BALTIC CONFERENCE
CHEMISTRY

27-28.MAY.2023

ONLINE

Book Of Abstracts

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PROLOGUE

Dear Colleagues,

On behalf of Student's Science Club for Chemistry at the University of Gdańsk, the Student's Science Club for Chemistry, the Students' Self-Government Council of the Faculty of Chemistry and the Doctoral Council of the Doctoral School of Natural Sciences of the University of Gdansk I extend my heartfelt appreciation to everyone who attended the Baltic Chemistry Conference.

Our esteemed event united bright minds from across the globe in the fields of chemistry, biomedical chemistry, biochemistry, environmental protection, and ecology. The insightful lectures delivered by Prof. Elżbieta Jankowska from the University of Gdańsk and Dr Chiara Da Pieve from the Institute of Cancer Research, UK, set a high bar for the scientific exchange and created a vibrant atmosphere of innovation.

We express our gratitude to our patrons for their generosity and support, which was instrumental in creating an enriching platform for all our participants.

The conference not only facilitated the presentation of ground breaking research but also fostered international collaborations and professional relationships. It is our hope that the insights gained and connections made during this conference will continue to inspire and influence your work.

As we reflect on the success of the Baltic Chemistry Conference, let's revisit the abstracts enclosed in this book and continue the discussions that were started. Each one represents the dedication, passion, and innovation of our global scientific community.

Thank you once again for your engagement and contributions to the success of this event. Here's to the advancement of science and to future collaborations.

Until we meet again at the next Baltic Chemistry Conference!

On behalf of the organisers of Baltic Chemistry Conference

MSc Mateusz A. Baluk

President of the Doctoral Council
of the School of Natural Sciences of the University of Gdansk

THE BALTIC SEA: EUROPE'S UNIQUE BODY OF WATER

The Baltic Sea, also commonly referred to as the Baltic, is a unique body of water possessing an array of distinctive features and environmental conditions. This sea is located in Northern Europe, stretching from the western shores of Denmark to the eastern fringes of Russia, and cradled by nine different countries: Denmark, Estonia, Finland, Germany, Latvia, Lithuania, Poland, Russia, and Sweden.

At approximately 1,600 kilometers (990 miles) long, the Baltic Sea covers an area of about 377,000 square kilometers (146,000 square miles), making it one of the largest brackish inland seas by area in the world. Its mean depth is 55 meters, with its deepest point being the Landsort Deep near Sweden, measuring 459 meters (1,506 feet).One of the most intriguing characteristics of the Baltic Sea is its brackish nature. Unlike most marine environments, the Baltic Sea has a low salinity level. This results from its semi-enclosed nature, with limited water exchange with the North Sea, and a significant influx of freshwater from numerous rivers that discharge into it. The salinity level varies across the Baltic, but on average, it stands at about 0.8% at the surface, significantly lower than the average salinity of oceanic waters, which is typically around 3.5%.

The low salinity, combined with the colder climate of Northern Europe, gives rise to a unique ecosystem. A variety of species adapted to these specific conditions inhabit the Baltic Sea. The most emblematic ones are perhaps the Baltic herring and the cod, which have been vital to the region's fishing industry for centuries. The sea also serves as an important resting and breeding ground for many species of birds, while its coastal regions host diverse flora and fauna. Another significant aspect of the Baltic Sea is its importance to the surrounding countries' economies. It has been an essential trading route for hundreds of years, connecting major ports like Kiel, Riga, Stockholm, and Gdansk. The sea also provides a wealth of resources such as fish, and more recently, offshore wind energy.

Moreover, the Baltic Sea is a significant focus of scientific research. Its unique properties make it a fascinating subject for studying marine biology, oceanography, and environmental science. Its sensitivity to environmental changes also makes it a crucial barometer for climate change. Issues like eutrophication, plastic pollution, and the impact of human activity on marine ecosystems are critical research topics in the Baltic region.

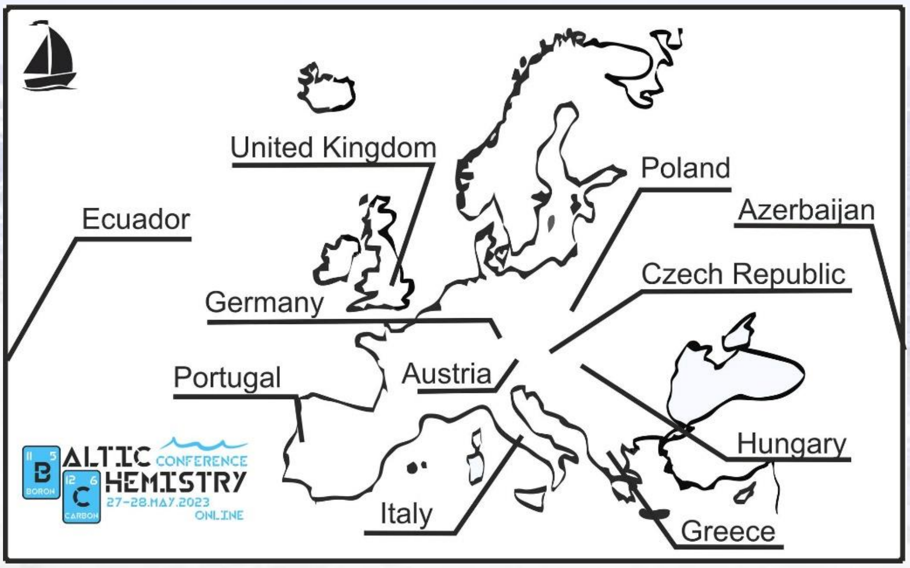
However, the Baltic Sea also faces considerable environmental challenges. Its limited water exchange with other bodies of water, combined with industrial and agricultural runoffs, has led to severe problems of eutrophication. This process is characterized by an excess of nutrients that cause harmful algal blooms and subsequent oxygen depletion in the water, endangering marine life.

In conclusion, the Baltic Sea is a uniquely brackish marine environment with rich ecological diversity and significant economic and scientific value. Its unique characteristics make it an interesting subject for various scientific studies. At the same time, it is a body of water under significant environmental stress, highlighting the importance of sustainable practices and ongoing research to understand and mitigate these challenges.

Author: Mateusz A. Baluk

ABOUT THE CONFERENCE

The Baltic Chemistry Conference held on the 27th and 28th of May 2023, was a remarkable gathering that united distinguished participants in a virtual setting. The conference was truly international, featuring attendees from 11 different countries, including Poland, Austria, Hungary, the Czech Republic, Greece, Italy, Germany, Azerbaijan, Portugal, Ecuador, and the United Kingdom. In total, we were honored to welcome 110 delegates representing 26 unique scientific institutions from around the world.



