programme of YISAC 2025

14:30	<b>TIA KRALJ</b> <i>Fungal Biosorption and Electrochemical Detection of Polystyrene Nanoplastics: Advancing Sustainable Remediation and On-Site Monitoring</i>	<b>SESSION V</b> <b>Environmental Analysis</b> <i>Moderators: Aleksander Kravos, Petr Rudolf</i>
14:45	<b>RASIM OMANOVIĆ</b> <i>Green SiO<sub>2</sub> surface modifications using ethanol extract from valorized fruit waste: enhancing methylene blue adsorption for sustainable water treatment</i>	
15:00	<b>AMAR KARADŽA</b> <i>Comparison of three different conifer species as bioindicators for the assessment of air pollution with metals</i>	
15:15	Coffee break	
15:30	<b>JERNEJ IMPERL</b> <i>Slovenian Dolomites as a Potential Source of Magnesium</i>	<b>SESSION V</b> <b>Environmental Analysis</b> <i>Moderators: Dominik Novák, Emma Paolin</i>
15:45	<b>ANNA WASILEWSKA</b> <i>To control or not to control? Optimization of the process of synthesis of metallic nanoparticles produced by green chemistry</i>	
16:00	<b>NEŽA KRALJ</b> <i>Study of chromophore-containing water-insoluble organic carbon in atmospheric aerosol particles</i>	
16:15	<b>IVAN KONJEVIĆ</b> <i>Electrochemical Impedance Spectrometry for Measuring Surface Tension Decrease on a Mercury Electrode</i>	
16:30	Closing of YISAC 2025	
20:00	Conference dinner Nebo Show Restaurant Tomšičeva ulica 2, 1000 Ljubljana	

# Scientific and social programme of YISAC 2025

**THURSDAY, July 3<sup>rd</sup>, 2025**

LOCATION: National Institute of Chemistry, Hajdrihova ulica 19, Ljubljana, Slovenia

TIME

**from  
10:00**

**City tour**  
National Institute of Chemistry, Ljubljana old town,  
boat ride on Ljubljanica river



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# SESSION I

## **Electrochemical Methods**

**Moderators:** *Alnilan Cristina Barros Lobato, Tijana Mutić, Mohanraj  
Sadasivam, Aleksandar Mijajlović*

## Activation and modification of 3D-printed WE, RE and CE used for electroanalysis of paracetamol

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Grzegorz Kowalski<sup>1,2\*</sup>, Łukasz Póltorak<sup>1</sup>, Karolina Kwaczyński<sup>1</sup>

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In recent years, 3D printing has become an essential tool in electrochemical laboratories. Among various techniques, fused deposition modeling (FDM) stands out as the simplest, most cost-effective, and widely accessible method, playing a key role in this field. Its broad applicability stems from several advantages: (i) it allows rapid prototyping, (ii) the costs of design creation and exploitation are low, (iii) the choice of printable materials is wide, and (iv) the printouts can take complex shapes [1]. FDM has been successfully implemented to fabricate various components of electrochemical sensors: working, reference and/or auxiliary electrodes [2], measurement cells [3], including complex shapes supporting liquid-liquid interfaces [4].

The presented research aimed to produce an electroanalytical platform as an alternative to the commercially available solid electrodes. The components of the sensor – holder, cell and electrodes were 3D printed using FDM technology. Electrodes were made from a commercially available conductive filament being a composite of poly(lactic acid) (PLA) and carbon black. Other components were made out of PLA. Due to the unsatisfactory electrochemical properties of the resulting printouts, they were subjected to an activation process. Characterization of the developed sensor was carried out using various techniques: cyclic voltammetry (in the presence of a redox probe – ferrocenemethanol), electrochemical impedance spectroscopy, scanning electron microscopy and 3D optical profilometry. The fabricated system was then used for electrochemical sensing of paracetamol, using differential-pulse voltammetry.

*The research was supported by funding from the National Science Centre (NCN) within the SONATA project (UMO-2022/47/D/ST5/02523).*

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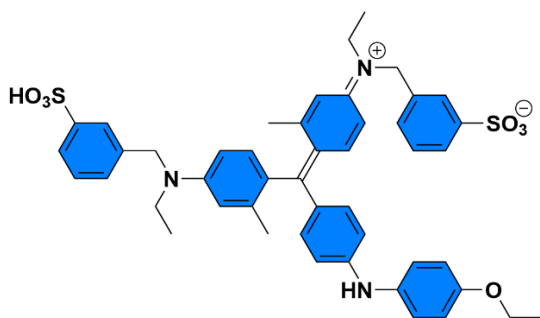
## Electroanalytical studies of Brilliant Blue G at the electrified water-organogel interface

Andrzej Krempiński<sup>1,2\*</sup>, Emilia Powalka<sup>2</sup>, Łukasz Półtorak<sup>2</sup>, Konrad Rudnicki<sup>2</sup>

Dyes are chemical compounds widely used across various fields. They play a crucial role in textile dyeing [1], analytical chemistry [2], and food coloring [3]. One such dye is Brilliant Blue G (BBG) (**Fig. 1**), an anionic dye commonly utilized for protein staining in electrophoresis and as a marker in biological research [4]. As the name suggests, its aqueous solutions absorb light in the range of 450 to 495 nm.

This study aimed to explore the electrochemical behavior of BBG at the macroscopic and miniaturized ITIES (interface between two immiscible electrolyte solutions) system. The latter was a formulation consisting of an aqueous electrolyte and an organic solution gelled using poly(vinyl chloride) (PVC). During the measurement involving microscopic ITIES, the gelled phase was paced in the plastic tip connected to a syringe with a threaded piston (used to control

the ITIES positions). Initial experiments aiming at ITIES characterization were performed using tetraethylammonium cation (TEA<sup>+</sup>) as a model ion to optimize detection parameters. Subsequently, the electrochemical detection of BBG was investigated by analyzing its interfacial transfer properties. The findings of this study may contribute to the development of novel dye detection methods at soft liquid interfaces.



**Figure 1.** Chemical structure of BBG.

**Acknowledgements:** This project was financially supported by the National Science Center (NCN) in Krakow, Poland (Grant no. UMO-2022/45/B/ST4/0218).

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## Thin Organic Film Electrodes as a Promising Tool for The Investigation of The Anticancer Drug Docetaxel

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Valentin Mirceski<sup>1,3</sup>, Mariola Brycht<sup>1</sup>

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Electrochemical techniques constitute a powerful and reliable tool for establishing a robust platform to investigate physicochemical traits of anticancer agents – most notably their redox behavior and lipophilicity. Among them, thin organic film electrodes (TOFEs) have emerged as promising tools for studying charge transport (electron and ion) across liquid | liquid interfaces, redox behavior within a thin lipophilic membrane, and specific interactions at the liquid | liquid interfaces. In a typical TOFE system, electrochemical reactions occur simultaneously at two interfaces: the electrode | membrane, where redox transformations of the mediator take place, and the membrane | aqueous solution, where ion transfer between phases occurs. Despite their simplicity and significant analytical potential [1,2], TOFE systems are rarely used, particularly in the analysis of anticancer drugs.

In this study, the TOFE system was optimized, including the selection of the composition of both the organic and aqueous phases, as well as the choice of substrate for depositing the thin organic film. The optimized TOFE setup was then applied for the indirect investigation of docetaxel (DTX), an anticancer drug from the mitosis inhibitors group, whose direct electrochemical analysis is not feasible due to its high oxidation potential at the solid electrode. Electrochemical studies using cyclic voltammetry and square-wave voltammetry demonstrated that the presence of DTX significantly suppresses the signal of the redox marker.

The system exhibits a linear analytical response in the DTX concentration range of 10.0–100.0  $\mu\text{mol L}^{-1}$ , satisfactory sensitivity, and low limits of detection and quantification. The results confirm that the TOFE system is a promising tool for the indirect determination of anticancer drugs and for studying their interactions under conditions that mimic biological environments.

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## Electroanalytical Determination of Penoxsulam on a Boron-Doped Diamond Electrode

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Boron-doped diamond electrode (BDDE) has become increasingly popular in electrochemical research due to its exceptional properties, such as a wide potential window, low and stable background current, excellent chemical and mechanical stability, and resistance to surface fouling [1]. These advantages make BDDE highly suitable for the detection of various environmental contaminants, including pesticides, which pose a growing threat to soil and water quality. In particular, the increasing environmental burden caused by widespread pesticide usage highlights the need for sensitive and selective detection methods.

Modern agriculture extensively uses plant protection products, including herbicides and fungicides, which, despite their effectiveness, pose significant environmental risks due to soil and water contamination. Consequently, the development of sensitive analytical methods for detecting these compounds has become increasingly important. One such compound is penoxsulam, a triazolopyrimidine herbicide that inhibits acetolactate synthase and effectively suppresses weed growth in cereal crops [2], whose usage has seen expanding in recent years.

In this study, the electrochemical behavior of penoxsulam was investigated by cyclic voltammetry (CV) using a BDDE. Its electrochemical activity was examined over a wide pH range (2.0–12.0) in Britton-Robinson buffer as the supporting electrolyte. CV experiments revealed that penoxsulam is electrochemically active across the entire tested pH range, with the highest oxidation signal observed at pH 2.0. The electrode process characteristics and the type of current involved were also characterized. Further studies confirmed an irreversible, diffusion-controlled electrode process of penoxsulam on the BDDE under optimal conditions. Additionally, a quantitative determination method was developed employing differential pulse voltammetry (DPV). For quantitative analysis, both pH of BRB and DPV operating parameters were optimized. A calibration curve was established, and key validation parameters, including the limit of detection, limit of quantification, sensitivity, accuracy and precision, were determined. Potential interferences from common coexisting substances (ions and pesticides) were evaluated, and the successful applicability of the developed method to environmental sample analysis was demonstrated.

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## Amino-acid Functionalized Mesoporous Silica Thin Film: A Promising Platform for Electrochemical Capture and Sensing of Polystyrene Nanoplastics

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Plastics, as persistent environmental contaminants, can degrade through a combination of physical, chemical, and biological processes into smaller fragments known as nanoplastics (NPs). Due to their nanoscale dimensions, NPs are capable of penetrating biological membranes and cellular structures, posing potential risks to both environmental and human health. However, their detection and monitoring present considerable technical challenges, typically requiring time-intensive procedures and sophisticated instrumentation [1]. Herein, we report for the first time a novel sensing platform based on a mesoporous silica thin film functionalized with proline for the electrochemical capture and detection of polystyrene NPs (PSNPs). Initially, a mesoporous silica thin film was deposited onto a screen-printed gold electrode via electrochemically assisted self-assembly [2]. Subsequently, epoxide functional groups were introduced onto the surface, followed by immersion of the modified electrodes in a proline solution. The modification process was systematically monitored and characterized using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

The sensing mechanism relies on two principal effects: the affinity of the immobilized amino acid residues for PSNPs [3], and the application of a positive potential to enhance the electrostatic attraction of the negatively charged PSNPs (in 0.1 M KCl) toward the electrode surface. The combined effect led to a measurable decrease in CV current responses and an increase in charge-transfer resistance, as measured by EIS. Optimization of the accumulation potential and accumulation time resulted in a 25–30% decrease in relative current intensity. Given that NPs of different sizes exhibit distinct physicochemical properties and toxicological profiles, the influence of NPs size on sensor performance was evaluated. A clear trend emerged, wherein smaller particles (6.1 nm) produced a more pronounced current decrease compared to larger ones (25.6 nm). A calibration curve was established using CV measurements.

