Coalesce Research Group

APPROVED PROVIDER #782310

*Joint Event*

7th International Conference on

# Chemistry

&

5th International Conference on

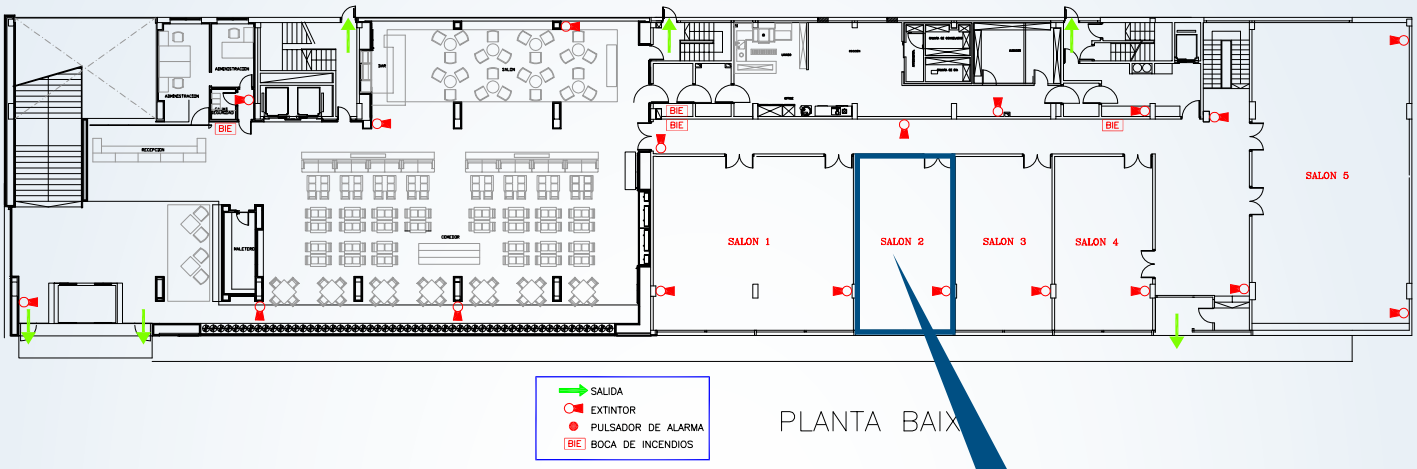
# Mass Spectrometry and Analytical Techniques

November 11-12, 2024
Barcelona, Spain

**Coalesce Research Group**
33 Market Point Dr,
Greenville, SC 29607, USA

**Contact Us:**
**Phone:** +1-718-543-9362

# Conference Hall




Conference Hall

# Scientific Program

**Monday**
**November 11, 2024**

7th International Conference on **Chemistry**

**&**

5th International Conference on

# Mass Spectrometry and Analytical Techniques

| Day 1 - November 11, 2024 | |
|---|---|
| Meeting Hall: Sala Forum B | |
| 09:00 - 09:45 | Registrations |
| 09:45 - 10:00 | Introduction |
| Keynote Presentations | |
| 10:00 - 10:40 | Designing Bimetallic Catalysts for Energy and Environment |
| | **Jaroslaw Polanski, University of Silesia, Poland** |
| 10:40 - 11:20 | Sustainable Transportations: Performance Additives for Lubricating Oil - Synthesis and Evaluation |
| | **Pranab Ghosh, University of North Bengal, India** |
| Networking & Refreshments: 11:20 - 11:40 @ Foyer | |
| 11:40 - 12:20 | Applications of Vanadium and Tantalum Single-Site Catalysts in Heterogeneous Catalysis |
| | **Stanislaw Dzwigaj, Sorbonne Universite, France** |
| Oral Presentations | |
| Session Chair: | **Stanislaw Dzwigaj, Sorbonne Universite, France** |
| Session Chair: | **Pranab Ghosh, University of North Bengal, India** |
| **Sessions:** | Mass Spectrometry Imaging \| Mass Spectrometry in Proteome Research \| UV, IR and Ion Spectroscopy\| Mass Spectroscopy in Clinical Science \| Organic and Inorganic Chemistry \| Medicinal and Clinical Chemistry \| Analytical and Surface Chemistry \| Physical Chemistry \| and Theoretical Chemistry \| Biochemistry \| Nano Chemistry |
| 12:20 - 12:45 | Characterization of Isolated Strains of Micro Organisms from Minerial Mountain and Spring waters from France, England, South Korea, Japan, The Netherlands and Bulgaria |
| | **Nedyalka Valcheva, Thrace University, Bulgaria** |
| 12:45 - 13:10 | Vapour-Phase Condensation of Ethanol into 1-Butanol Over Mg-Al(-M) Oxide Catalysts (M: Y, La, Ce) |
| | **K.V.Valihura, Institute of Physical Chemistry of National Academy of Sciences of Ukraine, Ukraine** |
| Group Photo: 13:10 - 13:20 | |
| Lunch 13:20 - 14:30 @ Restaurant | |
| 14:30 - 14:55 | Native Electrospray Ionization Mass Spectrometry (ESI-MS) in the Assessment of Novel DNA Ligands |
| | **Alberto Ongaro, University of Padua, Italy** |

# Scientific Program

**Monday**
**November 11, 2024**

7th International Conference on **Chemistry**

**&**

5th International Conference on

# Mass Spectrometry and Analytical Techniques

| Poster Presentations | |
|---|---|
| 14:55 - 15:15 | Method Optimization to Analyse Organic Acids in Urine Samples by GC-MS in a Clinical Laboratory |
| | **Laura Conesa, Vall d'Hebron Hospital, Spain** |
| 15:15 - 15:35 | Profiling Polysorbate 80 Components Using Comprehensive Liquid Chromatography–Tandem Mass Spectrometry Analysis (LC-MS/MS) |
| | **Yutaka Konya, Shimadzu Techno-Research, Japan** |
| 15:35 - 15:55 | Sorption Activity of Surfactant Modified Natural Armenian Zeolites Regret to Metals Removal from Natural Aquatic Systems |
| | **Alla Manukyan, Armenian National Agrarian University, Armenia** |
| 15:55 - 16:15 | Induction Heating Catalysis in $CO_2$ Methanation |
| | **Tomasz Siudyga, University of Silesia, Poland** |
| Networking & Refreshments 16:15 - 16:35 @Foyer | |
| 16:35 - 16:55 | Assessment of Antioxidant Activity of Piperazine-1,3,5-Traizine Dual Agents for FAAH and 5-HT6 Serotonin Receptor Ligands |
| | **Malgorzata Starek, Jagiellonian University Medical College, Poland** |
| 16:55 - 17:15 | Comprehensive Procedure for Monitoring Environmental Hazards Resulting from Antibiotic Contamination |
| | **Monika Dabrowska, Jagiellonian University Medical College, Poland** |
| 17:15 - 17:35 | Biomimetic Spinning of Crosslinked and Functionalized Spider-Silk Proteins with Multiarm Polyethylene Glycol |
| | **Viktors Romanuks, Latvian Institute of Organic Synthesis, Latvia** |
| 17:35 - 17:55 | Characterization of Bacterial Strains Isolated from the hypothermal Spring "Kariera" in the Area of Yablkova Village, Dimitrovgrade Municipality, Haskovo Region, Bulgaria |
| | **Denis Haralanov, Vocational High School, Bulgaria** |
| 17:55 - 18:15 | Characterization of Bacterial Strains Isolated from the hypothermal Spring "Osmanova Chehma" in Yablkova District, Dimitrovgrade, Region Haskovo, Bulgaria |
| | **Diyana Danailova, Vocational High School, Bulgaria** |
| 18:15 - 18:35 | Database with Integrated Machine Learning Aided Catalyst Design |
| | **Uladzislau Zhdan, University of Silesia, Poland** |
| Day-1 Concludes followed by Award Certifications | |

# Virtual Program

**Monday**
**November 11, 2024**

7th International Conference on **Chemistry**

**&**

5th International Conference on

# Mass Spectrometry and Analytical Techniques

| Virtual Presentations<br>Day-01 : November 11, 2024 (GMT) | |
|---|---|
| 10:00 - 10:15 | **Introduction** |
| **Presentations** | |
| 10:15 - 10:40 | Computer-Assisted Synthesis of Pyrrolo[4,3,2-de] Quinolinone Derivatives by Suzuki Coupling<br>**Barbara Bruni, Universidade de Lisboa, Portugal** |
| 10:40 - 11:05 | Eco-Friendly Dishwashing Liquid from Orange and Banana Peels: A Sustainable Solution to Chemical Pollution<br>**Kairatova Elina Kairatovna, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 11:05 - 11:30 | Environmental Justice in Industrial Cities: Addressing Health Inequalities in Atyrau, Kazakhstan Through Targeted Air Pollution Mitigation<br>**Symbat Bolatova, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 11:30 - 11:55 | Design and Analysis of an Innovative Enzymatic-Filter (E.F) for Purifying Air Contaminated with Sulfur Dioxide ($SO_2$)<br>**Zhanerke Yerbolatova, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 11:55 - 12:20 | Study of Properties of Magnetized Water<br>**Amangeldy Nuriya, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 12:20 - 12:45 | Possible Application of Quarks<br>**Muslim Zhasulanuly, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 12:45 - 13:10 | Effective Adsorbent for Iron, Lead, Zinc Ions<br>**Alihan Doskaliev, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 13:10 - 13:35 | AI-Optimized Algae Cultivation for Sustainable Biodiesel Production<br>**Sailau Adina Nurlankyzy, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 13:35 - 14:00 | Magnetized Nanotechnology for Oil Spill Cleanup: Evaluating the Efficiency of Ferrofluid-Mediated Oil-Water Separation<br>**Andossova Aizere, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 14:00 - 14:25 | Potential Application of Innovative Solid Waste Materials for Adsorptive Removal of Toxic Phenol from Wastewater for Ensuring Cleaner Environment and also for Generating Circular Economy<br>**Ashanendu Mandal, University of Calcutta, India** |
| Day-1 Virtual Conference Concludes | |

# Virtual Program

**Tuesday**
**November 12, 2024**

7th International Conference on **Chemistry**

**&**

5th International Conference on

# Mass Spectrometry and Analytical Techniques

| Day-02 : November 12, 2024 (GMT) | |
|---|---|
| 10:00 - 10:15 | **Introduction** |
| **Presentations** | |
| 10:15 - 10:40 | Natural Cleaner: Innovative Household ECO Detergent<br>**Amangoskyzy Ayaulym, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 10:40 - 11:05 | Sustainable Biofuel Production from Plant Waste *via* Secondary Processing Techniques<br>**Kenzhebai Adilbek Azamatul, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 11:05 - 11:30 | Microscale Evolution of Two LDPE Trilayer Films: Influence of Stabilizer Placement on Accelerated Aging Monitored by FTIR and UV Analysis<br>**Meriam Imane Babaghayou, Ecole Normale Supérieure Laghouat, Algeria** |
| 11:30 - 11:55 | Production of Environmentally Friendly Textile Fabrics from Banana Waste<br>**Al-Aziza Lukpanova, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 11:55 - 12:20 | Natural Sorbents Purification of Water from Chemical Contamination by Synthetic Detergents<br>**Gulziya Beisenbekova, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 12:20 - 12:45 | Natural Bark Fibers as Reinforcement in Polymer Composites: A Review of Characterization Techniques<br>**Sivasubramanian Palanisamy, PTR College of Engineering and Technology, India** |
| 12:45 - 13:10 | The Water Filter "AnsAqua"<br>**Kabdelova Ansagan, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 13:10 - 13:35 | Land Restoration: Innovative Bioremediation using Indigenous Bacteria<br>**Dilnaz Nagim Nurzhankyzy, Nazarbayev Intellectual School in Direction of Chemistry and Biology, Kazakhstan** |
| 13:35 - 14:00 | Distinctive Properties of Non-Equilibrium Dynamic Plasmachemical Systems<br>**Daniil Tretiakov, Taras Shevchenko National University of Kyiv, Ukraine** |
| 14:00 - 14:25 | Exploring the Calming and Pain-Relief Effects of Plant-Derived Terpenes (Pdt): A Natural Approach to Therapeutics<br>**Aziza Abatova, Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan** |
| 14:25 - 14:50 | Thiazine 1,1-dioxide Derivatives as Potential Anticancer Agents<br>**Aleksandrs Pustenko, Latvian institute of organic synthesis, Latvia** |

| | |
|---|---|
| 14:50 - 15:15 | Discovery of Aromatic Sulfonamides as Potential Human Carbonic Anhydrase Inhibitors and its Emerging Role as Antiepileptic Agents |
| | **Abha Mishra, National Institute of Pharmaceutical Education and Research, India** |
| 15:15 - 15:40 | Determination of Perchlorate in Foodstuff |
| | **Olga Pardo Marín, Universitat de València, Spain** |
| 15:40 - 16:05 | The Use of Gas Discharge Imaging (Gdv), Spectrophotometry and Gc-Ms Methods to Study the Effect of Organic Fertilizers on the Quality of Leafy Vegetables |
| | **Svetlana Motyleva, Strogoorganic Online Gardening School, Russia** |
| Program Concludes followed by Vote of Thanks | |

# *Day-1*
# *Keynote Presentations*

# DESIGNING BIMETALLIC CATALYSTS FOR ENERGY AND ENVIRONMENT

**Jaroslaw Polanski**
*University of Silesia, Poland*

## Abstract

**Background:** People are interested in drugs and materials, the agents that manipulate the environment. With climate change emerging as a significant challenge, developing materials for energy and environmental sustainability has become a primary focus in materials design. Various catalytic and biocatalytic methods have been pioneered to reduce industrial processes' toxicity and environmental impact. Key areas of interest include green and sustainable chemistry, $CO_2$ conversion and functionalization, energy storage or biomass conversion.

**Objective:** This lecture will cover novel approaches to materials design using deep chemistry methods aimed at advancing predictive green and sustainable chemistry. We will discuss the idea of bimetallic catalysis. To explore the impact of drug design on molecular design, we introduce the concept of a privileged metal combination in bimetallics.

**Methods:** We recently developed a novel method called *nano-transfer* for bimetallic materials preparation. We used this in various processes for environment and energy.