Over the two-day conference, 32 insightful presentations and 41 intriguing poster communication were delivered. These were spread across six sessions, each providing a platform for the exchange of groundbreaking ideas and fostering international collaborations in the fields of chemistry, biomedical chemistry, biochemistry, environmental protection, and ecology. The presentation sessions occurred in an online meeting, enabling speakers to either share a pre-recorded video or present a live lecture. Following each presentation, a live discussion was held, allowing further engagement and detailed exploration of the presented topics. Poster announcements, on the other hand, were divided into two parts: a five-minute video presentation showcasing the poster and a two-hour live discussion providing an avenue for deeper understanding and queries.

Among the 26 scientific institutions represented, there were both universities and research institutions, including but not limited to the University of Gdańsk, University of Vienna, Georg-August-University Göttingen, University of Camerino, Universidade NOVA de Lisboa, and the Institute of Cancer Research. Each institution brought its unique insights and contributions to the event, thus enriching the scientific discourse.

We extend our heartfelt gratitude to everyone who made the conference a success, especially the attendees and presenters who offered their innovative research and enriched the scientific discussions. Your active participation and invaluable contributions played a crucial role in making this conference a hub for intellectual exchange and innovation. The insights and connections fostered during the Baltic Chemistry Conference have undoubtedly spurred future research and collaborations. We hope the knowledge gained and shared at this conference will prove useful in your future endeavors.

Once again, thank you for making the Baltic Chemistry Conference a remarkable success. We look forward to welcoming you at our next event

ORGANISING COMMITTEE

The Baltic Chemistry Conference was organised by an agreement of three organisations from the University of Gdansk - the Student's Science Club for Chemistry, the Students' Self-Government Council of the Faculty of Chemistry and the Doctoral Council of the Doctoral School of Natural Sciences of the University of Gdansk.

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SCIENTIFIC COMMITTEE

Prof. Henry Pinto
(Yachay Tech University, ECUA)

Henry Pinto obtained his PhD in Physics in the field of Condensed Matter Physics and Quantum Mechanical simulations at the Department of Physics at the National University of Ireland in Cork and Tyndall National Institute, Ireland, in 2006. During his PhD studies he was the winner of the BOC Postgraduate Bursary Award for his research. Through his scientific career, Dr. Pinto has been doing research in world class centers like: Aalto University, Finland; Nagoya University, Japan and Liverpool University, UK. From 2010 until 2016 Dr. Pinto was a Research Professor in the Interdisciplinary Center for Nanotoxicity at Jackson State University, USA. From 2016 Dr. Pinto is a professor at the School of Physical Sciences and Nanotechnology at Yachay Tech University and the head of the CompNano Group. Dr. Pinto's main scientific interests are in Condensed Matter Physics and Computational Materials Science applying cutting-edge theoretical and computational methods together with the best available computing resources. He has special interest in the understanding of the nanoworld phenomena from a theoretical perspective in close collaboration with experimentalists. His main research topics include: electronic structure calculations, magnetism and strong correlated systems, mineral and metal-oxide surfaces and interfaces, polymers and metal/polymer interfaces, scanning tunneling microscopy simulations, nanomanipulation, molecular electronics, point defects and high performance computing

Dr Elżbieta Adamska
(University of Gdansk, PL)

Dr Elżbieta Adamska is part of the Department of Analytical Chemistry of the Faculty of Chemistry at the University of Gdansk. Her scientific interests concern the synthesis of nanoparticles with optical properties that have potential application in percutaneous permeability studies. She is the author and co-author of 19 scientific and popular science publications and about 80 national and international conference presentations. She obtained her bachelor's degree in 2015 and in 2017 a master's degree. She graduated as PhD in 2022 at the Faculty of Chemistry of the University of Gdańsk. She also completed foreign scientific internships at the Beijing Institute of Technology (China), University of Belgrade (Serbia) and Helmholtz-Zentrum Hereon (Germany).

Dr Aamod Desai
(University of St. Andrews, UK)

Dr Aamod Desai completed his PhD from IISER, Pune (India) and is currently working as a postdoctoral research fellow at the University of St Andrews (UK). Apart from the core training as material chemist in metal-organic frameworks (MOFs), he has worked in the field of electrode materials for rechargeable battery technologies, such as Li-ion and Na-ion batteries.

Dr Maria Madej
(Jagiellonian University, PL)

Maria Madej is a PhD researcher in Department of Analytical Chemistry at the Faculty of Chemistry, Jagiellonian University in Kraków, Poland. She received her PhD degree in 2021. Her research is related to the development of voltammetric (bio)sensors intended for the determination of antidepressants in environmental and biological samples. She focuses especially on searching of new materials for the modification of solid electrodes, including zeolites, metal-organic frameworks or polymers deposited in cold plasma reactors.

Dr Daria Grzywacz
(University of Gdansk, PL)

Daria Grzywacz is an assistant professor at the Department of Organic Chemistry, at the University of Gdansk. She conducts scientific research in the fields of organic chemistry and biology, with a particular focus on glycochemistry, as well as heterocyclic compounds that exhibit OLED emitter properties and act as photosensitizers/photocatalysts in the hydrogen production reaction. Her research interests encompass the chemistry of carbohydrates, especially their combination with triterpenoid and spirostan saponins that demonstrate biological activity, such as diosgenin and betulin. Additionally, her research interests include synthesizing and evaluating glycosylated antimicrobial peptides (gAMP) for their antifungal, antibacterial, and hemolytic activity.

Dr Daria Krefft
(University of Gdansk, PL)

Dr Daria Krefft is an assistant professor at the Department of Molecular Biotechnology at the Faculty of Chemistry of the University of Gdańsk. As part of her research, she dealt with gene cloning, as well as overproduction, purification and testing the properties of many proteins, including fluorescent proteins and luciferase, thermostable restriction endonucleases, and polyepitopic proteins with potential pro-regenerative properties.

Dr Catarina S. Lobo
(Institute of Cancer Research, UK)

Catarina S. Lobo is a postdoctoral research fellow working at The Institute of Cancer Research in London and her work is focused on photoimmunotherapy and PET imaging of neuroblastoma. Catarina completed her PhD in Medicinal Chemistry at University of Coimbra, Portugal, in 2021. Her PhD thesis was focused on photodynamic therapy, immunotherapy, and imaging techniques. Before joining ICR, Catarina worked as a researcher at LaserLeap Technologies. Catarina is a co-founder of Molecular Junior Enterprise.

Dr Eng Aleksandra Pieczyńska
(University Of Gdansk, PL)

Assistant professor at the Department of Environmental Technology, Faculty of Chemistry, University of Gdańsk. Scientific interests include the synthesis and characterization of new nanomaterials and their application for the degradation of resistant micropollutants and the generation of useful chemicals by photocatalytic and photoelectrocatalytic processes.