This study represents a significant advancement in the electrochemical capture and sensing of PSNPs and provides a foundation for future development, particularly toward on-site monitoring of polystyrene and other nanoplastic materials in aquatic environments.

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## Toward Smart Battery Diagnostics: Printed Sensors for Real-Time Monitoring of Transition Metal Dissolution

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Lithium-ion batteries (LIBs) play a crucial role in modern energy storage systems, yet their lifespan and capacity are significantly affected by various degradation mechanisms. One of the most impactful degradation processes is the dissolution of transition metals from the cathode active material into the electrolyte, which leads to performance decay and reduced cycle life. For instance, manganese (Mn) dissolution from  $\text{LiMn}_2\text{O}_4$  (LMO) cathodes and nickel (Ni) dissolution from NMC ( $\text{LiNi}_x\text{Mn}_x\text{Co}_x\text{O}_2$ ) cathodes are critical issues that compromise battery longevity.

To mitigate these effects, monitoring these degradation mechanisms in real-time could enable proactive measures to extend battery life. In this study, we propose an integrated sensor setup within the cell to detect dissolved transition metals. Previous research has demonstrated the feasibility of detecting Mn dissolution from LMO cathodes using such sensors. The next step involves quantifying Mn concentrations using a printed sensor, including a functional sensing layer. Furthermore, we explore the adaptability of this sensor for detecting other transition metals, such as Ni from NMC cathodes, by incorporating a Ni-selective sensing layer.

This approach offers a promising pathway for real-time degradation monitoring, ultimately contributing to enhanced battery management and prolonged cycle life.

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## Enhancement of cobalt hydroxide electrochemical performance through morphology control and composite formation

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First-row transition metal layered double hydroxides (LDH), such as  $\text{Co}(\text{OH})_2$ , have been widely studied due to their pseudocapacitive properties. These materials are characterized by fast, reversible redox reactions, multiple electron transfer ability, and the presence of various oxidation states, all of which enhance their energy storage performance [1]. The layered structure of  $\text{Co}(\text{OH})_2$ , with cobalt cations embedded within hydroxide sheets, facilitates efficient anion exchange, thereby increasing the accessibility of  $\text{Co}^{2+}$  sites to electrolyte ions [2]. Despite these advantages, pseudocapacitors are limited by low capacitance, poor electrical conductivity, and restricted voltage windows. To overcome these limitations and enhance material performance, improvements in morphology, pore size distribution, mass transport pathways, and redox site exposure are needed.

Understanding the morphological and structural properties of materials is essential for analyzing their diffusive behavior, as they significantly influence ion diffusion. For cobalt hydroxide, the hexagonal hydrotalcite-like structure, characterized by lower skeletal density and larger basal plane spacing, outperforms the monoclinic cobalt carbonate hydroxide structure, achieving an order of magnitude higher electrochemical capacitance. Furthermore, the hydrotalcite structure can be utilized for nanocomposite formation. Using  $\text{CoAl-LDH}$ , it is possible to increase capacitance by expanding the interlayer spacing through organic anion intercalation [3]. Utilizing ion exchange, we form a nanocomposite with gold nanoparticles incorporated in the space between hydroxide layers, preserving the LDH structure while further enhancing capacitance. The resulting morphologies and structural variations significantly influence the electrochemical behavior of the material, which we observe through *in-situ* X-ray absorption fine structure (XAFS) spectroscopy at the Co K-edge. The monoclinic cobalt carbonate undergoes minimal changes in the Co oxidation state, indicative of surface-limited redox activity, while hydrotalcite-like cobalt hydroxide exhibits pronounced shifts in the Co K-edge position, indicating oxidation of Co-metal throughout the bulk.

**Acknowledgments:** This research received financial support from the Slovenian Research and Innovation Agency (ARIS) under the research programs P2-0412, P1-0112, and research project J2-50058. We acknowledge DESY (Hamburg, Germany), a member of the Helmholtz Association HGF, for the provision of experimental facilities at PETRA III (beamline P65, project I-20230893 EC, and I-20240152 EC) and P65 beamline staff for the support during the XAFS experiment.

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## Post-Deposition Treatment of Graphite-Based Working Electrode

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Miniature electrochemical sensors (ES) can be used for the rapid, low-cost and sensitive detection of pollutants in water. They consist of a counter (CE), a (quasi-)reference (RE) and a working electrode (WE) as well as electrical contacts integrated on a selected substrate. The electrical contacts that are exposed to the solution during the measurements need to be covered with a protective layer to prevent short circuits. This layer is usually deposited in the last step of the ES production and requires an additional treatment that could affect the properties of other the ES components, especially the WE. We investigated the effects of the post-deposition treatments on the chemical composition, microstructure and conductivity of the graphite-based WE and the electrochemical performance of the resulting ESs.

The components of the ES on alumina substrate were prepared by screen printing and subsequent firing of platinum CE, RE and electrical contacts at 1000 °C in air, and graphite-glass composite WE at 850 °C in argon. We investigated two commercially available polymers for covering the electrical contacts, one that requires annealing at 150 °C in air and one that is cured by exposure to UV light for 10 min with a 400 W iron-doped metal halide UV lamp.

The additional temperature or UV- treatments of the WE have minimal impact on the surface morphologies investigated by AFM and the sheet resistance, which was around 9  $\Omega/\text{sq}$  for all samples. However, the XPS analyses show that the temperature-cured WE (TC) had a 3-fold higher O/C ratio than the as-prepared WE (AP) or the UV-cured WE (UVC). The electrochemical response of the ESs was analyzed by cyclic voltammetry in a model solution of 5 mM  $\text{Fe}(\text{CN})_6^{3-/4-}$  in 0.1 M phosphate buffer (pH=7). All electrodes exhibited good reversibility, with AP and UVC showing similar current response and peak-to-peak potential separation, confirmed by similar electrochemically active surface area ( $A_{\text{ecsa}}$ ) values of 0.6  $\text{cm}^2$  and electron transfer rate ( $k^0$ ) of  $7 \times 10^{-3}$  cm/s, while the response of TC was significantly lower, with  $A_{\text{ecsa}}$  dropping to 35 % and  $k^0$  to 22 % of AP values. The lower response is likely due to the oxygen at the graphite electrode. Furthermore, TC also exhibited an additional peak at -0.7 V, corresponding to the reduction of the bound oxygen observed on WE by XPS. We demonstrate that with a single cathodic scan to -1.5 V, the electrochemical response of TC can be improved while the response of AP and UVC remains the same. Conditioning with a cathodic scan also resulted in a higher surface roughness of the WE for all samples. These results indicate that the improvement of the electrochemical properties of TC does not correlate significantly with changes in surface roughness, while it is strongly influenced by the oxygen content.

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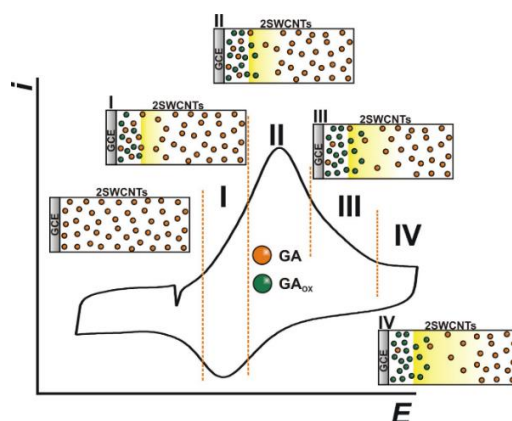
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## Mechanistic Insights into the Electrochemical (Ir)Reversibility of Gallic Acid at Carbon Nanotube Electrodes

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In this study, the electrochemical behavior of gallic acid (GA) is investigated using cyclic voltammetry on a glassy carbon electrode modified with single-walled carbon nanotubes (SWCNTs/GCE). The study provides a mechanistic insight into the observed electrochemical phenomena. It was found that the voltammetric response of gallic acid can range from irreversible to reversible, depending on parameters such as the thickness of the modifying layer, the ionic strength of the buffer and the scan rate. Given the counterintuitive nature of some results previously predicted by other authors [1, 2], such as unexpected trends in the current response with varying ionic strength of the buffer and the undefined electrochemical activity of the single-walled carbon nanotubes, the focus of the investigation was placed on processes occurring within the porous layer of the SWCNTs. By distinguishing between the processes in the bulk solution and those in the porous layer of SWCNTs, unusual  $\log v$  vs.  $\log i$  slopes of 0.5 to 1.8 were observed, along with atypical variations in the  $\log v$  vs.  $E_{\text{peak}}$  relationship. These dependencies were found to be strongly influenced by the degree of electrochemical reversibility. The results suggest that the voltammetric behavior is governed by a complex mass transport regime involving both thin-layer effects and retarded diffusion. Finally, the apparent (ir)reversibility of gallic acid is discussed in this context and the number of electrons exchanged during oxidation (peak at  $\sim 0.4$  V) is estimated to be two.



**Figure 1:** Mechanistic insight into the distribution of GA and GA<sub>ox</sub> in a 2SWCNT/ during cyclic voltammetry.

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## Electroanalytical studies with electrode printed using direct ink writing

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The importance of additive manufacturing grows in chemical laboratories [1]. Among the 3D printing technologies used, fused deposition modelling (FDM) is the most popular due to its low cost and user friendliness. The availability of filaments holding particular properties is limited. Although electricity-conductive filaments are available on the market, these frequently offer poor conductivity or require multistep surface activation [2]. An alternative 3D printing method is known as Direct Ink Writing (DIW). The main difference (FDM vs DIW) lies in the extrusion process. In FDM, the hardware melts filament, while DIW uses viscous inks that are extruded through a nozzle under applied pressure. The preparation of the viscous inks, in many cases, is very straightforward as it is based on the mixture of a binder and functional additive. From the electrochemical point of view, conductive inks can be used for e.g. printing electrical components or entire energy storage devices. This was reported by a few groups, especially focused on printing parts or even entire energy storage devices [3], [4], [5]. To the best of our knowledge, very little effort was given to the application of DIW in electroanalysis. In this work, conductive ink was prepared by mixing graphite, silicone, and chloroform, acting as conductive additive, binder, and viscosity modulating agent, respectively. Formulated ink was used to print cylindrical electrodes, further used for electroanalytical and energy storage applications. Electrodes were electrochemically characterized, and their surface was further inspected via scanning electron microscopy, optical profilometry, contact angle measurements, and energy-dispersive X-ray spectroscopy. The electrode electrochemical activation methods were developed, and significantly improved the electroanalytical performance of the electrode surface. Printed electrodes were used in the detection of cocaine in the presence of adulterating substances (frequently found in real samples) and were also tested in Li-ion battery configurations. Low-cost and easy DIY manufacturing of inks is considered a sound advantage of the proposed method.