**Results:** We described a variety of bimetallics for efficient low-temperature $CO_2$ to $CH_4$ conversion, such as nano-Ru/Ni with inductive heating catalyzed and ultra-low temperature conversion. Bimetallic systems also appeared to be efficient for biomass conversion or acetal synthesis. Finally, we will demonstrate how insights from bimetallic research have inspired a novel energy storage system.

**Conclusion:** Bimetallic catalysis can be a powerful approach in the energy and environment.

**Acknowledgements:** The research activities co-financed by the funds granted under the Research Excellence Initiative of the University of Silesia in Katowice, Poland. We also acknowledge the financial support of NCN Krakow, OPUS 2018/29/B/ST8/02303.

## Biography

Jaroslaw Polanski has a background in Chemistry from the Silesian Technical University of Technology in Gliwice and is a Professor of Organic Chemistry at the University of Silesia in Katowice, Poland. He is an expert in drug and materials design, developing an early self-organizing neural network architectures for molecular design, designing original catalysts for energy and environment, a novel system for energy storage, and several libraries of would-be drug candidates.

# SUSTAINABLE TRANSPORTATIONS: PERFORMANCE ADDITIVES FOR LUBRICATING OIL SYNTHESIS AND EVALUATION

**Pranab Ghosh**

*University of North Bengal, India*

## Abstract

Lubricating oil, also called base oil, is the basic building block of a lubricant. They are complex mixture of paraffinic, aromatic and naphthenic hydrocarbons with molecular weights ranging from C20-C70 (boiling range 622-673K). The lubricating oils in addition to primarily reducing the friction and wear, they provide assorted functions like dissipation of heat, prevention of corrosion and cushioning the shocks.

As the development has speeded up in a field of engine and transmission technologies which in turn demands an equally modern lubricant that complies with every possible requirement to produce maximum efficiency. Therefore, to produce such desired output from the said lubricant, oil needs some functional materials which may enhance the performance of the base oil tremendously. There are different types of additives which are used in petroleum base oils: i) Pour Point Depressant (PPD), ii) Viscosity Index Improver (VII) or Viscosity Modifier (VM), iii) Friction Modifier (FM), iv) Anti-wear Additive (AW), v) Detergent, vi) Antioxidant (AO), vii) Extreme Pressure Additive (EP), vii) Dispersant, viii) Anti-foaming Agent, ix) Rust and Corrosion Inhibitor.

The conjoint action of base oil and additives maintain superior machine functionality and lessen the possibility of recurrent malfunctions, which enables flat-level operations. In the modern world, the price of crude oil is increasing along with reservoir depletion. Therefore, maintaining a clean atmosphere is a serious obligation.

After careful scrutiny of literatures, it has made us to realise that, since many countries including India are producing an abundant of non-edible vegetable oils like Castor oil, Karanja Oil, Jatropha oil etc. and if such scale can be realized to the lubricating industries then it will bring down the dependency on petroleum based products, making a sustainable environment. Lots of work has been done by our group and many of them are in progress in this direction, some of them will be discussed in the presentation.

## Biography

Pranab Ghosh -Professor in Chemistry and Director, Research and Development Cell (additional charge) of the University of North Bengal, Darjeeling, INDIA. His Subject of Specialization is Organic Chemistry and Area of Research Interest is: Natural Product Chemistry, Organic Synthesis and synthetic Methodology, Polymer Chemistry and Lube oil additives. Professor Ghosh has guided 37 Ph.D. students to receive their PhD degree. So far, his group has published around 300 Research papers and patented 6 innovations. About 20 book chapters/books of his research group have published with publishers like, Springer, Bentham, Elsevier, Taylor and Francis, Wiley etc. Research paper of his group "β-Cyclodextrin: A supramolecular catalyst for metal free approach towards the synthesis of 2-amino-4,6-diphenyl -nicotinonitriles and 2,3-dihydroquinazolin -4(1H) -one", has ACCEPTED AS 'HOT ARTICLE' for the year 2021-2022 in Royal Society of Chemistry Journal." RSC Adv., 2021, 11, 1271–1281. Prof Ghosh has selected as the "Research Fellow" of INTI International University, Malaysia for two years. December 2023 to Dec 2025. He is the Recipient of UGC Mid-Career Award 2019. He is also the Convenor of CRSI NORTH BENGAL LOCAL CHAPTER Professionally he is with more than 25 yrs of teaching and about 7 yrs of Industrial experience. As an Administrator he has served the University of North Bengal in different capacities including, as the Registrar for 2 yrs. He is the President of the Institution`s Innovation Council (IIC), NBU since 2018.

# APPLICATION OF VANADIUM AND TANTALUM SINGLE-SITE ZEOLITE CATALYSTS IN HETEROGENEOUS CATALYSIS

**Stanislaw Dzwigaj**

*Sorbonne Universite, France*

## Abstract

The metal ions well dispersed at zeolite framework are considered to be active sites of catalytic processes. Therefore, the incorporation of these metals into zeolites as isolated tetrahedral sites appears to be the important task. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions results in the reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite. During my keynote talk the design of single-site zeolite catalysts with transition metal will be described and characterized by different physical techniques both at the macroscopic (XRD, BET, TPR, TEM) and molecular level (FT-IR, NMR, DR UV-Vis, XPS, EPR, XAFS). The application of metal single-site zeolite catalysts in environmental catalysis will be discussed. This two-step postsynthesis method applied in this work allowed obtaining vanadium and tantalum single-site zeolite catalysts active in different catalytic processes such as oxidative dehydrogenation of propane into propene, selective catalytic reduction of $NO_x$ to $N_2$, production of 1,3-butadiene from renewable sources, including ethanol obtained from biomass. Their catalytic activity strongly depended on the speciation and amount of vanadium or tantalum incorporated into zeolite structure as well as their acidity.

## Biography

Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris) he obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements, he received the title of professor. His published work includes more than 170 papers published in reputable international journals.

# *Day-1*
# *Oral Presentations*

# CHARACTERIZATION OF ISOLATED STRAINS OF MICROORGANISMS FROM MINERAL, MOUNTAIN AND SPRING WATERS FROM FRANCE, ITALY, ENGLAND, SOUTH KOREA, JAPAN, THE NETHERLANDS AND BULGARIA

**Nedyalka Valcheva**

*Thrace University, Bulgaria*

## Abstract

The aim of the present work is to isolate, identify and investigate the species of bacteria from medicinal, mountain and spring waters in the area of Paris, France, Rome, Italy, London, England, Busan, South Korea, Tokyo, Japan, Amsterdam, the Netherlands and in Bulgaria. 126 bacterial strains were isolated and their colonial and morphological characteristics were determined and the study strains were identified. The data show that the isolated 9 strains from the hypothermal healing spring waters in the Paris area, France were identified as N. Valcheva - *Lisinibacillus pakistanensis*, *Serratia marcescens* (four strains), *Staphylococcus hominis, Staphylococcus haemoliticus, Bacillus pumilus* and *Bacillus cereus*. The isolated strains from thermal healing springs in Saturnia, Tuscany region and Fontana di Trevi in Rome, Italy were identified as N. Valcheva - *Tiobacillus Ferrooxidans, Staphylococcus cohnii*, from a hypothermal spring in the London area as N. Valcheva - *Aeromonas caviae, Pseudomonas chlororaphis*, from a mountain spring in the region of Busan, South Korea, was identified as N. Valcheva - *Bacillus safensis, Staphylococcus cohnii, Pseudomonas chlororaphis, Staphylococcus cohnii*. From a mountain geothermal spring in the region of Tokyo, Japan, strains were identified as N. Valcheva - *Bacillus safensis , Phellodendron chinense, Aeromonas caviae, Pseudomonas japonica*. The strains identified in the Amsterdam area, the Netherlands were identified as N.Valcheva&A.Atanasova-*Aeromonas viridans*, N.Valcheva & V.P.Panteleev - P. japonica, N.Valcheva&V.V. Panteleev - *Aeromonas salmonicida*, N.Valcheva&A.V. Panteleev - Aeromonas caviae, N.Valcheva&L.A.V. Panteleeva - Phellodendrom chinense. The strains from Bulgaria were identified from 100 hypothermal, thermal and common springs from 11 regions and belong to the following 14 genera: *Bacillus, Brevibacillus, Geobacillus, Aeromonas, Klebsiella, Pseudomonas, Staphylococcus, Stenotrophomonas, Serratia, Nocardia, Trichosporon, Azoarens, Lisinbacillus, Rodococcus* . All 1-time strains were isolated from sources. The difference in the type of strains identified can be explained by the influence of the composition of the water, the type of soil and rocks through which it passes, the temperature, the pH of the environment and the different geographical location

# VAPOUR-PHASE CONDENSATION OF ETHANOL INTO 1-BUTANOL OVER MG-AL(-M) OXIDE CATALYSTS (M: Y, LA, CE)

**K.V. Valihura**

*Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Ukraine*

## Abstract

**Background:** Conversion of ethanol (EtOH) into 1-butanol (BuOH) via the Guerbet coupling received wide attention due to the sufficient supply of bio-EtOH and the versatile applications of BuOH. One of the promising catalysts for this process are $MgO\text{-}Al_2O_3$ systems with advanced acid-base properties.

**Objective:** The study on the influence of modifier nature of rare earth elements on physicochemical characteristics and catalytic properties of Mg-Al(-M) oxide systems (M: Y, La, Ce) in the vapour phase condensation process of EtOH with the obtaining of BuOH.

**Methods:** Samples were characterised by X-ray diffraction, low-temperature N2 ad(de)sorption, and temperature-programmed desorption of $NH_3$ and $CO_2$. Catalytic studies were carried out in a flow reactor under atmospheric pressure with a fixed bed catalyst at 275–400°C, WHSV 0.14 $g \cdot gcat^{-1} \cdot h^{-1}$.

**Results:** The highest selectivity values for BuOH formation are achieved at 275 °C. With increase of operation time the selectivity decreases significantly in the presence of the investigated $MgO\text{-}Al_2O_3$ based catalysts except of Mg-Al-Y sample. For Y-modified system the initial selectivity for BuOH is 77% and after 6 h on stream it remains at the level of 75%. For Mg-Al-La the noticeable formation of side heavy $C^{5+}$ condensation products was observed and for Mg-Al-Ce sample the significant amount of unconverted intermediate product acetaldehyde, which increases with operation time, was detected.

**Conclusion:** Mg-Al-Y-oxide catalyst was established to have the highest selectivity for the target product BuOH, as well as the stability of operation over time. The positive effect of yttrium consists in the formation of additional acidic and basic surface sites.

## Biography

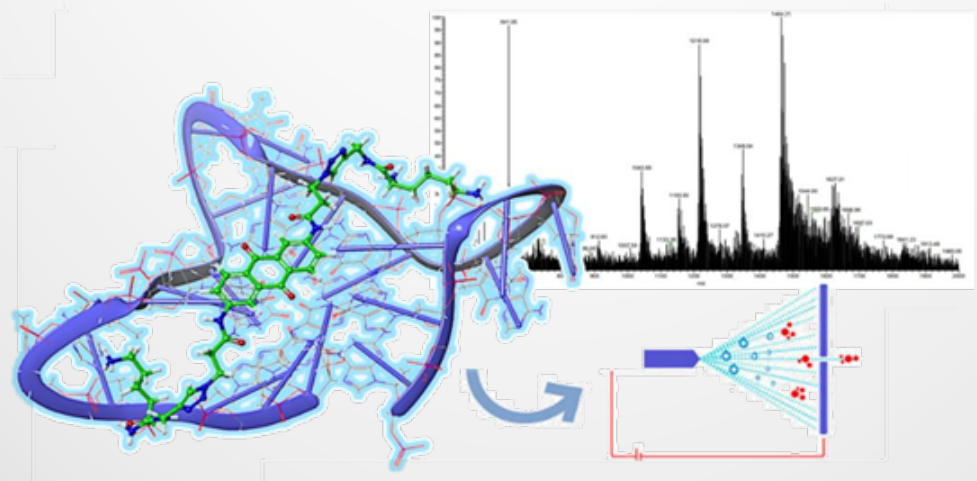
K.V. Valihura defended the thesis "Effect of the composition of Mg(II), Al(III), Zr(IV) oxide systems on their catalytic properties in the processes of gas-phase conversion of ethanol and 1-butanol with doubling of the carbon chain", scientific supervisor Dr.Hab. S.O. Soloviev. She holds the position of a Researcher in a Department of Catalytic Oxidative-Reductive Processes, L.V. Pisarzhevskii Institute of Physical Chemistry of the NASU and currently she is a Visiting Researcher at the Department of Chemical and Environmental Engineering of Higher School of Engineering, University of Seville, Spain.

# NATIVE ELECTROSPRAY IONIZATION MASS SPECTROMETRY (ESI-MS) IN THE ASSESSMENT OF NOVEL DNA LIGANDS

**Alberto Ongaro**
*University of Padua, Italy*

## Abstract

The deoxyribonucleic acid (DNA) is a macromolecule containing the genetic code of organisms and is usually found in its canonical form called double-stranded (ds) DNA formed by two DNA strands held together by Watson-Crick-type base-pairs. Targeting precise sequences of dsDNA with small molecules is a matter of great interest for the medicinal chemist as it causes a variety of significant biological responses, however its peculiar size and the high level of similarity among sequences make it an elusive target for selective drug action. Structures that disobey the Watson-Crick canon are described as non-canonical and provide for less common base pairing patterns. One of the most studied non-canonical forms is the G-quadruplex (G4) which appears in guanine-rich sequences and is present in several genomes, from viruses to humans. Due to their peculiar localisation, the induction of G4 formation or G4 stabilisation with small molecules represents a strategy for interfering with crucial biological functions. Studying the DNA-recognition event by small molecules, at the molecular level with the aim of fully understanding the pharmacological effects induced is challenging. Native electrospray ionisation mass spectrometry (ESI-MS) is a very powerful tool to study these non-covalent assemblies. Quantitative parameters obtained from ESI-MS studies, such as binding affinity (BA), equilibrium binding constant and sequence selectivity represent valuable information for the evaluation of new potential DNA ligands.In the past years, we took advantage of this technique for the evaluation of various new ligands for the recognition of ds or G4 DNA and three different works will be presented. We first applied the Native MS tehcnique for the assessment of a new ametantrone derivative designed to selective recognize palindromic dsDNA sequences which demonstrated its ability to promote the apoptosis on cancer cell lines.In a second work, a set of 6 mono and one di-substituted propargylamine anthracene derivatives was studied identifying a new G4-selective ligand. In the last presented work, we took advantage of the technique to screen seven newly synthesized amino acid-anthraquinone click chemistry conjugates for their ability to interact with human telomeric G4, for five of the seven compounds a marked selectivity for G4 over dsDNA was detected.