Dr Karolina Plecyk
(Warsaw University, PL)

Adiunct at the University of Warsaw, Chemistry Department. My work is focused on organic chemistry with elements of biophisics and biochemistry. My main research is based on synthesis of mRNA 5′ cap analogs and their application in biochemical and physicochemical studies on the mechanisms of translation initiation, splicing, intracellular transport and mRNA stability in eukaryotic cells; Synthesis and biochemical studies of nucleotide inhibitors of protein biosynthesis of potential therapeutic importance in neoplastic diseases and synthesis of cap analogs improving RNA properties for therapeutic and biotechnological applications

Dr Joanna Żebrowska
(University Of Gdansk, PL)

Ph.D. from the Faculty of Chemistry, University of Gdansk, graduated LiSMIDoS at the Faculty of Biotechnology University of Gdansk-Medical University of Gdansk. Assistant Professor at the Department of Molecular Biotechnology, Faculty of Chemistry at the University of Gdansk. Research area: purification of polyepitopic proteins with therapeutic and regenerative proteins, design and cloning synthetic genes, bacteriophage proteins, chemical synthesis cofactor analogues for Thermus family enzymes, engineering DNA-recognition specificity of enzymes, biochemical and physico-chemical properties of the enzymes.

SPECIAL GUESTS

Prof. Dr Hab. Elżbieta Jankowska
(University Of Gdansk, PL)

Elżbieta Jankowska is an employee of the Department of Biomedical Chemistry, Faculty of Chemistry, University of Gdańsk. She received her PhD degree in 2001, and in 2013 she was awarded with a habilitation degree in chemical sciences. In 2015, she was promoted to the position of Associate Professor at the University of Gdańsk. Her scientific interests include primarily peptides, polypeptides and proteins. She deals with the study of their structure, in particular conformational changes that accompany the processes of oligomerization and aggregation of these biomolecules. Since her postdoctoral internship in 2003-2004, at the University of Texas Health Science Center in San Antonio, USA, the focus of her interest has been the proteasome, a multiprotease responsible for the degradation of most cellular proteins, including damaged ones, which are precursors of toxic oligomeric forms. The current research focuses on the design of modulators capable of accelerating the degradation of oligomers by the proteasome. Dr. hab. Elżbieta Jankowska managed 4 projects awarded by the National Science Center and worked in 3 other research projects. She is the co-author of 54 scientific articles, her papers have been cited 999 times, and the Hirsch index is 18.

Dr Chiara Da Pieve
(Institute of Cancer Research, UK)

I am a senior radiochemist in the Preclinical Molecular Imaging group, Division of Radiotherapy and Imaging at the Institute of Cancer Research, London, UK. I received my PhD degree in 2005 from the Inorganic Chemistry department, University of Zuerich (Switzerland). From my master's degree at the University of Padua (Italy), through my PhD and to my postdoctoral position at the Open University (UK), I worked with metal and radiometal ions, and biomolecules (DNA aptamers, peptides and proteins) focusing on the preparation of coordination compounds for medical applications.

Currently I am involved in the development and production of targeted radioactive probes for the imaging and therapy of cancer. My scientific interests include peptides, small proteins, full size antibodies, chelators (for radiometals) and bioconjugation techniques. I spend my working days preparing, analysing, and purifying various protein-chelator conjugates which are then radiolabelled with the most suitable radioactive label for preclinical assessment.

Opening lecture by Prof. Dr Hab. Elżbieta Jankowska

Title: “Can amyloidogenic forms of proteins be removed from our body?”

Abstract: Human 20S proteasome provides cells with a cleaning system, removing mutated, misfolded, and oxidatively damaged proteins. During aging, the effectiveness of the proteasome system gradually declines. Impaired proteasome function leads to the accumulation of abnormal proteins and their aggregation, which in turn contributes to the development of aging symptoms, such as cataracts or changes in skin pigmentation, as well as severe illnesses, for instance, amyotrophic lateral sclerosis and Alzheimer's and Parkinson's diseases. A promising therapeutic strategy to delay the onset of age-related disorders could be proteasome activation. This approach is growing in popularity, but so far little is known about the mechanism of 20S stimulation by small molecules, hence the lack of good leading structures for the design of activators.

A few years ago, we had our first success in developing proteasome activators. We obtained a compound named Blm-pep and a dozen of its analogs, which turned out to be effective in

stimulating human proteasome. These peptides enhanced degradation not only of small fluorogenic substrates but also of model proteins, including those involved in neurodegeneration, such as α-synuclein and Tau protein. However, the compounds had negligible resistance to proteolytic enzymes. In order to increase their stability in human serum, we transformed them into peptidomimetics by replacing natural amino acids with their N-methylated versions or introducing a peptoid bond. In addition, to ensure cell permeability, peptidomimetics were grafted with a cell penetrating moiety. These modifications turned out to be effective, allowing to obtain very promising, effective, proteolytically stable and cell-permeable compounds. They can become leading structures in the design of therapeutics that are a response to aesthetic and medical problems related to aging process.

Opening lecture by Dr Chiara Da Pieve

Title: "PET imaging is a non-invasive technique that uses radioactive probes for the detection of various diseases and the evaluation of organ functionality"

Abstract: In the last years, following the fast development of immunotherapy and to meet the need of personalized medicine, protein-based PET probes design and use is in its fastest-growing phase. Such radioactive agents contain radioactive metals and the most suitable chelators and are prepared by applying conjugation techniques.

Before translation to the clinical setting, each radioactive agent is preclinically tested (in vitro and in vivo) to assess the pharmacokinetics and biodistribution properties. The talk is covering the basic principles and steps followed for the preparation of PET probes and their assessment.

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We would like to thank our patrons sincerely, thanks to their support our conference has become known in the international scientific world.

Uczelnie Fahrenheita

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Thanks to the collaboration with the Journal of Young Researchers PROGRESS,
Baltic Chemistry Conference speakers can publish their papers free of charge.

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ORAL COMMUNICATIONS

Oral messages were distributed over six sessions. The presentation sessions took place in an online meeting, where speakers could share a video recording or present a live lecture. After each presentation there was a live discussion with the speaker about the communication.

TITLE

Occurrence of estrogens and tetracyclines in the European aquatic environment

AUTHORS

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ABSTRACT

Nowadays, humanity is facing a shortage of drinking water, which is related on the one hand to climate change and on the other hand to the increasing pollution of surface and groundwater caused by human activity. Among the plethora of chemicals released into the environment, much attention is paid to emerging contaminants, such as hormones and antibiotics. Estrogens and tetracyclines can enter the environment through domestic sewage disposal and fertilisation of fields with animal manure. It was noted that areas characterized by intensive animal husbandry and a high population density are main sources of estrogen emissions into the environment [1]. It is also significant in this regard that there are no legal restictions about amount of tetracyklines and estrogens released from wastewater treatment plants, therefore they are constant present in aquatic environment in ng/L or µg/L.