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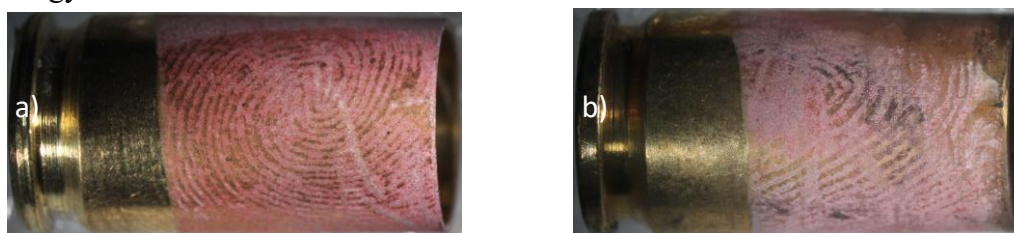
## Visualization of Latent Fingerprint with Poly(Neutral Red) and Study of its pH Dependence

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Sára Hermochová<sup>1\*</sup>, Jana Herinková<sup>1</sup>, Gabriela Broncová<sup>1</sup>

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The electrochemical visualization of latent fingerprints (FPs) on metallic substrates offers a rapid and field-applicable alternative to traditional cyanoacrylate fuming [1]. This study focuses on the use of poly(neutral red) (PNR) for the visualization of sebaceous FPs deposited on metallic surfaces, including fired cartridge cases. The PNR film was deposited by cyclic voltammetry and selectively forms around the FP residue (Fig. 1), producing a negative image of ridge details. We also investigated the effect of the pH of the supporting electrolyte on film formation and visualization quality. Several supporting electrolytes with pH values in range 5–8 were tested under identical electrochemical conditions on a brass substrate (–200 to +500 mV vs. Ag/AgCl, scan rate 50 mV/s, 4–8 cycles). The resulting PNR films showed noticeable differences in color, homogeneity, and visualization quality depending on the pH of the supporting electrolyte. The best fingerprint visualizations were obtained at pH 7, where the polymer film exhibited optimal coverage and clear differentiation of the ridge patterns. At lower or higher pH values, the films were either too thin, uneven, or resulted in poor visualization. These findings were supported by optical microscopy and profilometry. The results underline the importance of pH and electrolyte selection in optimizing the electrochemical visualization of fingerprints using PNR and contribute to the development of reliable and safe forensic methodology.



**Figure 1:** Poly(neutral red) around the fingerprint on the brass cartridges: a) before and b) after firing.

### Acknowledgements

This project Advanced Techniques of Visualization of Dactyloscopic Traces, VK01010022, was supported by the Ministry of the Interior of the Czech Republic from the Program Open Calls for Security Research 2023–2029 (OPSEC).

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*30<sup>th</sup> Young Investigators' Seminar on Analytical  
Chemistry (YISAC 2025)  
June 30<sup>th</sup> – July 3<sup>rd</sup>, Ljubljana, Slovenia*

# SESSION II

## **Chromatography**

Moderators: *Tia Kralj, Špela Pok*

## Antioxidant and antimicrobial properties of blackberry extract

Branka Ružičić<sup>1\*</sup>, Biljana Pećanin<sup>1</sup>, Dragana Grujić<sup>1</sup>, Blanka Škipina<sup>1</sup>, Aleksandar Savić<sup>1</sup>, Mitja Kolar<sup>2</sup>, Drago Kočar<sup>2</sup>, Sandra Dedijer<sup>3</sup>

The growing demand for sustainable and health-conscious materials has driven interest in agro-industrial by-products as natural sources of bioactive compounds. In this study, blackberry pomace, rich in polyphenols and anthocyanins, was examined as a functional ingredient for textile printing applications. Figure 1 shows the research project in graphical form. The natural dye was extracted by maceration with 80% methanol, followed by ultrasound-assisted extraction to improve the yield of active components. The extract showed strong antioxidant capacity, confirmed by FRAP (1,200  $\mu\text{mol Fe}^{2+}/\text{g}$ ), ABTS<sup>+</sup> (570  $\mu\text{mol TE/g}$ ), and DPPH (170  $\mu\text{mol TE/g}$ ) tests. Total monomeric anthocyanins reached 3.59 mg/g dry extract, of which 0.72 mg/g (20 %) remained in the form of ionised flavylum. The extract also showed a total phenolic content of 61.63 mg GAE/g dry extract, of which 43.65 mg GAE/g flavonoids. Antimicrobial activity, assessed by the agar dilution method, showed inhibitory effects against *Staphylococcus aureus* and *Escherichia coli* (MIC 10 mg/mL, MBC 20 mg/mL), while *Candida albicans* showed no sensitivity at concentrations up to 20 mg/mL. These results highlight the potential of blackberry pomace extract as a sustainable source of natural antioxidants and antibacterial agents for functional textile applications. Its dual functionality and natural origin make it suitable for integration into eco-friendly printing pastes and smart textiles designed for use in healthcare, hygiene, or protective products.

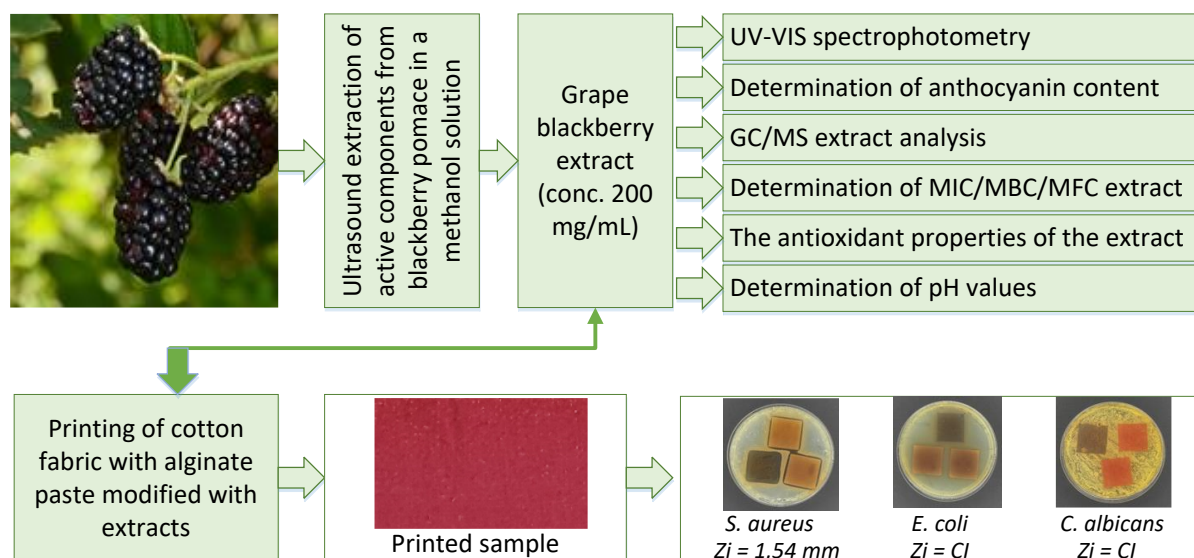


Figure 1: Graphical abstract

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## Deep Eutectic Solvents for Efficient and Sustainable Extraction of Bioactive Compounds from Slovenian Apple Peels

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Nika Marija Murenc<sup>1</sup>, Maša Islamčević Razboršek<sup>1\*</sup>

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In this study, the extraction efficiency of deep eutectic solvents (DESs) for isolating bioactive compounds from apple peels of four Slovenian cultivars (Gala, Idared, Topaz, and Carjevič) was investigated. The DESs were synthesized using choline chloride or menthol as hydrogen bond acceptors (HBAs) and various hydrogen bond donors (HBDs), including propane-1,2-diol, acetic acid, lactic acid, and levulinic acid. For comparison, 56% ethanol was used as a conventional solvent. The phytochemical profiles of the extracts were determined using high-performance liquid chromatography with UV detection (HPLC-UV), while antioxidant activities were assessed spectrophotometrically using TPC, ABTS, FRAP, and DPPH assays. The following phenolic compounds were identified in all extracts: rutin, phloridzin, chlorogenic acid, caffeic acid, quercetin-3-*O*-glucopyranoside, quercetin-3-*O*-galactoside, kaempferol-3-*O*-glucoside, kaempferol-3-*O*-rutinoside, and isorhamnetin-3-*O*-rutinoside. Although 56% ethanol generally achieved the highest overall extraction efficiency, certain DESs—particularly DES1 (choline chloride–propane-1,2-diol) and DES2 (choline chloride–lactic acid)—demonstrated comparable or even superior extraction performance for specific phenolic compounds. Ethanol extraction yielded the highest contents of isorhamnetin-3-*O*-rutinoside (0.93 mg/g dry weight (DW), cultivar Carjevič) and quercetin-3-*O*-galactoside (0.85 mg/g DW, cultivar Gala). Among the DESs, DES1 proved most effective for the majority of target analytes, including chlorogenic acid (0.53 mg/g DW), caffeic acid (0.15 mg/g DW), rutin (0.08 mg/g DW), quercetin-3-*O*-glucopyranoside (0.16 mg/g DW), and quercetin-3-*O*-galactoside (0.76 mg/g DW) in Gala; phloridzin (0.18 mg/g DW) in Idared; and kaempferol-3-*O*-rutinoside (0.02 mg/g DW) in Carjevič. DES2 exhibited the highest efficiency for isorhamnetin-3-*O*-rutinoside (0.67 mg/g DW, Gala), while DES3 was most effective for kaempferol-3-*O*-glucoside (0.26 mg/g DW, Gala).

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## Application of a multidisciplinary approach combining sensory and TD-GC-MS-O analysis for the characterization of VOCs emitted by ancient Egyptian mummified bodies

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Ancient Egyptian mummification is a mortuary practice with spiritual significance that aims to preserve the body for the successful transition of the soul into the afterlife. Various balms, oils, gum resins and waxes were used to preserve the body and its organs, and different techniques were used between and within historical periods and social classes. Nowadays, a large number of mummified bodies is being excavated and stored, and most of the ones in museum collections have been treated. Therefore, conservation products and/or pesticides, such as plant oils and various synthetic pesticides, are often present alongside the original materials.

This study explores a selection of nine ancient Egyptian mummified bodies and proposes an innovative multidisciplinary approach to study the volatile organic compounds (VOCs) emitted by combining traditional techniques with olfactory analysis. In particular, we combined sensory analysis, chemical analysis with thermal desorption-gas chromatography coupled with mass spectrometric and olfactory detection (TD-GC-MS-O), and microbiological investigation [1].

The main result from the study is the different type and concentration of volatiles emitted by the mummified bodies stored in different areas of the museum, highlighting higher amounts and variety of volatiles for those stored in the display cases in the exhibition area. The chemical analysis allows to classify the volatiles into four main categories based on their origin: the original mummification materials and their degradation (Acetic acid,  $\alpha$ -Pinene); plant oils used for conservation treatments (D-Limonene, (E)-Cinnamaldehyde); synthetic pesticides (1,2-Dichlorobenzene, 1,4-Dichlorobenzene); and microbiological deterioration (Octanol, 2-Heptanone). The majority of the compounds identified with mass spectrometry were also identified with olfactory detector, allowing to determine the olfactory profile of each mummified body under investigation. Although some compounds can be assigned to more than one origin group, as some oils used in the embalming process have recently also been used as insect repellents, this study demonstrates the possibility to classify the different compounds on the basis of chemical and olfactory analysis of the volatiles.

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## How will water contaminants dissipate in marine environment? Sorption versus photodegradation

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Water contaminants, such as pesticides, pharmaceuticals, and personal-care products, get exposed to various abiotic processes in natural marine environment that trigger their dissipation. Photolabile contaminants are likely to undergo photodegradation converting into related transformation products. Non-polar contaminants are, on the other hand, prone to sorption. Yet others may due to absence of chromophoric structural moieties and hydrophilicity persist unchanged in aqueous medium. These contaminants could be seen as the most problematic, especially if they exhibit elevated ecotoxicities to marine organisms [1].