## Biography

Alberto Ongaro always loved chemistry, which is why he first obtained in 2015 a Bachelor's degree in Chemistry at the University of Venice and then in 2017 a Master's degree in Chemistry at the University of Padua. After graduation, he worked for one year as an early-stage researcher and then he decided to pursue a Ph.D. in Precision Medicine at the University of Brescia which ended in 2021. For three years, he is continuing his research experience in academia with post-doctoral positions at the Department of Pharmaceutical and Pharmacological Sciences of the University of Padua. He specialised in Medicinal Chemistry and Organic Chemistry with a focus on the synthesis and the study of interaction of small molecules with macromolecules such as proteins and nucleic acids.

# *Day-1*
# *Poster Presentations*

# METHOD OPTIMIZATION TO ANALYSE ORGANIC ACIDS IN URINE SAMPLES BY GC-MS IN A CLINICAL LABORATORY

## Laura Conesa

*Vall d'Hebron Hospital, Spain*

## Abstract

**Background:** Organic acids (OA) play an important role in human metabolic processes since they are related to a group of inborn errors of metabolism, characterized by the accumulation of these analytes mostly in urine. Identification and quantification of these compounds provide valuable information about the physiological condition of metabolic processes. Gas chromatography-mass spectrometry (GC-MS) is the gold standard method to screen organic acidurias, involving challenging steps of sample preparation and derivatization prior to injection.

**Objective:** To optimize the liquid-liquid extraction process of OA in urine samples from the current method used in our laboratory, and to develop a quantitative method to analyse them by GC-MS.

**Methods:** Optimization process comprise the improvement of the extraction yield by testing several combinations of different volumes of sample, compositions and volumes of polar solvents, as well as the number of extraction steps. Regarding instrumental method, a temperature gradient (50-290°C) for 36 min per sample and scan mode were performed (50-500 m/z). For quantification, certified standards with their corresponding internal standards were used to create calibration curves for 34 compounds. Measuring ranges were adjusted to cover the clinically relevant concentrations. Target and reference ions were defined for each analyte and libraries were employed for identification.

**Results:** Pre-treatment was optimized by reducing original sample volume to 250 µl and adding methanol. Extraction steps were reduced from 4 to 2 (ethyl acetate). The new extraction conditions ensured equivalent areas in most of the tested analytes. Calibration curves showed good linearity (r2>0.99). Compounds with no standards available were semi-quantified with external controls acting as standards.

**Conclusion:** The strategy proposed optimizes resources and technical staff time. Quantification of OA with certified standards improves diagnosis and management of patients. To apply this methodology in clinical practice is still needed an extended validation in terms of reproducibility, robustness and clinical concordance.

## Biography

Laura Conesa was graduated in chemistry and master in chemical pharmacology. Always has been interested in medicinal chemistry, so she developed her PhD focussed on the design and synthesis of biological compounds with potential anticancer activity. She attended some symposiums and conferences related to this field and started working in the clinical laboratory of Vall d'Hebron Hospital in Barcelona four years ago. At the present time, she continues working in the area of chromatography and mass spectrometry, managing the identification/quantification of analytes related to health, such as drugs, vitamins, trace elements, organic acids or hormones. The complexity of the hospital leads her to be aware of the recent advances and to develop new methodologies to incorporate novel analysis in the catalogue of services.

# PROFILING POLYSORBATE 80 COMPONENTS USING COMPREHENSIVE LIQUID CHROMATOGRAPHY–TANDEM MASS SPECTROMETRY ANALYSIS (LC–MS/MS)

**Yutaka Konya**

*Shimadzu Techno-Research, Japan*

## Abstract

**Background:** Polysorbate 80 (PS80) is an amphipathic, nonionic surfactant most commonly used in pharmaceutical protein formulations and is composed of fatty acid (FA) esters of polyethoxylated sorbitan. However, commercial PS80 products contain substantial amounts of by-products. The development of simple and reliable methods for PS80 component analysis is challenging given the inherent heterogeneity.

**Objective:** To develope a comprehensive liquid chromatography–tandem mass spectrometry (LC–MS/MS) method to profile the components of PS80.

**Methods:** Semi-comprehensive LC–MS/MS analyses of 11 subspecies in three commercial PS80 products were performed to estimate the average degree of polymerization of the ethylene oxide units (Avg-n) in the molecules. Furthermore, three subspecies (polyoxyethylene sorbitan monoester, polyoxyethylene isosorbide monoester, and polyoxyethylene monoester) were analyzed to estimate the composition ratios of the seven ester-bonded FAs present in PS80.

**Results:** The Avg-n values of five polyoxyethylene sorbitan esters (none, mono, di, tri, and tetra), three polyoxyethylene isosorbide esters (none, mono, and di), and three polyoxyethylene esters (none, mono, and di) were 26.5–30.6, 12.1–14.6, and 11.4–15.8, respectively. These values were comparable regardless of the number of ester-bonded FAs. Each product had a similar FA composition ratio regardless of the differences in the subspecies.

**Conclusion:** We developed an LC–MS/MS method to evaluate PS80 components using two techniques; contour plot and semi-comprehensive MRM analysis. The former remarkably revealed the abundance of each component and the elution pattern of each subspecies, while the latter allowed for a more accurate calculation of the degree of polymerization of POE compared with other methods reported so far. These results indicate that the developed method is useful for quality control of PS80 formulations.

## Biography

Yutaka Konya received his PhD degree on the theme of rapid analytical method development for unlabeled chiral amino acids (https://doi.org/10.1016/j.chroma.2018.10.004). Following the paper describing the contents of this poster (https://doi.org/10.1002/rcm.9438), Konya et al. also carried out vigorous research on oxidative decomposition products and enzymatic decomposition products of PS80, and identified several hitherto unknown oxidative decomposition products, as well as elucidated the variation associated with oxidation treatment time (https://doi.org/10.1002/rcm.9715).

- Research Interest: Mass spectrometry, Chiral amino acid analysis

# SORPTION ACTIVITY OF SURFACTANT MODIFIED NATURAL ARMENIAN ZEOLITES REGRET TO METALS REMOVAL FROM NATURAL AQUATIC SYSTEMS

**Alla Manukyan**

*Armenian National Agrarian University, Armenia*

## Abstract

The pollution of the natural aquatic systems by harmful contaminants is one of the most worrying problems in the modern world because the pollution of the natural aquatic systems leads to negative effects on the quality of the environment, life and quantity of aquatic system's animals, as well as human life quality, globally. One of the easiest, highly effective and non-expensive technologies is adsorption, especially if there are local deposits of the natural alumosilicate clays. In this paper the effectiveness of anionic surfactant sodium dodecyl sulfate surfactant-modified zeolite (SMZ) samples for the removal of metals from aqueous samples of Rivers Shnogh and Akhtala (Armenia) is presented. It has been shown that after purification of water samples by usage of SMZ the concentrations of metals in multi-component system of Shnogh and Akhtala Rivers water samples sharply decrease, showing high adsorption ability of SMZ regret to metals. Particularly, the concentration of copper decreases in 33.3%, the concentration of manganese- in 16.5%, the concentration of cobalt- in 25.4% and the concentration of zinc- in 31.0%. It must be noted that in natural aquatic systems different types of inorganic and organic compounds exist all of which participating in sorption process on the surface of SMZ. Therefore, the obtained data of metals removing in the conditions of competition sorption are quite good results. Thus, SMZ can be suggested as effective purification agents for sorption of metals contaminants from different types of aqueous mediums in general. The comparison of obtained data with metals removing effectiveness of natural (non-modified) zeolites reveals that due to modification the metals removal effectiveness doubles in average, which justified modification itself.

## Biography

Alla Manukyan has completed her PhD in Chemical Sciences in Yerevan State University. She has worked as Head of Central Analytical Laborotary in Lernametalurgiai Institute CJSC for 20 years, 2004-2009 as a chemist –analyst, 2009-2016 as a senior chemist-analyst, 2016-2018 as an assisstant head of laboratory and since 2018 she has been Head of the Central Analytical Laboratory of the above mentioned institute.

She has published over 10 papers in reputed journals and has received two patents ('Quantitative method of Determination of Chromium', 2013 and 'Purification Method for Waste Water Containing Ions of Copper and Molybdenum', 2018). She has participated in two grant projects and currently working on a third one.

# INDUCTION HEATING CATALYSIS IN $CO_2$ METHANATION

**Tomasz Siudyga**

*University of Silesia, Poland*

## Abstract

**Background:** Carbon oxides are harmful greenhouse gas that cause climate change and threaten human well-being. Ongoing efforts are being made to reduce greenhouse gas emissions from industrial and household sources, but replacing fossil fuels is a complex issue. Novel technologies generally aim for carbonless energy production, but require continuous improvement, e.g. hydrogen as a potential fuel is still under development. To address this dependency, e-fuels are being developed to replace fossil fuels. These fuels are produced using renewable or decarbonized electricity, where hydrogen reacts with carbon dioxide. New materials are being developed to create, store, and manipulate e-fuels. Induction heating catalysis (IHC) significantly enhances heat transfer improving reactor hydrodynamics, and preventing slow heating/cooling rates.

**Objective:** The presented research aimed to evaluate the potential for scaling up the $CO_2$ methanation nano-catalysts and the possibility of their use in a variant of induction-assisted catalysis.

**Methods:** We fabricated different Ni-based carriers using sintering or 3D printing techniques to support nanoparticles of different active metals by the nano-transfer method. We studied the properties of the prepared catalysts using various techniques, and we tested their catalytic activity in a laboratory scale.

**Results:** Catalytic systems containing mixtures of Pd and Re nanoparticles on Ni carrier appeared to be especially interesting. We compared their reactivity with catalyst in form of powders. During testing catalytic systems in low-temperature-IHC $CO_2$ methanation, we discovered that a high $CO_2$ methanation activity is closely associated with the oxide-passivation of the surface structures. Our research indicates that nano-Pd, Re/Ni catalysts are coking resistant, while IHC variant allowed for 58°C reduction in reaction temperature.

**Conclusion:** The studies revealed that nano Pd,Re/Ni catalysts show good resistance to carbon deposition formation on the surface. They also demonstrated the possibility of using inductive heat transfer to the catalytic bed, which also results in lower reaction temperatures compared to conventional heating. The supports used also offer the opportunity for easier scaling-up the process.

**Acknowledgements:** The research co-financed by the funds granted under the Research Excellence Initiative of the University of Silesia in Katowice, Poland. We also acknowledge financial support of NCN Krakow, OPUS 2018/29/B/ST8/02303.

## Biography

Tomasz Siudyga has a background in Chemistry from Maria Curie-Sklodowska University in Lublin (Poland) and he is an Associate Professor at University of Silesia in Katowice, Poland. He is an expert in heterogenous catalysis, novel materials for energy storage and waste management.

# ASSESSMENT OF ANTIOXIDANT ACTIVITY OF PIPERAZINE-1,3,5-TRAIZINE DUAL AGENTS FOR FAAH AND 5-HT6 SEROTONIN RECEPTOR LIGANDS

## Małgorzata Starek

*Jagiellonian University Medical College, Poland*

## Abstract

**Background:** Alzheimer's disease (AD) is a neurodegenerative disease, which accompanying progressive cognitive decline via the accumulation of amyloid beta (Aβ) plaques and tau protein tangles leading to death, while available drugs are not able to inhibit AD progress. Although the mechanisms of AD are not fully understood, key pathogenic factors include oxidative damage, inflammation, neurotransmitter abnormalities, and deregulation of cellular signaling pathways. Recent trends in search for new drugs promote compounds that regulate on more than one protein target involved into the complexed etiology of AD.

**Objective:** To examine the antioxidant activity of a series of piperazine-1,3,5-traizine dual agents for FAAH and 5-HT6 serotonin receptor ligands (with therapeutic perspectives against AD).

**Methods:** In previous research, a series of ten piperazine-1,3,5-triazines was identified as potent dual ligands of the 5-HT6 serotonin receptor and the fatty-acid amide hydrolase 1 (FAAH), both indicated as attractive AD-targets. From a therapeutic point of view, additional antioxidant effects are desirable to inhibit neurodegeneration causes and progress. There are many methods for determining antioxidant activity. Four methods were selected for the study; these are: DPPH free radical scavenging assay, iron(III) ion reduction, phosphomolybdenate method and iron ion chelation.

**Results:** The obtained results suggest that most of the new tested substances did not show a strong antioxidant effect. However, there are some that, in two of the above-mentioned methods, showed more beneficial antioxidant properties than ascorbic acid.

**Conclusion:** Promising preliminary research results indicate the possibility of enhancing the therapeutic effect of the tested compounds, and the proposed tests for determining antioxidant potential may be used in further studies.

## Biography

Małgorzata Starek (employee of the Department of Inorganic and Pharmaceutical Analytics, Faculty of Pharmacy, Jagiellonian University Medical College, Poland, as an assistant professor) conducts scientific activities related to the optimization of chromatographic and spectrometric conditions towards the analysis of active substances. The conducted research includes qualitative and quantitative analysis of compounds with biological activity and finished products, stability tests in variable environmental conditions, determining the degradation paths of compounds, quality control of drugs and dietary supplements. She also conducts research on the possibilities of modifying physicochemical properties (e.g. lipophilicity) as well as routes of administration of medicinal substances (e.g. nanomaterials).

# COMPREHENSIVE PROCEDURE FOR MONITORING ENVIRONMENTAL HAZARDS RESULTING FROM ANTIBIOTIC CONTAMINATION

**Monika Dąbrowska**

*Jagiellonian University Medical College, Poland*

## Abstract

**Background:** In recent years, concerns about the presence and detection of toxic agents in ecosystems have increased rapidly. For a long time, water pollution was assessed solely on the basis of specialized chemical analyses, but experience has shown that this approach is insufficient. The use of biological methods to assess environmental contamination indicates an important new alternative to assessing direct or diffuse contamination resulting from the presence of pharmaceuticals in the environment, potentially indicating the impact of this presence on human health.