According to Commission Implementing Decision 2018/840, which was valid until 25.07.2022, three estrogens were on the Union-wide monitoring substance watch list [2]. Monitoring of these pollutants in the aquatic environment was carried out in most of Western Europe countries. In Eastern Europe, monitoring was not carried out in many countries [3]. The average level of estrogen contamination in water was 0-10 ng/L and for tetracycline contamination 0-20 ng/L in most environmental samples tested [3]. Such levels of estrogen and antibiotic concentrations in the aquatic environment pose a serious threat to the functioning of animals closely associated with water [3].

The development of wastewater treatment technologies and the application of good agricultural practices can improve water quality when contaminated with estrogens and tetracyclines [4,5,6]. The Commission of the European Union should consequently lead to appropriate regulations to control the concentration of estrogens and tetracyclines in the effluent of wastewater treatment plants.

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[5] Rechsteiner D, Wettstein FE, Warren BP, Vermeirssen ELM, et al. (2020) Natural estrogens in surface waters of a catchment with intensive livestock farming in Switzerland. Environ Sci Process Impacts 22: 2244–2255.

[6] Zhou X, Cuasquer GJP, Li Z, Mang HP, Lv Y (2021) Occurrence of typical antibiotics, representative antibiotic-resistant bacteria, and genes in fresh and stored source-separated human urine. Environ Int 146: 106280.

TITLE

Synthesis and characterization of $ZnGa_2O_4$:Cr^{3+} nanoparticles showing persistent luminescence

AUTHORS

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ABSTRACT

Materials that have the ability to emit light after irradiation have been known for centuries. This phenomenon is known as Persistent Luminescence (PL), and has been extensively researched in recent years. These materials have even been used in many daily life materials e.g. in the production of glow-in-the-dark toys and safety signs [1]. However, with the advancement of nanotechnology, PL continues to be a intensively studied area of research. One of the most promising developments in this field is the use of Persistent Luminescence Nanoparticles (PLNPs), which have a wide range of potential applications in biosensors, photodynamic therapy, and bioimaging [2]. ZnGa2O4 doped with Cr3+ ions is one such material that has been thoroughly investigated due to its long-lasting luminescence and emission band located within the first biological window range, making it suitable for multiple biological applications [3].

In this presentation, preliminary research results on ZnGa2O4 nanoparticles doped with various concentrations of Cr3+ ions will be shown. The synthesized materials were obtained using two different methods: hydrothermal and sol-gel. We have also examined the decay times of long-lasting luminescence and the excitation and emission spectra of PLNPs. The structure and morphology of the nanomaterials have been confirmed using powder X-ray diffraction (XRD), and transmission electron microscopy. The sizes of synthesized PLNPs in aqueous colloids were determined using dynamic light scattering method (DLS).

The research was funded by the National Science Center's Opus grant No. 2022/45/B/ST5/00604

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[3] Lin X. Song L. Chen S. Chen X. Wei J. Huang G. Yang H. (2017) Kiwifruit-like Persistent Luminescent Nanoparticles with High-Performance and in Situ Activable Near-Infrared Persistent Luminescence for Long-Term in Vivo Bioimaging. ACS Appl. Mater. Interfaces 9: 41181-41187.

TITLE

Preliminary electrochemical studies of newly synthesized metallocarbonyl complexes with imides.

AUTHORS

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ABSTRACT

The chemistry of organometallic transition metal complexes of biologically important ligands is a field of research within the relatively new branch of organometallic chemistry and bioorganometallic chemistry.

Succinimides have a diverse range of biological functions, which is of interest to many scientists. In my university laboratory, methods of introducing the $CpFe(CO)_2$ group ($Cp=\eta_5$ -C_5H_5) into such ligands containing acidic NH bonds were developed, based on the photochemical substitution of iodide in $CpFe(CO)_2I$ leading to the formation of 3-substituted metallocarbonyl complexes (Fe, Ru) with maleimide and succinimide ligands (Fpm, Rpm and Fps). These complexes were obtained in the presence of K[sub]2[/sub]CO[sub]3[/sub] during the reaction of oxa-Michael $CpM(CO)_2$ (1-maleimidato) (M = Fe, Ru) with alcohols (MeOH, EtOH). Metallocarbonyl complexes containing succinimides can serve as modern compounds overcoming antibiotic resistance. One of the ways of pharmacological action of this type of compounds are redox reactions leading to the disruption of cellular processes.

One of the commonly used electrode materials for the electrochemical analysis of organic compounds is glassy carbon. Glassy carbon is electrochemically inert, dense and hard as glass, impervious to gases and liquids, and has a large potential window.

The aim of the presented work was to determine the electrochemical activity of newly synthesized imide complexes such as Fpm, Rpm and Fps.

The characteristics of the working glassy carbon electrode were determined in a solution of the standard Fe(III)/Fe(II) redox system using cyclic voltammetry (CVC) and electrochemical impedance spectroscopy (EIS). Determination of the topographic properties of the GC electrode surface was carried out using an atomic force microscope (AFM). The electrochemical properties of the imide complexes were studied in Britton-Robinson buffer solutions at different pH 5, 7 and 10 using cyclic voltammetry (CVC) and electrochemical impedance spectroscopy (EIS).

TITLE

Sustainable aviation fuel production from waste: Current status and challenges

AUTHORS

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ABSTRACT

The aviation industry is expanding rapidly and is an important contributor to the global economy. However, reducing carbon emissions in the aviation sector is an ongoing issue, and sustainable aviation fuels (SAFs) are expected to be crucial in achieving initial reductions in CO2 emissions by 2030 and significant reductions by 2050. Several waste-to-energy technologies can convert waste feedstocks, including used cooking oils (WCOs), agricultural residues, and food and plastic waste, into biojet fuels [1, 2]. The hydroprocessed esters and fatty acids (HEFA) pathway is a mature technology for converting oleochemical feedstocks, including WCOs, into aviation biofuel and will continue to dominate in the near future. In addition, the gasification-Fischer-Tropsch (FT) pathway utilizes catalytic syngas conversion over various catalysts and covers any feedstock type. The main challenges of the FT-SPK pathway include the economic viability of bio-based feedstocks concerning the required gasification technology and syngas clean-up methods. Around the world, a vast quantity of agricultural biomass is generated, with the main waste products being wheat and rice straw, corn stover, and sugarcane bagasse. The alcohol-to-jet (ATJ) route is a potential pathway for producing biojet fuels from starch-rich or lignocellulose-based biomass feedstocks in the near future [3]. Evaluations of the technology and economics show that using agricultural biomass for biofuel production through thermochemical methods could be feasible in the near future. However, producing biofuels efficiently and cost-effectively still faces challenges in the energy market, a lack of supportive policies and financial incentives, and a scarcity of knowledge about the necessary equipment [4]. Finally, food and plastic waste could serve as alternative feedstocks for SAF production. Instead of landfilling or burning, utilization of the organic fraction of these types of wastes could be used for biojet fuels production through several methods, including pyrolysis, gasification, co-pyrolysis, and hydrothermal liquefaction (HTL). Nevertheless, more research and development are required as most of these advanced technologies are not yet commercialized [5].