In this study we addressed the environmental fate of 20 water contaminants with different uses, chemical polarity, and photoactivity (Figure 1). The 20  $\mu\text{g L}^{-1}$  multicomponent aqueous test solutions of all target contaminants were subjected to photoirradiation emitted from filtered 125 W Hg lamp (wavelengths above 300 nm). The results show that only 8 contaminants underwent photodegradation while others remained unchanged. Next, sorption was tested in modified Erlenmeyer flasks containing 10 g  $\text{L}^{-1}$  of solid material (30–120  $\mu\text{m}$  fraction), namely, real marine sediments from Gulf of Trieste, Slovenia, as well as their major constituents, i.e., natural minerals quartz, calcite, aragonite, dolomite, muscovite (mica), and clinocllore. Slight dissipation tendency was observed only for neotame, ramipril, and 2-mercaptobenzothiazole. If not readily biodegraded, most tested contaminants can be viewed as persistent as they would remain in the seawater unchanged by abiotic processes.

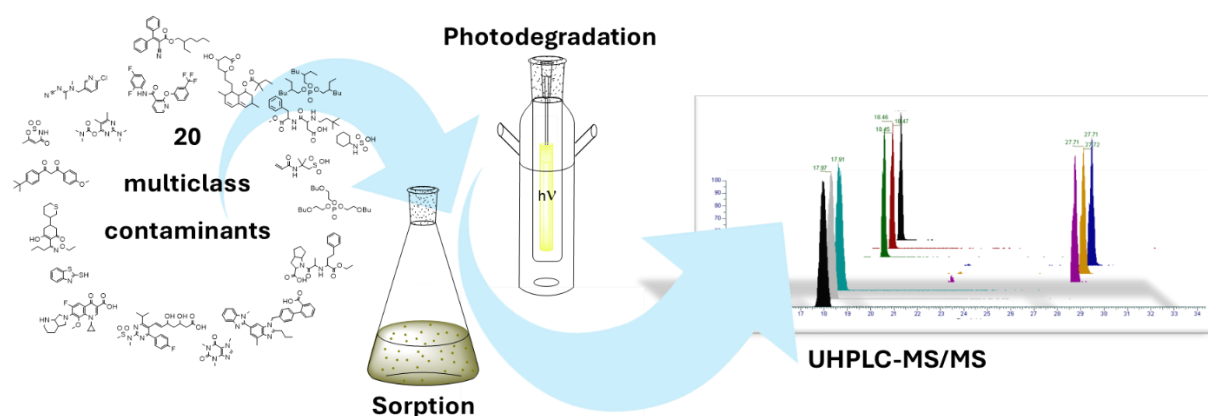


Figure 1: Study overview

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## Phospholipid Determination in Lecithin: A Standard-free Approach

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Phospholipids are amphiphilic molecules with different polar head groups and non-polar fatty acid tails that differ in length and saturation. As essential components of cell membranes, they form bilayers in all living organisms. Their unique structural properties enable applications as natural emulsifiers and encapsulating agents in pharmaceutical, food and cosmetic formulations, where they facilitate the formation of micelles and liposomes to improve the stability, bioavailability and delivery of active ingredients [1]. A common natural source of phospholipids in the industry is lecithin. The performance of lecithin in different formulations is highly dependent on its phospholipid composition. Differences in head group type and fatty acid saturation affect the type of structures lecithin can form and its emulsifying behavior. Therefore, the characterization of the phospholipid profile of lecithin is essential to ensure the stability and functionality of the final product [2].

The analysis of phospholipids is usually based on commercial reference standards. However, the high structural diversity of phospholipids requires numerous standards to cover all possible variants in complex mixtures such as lecithin. Given the cost, limited availability and time required for extensive comparisons, this approach is often inefficient and impractical [3].

In this study, we developed and optimized a qualitative method for the determination of phospholipids in lecithin without the use of reference standards. Reversed-phase high-performance liquid chromatography was coupled with high-resolution mass spectrometry to separate and detect the phospholipid species. Molecular ions were recorded in full scan mode and analyzed using a custom Python script that generated a list of possible phospholipid structures for each  $m/z$  value. The identification was confirmed by matching the MS/MS fragmentation patterns with the theoretical predictions.

The proposed method provides a reliable, cost-effective alternative for phospholipid profiling in complex lipid matrices and demonstrates that standard-free identification is possible using high-resolution analytical tools in combination with computational support.

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## Use of deep eutectic solvents for the analysis of white mulberry (*Morus alba*) samples

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Historically, *Morus alba* (white mulberry) has been extensively used in traditional Chinese medicine, in addition to its role in sericulture [1]. It is a rich source of bioactive compounds that exhibit a variety of physiological and pharmacological effects. However, the organic solvents conventionally used for extracting these compounds pose environmental and health concerns due to their toxicity [2]. Deep eutectic solvents (DESs) offer a potential green alternative. DESs are mixtures of two or more organic or inorganic compounds, which liquefy under optimal conditions to form a stable eutectic. These solvents are held together by hydrogen bonds, where one compound serves as a hydrogen bond acceptor (HBA) and the other as a hydrogen bond donor (HBD) [3].

This study aimed to assess the efficiency of selected DESs compared to conventional organic solvents for the extraction of bioactive compounds from white mulberry. For this purpose, a high-performance liquid chromatography with diode-array detection (HPLC-DAD) method for the determination of selected polyphenols (gallic acid, caffeic acid, p-coumaric acid, rutin and resveratrol) was developed and partially validated, examining parameters such as linearity, repeatability, limit of detection, limit of quantification, accuracy and selectivity. Bioactive compounds were extracted from white mulberry samples using ultrasound-assisted extraction (UAE). The determined optimal conditions were: DES with 1:2 molar ratio (HBA:HBD), 20% added water to DES, 80 °C and 30 minutes. Six different DESs based on choline chloride (ChCl) as the HBA were prepared, using glycerol, ethylene glycol, propane-1,3-diol, butane-1,4-diol, urea, and glucose as HBDs. Methanol was used as the conventional organic solvent for comparison. Extracts were prepared from the branches, leaves and fruits of white mulberry, and extraction efficiencies were evaluated using the developed HPLC-DAD method, along with measurements of total phenolic content (TPC) and total flavonoid content (TFC). The results demonstrated that DESs, particularly those based on polyalcohols as hydrogen bond donors, were the most efficient for extractions. For branches and leaves, the ChCl/glycerol DES yielded the highest efficiency, while for fruits, the ChCl/ethylene glycol DES was the most effective. In most polyphenol extractions, at least one DES achieved comparable or higher extraction efficiencies than methanol, except in the case of flavonoids, where DES yields were generally lower. These findings highlight the potential of using DESs as an alternative procedure for the green and efficient extraction of polyphenolic bioactive compounds from plant materials such as white mulberry.

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## Method development for the chromatographic separation and extraction of organic UV filters from seawater samples

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Matevž Polak<sup>1</sup>, Helena Prosen<sup>1\*</sup>

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Organic UV filters are widely used as active ingredients in sunscreens and are also present in a variety of consumer products such as cosmetics, plastics, paints, and textiles. These compounds are of growing environmental concern due to their persistence, bioaccumulative potential, and especially their chronic toxicity. Several UV filters have been identified as endocrine-disrupting chemicals (EDCs), capable of interfering with hormonal systems in aquatic organisms and potentially affecting human health. Although some of these substances are already partially regulated, they continue to be frequently detected in various aquatic environments. Their presence is primarily attributed to discharges from wastewater treatment plants, improper waste disposal, and direct release into water bodies through recreational activities and washing off the skin in the case of sunscreen products [1,2].

Because of their frequent occurrence in aquatic environments, the aim of this work was to develop an extraction method for sample preparation, as well as a chromatographic method for the qualitative and quantitative analysis of seawater samples. The target analytes included eight commonly used organic UV filters: 5-methylbenzotriazole, dimethylbenzotriazole, octinoxate, oxybenzone, octocrylene, avobenzone, 4-methylbenzylidene camphor, and benzophenone-4, which are the most common UV filters used in cosmetic products. The chromatographic method was developed on an HPLC-DAD system using gradient elution, with methanol and 0.1% formic acid in Milli-Q water as the mobile phases. Detection was performed at two wavelengths – 285 and 330 nm. For sample preparation, a solid-phase extraction (SPE) method was optimized using a C8 cartridge, with various extraction parameters adjusted to achieve the highest possible recoveries. This method is designed to concentrate the analytes from seawater samples, where they are typically present at very low concentrations, thereby improving the sensitivity and reliability of the subsequent chromatographic analysis.

Method was applied to the determination of selected UV filters in Slovenian seawater, where these compounds are seldomly monitored [3].

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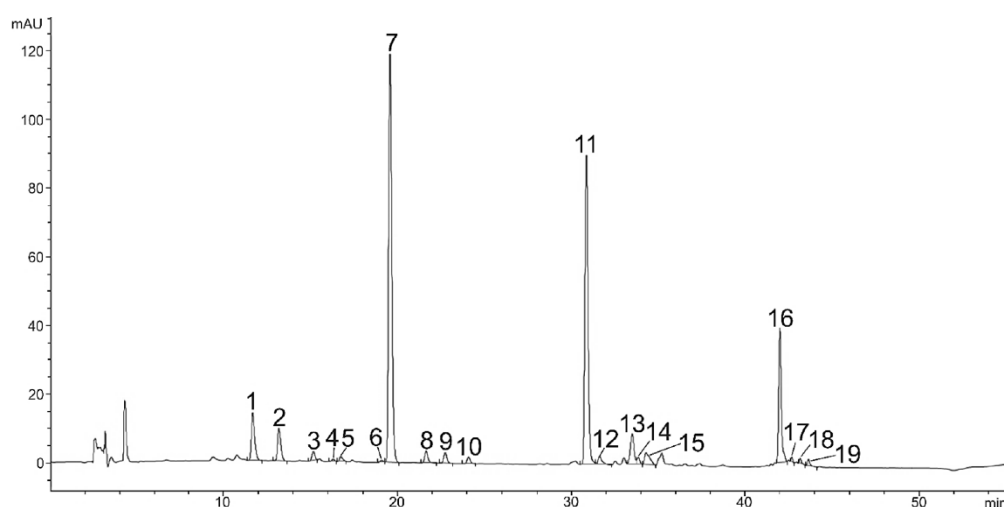
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## Pigment analysis in the alga *Haematococcus pluvialis*

Veno Jaša Grujić<sup>1,2</sup>, Maša Islamčević Razboršek<sup>3</sup>, Jana Ambrožič-Dolinšek<sup>1,2\*</sup>

*Haematococcus pluvialis* is a unicellular freshwater alga known for its high content of bioactive compounds, especially carotenoids, which are powerful antioxidants. In this study, the pigment composition in both life stages of the alga was compared, focusing on the less studied green vegetative stage. The pigments were analyzed by HPLC-DAD and LC-QTOF-MS. In the green stage, 16 pigments were identified (Figure 1), accounting for a total of 8.86 mg g<sup>-1</sup> DW, with chlorophyll a and its derivatives accounting for 59% (5.24 mg g<sup>-1</sup> DW) and free carotenoids 41% (3.62 mg g<sup>-1</sup> DW). In contrast, secondary carotenoids, especially astaxanthin esters, dominated in the red stage. Of the 37.86 mg g<sup>-1</sup> DW of pigments in the red stage, monoesters accounted for 82% (the most abundant group), followed by diesters (12%) and free carotenoids (6%). These results improve the understanding of pigment dynamics in *H. pluvialis* and support the optimization of cultivation. Insights into the green stage enable more targeted growth conditions to enhance the biosynthesis of precursors essential for astaxanthin accumulation during the red stage.