**Objective:** To acquire new and supplement existing knowledge about the fate of selected biologically active substances in the environment, their behavior in the aquatic environment, and potential ecotoxicity, as well as an attempt to select potentially toxic products formed during phototransformation of parent substances.

**Methods:** We proposed the procedure using a battery of bioindicators: Thamnotoxkit (*Thamnocephalus platyurus*), Daphtoxkit, (*Daphnia magna*) and LumiMARA, a "toxic fingerprint" test based on a series of microbial strains. In addition, *Danio rerio* embryos and larvae were used to study acute embryonic toxicity *in vivo*. The usefulness of this model results from the great similarity of the phenomena occurring in this species to those occurring in the human body. *In vitro* cytotoxicity studies were also carried out, using the biosynthetic or enzymatic activity of cells to assess the cytotoxic response.

**Results:** The results of studies conducted on selected cephalosporin antibiotics clearly indicate an increase in the toxicity of mixtures of the drug and its photodegradation products.

**Conclusion:** The presented procedure is based on the 3R principle (Replace, Reduce, Refinement) which concerns e.g. the ethical approach to the use of animals in scientific research, and is the foundation of ethical practices in toxicology. Assessment of hazards of xenobiotics in various elements of the environment is necessary for their proper and safe use and degradation.

## Biography

Monika Dąbrowska has her expertise in comprehensive drug analysis. Scientific activity is related to the optimization of chromatographic systems for the analysis of biologically active substances, stability studies in variable environmental conditions taking into account e.g. the influence of redox factors, metal ions, UV-Vis radiation and determining the degradation paths of the analyzed compounds as well as kinetic studies. She conducts extensive research on the possibilities of bioremediation of xenobiotics and analysis of environmental hazards resulting from the presence of antibiotics in the environment using, among others, bioindication tests, in vivo studies (Danio rerio) and in vitro cytotoxicity tests, as well as in silico analyses.

# BIOMIMETIC SPINNING OF CROSSLINKED AND FUNCTIONALIZED SPIDER-SILK PROTEINS WITH MULTIARM POLYETHYLENE GLYCOL

**Viktors Romaņuks**

*Latvian Institute of Organic Synthesis, Latvia*

## Abstract

**Background:** Spider silk stands out due to its impressive mechanical attributes, such as tensile strength and flexibility, which are difficult to fully replicate in synthetic materials. The synthetic version often has a lot worse physical properties than its natural counterpart. By utilizing bioconjugation techniques, particularly with polyethylene glycol (PEG), we are exploring ways to impact and enhance the mechanical properties and resilience of synthetic spider silk.

**Objective:** This study aimed to improve the performance of synthetic spider silk by applying multiarm PEG bioconjugation, thereby enhancing fiber solubility, spinnability, and mechanical properties while addressing sensitivity to environmental impact.

**Methods:** We engineered spider silk proteins (spidroins), by replacing the C-terminal domain with a cysteine residue to enable maleimide-thiol click-reactions with multiarm PEG. Proteins from *N. clavipes* and *E. australis* were selected for bioconjugation with PEG (2-arm to 8-arm). Fibers were spun under biomimetic conditions, with pH adjustments used to induce polymerization.

**Results:** The 8-arm PEG bioconjugates significantly improved fiber strength, achieving tensile strengths up to four times greater than other synthetic silk fibers based on the same spidroins. Under high humidity, the fibers demonstrated increased extensibility. However, lipid-mimicking coatings led to a reduction in tensile strength and lower spin-ability, implying that lipid coating must be applied after spinning.

**Conclusion:** Multiarm PEG bioconjugation proves to be a viable method for enhancing the mechanical properties of synthetic spider silk. Although further improvements are needed, particularly in replicating the lipid layer, this approach offers a strong foundation for developing more durable and high-performance synthetic fibers, also allowing us to modify spidroins with different compounds.

## Biography

Viktors Romaņuks he has a master's degree in chemistry and currently, he pursuing a Ph.D. at the University of Latvia. For the past five years, I have been working on artificial spider silk research in all of its stages. His main field of expertise is bioconjugation via click-chemistry. Over time he started to acquire knowledge and experience in protein production and fiber wet-spinning. Our research group has published initial results, where he main author, and also we have patented our spinning methodology. From that patent, we started a start-up firm, where now I am part of the stakeholders.

# CHARACTERIZATION OF BACTERIAL STRAINS ISOLATED FROM THE HYPOTHERMAL SPRING "KARIERA" IN THE AREA OF YABLKOVO VILLAGE, DIMITROVGRAD MUNICIPALITY, HASKOVO REGION, BULGARIA

**Denis Haralanov**

*Vocational High School, Bulgaria*

## Abstract

Bulgaria is a country in Europe that has the second largest number of mineral springs after Iceland. The number of mineral springs is 225. From the tests and research done, it can be seen that there are almost no pathogenic microorganisms in the healing mineral spring waters. In ordinary springs that are not controlled by chemical and microbiological laboratories, pathogenic microorganisms are observed in almost all springs. The purpose of the present work is to isolate and identify microorganisms from the hypothermal spring " Kariera" in the Yablkovo region and to examine them for pathogenic microorganisms according to Ordinance No. 9 on the quality of water for drinking purposes.

In many of the unexplored springs, microorganisms with valuable biological properties have been isolated. These microorganisms are used in medicine, pharmacy, biotechnology, agriculture, food industry, household, etc.

# CHARACTERIZATION OF BACTERIAL STRAINS ISOLATED FROM THE HYPOTHERMAL SPRING "OSMANOVA CHESHMA" IN YABLKOVO DISTRICT, MUNICIPALITY. DIMITROVGRAD, REGION HASKOVO, BULGARIA

**Diyana Danailova Grozeva**

*Vocational High School, Bulgaria*

## Abstract

Bulgaria is a country in Europe that has the second largest number of mineral springs after Iceland. The number of mineral springs is 225. From the tests and research done, it can be seen that there are almost no pathogenic microorganisms in the healing mineral spring waters. In ordinary springs that are not controlled by chemical and microbiological laboratories, pathogenic microorganisms are observed in almost all springs. The purpose of the present work is to isolate and identify microorganisms from the hypothermal spring "Osmanova Cheshma" in the Yablkovo region and to examine them for pathogenic microorganisms according to Ordinance No. 9 on the quality of water for drinking purposes.

In many of the unexplored springs, microorganisms with valuable biological properties have been isolated. These microorganisms are used in medicine, pharmacy, biotechnology, agriculture, food industry, household, etc.

# DATABASE WITH INTEGRATED MACHINE LEARNING AIDED CATALYST DESIGN

**Uladzislau Zhdan**

*University of Silesia, Poland*

## Abstract

**Background:** Properties and descriptors are two forms of molecular in silico representations. Properties can be further divided into functional, e.g., catalyst or drug activity, and material, e.g., Xray crystal data. Millions of real measured functional property records are available for drugs or drug candidates in online databases. In contrast, there is not a single database that registers a real conversion, TON or TOF data for catalysts. All the data are molecular descriptors or material properties, which are mainly of a calculation origin.

**Objective:** To build a database of experimental data, surface properties of heterogeneous catalysts and data about their reaction conditions.

**Methods:** The data comes from primary literature sources and general databases: Reaxys, ResearchGate, the Web of Science, etc. The database has a set of data for the physical properties of catalysts, e.g., absorbed metal species, support, metal loading ratio or the Bruanauer–Emmet–Teller surface area. Furthermore, the database also includes functional properties, i.e., the reaction data such as substrates, conversion rates, products, selectivity/yield rates, reaction temperature, pressure, catalyst/substrate mass, turnover frequency (TOF) values, gas hourly space velocities/weight hourly space velocities (GHSV/WHSV), flow gas compositions and flow rates.

**Results:** The Catalyst Metadata Database (CMD) successfully compiled an extensive dataset on the physical and functional properties of heterogeneous catalysts. The database covers essential physical and functional data.

**Conclusion:** The CMD offers a unique and valuable repository of experimental data on heterogeneous catalysts. By incorporating real-world data on catalyst performance and reaction conditions, CMD enhances the ability to analyze, model, and predict catalyst behavior in practical applications. This could accelerate research in catalyst design, optimization, and industrial scaling.

## Biography

Uladzislau Zhdan is a researcher focused on heterogeneous catalysis and materials science. His work is dedicated to understanding and optimizing heterogeneous catalysts, contributing to advancements in the fields of green chemistry and industrial applications. Zhdan's expertise spans the study of property prediction of materials and drugs using machine learning methods. A significant part of his research involves creating comprehensive databases that compile real-world experimental data on catalysts, such as the Catalyst Material Database (CMD). Zhdan's contributions are not only advancing scientific understanding of catalytic material property prediction but also his research aimed at developing new methods of drug and material design.

# *Virtual - Day 1 Presentations*

# COMPUTER-ASSISTED SYNTHESIS OF PYRROLO [4,3,2-de] QUINOLINONE DERIVATIVES BY SUZUKI COUPLING

## Bárbara Bahls

*Universidade de Lisboa, Portugal*

## Abstract

**Background:** The pyrrolo[4,3,2-de]quinolinone (PQ) scaffold is present in natural alkaloids that show different biological activities, such as cytotoxicity against cancer cell lines and inhibition of topoisomerase I. A possible mechanism of anticancer activity of PQ compounds is the targeting of G-quadruplex (G4) nucleic acids. G4s are secondary DNA/RNA structures formed in guanine rich sequences which are involved in regulation of gene replication, transcription and translation. Over the years, many small molecules have been developed to target G4s, particularly in promoters of oncogenes but none has yet reached the clinic. To overcome this impasse, new chemical scaffolds like PQ must be explored.

**Objective:** To synthesize by Suzuki coupling new derivatives of the PQ core.

**Methods:** The PQ core was synthesized following the procedure of Yang et. al. Then, DFT calculations were used to explore the mechanism and reactivity of this scaffold with a simple boronic acid, using three different solvents: dioxane, dimethoxyethane and methanol. Reactions were reproduced in small scale and analyzed by HPLC-ESI-MS to validate the in silico studies.

**Results:** The PQ core was synthesized in 3 steps with a global yield of 18%. The reaction mechanism was studied in silico and the energies of intermediates calculated showed that the polarity of the solvent can interfere with the energy barriers of the reaction. The TIC of reaction mixtures shows the formation of the desired product and validates the *in silico* studies.

**Conclusion:** In silico studies indicated methanol as the best solvent to perform the Suzuki Coupling with pyrrolo[4,3,2-de]quinolinone. Preliminary synthetic reactions confirm the in silico studies but additional experiments are needed to improve the yield.

## Biography

Bárbara Bahls has an integrated master in Pharmaceutical Sciences from Universidade Federal do Paraná (Brazil) and a master in Medicinal and Biopharmaceutical Chemistry from Faculty of Pharmacy in Universidade de Lisboa (FFUL). Currently, she is a PhD student in Medicinal Chemistry at FFUL with a scholarship from FCT (2023.01798.BD) and a member of the project "Inquiring the druggability of DNAG4-helicase interactions with small molecules" funded by FCT (2022.06099.PTDC). She has training in organic and computational chemistry. She has experience in the pharmaceutical industry in quality control. Her research interests focus on G-quadruplexes, cancer treatment and applying energy calculations in synthesis optimization. Her combined expertise in multiple areas leads her to innovative approaches to solving challenging problems.

# ECO-FRIENDLY DISHWASHING LIQUID FROM ORANGE AND BANANA PEELS: A SUSTAINABLE SOLUTION TO CHEMICAL POLLUTION

**Aktayeva Adiya Kizatovna and Kairatova Elina Kairatovna**

*Nazarbayev Intellectual School of Chemistry and Biology in Atyrau, Kazakhstan*

## Abstract

**Background:** The ever-growing problem of environmental pollution due to the use of chemical-based cleaning agents across regions is reinforcing sales. Most of the dishwashing liquids sold in supermarkets have dangerous substances that provide water contamination and damage to aquatic ecosystems. It is necessary that we start exploring natural, biodegradable alternatives in order to join global the reduce pollution and promote sustainability initiatives. This naturally occurring oil and enzyme mix amace for a possible sustainable resolution from the orange peel with high natural oils, in addition to elements of banana peels. The aim of this project is to turn waste derived from the peeling process with fruits into a powerful, ecologically sound skin care dishwashing liquid.

**Objective:** To design, develop and test an orange peel based dish washing detergent that is both effective in cleaning the dishes at minimal environmental cost.

**Methods:** The study commenced with the collection of fresh orange and banana peels, which were subsequently cleaned, dried, and ground into a fine powder to maximize surface area for extraction. The powdered peels were then boiled in distilled water for a specified duration to facilitate the release of essential oils and enzymes, crucial for the cleaning efficacy of the dishwashing liquid.

Reetha (soapnut) was incorporated as a natural surfactant due to its proven effectiveness in creating lather and removing grease. In addition to the peel extracts, fresh lemon juice was added for its antibacterial properties and pleasant fragrance. The mixture was thoroughly stirred to ensure uniform distribution of components.

Subsequent to preparation, the resulting liquid was subjected to a series of controlled tests against common kitchen greases and food residues on glass and ceramic dishes. A standardized grease removal test was employed to quantify cleaning efficiency, comparing the eco-friendly formulation against commercial dishwashing agents. Data collected included the percentage of grease and residue removed, toxicity assessments, and biodegradability analyses to evaluate the overall environmental impact of the product.

**Results:** Preliminary testing revealed that, compared to commercial products, the orange and banana peel liquid cleaned between 75-85% of grease and food contaminants ever-so-slightly less effective than mainstream brands but a relatively normal rate for household cleaning. The formulation also presented low toxicity, biodegradability and ecological flashpoint as advantages when compared to the traditional products.

**Conclusion**: Fruit-derived ecofriendly dishwashing liquid for cleaning efficacy and environmental sustainability. It may be made more competitive with chemical-based cleaners through ongoing improvements in formulation. This could help with efforts to minimizes chemical pollution and waste when uses fruit peels!, promoting it will support sustainability.