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TITLE

Synthesis of cycloalkylacetophenones in the presence of nano-sized $ZnCl_2$

AUTHORS

G.Z.Haydarli (1), N.R.Dadashova (1), S.T.Shahmuradov (1)

AFFILIATION

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ABSTRACT

In industrialized countries, the production of antioxidants, stabilizers, additives and plasticizers is preferred over the production of polymeric materials, rubbers and oils. Alkylphenol-based chemical compounds have a special place in these chemical additives. The most important advantage of this type of chemical additives is its resistance to light, oxygen and temperature. For this reason, today, alkylphenol-based additives are used large part of the chemical industries.

In this paper, 2-cycloalkyl-4-methylphenols were obtained from catalytic alkylation reactions of para-cresol and the cyclodimers of isoprene. the synthesized 2-cycloalkyl-4-methylphenols are involved in the Friedel-Crafts acylation reactions with acetic acid (AcOH) in the presence of nano-catalytic system to obtain methylcyclohexylacetop-henones.

In order to obtain 2-cycloalkyl-4-methylphenols, we studied the alkylation reaction of p-cresol with diprene (DP), dipentene (DPT) and their mixture in the presence of KU-23. Acylation of 2-cycloalkyl-4-methylphenols (CAP) with acetic acid.

Acetophenons are synthesized by acylation reactions of 2-cycloalkyl-4-methylphenols with acetic acid in the presence of nano-sized ZnCl2.

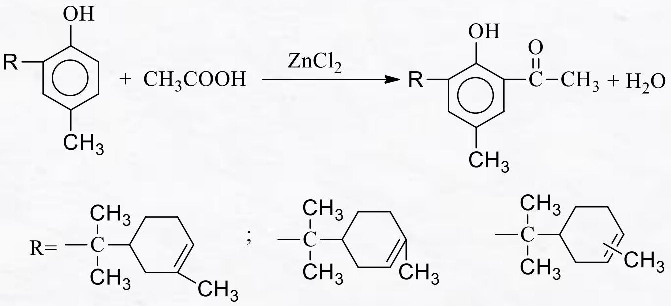

Fig. 1. Acylation rections of 2-cycloalkyl-4-methylphenols with acetic acid in the presence of nano-sized ZnCl2

Optimal conditions were found (temperature 130-140 °C, duration of the reaction 5-6 h, molar ratio of the initial components 1:1, the amount of catalyst 12-15%) for the alkylation process of p-cresol with diprene, dipentene and their mixture (fr.160-180 °C) in the presence of the catalyst KU-23;

The reaction of 2[3(4)-methylcyclohexen-3-yl-isopropyl]-4-methylphenols with AcOH in the presence of nanostructured $ZnCl_2$ at a temperature of 140°C, a reaction time of 30–40 minutes, and a 1:2 molar ratio of CAP to AcOH was used to obtain cycloalkylacetophenones with yields 65.6-68.4%.

Synthesized cycloalkylacetophenones have been tested as an environmentally safe additive in diesel fuel.

TITLE

Immobilization of Agaricus bisporus Polyphenol Oxidase 4 on mesoporous silica: towards mimicking key enzymatic processes in peat soils

AUTHORS

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ABSTRACT

The development of methods for the structure elucidation of riverine humic-derived iron-complexes is challenging but an essential task at the present time since they play a pivotal role in maintaining the productivity of marine ecosystems. Low-molecular-weight phenolic compounds represent the most important group of iron-carrying humic substances in peatland-influenced rivers. These compounds may be converted into multidentate Fe-binding ligands via the activity of polyphenol oxidases produced by soil bacteria.[1] In order to develop an accurate model system for the formation of these iron-chelating ligands we focus our studies on the immobilization of a functional mushroom tyrosinase, Agaricus bisporus Polyphenol Oxidase 4 (AbPPO4, 65 kDa)[2] on mesoporous Santa Barbara Amorphous type material #15 (SBA-15, pore size: 8.5 nm). The enzyme adsorption isotherm was obtained at 4 °C and pH 7.4, resulting in a maximum amount of 7.2 µmol of immobilized AbPPO4 per gram of non-modified SBA-15. To verify that the tyrosinase preserved its catalytic performance throughout the immobilization process, enzymatic activity tests were developed following the oxidation of L-tyrosine (2 mM) by UV-vis spectroscopy (λ = 475 nm). The influence of the surface charge of the silica support on the loading efficiency of AbPPO4 was evaluated through functionalization of SBA-15 with a positively charged amino-silane, 3-Aminopropyltriethoxysilane (APTS), introduced through a post-grafting strategy.[3]

When the specific enzymatic activity of the obtained catalyst (SBA15-NH2-Tyr) was compared with the free enzyme a considerable decrease in the catalytic performance of the immobilized AbPPO4 was observed. This apparent drop in activity could be attributed to absorption of the reaction product Dopachrome in the mesopores, which was removed after several washings. The oxidation of other phenolic compounds (4-tert-butylcatechol, dopamine and tyramine) was followed by 13C-NMR, HPLC/MS and UV-Vis using AbPPO4 loaded on non-functionalized SBA-15 (20% w/w), which allowed to elucidate the structure of different oxidized products. This catalyst (SBA15-Tyr-20) exhibited enhanced stability over a wide range of pH and temperatures compared to the free AbPPO4, retaining enzymatic activity after 10 cycles of reuse and up to 66% of its initial biocatalytic performance after 6 months of immobilization. The results obtained point to the possible use of SBA15-Tyr-20 for the preparation of a column-type bioreactor to mimic specific processes in the soil and allow structure elucidation of humic-derived iron- complexes.

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TITLE

Research progress on speciation analysis of arsenolipids in seafood and its associated health risk

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ABSTRACT

Arsenic (As) is one of the most toxic elements, its contamination is a major global environmental problem due to the presence of inorganic arsenic in drinking water and the resulting chronic health effects such as cancer, cardiovascular disease and diabetes. It is present in both organic and inorganic forms and compounds. The interest in arsenic toxicity has been mainly focused on inorganic forms, while the organic ones were considered non-toxic. However, in recent years it has been shown that organic forms can also show toxicity and in the case of arsenolipids comparable or even higher than inorganic forms.

Marine products are one of the largest sources of arsenic in the human diet and over 50 different forms and compounds of this element have been identified in them. They may contain compounds such as: arsenites, arsenates, methylarsonic acid (MMA), dimethylarsinic acid (DMA), arsenobetaine, arsenocholine, arsenosugars and arsenolipids. Marine organisms, such as fish, shellfish and seaweed, are high in total arsenic, but more than 90% of it occurs in organic forms.

The total arsenic content is not sufficient to determine toxicity and accurately determining the myriad forms in which arsenic occurs in food is a major challenge for food safety authorities and institutions. The current regulations and restrictions regarding the exposure to arsenic mainly focus on its inorganic forms. In Europe, there is and is used a standardized method for the analysis of inorganic arsenic forms, but such a method for the organic forms of arsenic has not yet been published.