**Figure 1:** HPLC-DAD chromatogram (475 nm) of chlorophylls and carotenoids in green vegetative stage, Neoxanthin (1), Violaxanthin (2), Astaxanthin (3), Adonixanthin (4), Astaxanthin isomer (5), Zeaxanthin (6), Lutein (7), Lutein isomer (8), Lutein isomer (9), Lutein isomer (10), Chlorophyll *b* (11), Chlorophyll *b* derivate (12), Chlorophyll *a* (13), Chlorophyll *a* derivate (14), Echinonone (15), *B*-Carotene (16), Not identified (17), Not identified (18), Not identified (19).

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*30<sup>th</sup> Young Investigators' Seminar on Analytical  
Chemistry (YISAC 2025)  
June 30<sup>th</sup> – July 3<sup>rd</sup>, Ljubljana, Slovenia*

## SESSION III

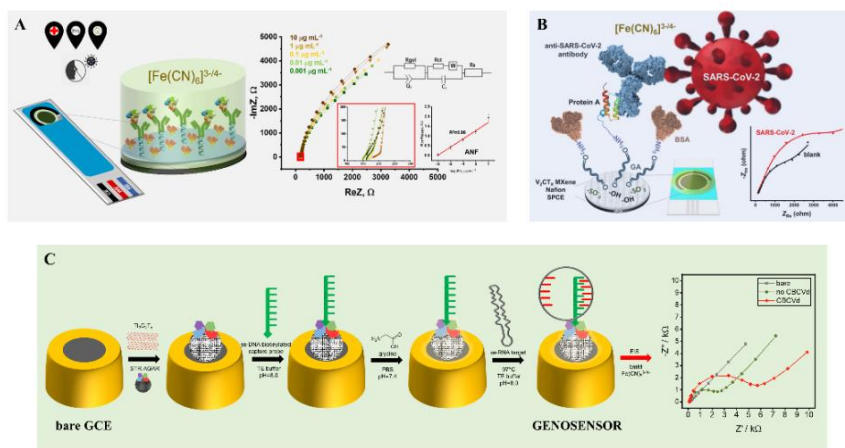
# Electrochemical Sensors

Moderators: *Maksimiljan Dekleva, Josipa Dugeč*

# Affinity-based Strategies for Electrochemical Detection of Viruses and Viroids

Alnilan Lobato<sup>1,2\*</sup>, Ivan Konjević<sup>1,3</sup>, Samo B. Hočevar<sup>1</sup>, Nikola Tasić<sup>1</sup>

Viruses are small infectious agents composed of nucleic acids (DNA or RNA) enclosed in a protein coat, whereas viroids are small, single-stranded circular RNAs without protein coating. Viruses can cause diseases in humans, plants, and animals, and are capable of causing global pandemics; in contrast, viroids infect only plants, which can lead to severe agro-economic losses. Conventional molecular biology techniques offer reliable virus and viroid detection but are often time-consuming, expensive, and require sophisticated laboratory infrastructure. Alternatively, electrochemical biosensors promise rapid, sensitive, and point-of-care alternatives, though improvements in selectivity and stability are still needed. Here we present two electrochemical immunosensors targeting the SARS-CoV-2 spike protein [1,2] and one genosensor for detecting the *Citrus bark cracking viroid* (CBCVd) [3], shown in Figure 1. These sensors use affinity-based detection by measuring specific interactions between immobilized biological recognition elements and target analytes using faradaic electrochemical impedance spectroscopy to achieve high sensitivity.



**Figure 1:** Schematics of electrochemical biosensors: (A, B) immunosensors for SARS-CoV-2; (C) genosensor for CBCVd. Adapted from [1–3].

## Acknowledgements

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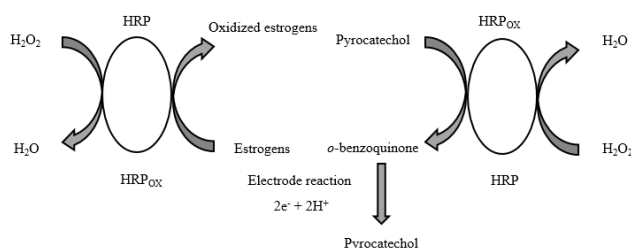
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## Analytical Characteristic of a Biosensor Based on Horseradish Peroxidase for Electrochemical Determination of Estrogens

Gabriela Satora<sup>1\*</sup>, Maria Madej<sup>1</sup>, Jolanta Kochana<sup>1</sup>

Estrogens, including estradiol, estriol, and estrone, play crucial role in different physiological processes in the human body. Disorders of estrogens levels can have serious health consequences. For this reason, the development of analytical techniques that provide fast and sensitive detection of these hormones in biological samples is of great importance.

The studied biosensor was based on enzyme, horseradish peroxidase (HRP), as a recognition element. It was immobilized in a matrix containing multi-walled carbon nanotubes, metal-organic framework JUK-2, and gold nanoparticles. Since the products of enzymatic oxidation of estrogens are not electroactive, the detection strategy was based on the competition for the enzyme's active site between estrogens and pyrocatechol which was present in the system at a constant concentration. To ensure enzyme reversibility a constant amount of hydrogen peroxide was also added to the electrochemical cell. The analytical signal was related to the reduction of *o*-benzoquinone produced during the enzymatic reaction. The principle of the biosensor's operation is shown in Figure 1. Conducted studies demonstrated that the HRP-based biosensor showed electrochemical response towards each of the estrogens. Therefore, analytical parameters (sensitivity, limit of detection and limit of quantification) were determined for each estrogen separately. Reproducibility of the signal was also examined. After that, multi-component samples were analysed: a synthetic sample simulating the concentration of all three estrogens in a woman's blood during the third trimester of pregnancy, the analogous sample prepared in a biological matrix and a real sample - the pharmaceutical preparation Alpicort E. The obtained relative errors were within the  $\pm 4\%$  range indicating the potential of practical application of the studied biosensor for the determination of estrogens.



**Figure 1:** Schematic representation of the studied biosensor.

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## Design and synthesis of neodymium-oxide for effective electrochemical detection of hazardous pesticide carbofuran

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Over the last two decades, as the population has grown and the demand for agricultural products has increased, the use of pesticides in fruit and vegetable production has risen significantly [1]. Carbofuran (CBF), a widely used carbamate pesticide, poses significant risks to human health due to its persistence and poor degradability, leading to soil and water contamination [2]. Consequently, the development of a sensitive and reliable sensor for CBF detection is crucial for environmental monitoring. In this study, neodymium oxide (Nd<sub>2</sub>O<sub>3</sub>) nanoparticles, synthesized via a single-step hydrothermal method, were utilized for the first time as a carbon paste electrode (CPE) modifier to enhance the electrochemical detection of CBF. Comprehensive morphological and electrochemical analysis confirmed that Nd<sub>2</sub>O<sub>3</sub> incorporation significantly improved the electrocatalytic response. The resulting sensor exhibited a broad linear detection range (3–200 µM), low detection (0.813 µM) and quantification limits (2.711 µM), and high sensitivity (0.8 µA µM<sup>-1</sup>cm<sup>-2</sup>). Its practical applicability was successfully demonstrated in real sample analysis, achieving excellent recovery rates and validation via UV-Vis spectroscopy. This study highlights the potential of Nd<sub>2</sub>O<sub>3</sub>-modified electrodes as a promising platform for effective CBF monitoring in environmental samples.

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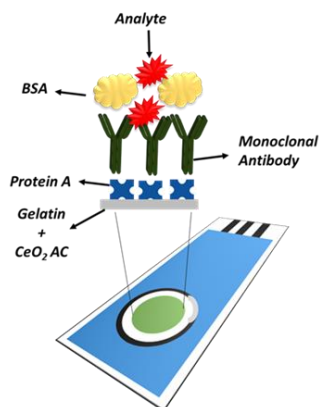
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## Label-Free Electrochemical Immunosensor Based on Gelatin-CeO<sub>2</sub> Nanocomposite for Sensitive Detection of Insulin

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Insulin, a polypeptide hormone (5808 Da), plays a key role in the homeostasis and regulation of glucose in the blood [1]. Detection of insulin alongside other diagnostic biomarkers is important as it can distinguish between type I and type II diabetes [2]. Monitoring insulin levels can improve glycemic management for the proper administration of insulin [3]. Herein, we report an electrochemical label-free immunosensor developed on a disposable supporting screen-printed carbon electrode for the detection of insulin in the picomolar concentration range. The biosensor comprises activated carbon-supported cerium oxide encapsulated within a gelatin layer, the latter also serving as a support for further binding of the biorecognition elements. It has been observed that the gelatin matrix enhances the stability of both the (electro)catalytic layer and biorecognition elements, in addition to an improved overall electroanalytical performance of the immunosensor. The electrochemical detection mechanism is based on the decrease of the current signal upon binding of the insulin with monoclonal antibodies when measured by square-wave voltammetry. The sensor exhibits a linear response toward insulin in the concentration range of 1 - 100 pM in a phosphate-buffered saline. This work showcases the sensitive and selective detection of insulin at the picomolar level with a simple immunosensor architecture and sensing strategy.



**Figure 1:** Schematic representation of the immunosensor design.

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## Preparation and application of a molecularly imprinted polymer for indirect electrochemical sensing of acetamiprid

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Acetamiprid (ACM) is a commonly used neonicotinoid insecticide with potential neurotoxic effects on non-target organisms, including pollinators and humans. Its frequent presence in surface waters and agricultural products requires development of sensitive, fast, and reliable detection methods [1]. Electrochemical techniques offer a rapid, low-cost alternative to conventional chromatographic methods, with additional advantages of portability and fast response times, which make them well-suited for on-field sensing platforms [2]. Since ACM is electrochemically inactive within the potential window of carbon-based working electrodes (WE), a molecularly imprinted polymer (MIP) was applied as a selective recognition element on the WE surface, enabling its indirect electrochemical detection.

Key parameters for bulk MIP synthesis including monomer type, solvent, prepolymerization conditions, and reagent ratios were systematically optimized. MIP with the best binding and selective properties (imprinting factor 2.12 and binding capacity 7.14  $\mu\text{mol/g}$ ) was selected for further characterization. The adsorption properties of the resulting material, studied using UV–Vis spectroscopy, exhibited Langmuir–Freundlich binding behavior and pseudo-second-order adsorption kinetics. MIP was subsequently used to modify the WE for indirect ACM detection, based on signal suppression of the redox probe (ferricyanide/ferrocyanide, HCF) after WE incubation in the analyte solution. Preliminary characterization was performed using cyclic voltammetry on screen-printed carbon electrodes, as well as on a conventional three-electrode system with a glassy carbon electrode (GCE). The most pronounced change in anodic peak current in 5 mM HCF was observed after a two-layer drop-casted modification of the GCE using a 5 mg/mL MIP suspension. Selectivity was evaluated in the presence of structurally related neonicotinoids. Scan rate study confirmed a decrease in the electroactive surface area of the WE after ACM exposure, consistent with the observed signal suppression. Quantification using differential pulse voltammetry was carried out over the 1–100  $\mu\text{M}$  range, yielding good linearity between the signal change ( $\Delta I$ ) and  $\log c$  ( $R^2 = 0.989$ ), based on four calibration points, and a calculated limit of detection (LOD) of 1.06  $\mu\text{M}$ . Further work will focus on improvement of LOD by incorporating conductive nanomaterials and optimizing the MIP particle size.

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## **Electrochemical Sensors for the Forensic Detection of New Psychoactive Substances**

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The rapid emergence and structural diversity of new psychoactive substances (NPSs) present ongoing challenges in forensic analysis. These compounds often evade standard detection methods, necessitating the development of alternative analytical strategies [1]. This work explores electrochemical techniques as efficient, cost-effective and portable tools for detecting selected NPSs, namely synthetic cathinones and aminoindanes.