# ENVIRONMENTAL JUSTICE IN INDUSTRIAL CITIES: ADDRESSING HEALTH INEQUALITIES IN ATYRAU, KAZAKHSTAN THROUGH TARGETED AIR POLLUTION MITIGATION

**Symbat Bolatova**

*Nazarbayev Intellectual School of Chemistry and Biology in Atyrau, Kazakhstan*

## Abstract

**Background:** Air pollution disproportionately affects vulnerable groups, including women, children, and low-income families, particularly in industrial cities. In Kazakhstan's Atyrau, an oil and gas hub, pollutants like hydrogen sulfide and PM2.5 from industrial activities pose significant health risks. Despite national efforts to improve air quality, there is a gap in addressing the specific needs of these populations. This study aims to highlight the local impacts and propose solutions to reduce health inequalities and promote sustainable development.

**Objective:** The objective of this research is to assess the impact of air pollution on socially vulnerable populations specifically women, children, and low-income families in Atyrau, Kazakhstan, by analyzing health outcomes related to pollutants such as hydrogen sulfide and PM2.5. The study aims to propose targeted interventions, including government policies and community-based solutions, to mitigate health inequalities and enhance public awareness for improving air quality in industrial regions.

**Methods:** This research utilizes a mixed-method approach to explore the effects of air pollution on vulnerable populations in Atyrau, Kazakhstan, combining quantitative and qualitative data for a comprehensive analysis.

Quantitative data was collected through structured surveys administered to over 120 residents from low-income households, women, and families with children. The survey focused on key health indicators, including respiratory diseases, headaches, reproductive health issues, and general well-being, while also examining socio-economic factors such as income levels, housing conditions, and proximity to industrial sites. Questions on awareness of air pollution and access to healthcare were included to assess community understanding and resources available to mitigate the risks.

Qualitative data was gathered through semi-structured interview with healthcare professional, who provided detailed insights into the prevalence of pollution-related diseases such as asthma, bronchitis, and other respiratory conditions in vulnerable groups. Her expertise helped to contextualize the survey findings and identify key areas for intervention.

In addition to primary data collection, the research involved a comprehensive review of secondary sources, including environmental reports, air quality data, and public health records, to correlate pollution levels with health outcomes. This combined approach allows for a thorough understanding of the local context and the identification of practical solutions to address the health inequalities linked to air pollution in Atyrau.

**Results:** The results indicate that air pollution in Atyrau disproportionately affects vulnerable populations, with over 65% of surveyed women, children, and low-income families reporting respiratory issues, and women's reproductive health problems. Health professionals confirmed a rise in pollution-related illnesses, particularly among children and pregnant women. The study highlights a lack of targeted

interventions and emphasizes the need for air quality monitoring, public health campaigns, and localized solutions to reduce health disparities.

**Conclusion:** The research concludes that air pollution in Atyrau significantly impacts vulnerable populations, particularly women, children, and low-income families, exacerbating health inequalities. The findings reveal a high prevalence of respiratory and reproductive health issues linked to pollutants such as hydrogen sulfide and PM2.5. Despite existing national efforts to improve air quality, there is a critical gap in addressing the specific needs of these groups. To mitigate these effects, targeted interventions, including government policies, public health campaigns, and practical solutions such as air purifiers in public spaces, are urgently needed. This study underscores the importance of addressing environmental justice in industrial regions and highlights the need for sustainable, community-focused strategies to protect at-risk populations. These solutions can serve as a model for other polluted industrial areas facing similar challenges.

# DESIGN AND ANALYSIS OF AN INNOVATIVE ENZYMATIC-FILTER (E.F) FOR PURIFYING AIR CONTAMINATED WITH SULFUR DIOXIDE ($SO_2$)

**Zhanerke Yerbolatova, Nurtas Tazhmagambetov and Asif Abbas Syed**

*Nazarbayev Intellectual School of Chemistry and Biology in Atyrau, Kazakhstan*

## Abstract

**Introduction:** BBB

The project aims to provide a detailed overview of the installation to better optimize the processes of air purification from sulfur dioxide, as well as to offer a relatively affordable and fast method of air purification.(Using the oxidative abilities of enzymes).

**Basic reactions:**

Oxidation of hydroquinone to 1,4-benzoquinone:

The enzyme oxidase, obtained from potatoes, catalyzes the oxidation of hydroquinone ($C_6H_4(OH)_2$) to 1,4-benzoquinone($C_6H_4O_2$). This process also involves interaction with molecular oxygen ($O_2$), which forms water ($H_2O$) as a by-product:

$C_6H_4(OH)_2+O_2 = C_6H_4O_2 + H_2O$

1. Formation of sulfurous acid:

• In an aqueous environment, sulfur dioxide partially dissolves and hydrates, forming sulfurous acid ($H_2SO_3$):

2.Reduction of 1,4-benzoquinone to 1,4-hydroquinone:

• Benzoquinone reacts with sulfurous acid, taking two electrons and two protons, which leads to the formation of 1,4-hydroquinone:

$C_6H_4O_2 + 2H^+ + 2E^- = C_6H_4(OH)_2$

3. Oxidation of $SO_2$ to sulfuric acid:

• During the reduction of benzoquinone, sulfur dioxide is oxidized. This can occur through subsequent stages, with the formation of intermediates such as hydrosulfite and sulfite, but the final product of $SO_2$ oxidation will be sulfuric acid:

$H_2SO_3 + [O] = H_2SO_4$

**Conclusion:** The data obtained make it possible to effectively apply this technique to purify the air from hydrogen sulfide in residential buildings, educational institutions, hospitals, as well as in industry.An operating hydrogen sulfide air purification system has been created, characterized by low energy consumption.The catalyst is not dangerous to the environment and humans, the process proceeds quickly at normal temperatures and pressures

# STUDY OF PROPERTIES OF MAGNETIZED WATER

**Amangeldy Nuriya and Amankos Symbat**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Plants play a critical role in oxygen production and ecological balance, yet their growth can be hindered by impurities in tap water. Magnetized water is proposed as a means to improve plant development by enhancing water properties that may boost fluidity and nutrient absorption.

**Objective:** This study aims to evaluate the effects of magnetized water on plant growth, particularly its impact on the growth rate and robustness of plants. The research compares the growth outcomes of plants irrigated with magnetized versus regular water. To collect and analyze information on magnetic fields, investigate the properties of water influenced by magnetic fields, monitor the impact of magnetized water on plant growth, and draw conclusions based on experimental results.

**Methods:** The methodology encompasses experimental observations, data analysis, and a comprehensive review of relevant literature. Plants were observed under conditions using both magnetized and non-magnetized water, with specific attention to growth rates, root development, and overall health. Additionally, the properties of magnetic fields, such as their influence on charged particles, were examined for their potential biological applications.

**Results:** Preliminary observations suggest that onions grown with magnetized water exhibit a faster growth rate and improved root establishment compared to those watered with non-magnetized water. Magnetized water showed reduced sediment formation and was effective in enhancing nutrient uptake without chemical additives. Additional benefits noted include improved water quality and potential positive effects on human health, as magnetized water is reported to aid in detoxification and alleviate various health issues.

**Conclusion:** The study supports the hypothesis that magnetized water positively influences plant growth and suggests practical applications for household and educational settings to boost plant development. The findings recommend using magnetized water for irrigation to enhance plant growth and for various health and domestic applications, including water treatment for appliances and personal care. Further research could explore the long-term effects and scalability of magnetized water use in agriculture.

# POSSIBLE APPLICATION OF QUARKS

## Muslim Zhasulanuly

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** This project explores quarks and the potential applications of different types of quarks. Quarks are a relatively recent topic in science, and their applications have not been extensively studied. There is limited understanding of their potential in the scientific community, and there are very few materials available in the term of this sphere. Understanding the properties and behavior of quarks is essential for advancing our knowledge of quantum and subatomic particle physics. It also plays a crucial role in sparking interest among non-expert readers in the more complex areas of physics. Quarks and other subatomic particles can provide valuable insights into the nature of all matter. Furthermore, exploring the potential applications of quarks may lead to innovations across various scientific fields. By shedding light on the properties and behavior of these particles, this research contributes to the broader exploration of practical applications in the subatomic world and paves the way for future technological advancements.

**Objective:** By studying their properties and behavior, this project aims to understand the hypothetical applications of these types of quarks. Additionally, it seeks to make information from scientific resources accessible to non-expert readers.

**Methods:** Information for the project was gathered through theoretical analyses, quantitative research, and qualitative studies. Although these methods save time, they significantly limit the researcher's hands-on experience, as there is no practical component involved. However, due to equipment limitations, this methodology was chosen. Additional literature was used as a source of information, including the works of scientists such as Karliner and Rosner, as well as documents from the CERN research organization. The information was carefully studied and translated into clear Kazakh. Due to the tight schedules of specialists, it was not possible to obtain primary data.

## Biography

Muslim Zhasulanuly is a dedicated researcher focusing on the properties and potential applications of quarks, aiming to advance the understanding of quantum and subatomic physics. Utilizing theoretical analyses, quantitative research, and qualitative studies, they translate complex English resources into accessible material for non-expert readers, drawing from experts like Karliner and Rosner and institutions like CERN. Due to equipment constraints, their research is based on theoretical models rather than practical experiments. This work not only seeks to enhance scientific knowledge of matter but also aims to spark interest in advanced physics among casual readers and contribute to technological advancements in academic community. By exploring quarks' practical applications, they are paving the way for innovations that could impact various scientific fields.

# EFFECTIVE ADSORBENT FOR IRON, LEAD, ZINC IONS

**Alihan Doskaliev, Yeraly Kanatuly and Nurzhanova Dariga**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Heavy metal contamination in natural water, largely from industrial waste, poses severe health risks as these metals accumulate rather than decompose. Common toxic metals, including iron, copper, lead, and zinc, enter water sources through industrial discharge, impacting communities across Kazakhstan. This study addresses the critical need to purify wastewater by removing such contaminants, with an emphasis on finding low-cost, effective adsorbents for this purpose.

**Objective:** The objective of this research was to evaluate the adsorption efficiency of three alternative adsorbents-clay, used tea leaves, and reeds-for removing iron, zinc, and lead ions from contaminated water.

**Methods:** We prepared 0.5 M solutions of the metal ions and assessed the adsorption efficiency by treating these solutions with the adsorbents. The effectiveness of each was compared by observing changes in metal ion concentrations post-treatment using a qualitative test with potassium hydroxide (KOH) solution.

**Results:** Our findings indicated that reeds were the most effective adsorbent among the three, contrary to our initial hypothesis that tea waste would yield the best results. In the presence of reeds, the precipitate that initially formed with metal ions in solution almost completely dissolved, indicating successful adsorption. Clay and tea waste showed limited effectiveness, with noticeable residues remaining after treatment.

**Conclusion:** Reeds demonstrated the highest adsorption efficiency for zinc, iron, and lead ions, thus being the recommended choice for wastewater treatment in this context. Although tea waste is reusable and environmentally benign, it proved less effective for these specific ions. Future research will explore additional low-cost adsorbents to enhance heavy metal removal further.

## Biography

Alihan Doskaliev is a student at the Nazarbayev Intellectual School of Chemistry and Biology in Atyrau, Kazakhstan. Together with his classmate, Yeraly Kanatuly, they conducted a research project to develop efficient and low-cost adsorbents for removing heavy metals like zinc, iron, and lead from wastewater. Under the supervision of their chemistry teacher, Dariga Nurzhanova, they investigated the potential of materials such as clay, reeds, and used tea leaves as effective adsorbents. Their study is especially significant given the environmental challenges in Kazakhstan, where industrial waste often contaminates water bodies with heavy metals. Through their experiments, the team found that reeds were the most effective adsorbent, surpassing their initial hypothesis. The project offers valuable insights into low-cost solutions for improving water quality and mitigating the harmful effects of heavy metal pollution on public health.

# AI-OPTIMIZED ALGAE CULTIVATION FOR SUSTAINABLE BIODIESEL PRODUCTION

**Ualikhan Yassaui Kubaidollauly, Yedil Kairzhan Shyngysuly, Sailau Adina Nurlankyzy and Asif Abbas Syed**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Given the urgent need for cleaner energy sources, this research focuses on harnessing the potential of algae as a biofuel feedstock while leveraging AI and IoT to optimize the production process. The goal is to explore a scalable, sustainable method for producing biodiesel from algae and contribute to global efforts toward reducing reliance on fossil fuels.

**Objective:** Use AI and IoT systems to monitor and automate critical environmental factors such as light intensity, temperature, and carbon dioxide levels to ensure maximum lipid production in algae.

**Methods:** The research begins by cultivating a high-lipid algae strain in a controlled environment, using sensors to monitor key variables such as light, temperature, pH, and $CO_2$ levels. AI and IoT technologies analyze this data to automatically adjust these conditions, optimizing algae growth for maximum lipid production. Once the algae reach peak biomass, they are harvested using filtration or centrifugation, then dried to preserve the lipid content. The lipids are extracted from the dried algae using solvent extraction, such as hexane, or advanced methods like supercritical $CO_2$ extraction.

Next, the lipids undergo transesterification, where they are mixed with methanol and a catalyst (e.g., sodium hydroxide) and heated to produce biodiesel and glycerol. The biodiesel is then separated from the glycerol and purified through washing and drying to remove impurities. Throughout the process, data on lipid yield, biodiesel conversion efficiency, and energy consumption are collected.

Real-time sensor data is analyzed to assess how the AI-optimized conditions impact algae growth and biofuel yield. The energy efficiency of the biodiesel production process is compared to traditional fuels, and a life cycle assessment evaluates environmental impacts. Finally, the scalability and economic feasibility of the algae-based biofuel system are examined for potential industrial applications.

**Results:** The research demonstrated that integrating AI and IoT technologies significantly optimized algae growth, resulting in higher lipid yields. The biodiesel produced from algae was energy-efficient and environmentally friendly, with favorable comparisons to traditional fuels. The process proved scalable and economically feasible for potential industrial biofuel production.

# MAGNETIZED NANOTECHNOLOGY FOR OIL SPILL CLEANUP: EVALUATING THE EFFICIENCY OF FERROFLUID-MEDIATED OIL-WATER SEPARATION

**Andossova Aizere and Asif Abbas Syed**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Oil spills pose significant environmental challenges, causing extensive harm to marine ecosystems and requiring costly and complex cleanup efforts. Traditional methods often fall short in fully removing oil from affected waters, leaving residual pollutants that can devastate local wildlife and habitats. In recent years, advancements in nanotechnology have opened the door to innovative solutions, one of which involves the use of ferrofluids liquids containing suspended ferromagnetic nanoparticles. These particles respond to magnetic fields, offering a potential method for separating oil from water by magnetizing the oil and using magnets to pull it out of the water.