At first the structural novelty of arsenolipids, their biosynthesis and possible roles in organisms, made them gain attention. However, in recent years, they attracted human health interest because of their high toxicity. Arsenolipids (AsLs) are mostly arsenohydrocarbons (AsHCs), arseno-fatty acids (AsFAs) and mono- and di-acyl arsenosugarphospholipids (AsPLs, AsSugPLs). The recent in vitro study of arsenolipids revealed that arsenohydrocarbons are, to a comparable degree with inorganic arsenic(III), cytotoxic to human liver cells and bladder, and that arseno-fatty acids are only 10-20 fold less cytotoxic to human liver cells than arsenohydrocarbons. Comparing in vitro toxicity of AsHCs with other organic arsenicals found in marine products, arsenohydrocarbons were at least 600 times more toxic than a glycerol arsenosugar and 20-25 times more toxic than DMA(V). Arsenolipids pass the in

vitro intestinal barrier model (Caco-2) and the blood-brain barrier (BBB) of fruit flies (in vivo) and porcine (in vitro) [1, 2, 3].

Arsenic occurs in the form of the water- and fat-soluble forms (arsenolipids) in foods. Previous speciation analysis studies focused mainly on water-soluble forms of arsenic. The analysis of the fat-soluble forms of arsenic remains largely unknown due to the lack of appropriate methods of their extraction, separation and detection. Therefore, the aim of the planned study is to develop an effective method of speciation analysis of fat-soluble arsenic forms - arsenolipids, using HPLC-ICP-MS.

The research is funded by ID-UB (Initiative of Excellence - Research University) Proposal No.: 054/13/SNŚ/0037

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TITLE

Analysis of brain cancer cells – Raman spectroscopy and imagining

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ABSTRACT

Raman spectroscopy enables us to determine the vibrational modes of molecules and thus to identify molecules. This technique is based on providing monochromatic light to the molecule, which then interacts with light. It results in a change of energy, that gives information about the molecule. [1] Raman spectroscopy and imaging have multiple applications. One of them is a diagnosis of diseases. Raman techniques are non-invasive to the sample and this fact creates a possibility of usage as a diagnostic method even during operations. To be able to develop a diagnostic tool it is necessary to know compounds, which presence or amount in cells indicates whether this cell is cancerous or not. This research hypothesizes that carotenoids might be such a compound. They are organic compounds, mostly pigments produced by plants and algae. In plants, carotenoids absorb light energy for photosynthesis. In the human body, they can be converted into retinol (vitamin A) and have antioxidant properties due to the support of transport, storage and metabolism of oxygen. Humans obtain carotenoids from their diet, especially vegetables and fruits like oranges or pumpkins. [2] Although, B-carotene has been found to increase the risk of cancer if taken in large amounts and the patient is a smoker or exposed to asbestos. [3]

Using Raman Spectroscopy and imaging for analysis of carotenoids in cells, I can figure out what is the amount of them in healthy and cancer cells and does it differ or not. If only this amount will be different, carotenoids would be recognized as Raman markers. Looking into the future, this research might contribute to developing a new diagnostic tool for cancer.

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TITLE

Portable biosensor with hybrid nanomaterial for POTC application

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ABSTRACT

Diabetes mellitus is a frequent, clinically complex condition characterized by a persistent rise in blood glucose levels brought on by decreased insulin production and/or peripheral insulin resistance. About 5–10% of all cases of diabetes are insulin-dependent type 1, which is defined as a failure in insulin production due to an autoimmune attack on pancreatic beta cells. The most common kind of diabetes sometimes referred to as non-insulin-dependent diabetes, is brought on by a confluence of genetic and environmental variables. This latter variety typically combines a background of insulin resistance at the level of skeletal muscle, liver, and adipose tissue with a relatively low insulin production that is caused by a gradual beta cell dysfunction [1].

Numerous types of portable glucose meters were created for the early diagnosis of diabetes mellitus and serum glucose control. Point-of-care testing also known as near-patient testing can be defined as an investigation taken at the time of the consultation with the patient. POCT can be carried out in a variety of locations by healthcare providers including pharmacies, clinics, ambulances, accident scenes, care facilities, and homes. Remote patient monitoring, made possible by POC testing devices, gives doctors access to nearly real-time views of critical patient information [2]. The usage of mobile devices at the point of care is a major factor in raising the standard of care's affordability, accessibility, and safety. This enables quick, easy, low-cost results and, as a result, immediate action after consultation with the doctor, without the need to leave the patient's place [3].

Herein, we present a novel Point-of-care biosensor based on novel hybrid material. The nanoplatform was used for the immobilization of glucose oxidase (GOx). A number of physicochemical and biochemical analyzes were performed, i.e. transmission electron microscopy (TEM), atomic force microscopy (AFM), Bradford analysis, electrokinetic analysis, non-invasive light scattering technique (NIBS), and polydispersity coefficient (PdI), which allowed the dispersion-morphological characterization of the proposed materials.

The resulting material was used to modify the SPE electrode. In order to carry out electrochemical measurements, the smallest potentiostat in tandem with a mobile device was used. Electrochemical tests were carried out using amperometry and cyclic voltammetry. Finally, the glucose detection was carried out in real glucose solutions, i.e. human serum or human blood

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TITLE

Research on the method of accumulation the energy obtained from a renewable source such as a photovoltaic panel in lithium-ion batteries

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ABSTRACT

Some of the key problems and challenges in modern civilization is the greenhouse effect and energy security (strategy of the European Union), competitiveness European economy and reduction of air pollution in cities. Development of modern ion-lithium batteries and improving the batteries ability for energy storage have strategic importance for Europe. The researches all over the world are working how to improve batteries parameters. From many proposition there are: exploring new battery materials or optimizing the existing battery components.

The presentation contains works related to the design and implementation of a new energy storage for a single-family house of 8 kWh. In order to choose the design of a new warehouse for a given application, Research Team have defined parameters such as: energy and power density, warehouse response time, lifetime, size, rate of return on investment, additional equipment, storage efficiency, energy consumption profile, energy tariff.

Designing an effective energy storage is a complex design, economic and legal issue. Before starting the design, it is necessary to recognize the scale and purpose of the warehouse and choose the appropriate technology. In order to improve the operating parameters of the energy storage, it is worth choosing at least one of the strategies energy storage design presented in this study.