Three electrochemical methods – potentiometry, voltammetry and electrochemical impedance spectroscopy (EIS) – were investigated with a focus on enhancing sensitivity and selectivity through tailored electrode design and surface modification. Potentiometric sensors based on ion-selective electrodes (ISEs) were optimized for biological sample analysis. Cation-exchanger-based membranes outperformed neutral carriers, offering improved detection limits. Coupling sensor arrays with chemometric analysis enabled reliable differentiation among structurally similar NPSs such as cathinones, aminoindanes and tryptamines.

Voltammetric sensing was enhanced via electrode modification with electropolymerized methoxyphenylthiophene oligomers, which facilitated the oxidation of electrochemically inactive 2-aminoindane and therefore improved sensor response. In parallel, EIS sensor was developed using graphite screen-printed electrodes modified with zwitterionic oligomers of 3-aminobenzoic acid. The hydrophilic and polar nature of this coating, along with potential hydrogen bonding interactions, resulted in improved selectivity for selected NPSs.

These findings demonstrate that electrochemical sensor performance can be significantly improved through appropriate material choices and surface modifications. These approaches offer promising openings for rapid, selective and field-deployable forensic drug screening.

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## Lanthan's Touch: Designing La-Dy<sub>2</sub>O<sub>3</sub>/MWCNT Sensor for Electrochemical Detection of Metol in Enviromental and Biological Fluids Samples

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Global water pollution is increasingly driven by persistent organic pollutants, notably nitrogen- and sulfur-based compounds. Among them, metol (MTL), an amine derivative used in pharmaceuticals and photographic processing, is particularly concerning due to its toxicity and resistance to biodegradation. Even at trace levels, MTL can accumulate in ecosystems, posing risks to both the environment and human health. [1,2]. In this study, a novel electrochemical sensor for MTL detection was developed using a glassy carbon electrode (GCE) modified with a La-Dy<sub>2</sub>O<sub>3</sub>/MWCNT nanocomposite. Dysprosium oxide (Dy<sub>2</sub>O<sub>3</sub>) was chosen for its thermal, chemical, and electrical stability, while lanthanum doping enhanced its electrocatalytic activity by promoting charge transfer through electronic structure modulation [3]. The La-doped Dy<sub>2</sub>O<sub>3</sub> was synthesized via a hydrothermal route, followed by composite formation with multi-walled carbon nanotubes (MWCNTs) using ultrasonication. Structural and morphological characterization of the synthesized materials was carried out using X-ray powder diffraction (XRPD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS), confirming the successful formation of the nanocomposite. The electrochemical performance of the modified GCE was evaluated for MTL detection using cyclic and square wave voltammetry. The sensor showed high sensitivity, with a linear range of 0.3–220 µM, a detection limit of 0.45 µM. Excellent selectivity was observed with negligible interference from common substances. Practical applicability was demonstrated in tap water, Mur River water, artificial urine, and human serum, with good recovery. Results correlated well with UV–Vis spectrophotometry, confirming accuracy and reliability in real-sample analysis.

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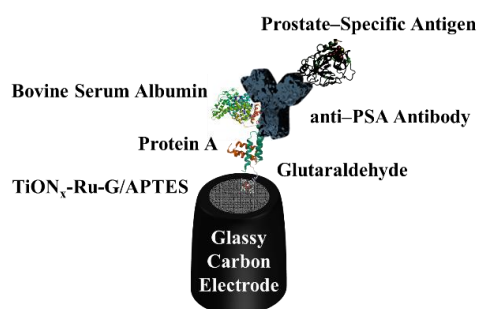
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## Electrochemical Detection of PSA Biomarker Using a Ruthenium-Decorated Titanium Oxynitride Nanocomposite-Based Immunosensor

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Prostate cancer is estimated to affect one in eleven men by the age of 74 [1], making it one of the leading causes of cancer-related deaths. Early diagnosis significantly enhances survival outcomes, primarily through the detection of specific biomarkers [2]. In this study, we developed an impedimetric immunosensor to detect prostate-specific antigen (PSA), the key biomarker associated with this cancer. The sensor is based on a glassy carbon substrate electrode modified with a composite material comprising conductive graphene-supported ruthenium-decorated titanium oxynitride nanoparticles as the electrocatalyst and (3-aminopropyl)triethoxysilane (APTES). Anti-PSA antibodies were immobilized onto the modified glassy carbon electrode using an optimized protocol involving APTES, glutaraldehyde, and Protein A, the latter enabling oriented binding of the antibodies (Figure 1). Each modification step was systematically optimized and characterized, resulting in a highly sensitive immunosensor capable of detecting PSA at clinically relevant concentrations. Furthermore, we discuss the results and challenges of transferring the developed immunosensor to a screen-printed carbon electrode, which offers benefits such as suitability for one-shot and point-of-care applications.



**Figure 1:** Design of the proposed immunosensor.

### Acknowledgements

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## SESSION IV

# **Optical and Surface Methods, Biochemistry**

**Moderators:** *Ibrahim Elrefaey, Sára Hermochová*

## Surface Characterization of $\text{ZnM}^{3+}$ Oxide Catalyst Supports by Physisorption and Chemisorption Methods

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Metal oxides such as zinc oxide, aluminum oxide ( $\text{Al}_2\text{O}_3$ ), and gallium oxide ( $\text{Ga}_2\text{O}_3$ ) are pivotal as catalytic supports, particularly in reactions like  $\text{CO}_2$  hydrogenation, where they influence both the activity and selectivity of the catalytic process [1]. The surface characteristics of metal oxides, including their acidity, basicity, and metal–support interactions, are key factors governing catalytic activity, selectivity, and stability, particularly in  $\text{CO}_2$  hydrogenation processes. Tailoring these properties through the design of mixed metal oxides, enables improved dispersion of active metal species, enhanced thermal stability, and precise modulation of surface reactivity. Such modifications facilitate a deeper understanding of reaction mechanisms by influencing the nature, distribution, and accessibility of active sites [2, 3, 4, 5].

We present the preparation of  $\text{ZnM}$  mixed metal oxide ( $\text{M} = \text{Al}^{3+}, \text{Ga}^{3+}, \text{In}^{3+}$ ) catalyst supports via hydrothermal treatment of a mixed metal hydroxide precursor. The hydroxides were synthesized via co-precipitation and subsequently thermally treated at various temperatures (400 °C, 550 °C, 700 °C, 850 °C, and 1000 °C) to obtain the corresponding mixed metal oxides with varying degrees of crystallinity. Temperature-dependent changes in crystallinity and surface area were evaluated using XRD and BET analysis, revealing increased crystallinity and a progressive decrease in surface area with rising calcination temperature. Morphological and elemental analyses were conducted using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDS), confirming homogeneous distribution of metal ions. Surface acidity was investigated using pyridine temperature-programmed desorption (TPD), and surface interactions with  $\text{CO}_2$  were assessed via *in situ* diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)  $\text{CO}_2$  adsorption/desorption studies. The findings highlight the potential of mixed metal oxide systems for advancing  $\text{CO}_2$  hydrogenation applications.

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## Using Multiparametric Surface Plasmon Resonance to determine the affinity of interaction between antigen and antibody

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Information about the affinity is crucial in various applications based on specific interaction between biomolecules, such as antigen and antibody, antigen and aptamer, enzyme and inhibitor etc. These applications include affinity biosensors, enzyme-linked immunosorbent assay (ELISA), drug design and screening, and many others [1]. These applications have gained relevant attention due to their expanding applications in biochemical detection, clinical diagnostics, food safety assessment and etc. The affinity and appropriate reactivity of biomolecules are essential for ensuring assay selectivity and sensitivity [1-2].

Several methods are used for studying this interaction, such as Western-blot, Bio-layer interferometry, ELISA, or Surface plasmon resonance (SPR) [2]. SPR is a label-free, optical biosensing technique that enables real-time monitoring of biomolecular interactions. SPR detects changes in the refractive index at the interface between a dielectric medium and a thin metal film, typically gold, as a result of analyte binding to the sensor surface. The major advantages of SPR include its label-free nature, minimal sample preparation, and potential for miniaturization and efficient screening [3–4]. Multiparametric SPR (MP SPR) is an enhanced version of SPR. Its improved goniometric design allows scanning over a wider range of refractive indices than standard SPR, enabling measurement of thicker layers and more complex systems [5].

This work was focused on the use of MP-SPR method for measuring of the interaction of specific antibodies with protein biomarker Pentraxin 3 associated with the intraamniotic inflammation. We also concentrated on the interaction of specific antibodies with protein HE-4 associated with ovarian carcinoma. We compared different types of modifications of gold sensors for the binding of antibodies.

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## Immobilisation of Tyrosine Protein Kinase Src on Magnetic Microparticles for Myelin Basic Protein Phosphorylation

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Zuzana Bilkova<sup>1</sup>, Marcela Slovakova<sup>1</sup>

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Phosphorylation is a very important post-translational modification of proteins in terms of their proper function and structure. A detailed study of protein phosphorylation can help clarify the pathogenesis of many diseases such as cancer or neurodegenerative diseases [1]. To study substrate phosphorylations, which are possible by various approaches, we chose the use of protein kinases. Protein kinases were conjugated with magnetic particles, with advantages such as easy and fast handling and separation from the mixture, and no contamination of the final product. For the best possible enzyme activity, we optimised immobilization conditions with various beads, also with the aim of minimising nonspecific sorption by using BSA [2].

The available particles with a carboxyl-modified surface were searched (Thermo Fisher, Chemicell, and Invitrogen). Phosphorylation of the peptide substrate by immobilised Src kinase was followed by analysis with MALDI-LTQ Orbitrap XL MS. The highest level of peptide phosphorylation (93.2% after 48 hours) was achieved with Src kinase immobilised on Sera Mag Speed Beads. In terms of storage stability, the activity of the immobilised enzyme after 4 weeks of storage was reduced by only 10.85%. Finally, the immobilised Src kinase was used to phosphorylate the native bovine myelin basic protein (MBP), known as an intrinsic disordered protein, which undergoes dynamic conformational ensembles with only a weak tertiary interaction. Naturally, MBP does not carry tyrosine phosphorylation [3]. Phosphorylation on tyrosines was demonstrated for soluble and immobilised Src protein kinase by MALDI-LTQ Orbitrap XL mass spectrometry and Western blot with immunodetection and pIMAGO detection.

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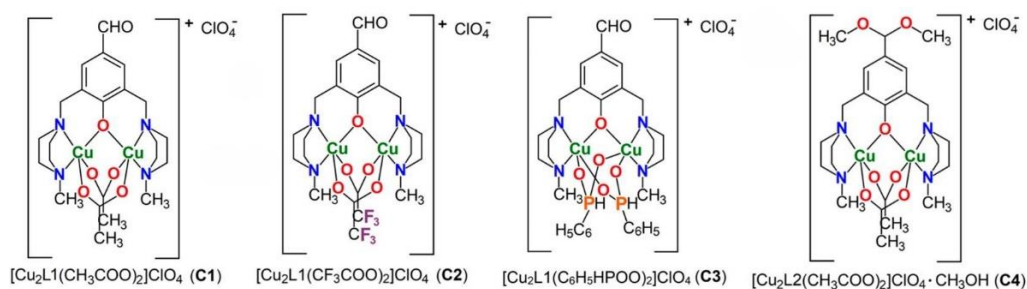
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## Biomimetic Copper Complexes

Michaela Bártová<sup>1\*</sup>, Milan Sýs<sup>1</sup>, Tomáš Mikysek<sup>1</sup>

In this work, four newly synthesized dinuclear copper(II) complexes (Fig. 1.) are presented as promising artificial enzymes mimicking the catalysis of natural enzymes such as laccase, tyrosinase, horseradish peroxidase or phenoxazinone synthase. These metalloenzymes have specific catalytic activities towards substrates like dihydroxyphenols, aminophenols, and phenylenediamines. For this reason, they either can play a role in degradation process of these toxic substances, or they can be a sensitive component of biosensors [1]. Unfortunately, biosensors constructed using natural systems are expensive and often provide low long-term stability. These problems could be solved, for example, by replacing enzymes with a biomimetic system, which could be the copper-based complexes mentioned at the beginning [2–4].