This study explores the effectiveness of this method by examining how varying amounts of ferrofluid and a strong neodymium magnet influence oil-water separation efficiency. By testing this approach on a small scale, the research aims to assess whether magnetized nanotechnology could provide a more efficient and environmentally friendly solution to oil spills, with potential implications for large-scale environmental remediation efforts.

**Objective:** To evaluate the efficiency of separating oil from water by using ferrofluids and a strong neodymium magnet, determining the optimal amount of ferrofluid required for maximum oil recovery and assessing the potential of this method for application in large-scale oil spill cleanups

**Methods:** The methodology for this study involves a controlled experiment to test the effectiveness of ferrofluid in separating oil from water. To begin, petri dishes are prepared with a standardized amount of water and oil, simulating an oil spill. Ferrofluid, containing ferromagnetic nanoparticles suspended in a carrier fluid, is then added to the oil in varying amounts to test the optimal quantity required for efficient separation.

Each dish is treated with different ferrofluid concentrations, ranging from no ferrofluid (control) to one and five drops. A strong neodymium magnet is placed in a plastic bag and passed through the oil layer to magnetize and extract the oil-ferrofluid mixture, leaving the water behind. Observations are recorded on the distribution of ferrofluid within the oil and any interactions with the water.

After extraction, the leftover oil volume is measured, and the efficiency of each setup is calculated using the formula:

Efficiency=1− (Volume of leftover oil / Volume of original oil Efficiency)

These values are averaged over multiple trials to ensure consistency, and results are plotted to compare efficiency across treatments. This method provides a preliminary assessment of the ferrofluid-magnet technique's potential for scalable oil spill remediation.

This structured approach allows for precise measurement, controlled conditions, and quantitative analysis of oil removal efficiency.

**Results:** In the results, it was found that the addition of ferrofluid significantly improved oil separation from water when using a neodymium magnet. The control group (no ferrofluid) showed minimal to no oil removal, with oil remaining largely unaltered on the water's surface. In contrast, petri dishes with one drop of ferrofluid demonstrated moderate separation, with a visible reduction in oil volume after magnet application. The efficiency, as calculated, showed that roughly 50-60% of the initial oil volume was removed in these tests.

Dishes with five drops of ferrofluid displayed the highest efficiency, achieving an average oil removal rate close to 90%. This setup allowed the magnet to capture a larger portion of the oil-ferrofluid mixture, leaving only a thin residue in the water. Visual observations also noted that as ferrofluid quantity increased, oil particles aggregated more uniformly, aiding magnetic separation. Efficiency data and graph plots confirmed that oil removal efficiency directly correlated with the amount of ferrofluid applied.

These findings indicate that ferrofluid, in sufficient quantities, could be a promising agent for oil spill remediation, offering effective separation on a small scale and potential for optimization in larger environmental applications.

**Conclusion:** This study demonstrates that using ferrofluid combined with a strong magnet significantly enhances oil spill cleanup efficiency in a controlled setting. Results suggest that increasing ferrofluid quantity improves oil removal rates, highlighting this approach's potential as an eco-friendly, scalable solution for mitigating environmental oil pollution.

## Biography

Andossova Aizere embodies dedication and ambition in every aspect of her academic journey. Her outstanding organizational skills and strong inner drive distinguish them from others. Over our time working together, I saw Andossova Aizere's remarkable talent for tackling complex chemical applications with both accuracy and confidence.

What truly left an impression was their 16-month commitment to in-depth research on the topic. Despite starting with impressive technical abilities, she continuously sought new knowledge and ways to improve. Her determination to thoroughly understand chemical experiments and enhance their skills was unparalleled among her peers.

# POTENTIAL APPLICATION OF INNOVATIVE SOLID WASTE MATERIALS FOR ADSORPTIVE REMOVAL OF TOXIC PHENOL FROM WASTEWATER FOR ENSURING CLEANER ENVIRONMENTAL AND ALSO FOR GENERATING CIRCULAR ECONOMY

**Ashanendu Mandal**
*University of Calcutta, India*

## Abstract

This research aims for adsorptive removal of phenol from wastewaters by solid waste materials viz. guava tree bark, rice husk, neem leaves, activated carbon from coconut coir, rice husk ash, red mud, clarified sludge from basic oxygen furnace and activated alumina. The characterizations of the adsorbents are performed by SEM, XRD, FTIR and BET analyzers. The experiments of phenol removal are carried out in batch process with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum phenol removal percentage was found with neem leaves used as adsorbent and it was 97.50%. The kinetics study shows that the pseudo-second order model is best fitted for all adsorbents except red mud. The kinetic modeling shows that the adsorption mechanism is supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggests that Freundlich isotherm model is best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm are best supportive for rice husk ash and clarified sludge respectively. The thermodynamics shows the spontaneity, randomness and endothermic/exothermic nature of the adsorption processes. The ANN modelings using Levenberg-Marquardt and Scaled Conjugate Gradient algorithms establish that the experimental and predictive data are within allowable range. The studies of scale-up designs, the regeneration of adsorbents and the safe disposal of used adsorbents show that these adsorbents can be used for commercial applications. Further, the column study of phenol removal is also carried out using the most efficient batch adsorbent neem leaves. The study concludes that the wastewater treatment for ensuring cleaner environment is commercially possible using solid waste materials as adsorbents, which in turn can also generate circular economy.

# *Virtual - Day 2 Presentations*

# NATURAL CLEANER: INNOVATIVE HOUSEHOLD ECO DETERGENT

**Amangoskyzy Ayaulym and Kossanov Rakhymzhan**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** In today's environmentally conscious world, there is a growing demand for sustainable, eco-friendly cleaning products. Conventional household detergents often contain harmful chemicals that can negatively impact human health and the environment. Natural alternatives, such as plant-based and biodegradable ingredients, have gained popularity. This project focuses on creating an innovative household eco-cleaner from natural resources, specifically watermelon rind, to reduce chemical pollution and provide a sustainable solution for everyday cleaning needs. The results of the experiments and research during the project prove it.

**Objective:** The primary goal of this study is to develop and test a natural cleaning product made from watermelon rind. The objective is to evaluate its cleaning efficiency, safety for household use, and environmental impact compared to commercially available chemical-based detergents.

**Methods: The study involved the following steps:**

1. Separation of the extract from the bark of the carob by physical methods.
2. Preparation of the eco-cleaner formulation by combining the rind extract with other natural ingredients, such as vinegar and essential oils.
3. Testing the cleaning efficacy on common household surfaces, such as glass, metal, and plastic, by comparing the results with a commercial detergent.
4. Environmental impact analysis by measuring biodegradability and the toxicity of waste materials.
5. Data was presented using comparative graphs and tables to illustrate the cleaning efficiency and environmental safety of the eco-cleaner versus chemical detergents.

**Results:** The eco-cleaner showed a 90% efficiency in removing dirt and stains from glass and metal surfaces, which was comparable to a leading chemical detergent, as illustrated in **Figure 1**. Moreover, the product was fully biodegradable within 30 days, with no toxic residues detected (**Table 1**). The environmental impact of the eco-cleaner was significantly lower, as demonstrated in the waste analysis graphs (**Figure 2**), where the eco-cleaner exhibited 80% lower environmental toxicity compared to its chemical counterpart.

| Cleaner | Time to Biodegrade (Days) |
|---|---|
| Eco-Cleaner | 30 |
| Chemical Cleaner | 180 |

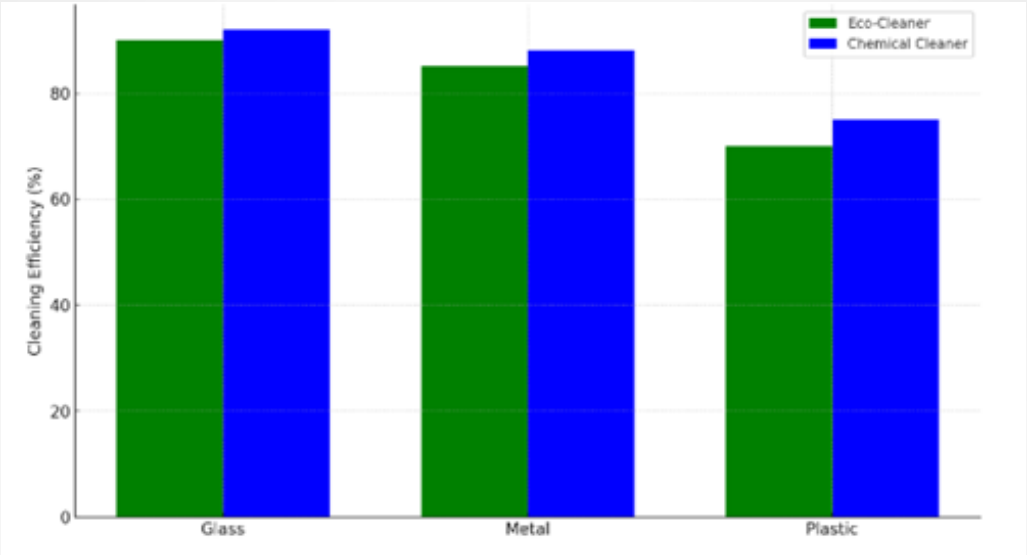



**Figure 1:** Cleaning Efficiency Comparison between the eco-cleaner and a chemical cleaner across different surfaces (glass, metal, plastic).

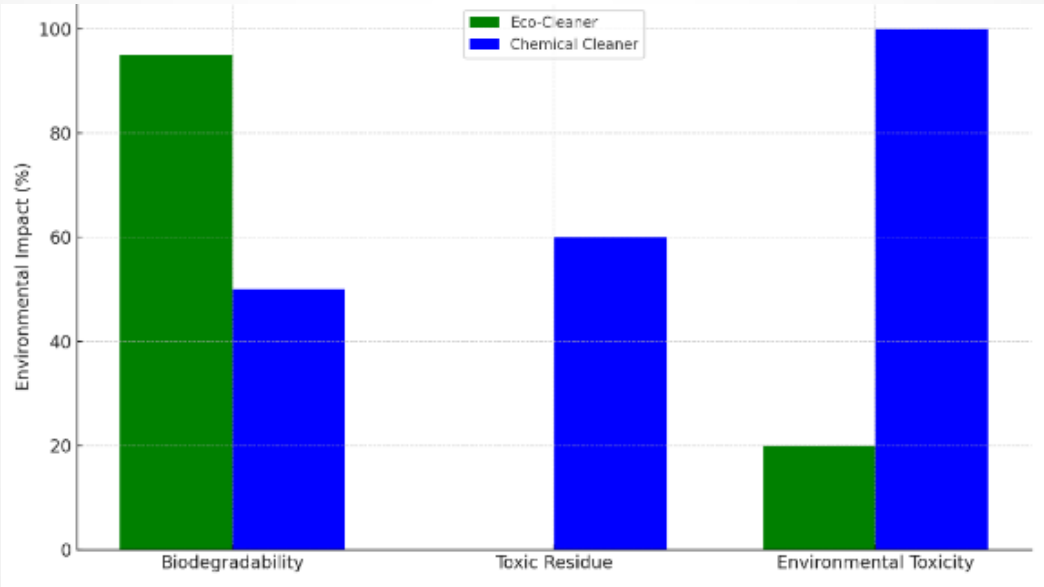



**Figure 2:** Environmental Toxicity Comparison between the eco-cleaner and a chemical cleaner, showing biodegradability, toxic residue, and overall environmental toxicity.

**Conclusion:** The results indicate that the natural eco-cleaner derived from watermelaon rind is an effective, safe, and environmentally sustainable alternative to traditional chemical household detergents. It offers a viable solution for reducing the ecological footprint of household cleaning products while maintaining cleaning efficiency. Further research could explore the scalability of this product for commercial use and the potential incorporation of other natural waste materials for enhanced performance.

# SUSTAINABLE BIOFUEL PRODUCTION FROM PLANT WASTE VIA SECONDARY PROCESSING TECHNIQUES

**Kenzhebai Adilbek Azamatuly, Abdulov Almir Alibekovich, Gulziya Beisenbekova and Asif Syed**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** The increasing demand for sustainable energy solutions has driven significant interest in biofuels as an alternative to fossil fuels. In regions like Atyrau, Kazakhstan, large amounts of plant waste, such as reeds, wood shavings, and dry branches, are produced as a byproduct of local industries and seasonal vegetation cycles. This biomass is often discarded or burned, contributing to environmental pollution and wasted potential. Biofuels, derived from organic materials, offer a promising way to address both energy and waste management challenges. The ability to convert plant waste into renewable fuel through secondary processing methods like fermentation and distillation not only reduces environmental harm but also provides a low-cost, locally sourced energy alternative. This research aims to explore the feasibility of utilizing abundant plant waste in Atyrau for biofuel production, contributing to the global push for renewable energy and aligning with sustainable development goals aimed at reducing reliance on fossil fuels and mitigating climate change.

**Objective:** The primary objective of this research is to evaluate the feasibility of converting plant waste, specifically reeds and wood shavings, into biofuel through secondary processing techniques such as fermentation, filtration, and distillation. The study aims to determine the efficiency, cost-effectiveness, and environmental sustainability of using these widely available organic materials as a renewable energy source. Additionally, the research seeks to optimize the biofuel production process, comparing the performance of reed-based and wood-based biofuels in terms of heat output, combustion properties, and overall viability as alternatives to traditional fossil fuels.

**Methods:** The primary objective of this research is to explore the feasibility of using secondary processing methods, such as fermentation, filtration, and distillation, to transform organic waste into biofuel. The study began by analyzing the chemical composition of the target biomass materials—reeds, wood shavings, and dry branches to assess their suitability as raw materials for biofuel production. Through literature review and preliminary experimentation, we identified that these materials contain substantial amounts of cellulose, lignin, and other organic compounds that are crucial for the biofuel production process.