TITLE

The stone that the chemists rejected – a practical overview on the selected methods of experimental data processing

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ABSTRACT

Experimental data, collected even with the highest performance instruments, prior to the analysis and interpretation is typically subjected to a so-called processing. In general, this term covers all types of operations in a result of which the recorded "crude" signal becomes more informative for the researcher. Yet, among possible procedures employed for this purpose, several being common for different measurement techniques appear to be especially popular. These includes, among others, reduction of noise (denoising), background correction or resolution of overlapping peaks [1,2]. Following the above hints, many commercial data analysis packages are supplemented with built-in routines dedicated to the aforementioned tasks. While such opportunity seems to be convenient for their users, it has one potential weakness, namely, the implemented default algorithms may turn out not to be the most effective ones. At the same time, the users may not be aware that very likely more adequate alternative for their needs remain available. In view of the latter, several firm techniques of data processing would be outlined and commented regarding their practical application. Great emphasis will be put on potent methods that, regrettably, are less frequently reported to be employed for the experimental data treatment in chemistry (as e.g. data smoother by Eilers [3]). In particular, performance and application of the fast Fourier transform (FFT) [4] and singular value decomposition (SVD) [5] shall be presented and discussed on the example of efficient spectroscopic signal analysis

Acknowledgments:
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TITLE

Evidence of Chemical Warfare Agent Soman Present in Urban Concrete Matrices – Development of Sample Preparation Method to Optimize Extraction of Pinacolyl Alcohol

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ABSTRACT

Since modern warfare assumes misuse of the banned chemical warfare agents primarily in urbanized areas, identification of their degradation products within contaminated concrete debris could represent a valuable source of forensic evidence of such misuse. Concrete is a specific type of solid matrix dominated by high alkalinity in terms of retrospective evidence of the use of chemical weapons. Most chemical warfare agents decompose rapidly in an alkaline environment. As time passes after the chemical attack, the presence of decomposition products will predominate in the sample. Pinacolyl alcohol (3,3-dimethylbutan-2-ol) is the final degradation product of a potent nerve agent soman.

In the current study, pinacolyl alcohol was examined in terms of its extraction from real concrete matrices. We compared observed recoveries of pinacolyl alcohol from ~10[sup]1[/sup]g bits of permanent formwork blocks under different sample preparation procedures. The aim of this study was to develop an optimized method for preparation of concrete samples contaminated by pinacolyl alcohol for subsequent chromatographic identification.

The tested parameters of sample preparation included choice of extraction agent, extraction temperature, extraction time, extraction mechanism, sample milling, sample storage time, sample storage temperature and pre-drying of concrete matrix. Observed recoveries for each selected set of parameters were calculated from measured pinacolyl alcohol concentration. Analytical technique was gas chromatography with flame ionization detection.

Data suggest that the optimized set of sample preparation parameters include using non-pre-dried concrete without sample milling nor storage delay. Polar aprotic solvents (in particular acetone) proved to be the best extraction agents used. The other extraction parameters were as follows: elevated extraction temperature (45 °C), prolonged extraction time (30 min.) and ultrasonication extraction. The observed recovery of pinacolyl alcohol for the optimized method was 77,5 % ± 17,9 %.

Despite the relatively high volatility of the analyte, a significant drop in the observed recovery was not recorded during the long-term measurement which indicates a significant physical-chemical affinity of the investigated alcohol to the material. This finding creates a promising hypothesis of a valuable sample in terms of evidence of the presence of a chemical warfare agent over time. The determined sample preparation method will serve as a reference for optimization of preparation of analogous samples consisting of other concrete matrix types and degradation products of other nerve agents.

TITLE

Raman imaging as a label-free diagnostic method for acute myeloblastic leukemia

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ABSTRACT

Leukemia is a group of hematologic malignancies caused by genetic aberrations occurring in stem or progenitor cells of the myeloid and lymphoid lineage. A crucial aspect of the fight against leukemia is proper diagnosis of all leukemia subtypes and targeted effective therapy. Raman imaging is a promising diagnostic tool, which enables the molecular characterization and differentiation of leukemia subtypes in clinical samples [1]. The aim of the study was to distinguish cells of acute myeloid leukemia (AML) of the THP-3 cell line from normal peripheral blood mononuclear cells (PBMCs) using Raman imaging combined with multivariate statistical chemometric analysis. Raman spectra of leukemia cells were compared with spectra of PBMCs, constituting the control group, in two spectral ranges: fingerprint (1800-600 cm $^{-1}$*) and the C-H stretching vibrations region (3030-2700 cm* $^{-1}$*). The results demonstrate that Raman spectra from the control group significantly differ from spectra of leukemic cells, especially in the intensity of the bands assigned to nucleic acids (792, 1582 cm*$^{-1}$ *and lipids (1445, 2846, and 2873 cm* $^{-1}$*). These results prove that Raman imaging can be consideredan innovative tool for the spectroscopic markers identification characterizing leukemia cells in clinical practice.*

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TITLE

Nonenzymatic glucose sensor based on PCA@MWCNT-CuO nanomaterial

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ABSTRACT

A major area of study in electrochemical and biosensor research is glucose sensing. Although there is no medical treatment that may entirely cure diabetes, glucose concentration is a significant signal for many diseases including endocrine and metabolic problems, as well as diabetes [1]. Improving the measurement of blood glucose concentration in diabetes patients is the primary way to monitor the disease. As a result, precise blood glucose monitoring has significant clinical consequences. Additionally, glucose is frequently employed in the food industry, pharmaceutical production, environmental monitoring, and biological process monitoring [1]. The fundamental principle of an electrochemical biosensor is based on monitoring the electrical changes at the conducting electrode surface upon integration of the enzyme, as they are directly correlated to the biocatalytic transformation of the substrate, resulting in the depletion of the reactant or the formation of product [2].

A phenolic derivative that is present in nature is called caffeic acid (3,4-dihydroxycinnamic). It occurs as a yellow substance, containing an acrylic and phenolic functional group. Because caffeic acid presents both reduced and oxidized o-hydroquinone/o-quinone pairs in its structure, it can be used in electrocatalytic reactions. The presence of its quinone redox probe, which enhances the flow of electrons between the analyte and the electrode, makes poly(caffeic acids) an advantageous material for electrochemical biosensor applications [3].

In this work, a hybrid nanomaterial magnetite@poly(caffeic acid) was developed. Using the unique qualities of each component, such as magnetite's magnetic stability and biocompatibility as well as PCA's capacity for electron transport, allowed the development of a novel hybrid material with beneficial features. Immobilizing glucose oxidase was accomplished using the developed nanomaterial (GOx).

The properties of the nanoplatform were determined by transmission electron microscopy (TEM), atomic force microscopy (AFM), Fourier transform infrared spectroscopy (FT-IR), Bradford assay, electrokinetic analysis (zeta potential), non-invasive light scattering (NIBS) and measurement of the polydispersity index (PdI). The screen-printed electrode (SPE), which was modified using this matrix, was employed in electrochemical testing to find glucose in real solutions.