**Figure 1:** The chemical structure of studied dinuclear copper(II) complexes (C1–C4).

The aim of our study was to electrochemically and spectrophotometrically characterize four copper complexes and subsequently monitor their catalytic activity towards selected substrates using spectrophotometry. Based on kinetic measurements, it was found that these complexes are able to mimic the catecholase activity, horseradish peroxidase-like activity, and phenoxazinone synthase-like activity of natural enzymes. The effect of water on their catalysis was also tested. The obtained results can be employed in design and development of new biomimetic systems serving e.g. in electroanalysis, degradation of pollutants, or drug synthesis.

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## Systematic development of LA-ICP-MS method for elemental analysis in organic-rich liquid samples

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Inductively coupled plasma mass spectrometry (ICP-MS) is one of the most advanced techniques for elemental analysis and is widely applied across a range of scientific and industrial disciplines. However, it faces significant limitations when dealing with organic-rich samples, such as oils. These samples can cause severe plasma instability and non-spectral interferences. Furthermore, they are often immiscible with water and typically require time-consuming microwave-assisted acid digestion. Laser ablation ICP-MS (LA-ICP-MS), primarily used for solid sample analysis, presents a promising alternative for the elemental analysis of such challenging liquid samples. In LA-ICP-MS, only a small amount of sample vapor is introduced into plasma, resulting in a significantly reduced impact on plasma stability. Since the application of LA-ICP-MS to liquid samples remains uncommon, it is necessary to develop a completely new methodology. This includes the selection of appropriate sample types (considering their volatility), the choice and design of the sample pad to minimize evaporation and stabilize the signal, and the overall optimization of the ablation process.

A key objective is to minimize concentration changes prior to laser ablation. This requires maximizing the droplet lifetime, which in turn depends on achieving a high contact angle between the droplet and the substrate. In our study, polytetrafluoroethylene was identified as the optimal support material due to its high contact angle and excellent chemical resistance. To investigate this phenomenon in greater detail, a mathematical model describing sessile droplet evaporation prior to laser ablation was developed [1]. It was also found that droplet lifetime can be significantly extended by placing the droplet into a circular hole with a diameter of 2 mm and a depth of 3 mm.

Subsequent work focused on optimizing the laser ablation conditions, including laser fluence, frequency, and the number of laser shots required for a stable signal. The optimal parameters were determined to be 100 laser shots at a frequency of 5 Hz. It was also observed that the optimal laser fluence depends on the sample matrix, therefore the effect of the internal standard was investigated. Additionally, various droplet volumes were tested, revealing that signal intensity is largely independent of droplet volume. Thus, small variations in droplet size do not significantly affect the analytical signal. Lastly, the developed method was applied to the elemental analysis of a set of motor oil samples.

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## Western Blot assay for Confirmation of Changes in CD44 Receptor Expression in Irradiated Lung-Derived Cells Treated with Hyaluronic Acid Nanoparticles

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Hyaluronic acid (HA) is a biopolymer naturally occurring in extracellular matrix and synovial fluids, widely studied for its biocompatibility. To date, only a few studies have investigated the potential of HA as a radioprotective agent. It has been demonstrated that HA exhibits radioprotective effect in the intestinal epithelium through a Toll-like receptor 4 (TLR4) and cyclooxygenase-2 (COX-2)-mediated mechanism [1]. However, HA's use as a radioprotective substance is limited due to its radiation-induced fragmentation into short, inflammatory units [2]. Nevertheless, HA in the form of nanoparticles exhibits improved stability and it has been proven that HA nanoparticles (HANPs), which were synthesized by optimized cross-linking of high-molecular weight HA are stable even upon irradiation and attenuate radiation-induced lung injury, particularly by modulating signaling pathways linked to fibrosis [3-4].

HA's key cell receptor is CD44, a ubiquitously expressed adhesion transmembrane glycoprotein that facilitates various biological activities, such as cell proliferation. CD44 is overexpressed in various types of cancer and is associated with poor prognosis and reduced response to radiation therapy [5].

This is why, in this work, we aimed to confirm the changes in CD44 expression in lung-derived cells after irradiation, with or without pre-treatment with HANPs. For the confirmation of reactivity of HANPs with CD44 we used Western Blot analysis with chemiluminescent detection. We optimized the method and the interaction was confirmed. Our results also show the potential of HANPs as carriers for radioprotective agents and anti-cancer drugs.

### Acknowledgment:

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June 30<sup>th</sup> – July 3<sup>rd</sup>, Ljubljana, Slovenia*

## SESSION V

# **Environmental Analysis**

**Moderators:** *Aleksander Kravos, Petr Rudolf, Dominik Novák, Emma  
Paolin*

## Investigating the Influence of Several Environmental Stressors on the Degradation of Non-weighted and Weighted Silk

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Ibrahim Elrefaey<sup>1\*</sup>, Matija Strlič<sup>1</sup>

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Silk fibroin represents a remarkable fibrous protein polymer celebrated for its exceptional properties, including strength, lustre, and biocompatibility [1]. Despite its historical significance and inherent beauty in textiles, silk remains susceptible to degradation through natural aging processes, potentially accelerated by traditional weighting practices involving metal salt treatments [2-4]. This study examines the degradation pathways of both non-weighted silk and tin-phosphate weighted silk when exposed to key environmental stressors: acidity, elevated temperature, and humidity. Through accelerated degradation experiments and a comprehensive analytical approach -including colour measurements, pH analysis, FTIR, SEM-EDS, XRD, SAXS/WAXS, contact angle analysis, viscometry, and tensile strength testing- we characterize the chemical and structural transformations occurring at multiple hierarchical levels within the silk fibres [5]. Our investigation specifically focuses on establishing relationships between these environmental conditions and resulting physical and chemical changes, while also evaluating how tin-phosphate weighting influences degradation pathways. The results of this research would contribute to developing improved preservation protocols for historical silk artifacts and optimizing silk performance in contemporary applications, advancing our understanding of protein polymer degradation in diverse environmental contexts.

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## Acidic emissions from PVC: A potential problem for museums and galleries

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Polyvinyl chloride (PVC) has been widely used since the 1920s in various industrial and consumer products. While PVC degradation has been extensively studied in the context of high temperatures, UV exposure, and outdoor conditions, these studies are less relevant to the conservation community, where optimal long-term storage is essential. PVC and its degradation represent a big challenge for museums and galleries. One of the main problems is the release of acidic emissions, which can damage valuable materials such as paper, textiles and leather, present in museums and archives. Understanding these emissions is therefore of the utmost importance for the preservation of the PVC object itself and the environment in which it is stored or displayed [1,2].

This study aimed to identify acidic compounds released during PVC thermal degradation, evaluate their role in indoor pollution, and provide deeper insight into hydrogen chloride (HCl) emission behavior. A modified Oddy test [3] was applied to evaluate emissions from various PVC materials and their potential to damage surrounding materials, using cellulose paper as a reference. Results showed that unplasticized and older PVC samples emitted more harmful compounds and caused greater reference material degradation compared to plasticized PVC.

Acidic gas emissions were assessed using the Markes Micro-Chamber/Thermal Extractor  $\mu$ CTE120 in surface emission mode. Samples were collected on pre-cleaned silica gel and charcoal sorbent tubes, then extracted and analyzed with ion chromatography equipped with a conductivity detector. To confirm the identity of the acidic species, ion-exclusion chromatography was also employed. Emission experiments were carried out at temperatures ranging from 80 to 120 °C, using sequential sampling. The data revealed a two-phase emission profile for HCl, with the second phase demonstrating a steady emission rate. Based on the calculated activation energy, HCl emission rates at room temperature were extrapolated and subsequently used to estimate the equilibrium concentration of HCl in a typical storage box.

Besides HCl, emissions of formic and acetic acids were detected and quantified. Notably, acetic acid concentrations correlated well with the cross-contamination test results. Nevertheless, further studies are required to elucidate the origins of these acidic compounds and to assess their role in the degradation process of PVC.

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## Fungal Biosorption and Electrochemical Detection of Polystyrene Nanoplastics: Advancing Sustainable Remediation and On-Site Monitoring

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Nanoplastics (NPs) are emerging contaminants of concern due to their ability to penetrate biological membranes and accumulate in ecosystems, posing a risks to environment and human health [1]. Despite great importance, the removal and monitoring of NPs remain challenging due to their size ( $< 1 \mu\text{m}$ ) and the limitations of conventional remediation and analytical methods, which often require separation step (e.g. filtration of particles). This work presents an innovative approach for both the remediation and electrochemical sensing for the detection of polystyrene nanoplastics (PSNPs). The biosorption potential of medicinal fungi biomass (*Trametes versicolor*), was evaluated using Eu-doped PSNPs. The use of *Trametes versicolor* for the biosorption of PSNPs from aquatic systems presents a promising biosorbent, offering a sustainable and readily available alternative for NPs mitigation [2]. The adsorption efficiency was systematically investigated under various operational parameters, including solution volume-to-biomass ratio, contact time, and adsorption mode (batch vs. column). Optimization of conditions led to a substantial improvement in removal efficiency up to 77.7%. The PSNPs analysis was carried out with the use of inductively coupled plasma atomic emission spectroscopy (ICP-OES) through Eu determination. Due to the complexity of instrumentation and high cost of europium-based NPs standards, a complementary electrochemical sensor was used for fast, cost-effective, and real-time alternative for PSNPs detection. Gold screen-printed electrodes (SPEs) were modified with a mesoporous silica thin film via electro-assisted deposition, followed by functionalization with epoxy silane and proline [3, 4] to enhance nanoparticle interaction. Using cyclic voltammetry (CV), the sensor enabled rapid and sensitive electrochemical detection of 6.1 nm PSNPs. When fungal biomass was introduced to the PSNPs suspension, a near-complete adsorption of PSNPs was detected without any evidence of interference with the SPE sensor. Adsorption kinetics and isotherm models were used for the evaluation of interaction mechanisms and sorption capacity of the fungal biomass toward PSNPs. This approach offers a promising tool for in-situ monitoring of NPs and contributes to the development of sustainable strategies for tracking and removal of plastic pollution in aquatic systems.

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## Green SiO<sub>2</sub> surface modifications using ethanol extract from valorized fruit waste: enhancing methylene blue adsorption for sustainable water treatment

Rasim Omanović<sup>1\*</sup>, Jasmina Sulejmanović<sup>1</sup>

Effective methods for wastewater recovery and reuse are essential [1]. This study presents a novel class of mesoporous silica-based sorbents, modified at room temperature (RT) with 70% ethanol extracts of lemon (L), grape (G), and pomegranate (P) peel waste, for wastewater purification. All sorbents showed increased affinity for methylene blue (MP) removal with rising pH (3-7), achieving maximum efficiencies at pH 7: 98.6% for SiO<sub>2</sub>-P-70%-RT, 97.7% for SiO<sub>2</sub>-L-70%-RT, and 99.0% for SiO<sub>2</sub>-G-70%-RT. Based on these results, an optimized adsorption procedure was developed for SiO<sub>2</sub>-G-70%-RT sorbent using a batch method, with optimal parameters: initial MB concentration (20 mg/L), pH (5 - 7), sorbent mass (25 mg), contact time (40 min), and solution temperature (20 ± 2 °C). Kinetic and isotherm studies suggest a mixed adsorption mechanism, best described by the pseudo-second-order and Freundlich models. Additionally, the sorbent demonstrated stable reuse over four cycles, with a maximum capacity of 50.6 mg/g. Characterization after modification and application confirmed successful performance via FTIR, SEM, EDS, and XRD analyses. This approach offers a cost-effective, sustainable alternative for dye removal and opens new avenues for similar sorbent development and process optimization using fruit waste extracts, particularly pomegranate and lemon, given their exceptionally high affinity for this cationic dye.