Two types of biomass were chosen for the study: (1) reed biomass and (2) wood shavings. The raw materials were subjected to fermentation at a controlled temperature of 30°C over a period of three days. This fermentation process was catalyzed using yeast, which facilitated the breakdown of the organic compounds present in the biomass. After fermentation, the mixtures underwent filtration to remove solid residues, followed by distillation to separate the liquid biofuel from any remaining impurities. The key focus was on optimizing the yield and quality of biofuel obtained from both types of biomass.

**Results:** The results of this research demonstrate the successful conversion of plant waste, specifically wood shavings and reeds, into biofuel through secondary processing techniques like fermentation, filtration, and distillation. The wood-based biofuel exhibited strong combustion properties and produced a high heat output, comparable to certain conventional fuels, making it a viable alternative ener-

gy source. In contrast, the reed-based biofuel showed lower combustion efficiency due to the presence of heavy organic compounds, indicating the need for further refinement. Economically, the production cost of the biofuel was significantly lower than market prices for traditional fuels, with an estimated cost of less than 150 KZT per liter. Environmentally, using plant waste as a renewable resource contributes to waste reduction and lower greenhouse gas emissions, highlighting the potential of biofuel as a sustainable energy solution. While the wood-based biofuel proved more effective, the reed-based fuel still shows promise with further optimization. This research indicates that plant waste holds significant potential as a cost-effective and eco-friendly biofuel source.

**Conclusion:** In conclusion, this research demonstrates the feasibility of converting plant waste into biofuel through secondary processing techniques. The findings suggest that biofuel derived from wood shavings is a viable and environmentally sustainable alternative to fossil fuels. Although reed-based biofuel was less efficient, further research and process optimization could unlock its potential as a renewable energy source. This study contributes to the development of biofuels as a cost-effective and eco-friendly solution for energy production, aligning with global sustainability goals.

# MICROSCALE EVOLUTION OF TWO LDPE TRILAYER FILMS: INFLUENCE OF STABILIZER PLACEMENT ON ACCELERATED AGING MONITORED BY FTIR AND UV ANALYSIS

**Meriam Imane Babaghayou**

*Ecole Normale Supérieure, Algeria*

## Abstract

**Background:** The durability of low-density polyethylene (LDPE) films used as greenhouse covers is critical for sustainable agricultural practices. Understanding the effects of stabilizer placement on the accelerated aging of these films can enhance their longevity.

**Objective:** This study investigates the accelerated aging of two trilayer LDPE films, focusing on the influence of stabilizer placement on their photodegradation characteristics and evaluating the microstructural changes they undergo.

**Methods:** Two trilayer films were fabricated: Film A, with stabilizers (Hindered Amine Light Stabilizers (HALS) and UV absorbers) positioned in the external layer, and Film D, with stabilizers in the middle layer. Both films underwent 33 days of artificial UV exposure, and microstructural changes were monitored using FTIR and UV-Vis spectroscopy, with a focus on carbonyl and vinyl group formation.

**Results:** Film D exhibited a 50% higher rate of carbonyl group formation after 12 days and a 117% increase in vinyl groups by the end of the aging period compared to Film A. These findings indicate that stabilizers in the middle layer are less effective in mitigating degradation, leading to increased formation of photodegradation products associated with Norrish Type II reactions. Specifically, the photo-initiated cleavage of the polymer backbone resulted in the generation of carbonyl and vinyl groups, which were more pronounced in Film D. Conversely, Film A showed greater crystallinity and UV absorbance, suggesting enhanced degradation resistance when stabilizers were placed in the outer layer. The results confirm that stabilizers are consumed more effectively in the external layer, providing better protection against photodegradation and reducing the incidence of Norrish Type II reactions.

**Conclusion:** The placement of stabilizers significantly influences the performance and longevity of LDPE films for agricultural applications. Optimizing stabilizer placement is essential for developing more resilient greenhouse covers, thus contributing to sustainable agricultural practices.

## Biography

Babaghayou Meriam Imane specializes in chemical engineering with a focus on sustainable materials and waste valorization. She earned her State Engineer degree in Chemical Engineering from Laghouat University in 2004, followed by a Magister degree in Chemistry in 2011 and a Ph.D. in 2017. Her research primarily investigates the degradation of polyethylene films and the development of new plastics and composites from waste materials. Since 2012, she has been a lecturer at the École Normale Supérieure (ENS) in Laghouat and currently serves as the Director of the Applied Chemical and Physical Sciences Laboratory. Dr. Babaghayou leads the Materials Science, Characterization, and Valorization research group, promoting innovative solutions for environmental sustainability. Her work embodies a commitment to advancing knowledge in her field while addressing the challenges of waste management and material longevity.

# PRODUCTION OF ENVIRONMENTALLY FRIENDLY TEXTILE FABRICS FROM BANANA WASTE

**Al-Aziza Lukpanova, Ayaulym Nurlan and Nurzhanova Dariga**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Environmental pollution and waste disposal are significant issues in Kazakhstan, where textile waste and food waste, like banana peels, contribute heavily to landfill accumulation. Annually, 7.5 million tons of clothing are discarded globally, with only a small percentage recycled. This study addresses the potential of combining recycled cotton and wool with banana peels to create a biodegradable fabric, which may mitigate environmental impact and reduce waste.

Objective: This project is aimed to develop a sustainable, biodegradable fabric by mixing recycled cotton and wool fibers with banana peels and evaluating the eco-fabric properties.

**Method:** In a laboratory setting, banana peels were collected from a school canteen and were cleaned, dried, ground, and combined with cotton and wool in various ratios. The resulting fabrics were tested for water absorption, abrasion resistance, dye retention, and oil resistance to assess durability and usability.

**Results:** The integration of banana peels with natural fibers significantly enhanced the biodegradability, water resistance, and moisture retention properties of the fabrics, while maintaining comfort and softness. Abrasion resistance was favorable, though durability remains below that of synthetic fabrics, highlighting areas for improvement.

**Conclusion:** This research underscores the viability of using agricultural waste like banana peels in textile production, presenting a meaningful advancement toward sustainable waste management and pollution reduction. With further development, this biodegradable textile could reshape the industry's approach to eco-materials, offering a scalable path to reduce the environmental footprint of fast fashion and textile waste.

# NATURAL SORBENTS PURIFICATION OF WATER FROM CHEMICAL CONTAMINATION BY SYNTHETIC DETERGENTS

**Gulziya Beisenbekova**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** In the city of Atyrau, there is a site known as "Tukhlya Balka" or the evaporation field, where all the city's waste, along with that of the Atyrau Oil Refinery (ANPZ LLP), is disposed of. This pond, located on the left bank on the outskirts of Atyrau, fills the surroundings with an unpleasant odor. ANPZ LLP takes a certain amount of water from the Ural River, uses it in technological processes, including equipment cooling, and then discharges the water, cleaned of industrial impurities, into the evaporation fields. To address this environmental issue, it was decided to use plant waste as natural sorbents: mandarin and orange peels, ground peels (nanomaterial), and kiwi and banana peels. This project was incorporated into the educational process as a mini-project titled "Methods of Water Purification" for 8th-grade students, taking into account their age-related abilities. Accessible materials and improvised items (household containers can readily replace laboratory equipment) were used.

**Objective:** Conduct an alternative study with students on water purification using readily available, inexpensive food waste such as tangerine and orange peels, as well as kiwi.

**Methods:** Raw Materials: plant waste – natural sorbents.

**Research Objects:** samples of water contaminated with synthetic detergents: 1) Liquid soap "Velvet Hands," 2) Dishwashing liquid "Fairy," 3) Shampoo "Pure Line," 4) Laundry detergent "Ariel."

**Academic Knowledge Used in the Lesson Includes:** Chemistry (adsorption, chemical composition of the outer part of plant waste), Biology (natural sorbents), Ecology (improving the aquatic environment from chemical pollutants), Physics (diffusion), Mathematics (calculations).

**Experimental Part:**

1. Before the experiment, add to the mass of the sorbent: 3 ml of water + 37 ml of detergent = 40 ml of mixture.
2. After the experiment, add 1 ml of the filtrate to 199 ml of water, bringing the total volume of the researched mixture to 200 ml.
3. The filtration time through natural sorbents for detergents: 1.5-2 minutes.
4. Determine the pH of the test samples before and after the experiment.
5. Measure the height of the foam before and after the experiment.

**Results:** When comparing the height of the foam before and after the experiments, the following results were obtained: 1) Banana, kiwi, and tangerine peels demonstrated good adsorption capacity for purifying water contaminated with liquid soap and the dishwashing liquid 'Fairy.' 2) Orange peels showed good adsorption capacity for purifying water contaminated with the dishwashing liquid 'Fairy,' the laundry detergent 'Ariel,' and the shampoo 'Pure Line'"

**Conclusion:** Thus, based on the properties of natural, unprocessed sorbents, water was purified from commonly used household detergents. Secondary water purification and its subsequent reuse are among the best solutions to the problem of water pollution.

## Biography

Beisenbekova Gulziya develops students' research skills through project-based work in her lessons. Students address local environmental issues with the teacher's support and deepen their academic knowledge in subjects such as chemistry, physics, biology, and mathematics. In her teaching process, Beisenbekova Gulziya applies STEAM education approaches, which help students develop divergent thinking skills. Her students find multiple ways to solve a single problem. Thanks to this creative approach, many of Beisenbekova Gulziya's students engage in scientific research projects and tackle local issues, contributing to the improvement of the ecological situation in the city of Atyrau."

# NATURAL BARK FIBERS AS REINFORCEMENT IN POLYMER COMPOSITES: A REVIEW OF CHARACTERIZATION TECHNIQUES

**Sivasubramanian Palanisamy**

*P T R College of Engineering and Technology, India*

## Abstract

In recent years, there has been a growing interest in fibers extracted from bark, which are often considered by-products or waste from other industries that utilize the outer, more lignified sections of plants for chemical extraction or discard them as useless.

As a result, studies focusing on the chemical composition (including cellulose, hemicellulose, and lignin content), thermal degradation, and mechanical properties of these fibers are increasingly prevalent, particularly regarding their potential application as short random fibers in polymer composites. This study aims to review the current research landscape to identify which bark fibers hold the most promise among the vast array of options available, particularly those that have received some attention in the literature.

A deeper characterization of these fibers could enhance their competitiveness against other types of fibers, such as those derived from bast, leaves, and other established production systems (like cotton, hemp, flax, and jute) that are already widely used in composite manufacturing. This potential for bark fibers remains largely unexplored.

## Biography

Sivasubramanian Palanisamy currently serves as an Assistant Professor in the Department of Mechanical Engineering at P T R College of Engineering and Technology, located in Madurai, Tamil Nadu, India. He holds a Ph.D. in the field of Mechanical Engineering from Kalasalingam Academy of Research and Education (KARE) situated in Krishnankovil, Srivilliputhur, Tamil Nadu, India. His research expertise encompasses a wide range of areas, including biocomposite materials, the characterization of fibers, fiber-reinforced polymer composites, hybrid composites, fiber-reinforced elastomer composites, the study of tribological behavior in composite materials, and 3D printing. He has an impressive publication record, having authored over 70 research papers in renowned international journals and contributed to 15 book chapters. Additionally, he has delivered 25 keynote/invited talks in his specialized research domains. In recognition of his expertise, He serves as a referee for numerous esteemed journals, including but not limited to Fibers, Biomass Conversion and Biorefinery, Engineering Science and Technology an International Journal, Applied Science and Engineering Progress, Tribology in Industry, Buildings, Processes, Sustainability, and Energies.

# THE WATER FILTER "ANSAQUA"

**Kabdelova Ansagan and Nurzhanova Dariga**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Access to clean water is essential for human health, and affordable filtration solutions are critical, particularly for rural and low-income areas in Kazakhstan. Industrial water filters can be expensive, creating barriers to clean water access, while untreated water sources heighten the risk of disease. This project addresses these issues by developing an affordable water filter, "AnsAqua," using natural and low-cost materials.

**Objective:** The project aimed to create a cost-effective water filter using eggshells as a calcium carbonate source to purify water while enriching it with essential ions.

**Methods:** We reviewed literature on water filtration and surveyed residents on their water filter preferences. Using eggshells, zeolite, and shungite as filter components, we prepared four filter prototypes. Each prototype was tested for its chemical purification capabilities and cost-efficiency, and analysis was conducted in a school laboratory using organoleptic and chemical methods.

**Results:** Among the prototypes, the optimal mixture was determined to be zeolite (40 g), shungite (80 g), and eggshells (40 g), resulting in a filter with effective purification at a cost of 200 KZT. Testing confirmed that the filtered water met safety standards, with reduced levels of iron, chloride, and nitrate ions and enriched levels of sulfate and phosphate ions.

**Conclusion:** The "AnsAqua" filter proves to be a viable, low-cost alternative to conventional filters, effectively purifying water while offering economic accessibility. Future goals include optimizing filter composition and investigating long-term usage efficiency. This filter provides an eco-friendly solution, reduces plastic use, and offers a practical clean water option for underserved communities.

# LAND RESTORATION: INNOVATIVE BIOREMEDIATION USING INDIGENOUS BACTERIA

**Dilnaz Nagim Nurzhankyzy and Kossanov Rakhymzhan**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

**Background:** Soil contaminated with oil poses a significant threat to ecosystems. It disrupts soil structure, water resources, and the life of plants and animals. Oil residues hinder the recovery of ecosystems and can also pose risks to human health. Current remediation technologies are often expensive and may lack efficiency. Therefore, bioremediation—using indigenous bacteria to cleanse contaminated land—has been proposed as an eco-friendly and effective alternative.

**Objective:** To utilize indigenous bacteria to degrade oil residues and restore soil to an environmentally safe condition.

**Methods:**

- Samples of contaminated and clean soil were collected, and the bacteria present in each were identified.
- The oil and heavy metal degradation abilities of these bacteria were tested in the laboratory.
- To accelerate the bioremediation process, the activity of indigenous bacteria was enhanced through a specially formulated nutrient medium.
- The levels of contaminants in the soil were monitored at various intervals to evaluate changes over time.

**Results:** Oil-contaminated soil was effectively treated with bacteria, transforming it into fertile soil ready for reintegration into the ecosystem. This soil was suitable for agricultural and greening purposes. Specific strains of bacteria, naturally present in the local ecosystem and effective at degrading oil, were identified and selectively utilized for bioremediation. These strains are now planned for use in cleaning other oil-contaminated areas. Preliminary results indicate that local bacteria can degrade up to 85% of the oil.

**Conclusion:** The study demonstrates that using indigenous bacteria is an effective method for the biological restoration of contaminated land. This approach is environmentally safe, relatively inexpensive, and practical for application. Areas treated with bioremediation are being restored and reintroduced into the ecosystem, potentially suitable for agricultural crops or other ecologically significant purposes. Step-by-step guidelines and protocols developed specifically for bioremediating oil-contaminated soil will be valuable for environmental organizations, industries, and government agencies. Future research should expand the study scale and implement industrial-level testing.

# DISTINCTIVE PROPERTIES OF NON-EQUILIBRIUM DYNAMIC PLASMA-CHEMICAL SYSTEMS

**Daniil Tretiakov and Valeriy Chernyak**

*Taras Shevchenko National University of Kyiv, Ukraine.*

## Abstract

**Background:** Plasma activation introduces significant energy-mass exchange, leading to non-equilibrium processes where non-equilibrium kinetics impact chemical transformations. L. Polak's work in the 1980s highlighted the diverse, unpredictable behaviors in such systems. This field has advanced microelectronics, diamond film growth, and nano-material synthesis. And goes back to at least the Miller-Urey experiment, conducted in 1953.

**Objective:** The article's main focus is to suggest a possible physical model for experimentally discovered effects, namely an impact of rotation direction on enantiomeric ratio of a treated substance. The effect and experimental methods were previously described in [1] and in [2].

**Methods:** A plasma-liquid system with a rotating gliding discharge was studied. The treated substances was studied for light polarization, UV spectroscopy and Mass-spectroscopy. The system plasma was characterized with optical spectral methods.

**Results:** The observed deviation does not contradict to known chemical laws, and are analogous to known technical processes. The study applied those principles to a system with pronounced rotational motion, and suggests a kinetic model explaining the experimental outcomes, namely: the generation of optically active substances from non-chiral precursors, and the change of polarization angle of initially chiral precursors. The study accounted for optimal particle interaction time, relative particle trajectory, molecule inertia tensor, and molecule shape.

**Conclusion:** The directional movement in dynamic plasma-liquid system can lead to a deviation of enantiomeric ratio which is not predicted for quasi-equilibrium systems. Dynamic systems have a number of mechanisms which might explain observed effect.

## Biography

Daniil Tretiakov was born in Kyiv, Ukraine, in 1994. He received the M.S. degree in radio physics and electronics from the Taras Shevchenko National University of Kyiv, Kyiv, in 2017, where he is currently pursuing the Ph.D. degree. His current research interests include plasma chemistry, synthesis of organic compounds, reforming of bio-fuel in plasma–liquid systems, and nonequilibrium plasma chemistry, recent interest in radio communication systems, electromagnetic warfare.

# EXPLORING THE CALMING AND PAIN-RELIEF EFFECTS OF PLANT-DERIVED TERPENES (PDT): A NATURAL APPROACH TO THERAPEUTICS

**Aziza Abatova, Khadisha Sagenova, Zhanzhetpes Mukhanova, Dana Amangeldi and Asif Abbas Syed**

*Nazarbayev Intellectual School of Chemistry and Biology, Kazakhstan*

## Abstract

The increasing prevalence of stress and respiratory-related disorders has driven a demand for natural and effective therapeutic agents. This project addresses the need for healthier, non-synthetic alternatives to relieve respiratory discomfort, focusing on the use of plant-derived terpenes. Specifically, cineole, a terpene extracted from cloves and cardamom, is explored for its respiratory benefits and therapeutic applications, including its potential to soothe coughs and alleviate related symptoms. This research aims to harness the aromatic and chemical properties of terpenes found in Syzygium aromaticum (clove) and Elettaria cardamomum (cardamom) to develop a natural cough candy formulation that provides respiratory relief. Additionally, the study explores the broader benefits of cineole as a natural remedy for alleviating cough-related symptoms and promoting overall respiratory health.

**Materials and Methods:** Ingredient Selection: Cardamom, clove, and honey were selected based on their documented stress-relief and calming properties. A balance between therapeutic effect and palatability was sought in the candy formulation.

**Extraction Process:** Cineole was extracted from cloves and cardamom using steam distillation:

- Boiler: Steam was generated to pass through cloves and cardamom.
- Distillation Unit: The steam carried essential oils, including cineole, which was then condensed.
- Separation: Cineole was separated from water and purified.

**Candy Formulation:** Multiple formulations were tested to optimize taste and therapeutic effect.

Testing: Sensory evaluations focused on taste, texture, and overall acceptability. The therapeutic effect was measured through subjective self-reports of relaxation and anxiety reduction

Results: The study demonstrates that terpenes, especially cineole and linalool, have notable anti-anxiety and analgesic effects when used therapeutically. Their antimicrobial properties also suggest effectiveness in reducing bacterial infections, offering both pain relief and general health benefits.

**Conclusions:** Plant-derived terpenes show significant promise as natural alternatives for anxiety and pain relief. Their therapeutic properties extend beyond relaxation to broader medical applications. Future research will focus on assessing the long-term affectivity and safety of these compounds.

# THIAZINE 1,1-DIOXIDE DERIVATIVES AS POTENCIAL ANTICANCER AGENTS

**Aleksandrs Pustenko**

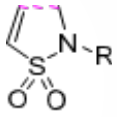
*Latvian Institute of Organic Synthesis, Latvia*

## Abstract

Diseases caused by malignant tumours are one of the leading causes of death in the world and one of the main factors in reducing the average life expectancy. The number of cases and mortality from cancer increases every year, therefore there is a need to develop new, innovative oncological drugs.

It is known that enzyme thioredoxin reductase (TrxR, EC 1.8.1.9) and carbonic anhydrases (CA, EC 4.2.1.1) inhibitors are defined as anti-cancer drug targets, yet there are no TrxR inhibitors in clinical trials and as far as we know there is only one compound as CA inhibitor in clinical trials.

Based on our experience we have designed thiazine 1,1-dioxide derivatives 1 as potential dual inhibitors of TrxR and CA.




1

**Acknowledgements:** This project has been funded by Recovery and Resilience Facility (RRF) (5.2.1.1.i.) grant Nr.41/OSI/PG.

# DISCOVERY OF AROMATIC SULFONAMIDES AS POTENTIAL HUMAN CARBONIC ANHYDRASE INHIBITORS AND ITS EMERGING ROLE AS ANTIEPILEPTIC AGENTS

## Abha Mishra

*National Institute of Pharmaceutical Education and Research, India*

## Abstract

**Background:** Epilepsy is a neurological disorder, affecting approximately 50 million people globally. Disruptions in brain ionic balance and pH shifts are central to its pathology. Human Carbonic Anhydrase II (hCA II) plays a crucial role in these disruptions. Recent studies have further elucidated the role of carbonic anhydrases in epilepsy, particularly through their influence on NMDA receptors and extracellular proton levels during seizures. Current antiepileptic drugs like Topiramate and Acetazolamide act through CA inhibition. This study aims to advance epilepsy treatment by new benzenesulfonamide derivatives as selective inhibitors of hCA II.

**Objective:** To design, and synthesize aromatic sulfonamide compounds as hCA II inhibitors and evaluate their potential as anticonvulsant agents.

**Methods:** A series of aromatic sulfonamide derivatives were synthesized using a tail approach. The compounds were characterized by ATR, HRMS, and NMR (1H and 13C). Drug design methodologies, including DFT computation, structure-based drug design, molecular docking were used. Inhibitory activities against hCA II were assessed, and the most effective inhibitors were further evaluated in a subcutaneous pentylenetetrazole (sc-PTZ) epilepsy model and assessed for acute toxicity. Structure-activity relationships linked structural features to inhibitory and anticonvulsant activity.

**Results:** The synthesized benzenesulfonamide derivatives exhibited inhibitory activity against hCA II, with inhibition constants (Ki) ranging from 0.09 to <10 nM. Among these compounds, C-11 was identified as the most potent inhibitor and showed 80% protection in the ScPTZ model. Toxicity assessment showed that the LD50 of the novel compounds was greater than 300 mg/kg body weight.

**Conclusion:** This study underscores the potential of hCA II inhibition as a therapeutic strategy for epilepsy. The identified compounds provide a basis for developing more effective, targeted treatments. Further preclinical and clinical evaluations are needed to confirm their therapeutic efficacy and safety.

## Biography

Abha Mishra is a dedicated Ph.D. Research Scholar in the Medicinal Chemistry department under the supervision of Dr. Kalyan kumar Sethi (Assistant professor) at NIPERGuwahati, Assam, India. She holds a B.Pharmacy from Bundelkhand University and an M.S.(Pharm.) in Medicinal Chemistry from NIPER, Raebareli. Abha has practical industry experience from an internship at Almelo Pvt. Ltd and work in API synthesis. She is currently working on the project entitled "Design, synthesis and pharmacological evaluation of Sulfonamide derivatives as human carbonic anhydrase inhibitors". Abha's contributions to academia are also noteworthy, with 7 published articles in journals, 2 patents, and 4 poster presentations at national and international conferences. With her solid educational background, rich industry experience, and active involvement in research and publications, Abha Mishra is undoubtedly positioned to make significant contributions to the chemistry, pharmaceutical, and research landscape.

# DETERMINATION OF PERCHLORATE IN FOODSTUFF

**Olga Pardo Marín**

*Universitat de València, Spain*

## Abstract

**Background:** Perchlorate is a stable, water-soluble ion that can be found in food due to both natural sources, such as atmospheric formation, and anthropogenic activities, including the use of certain fertilizers and the breakdown of sodium hypochlorite. Numerous toxicological studies have linked perchlorate exposure to adverse health effects, including thyroid tumors, reproductive toxicity, and fetotoxicity. In response to these health concerns, Commission Regulation 2023/915 has established maximum allowable levels of perchlorate in various food categories.

**Objective:** To develop and validate a methodology for the determination of perchlorate in foodstuff which present a maximum limit set in Commission Regulation 2023/915.

**Methods:** The method was developed involving extraction with acetonitrile (ACN) acidified to 0.1% with formic acid, followed by a clean-up step using dispersive solid-phase extraction (dSPE) with C18 and graphitized carbon black (GCB). Analysis was conducted via UHPLC-MS/MS with electrospray ionization in negative mode. Quantification was achieved using an internal standard calibration curve ranging from 0.5 to 20 ng/mL, employing an isotopically labeled perchlorate-18O4 internal standard at a constant concentration of 5 ng/mL.

**Results:** The method was validated according to the criteria established in SANTE 11312/2021 for samples of tea, cucurbitaceous crops, vegetables, and fruits. Accuracy was evaluated using fortified blank samples at three levels within the calibration curve, yielding recoveries from 70% to 129%. Intra-day precision ranged from 6% to 20%. The method's linearity was confirmed with regression coefficients of ≥ 0.99 and goodness-of-fit coefficients below 20%.

**Conclusion:** Validation results demonstrated that this method is accurate, reliable, and sensitive for the determination of perchlorate in food matrices. Future studies will extend this method's application to a wider range of food types and analyze various samples to facilitate a dietary risk assessment of perchlorate exposure.

# THE USE OF GAS DISCHARGE IMAGING (GDV), SPECTROPHOTOMETRY AND GC-MS METHODS TO STUDY THE EFFECT OF ORGANIC FERTILIZERS ON THE QUALITY OF LEAFY VEGETABLES

**Svetlana Motyleva, M. Gigadlo, M.Vinokur, E.Yamileva**

*Strogoorganic Online Gardening School, Russia*

## Abstract

**Background:** The assessment of the effect of fertilizers on the nutritional value of edible parts of plants is relevant. The applied fertilizers have an effect on the metabolic processes in plants, which leads to a change in their energy fields.

**Objective:** To study the energy activity, accumulation of vitamin K and accumulation of metabolites in leafy vegetable crops (Lactuca sativa L., Allium cepa L. and Ocimum basilicum L.) depending on the application of fertilizers in the form of concentrate, paste and granules.

**Methods:** Plants were grown under greenhouse conditions, in plastic vessels filled with peat with the addition of fertilizers at doses and methods of application recommended by the manufacturer. The leaves of plants at the stage of consumer maturity were examined. Direct determination of vitamin K (extraction with hexane) was carried out on a spectrophotometer SF-56 (Russia) at a wavelength of λ = 261nm. The Gas Discharge Visualization (GDV, Kirlian method) method was used in parallel. Plants were placed in an electromagnetic field of high intensity, and the luminescence formed around them was recorded using a GDV camera (manufacturer Biotechprogress LLC, Russia).The metabolites analysis was fulfilled on chromatograph GCMS-QP2010 SE, Shimadzu (Japan) by the method of gaschromate-mass-spectrometry (GC-MS). Capillary column DB-5HT. The temperature gradient during the analysis was 40-280°C; oven temperature progress from 40 to 130°C at 1 °C min-1, from 130 to 200°C at 2°C min-1, from 200 to 280°C at 4°C min-1 and holding at 280°C for 40 min; the temperature of the ion source - 200°C.

**Results:** Application of fertilizer in the form of concentrate for onion and basil plants contributes to the synthesis of the largest amount of vitamin K and leaves of these plants noted the greatest intensity of luminescence compared to the same indicators of plants grown on fertilizer in the form of paste and granules. Lettuce plants, on the contrary, have the highest intensity of luminescence and vitamin K when using fertilizer in the form of paste. The application of fertilizer in the form of granules for all the studied plants showed the lowest energy characteristics and vitamin K accumulation in the leaves. High correlations between the average luminescence intensity and vitamin K content in leaves of all investigated leafy vegetable species were revealed. More than 30 metabolites were identified by GC-MS in hexane extract. Fertilizers affect the quantitative content of palmitic, sageric acids and squalene.

## Biography

Svetlana Motyleva - head of the scientific laboratory, member of the All-Russian Mass Spectrometric Society. Mikhail Gigadlo is a scientist in the field of biophysics. Maria Vinokur and Elia Yamileva are the founders of the online gardening school Strogoorganic.

Coalesce Research Group

**Coalesce Research Group**
33 Market Point Dr,
Greenville, SC 29607, USA

**Contact Us:**
**Phone:** +1-718-543-9362
**Email :** info@coalesceresearchgroup.com,