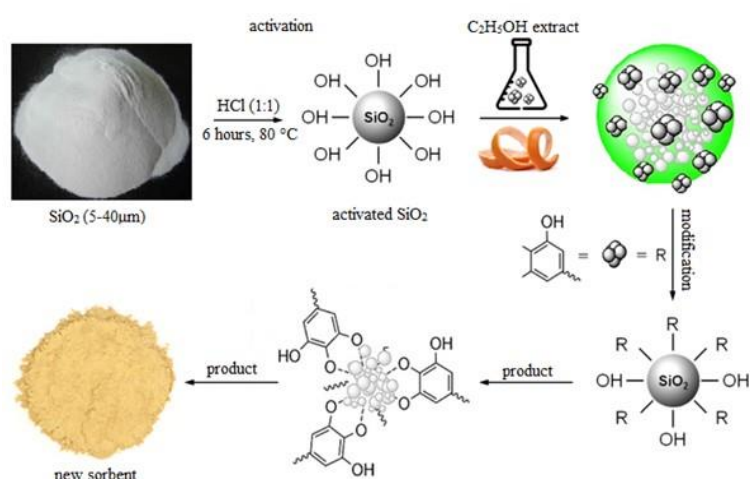


Figure 1. The SiO<sub>2</sub> modification process using ethanol extracts from grapefruit peel [2].

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## Comparison of three different conifer species as bioindicators for the assessment of air pollution with metals

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Interactions between humans and the environment represent a significant subject of research, especially in the context of the negative impacts of anthropogenic activities on air quality. In order to improve methods of environmental assessment, biomonitoring using natural bioindicators is becoming increasingly relevant, offering a more economical and accessible alternative to conventional monitoring methods. Conifer needles meet the basic requirements for bioindicators used in environmental monitoring, which are wide availability and ease of sampling [1]. In this research, the content of selected metals in different species of conifers was determined. All samples were prepared by dissolving in HNO<sub>3</sub> (65 %) and H<sub>2</sub>O<sub>2</sub> (30 %), and are prepared in triplicate. Before digestion, samples of conifers were air dried [2]. The content of Cr, Cu, Mn, Fe, Co, Ni, Cd, Pb and Zn in three different species of conifers *Picea abies* L., *Thuja plicata* D. and *Juniperus communis* L. from industrial location in Sarajevo, Bosnia and Herzegovina was examined. Metal concentration was determined using the flame atomic absorption spectrometry (FAAS). The concentration of Co, Ni, Cd, Pb were below the limit of detection (LOD) of FAAS. The metal content in the samples ranged from: < LOD-0,40 µg/g (Cr); (3,17-4,12) µg/g (Cu); (21,10-43,03) µg/g (Mn); (80,41-100,8) µg/g (Fe) and (12,92-25,86) µg/g (Zn). Pearson correlation coefficients between metals were also calculated to potentially provide some answers about the sources of metal emissions to the environment.

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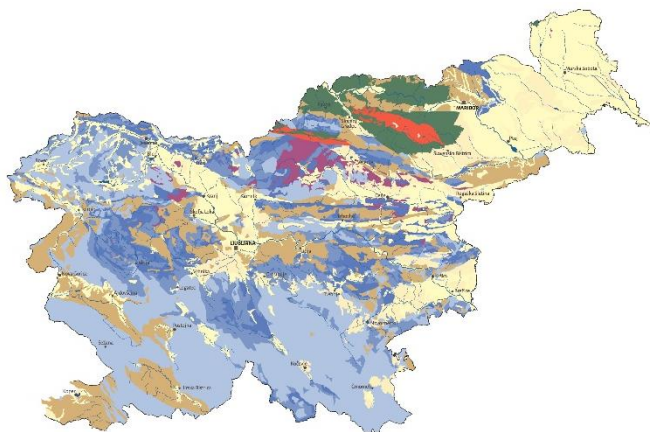
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## Slovenian Dolomites as a Potential Source of Magnesium

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The surface of Slovenia consists mainly of sediments and sedimentary rocks, of which limestone and dolomite are the most widespread (Figure 1). Dolomite deposits together cover about 10 % of Slovenia's territory [1]. Dolomite is a type of carbonate sedimentary rock. According to the molecular formula of its pure form  $\text{CaMg}(\text{CO}_3)_2$ , it contains 13.2 % magnesium by weight. This and its abundance compared to other mineral sources (such as magnesite and talc) make it an important source of magnesium [2]. As the demand for magnesium is constantly increasing due to its diverse industrial uses and new potential applications (e.g. energy storage), it has been categorised as a critical mineral resource [3]. In our study, a dolomite sample, identified as dolomite rock, was collected from a Slovenian quarry. The elemental composition of the sample was determined by microwave-assisted acid digestion and ICP-OES. The sample was found to be very pure dolomite, with the magnesium mass percentage close to the ideal value and the molar ratio between calcium and magnesium only slightly in favour of calcium ( $\text{Ca} : \text{Mg} = 1 : 0.96$ ). The sample was subjected to two hydrometallurgical processes – selective leaching and selective precipitation. The utilisation of differences in the solubility of calcium and magnesium salts led to a successful separation of the two elements and the production of magnesium-rich fractions.



**Figure 1:** Lithological map of Slovenia – shades of brown represent sediments; shades of blue represent sedimentary rocks. Darker blues indicate dolomite deposits. (Source: Geological Survey of Slovenia)

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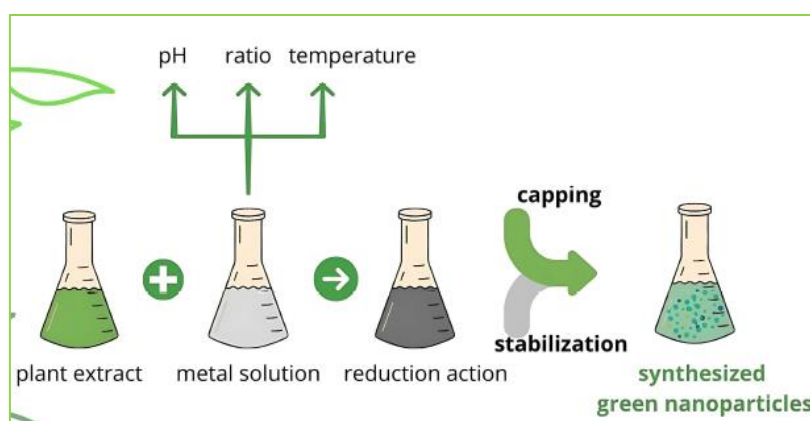
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## To control or not to control? Optimization of the process of synthesis of metallic nanoparticles produced by green chemistry

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In nanoparticle synthesis, particular attention is given to green methods, which are environmentally friendly and sustainable approaches utilizing natural materials and processes. The shape and size of nanoparticles directly influence their physicochemical properties, as smaller particles exhibit a higher surface-to-volume ratio, enhancing their reactivity [1]. Precise control over morphology and dimensions improves process efficiency, reduces energy consumption and raw material usage, and optimizes antimicrobial efficacy against bacteria and viruses, which is crucial for medical applications. Our study focuses on the physicochemical characterization of synthesized nanoparticles through UV-Vis spectroscopy, which confirms the formation of silver and copper nanoparticles, X-ray diffraction (XRD) for verifying their crystalline structure, and Transmission Electron Microscopy (TEM) for assessing morphology, size, and uniformity. The registered UV-Vis spectra confirm nanoparticle formation, while XRD diffractograms validate their successful synthesis. Nanoparticles with controlled size and shape exhibit excellent stability under various environmental conditions, making them highly suitable for diverse applications.



**Figure 1:** The step of nanoparticle synthesis using plant extract.

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## Study of chromophore-containing water-insoluble organic carbon in atmospheric aerosol particles

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Organic carbon is an important constituent of atmospheric aerosol particles, comprising a diverse array of compounds with various physical and chemical properties. Among these, light-absorbing organic compounds significantly influence radiative forcing due to their optical properties, impacting the climate. However, only about 40 % of organic compounds have been characterized on a molecular level. The poor chemical characterization, insufficient systematic research, and unknown sources of secondary-produced forcing agents are the cause of extremely high uncertainties in the estimation of radiative forcing by atmospheric aerosols. Therefore, it is crucial to characterize the organic compounds on a molecular level, especially those exhibiting chromophores and insolubility in water, i.e., water insoluble organic carbon (WIOC).

In this work, we will integrate a suite of state-of-the-art analytical techniques to address these gaps in the existing knowledge. The first step will be collecting atmospheric aerosol particles and developing optimized extraction methods tailored to chromophore-containing WIOC, which remain poorly investigated. Chromatographic techniques, hyphenated with mass spectrometry, will be used to separate and chemically identify the extracted compounds, enabling classification into distinct groups. Complementary spectroscopic analyses will focus on the detection of chromophore-containing species, which affect the atmosphere's heating. Despite the evolution of state-of-the-art instruments, challenges still persist in resolving the complex nature of WIOC compounds, due to their highly dynamic behaviour. Addressing these challenges and enhancing the resolution and sensitivity of the analytical methods are central goals of this research, ultimately aiming to enable comprehensive identification and characterization of WIOC species exhibiting chromophores.

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## Electrochemical Impedance Spectrometry for Measuring Surface Tension Decrease on a Mercury Electrode

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Ivan Konjević<sup>1,2</sup>, Kristijan Vidović<sup>1\*</sup>, Nikola Tasić<sup>1</sup>, Samo B. Hočevar<sup>1</sup>

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Atmospheric aerosols are suspensions of fine solid and/or liquid particles in the gas phase. They are crucial for atmospheric processes and influence human health and the global climate. Significant constituents of atmospheric aerosol particles are surface-active substances (SAS). Their unique structure involving hydrophobic and hydrophilic components causes their partition at the gas-liquid interface, thus lowering the particles' surface tension. SAS are expected to affect the particles' formation, growth, size distribution, and optical properties [1].

Measuring the surface tension of aerosol particles is of crucial importance for understanding atmospheric phenomena. Techniques like the Wilhelmy Plate, Du Noüy Ring, and Pendant Drop tensiometry are commonly used for bulk samples. However, the main drawback of these methods is their sensitivity to salt content, which introduces artefacts in the surface tension measurements. Changes of the surface tension caused by SAS can also be measured using electrochemical methods, which have several advantages, such as high accuracy, fast response time, and particularly low detection limits [1-3].

In this research, we are developing an electrochemical method for measuring the decrease in surface tension on a mercury electrode surface caused by the presence of SAS using electrochemical impedance spectrometry (EIS). EIS allows for the measurement of the double-layer capacitance, which is altered in the presence of SAS. By measuring the double-layer capacitance, the surface charge can be determined, which is, through the electrocapillary equation, directly correlated with the surface tension [3].

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