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TITLE

The use of microalgae to remove pharmaceutical residues from wastewater

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ABSTRACT

As a consequence of the development of medicine, there is an increase in the global use of pharmaceuticals that undeniably increase the comfort of people's lives. Nevertheless, this has led to a major concern as these drugs are entering the natural environment in an uncontrolled manner and pose a significant threat due to their potential ecotoxicity. The phenomenon of accumulation of pharmaceutical compounds in the environment is mainly due to the fact that conventional wastewater treatment plants are not designed to effectively remove them from household wastewater [1]. Not completely degraded, they are still chemically stable enough to get into surface waters, thus contaminating drinking water. They can accumulate in the tissues of living organisms and disturb their homeostasis. In addition, excessive consumption of antibiotics enhances the development of antibiotic resistance genes and the adaptation of resistant bacteria.

Modern methods of wastewater treatment from pharmaceuticals, based on advanced oxidation processes or photocatalysis, although efficient, have their disadvantages resulting primarily from high operating costs related to the consumption of energy and chemicals [2].

Thanks to their flexible metabolism, microalgae and cyanobacteria can be used in modern wastewater treatment systems containing pharmaceuticals. These compounds can be removed by bioaccumulation and biological biodegradation (as nutrients for biomass production). The process can use sunlight or artificial light, which will support both biomass growth and phytoremediation, as well as photodegradation. The process does not require the supply of chemicals—nitrogen, phosphorus and other microelements can be taken from wastewater, additionally, the produced biomass can be used, which makes the process economical and safe for the environment [3].

This paper examines the possibility of using selected strains of microalgae (Chlorella sp. 176) and cyanobacteria (Synechocystis sp. PCC 6803) to remove the anti-inflammatory drug—diclofenac and the antibiotic—amoxicillin, as exemplary pharmaceutical contaminants. The growth of biomass in the presence of pharmaceuticals and the degree of their removal, also taking into account photodegradation, were studied. Drug removal in the presence of microalgae was 40-70% for diclofenac and almost 100% for amoxicillin.

The cyanobacteria growth was inhibited from the beginning in the presence of antibiotic and removal of amoxicillin could have happened through adsorption on dead cells or photodegradation supported by dead cells or only photodegradation.

Nevertheless, the removal rates achieved were higher than those of conventional systems, indicating the possibility of applying microalgae to bioremediate wastewater containing pharmaceutical contaminants. Furthermore, microalgae do not contribute to increasing antibiotic resistance among bacteria. In conclusion, the single-celled photosynthetic organisms have big potential in removing the so-called emerging contaminants, which are a growing problem in the protection of water resources and the environment in general.

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TITLE

Evaluation of the potential for the release of unwanted organic compounds from polyethylene pipe and polyurea coating into water under simulated operating conditions

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ABSTRACT

Materials used to transport drinking water are required to comply with certain standards [1]. Drinking water distribution systems are made of various materials (steel, cast iron, plastics). At present, plastics, primarily polyvinyl chloride and polyethylene, are most commonly used for water distribution networks due to their durability and corrosion resistance. Unfortunately, these materials are not as resistant as assumed and are subject to operational aging, and their degradation contributes to the release of organic compounds that cause deterioration of drinking water quality. The answer to the need for quick repair solutions is trenchless techniques. These include the spray-in-pipe place (SIPP) technique [2-4]. Due to their properties, polyurea resins are a material potentially suitable for use as a polymer coating for pipe rehabilitation [5, 6].

The purpose of this study was to evaluate the potential for the release of unwanted organic compounds from pipes made of high-density polyethylene (HD-PE) and pipes rehabilitated with the tested polyurea resin (PM) into the drinking water transported by them. The study was carried out on a semi-technical model system, mimicking the conditions inside the water supply network, especially in its "dead spots" where water stagnation time is prolonged. The model station was supplied with treated water. Flowing and stagnant water samples taken from the model after a certain period of operation were analyzed. Sample preparation for analysis was carried out using solid phase extraction (SPE) and solid phase microextraction (SPME) techniques. Identification of the isolated compounds was performed using the technique of full two-dimensional gas chromatography coupled to mass spectrometry (GCxGC/ToF-MS).

The results revealed the presence of siloxane-like compounds used in personal care products in the feed water. Their presence in the treated water is of concern and should be further monitored. In the case of water after contact with polyethylene pipes, the presence of compounds described in the literature, which are released from the material as a result of degradation of antioxidant coatings, was observed. The results also indicate a high potential for the release into water of a wide range of organic compounds from the polyurea resin studied. Both volatile compounds were identified, as well as nitrogen-containing complex compounds among which amines were the main group. The results of the study confirmed that both materials studied are potential sources of secondary contamination of drinking water with soluble organic compounds.

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TITLE

Thermal treatment of photovoltaic panels: recovery of valuable components and risk mitigation

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ABSTRACT

Photovoltaic (PV) panels are a sustainable source of energy, but their end-of-life management poses a significant challenge due to the potential environmental impacts of their disposal. Thermal treatment is a promising approach for the recovery of valuable materials from used PV panels and energy recovery. However, the thermal treatment process also involves components that pose a risk of combustion of the photovoltaic panel, including Teflon, which can release harmful fluorine-containing substances into the environment.

In this presentation, we will show our studies on the thermal treatment of photovoltaic panels, with a focus on the risk of Teflon combustion and the recovery of valuable components. The results show that the thermal treatment process can be optimised to minimise the risk of Teflon combustion and the release of harmful substances. The efficient recovery of some components, such as glass, aluminium, and copper, is also possible through carefully optimised thermal treatment. To safely perform incineration, the procedure for screening photovoltaic panels containing Teflon was proposed. Furthermore, the procedure for its removal from the PV backings and a potential application of Teflon waste was proposed. The influence in variables of the thermal treatment process, such as the temperature and time of incineration, the orientation of the sample with respect to the elements of the furnace heating system, and the temperature gradient of the material during combustion was examined. It was shown that the listed parameters have a significant influence on the efficacy of the removal of carbon residue and the degree of fragmentation of the glass residue. During the studies, several advanced research methods, such as thermal analysis, thermal imaging, XRD and LIBS spectroscopy, as well as contact angle measurements, were employed.

In general, this presentation highlights the potential of thermal treatment as a sustainable approach to end-of-life management of photovoltaic panels, but the findings emphasise the importance of optimising the thermal treatment process to minimise the risk of Teflon combustion and maximise the recovery of valuable components and energy.

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Keywords: End-of-life management of photovoltaic panels, circular economy, Teflon combustion risk, thermal treatment of photovoltaic panels waste

TITLE

How can we improve curcumin for pharmaceutical applications?

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ABSTRACT

Curcumin (CUR) is a naturally occurring polyphenol, abundantly found in the rhizome of the Curcuma species, characterized by its intense yellow color [1,2]. The spectrum of its biological activity is very broad and includes anticancer, antimicrobial, antiamyloid, anti-inflammatory, and antioxidant activity, as well as it was proven an efficient photosensitizer in photodynamic therapy. However, albeit these favorable biological effects CUR is not clinically used. This is due to the unfavorable characteristics, most notably pharmacodynamic (poor bioavailability), pharmacokinetic (fast elimination from the system) and poor solubility in aqueous media. Because of that, new derivatives of CUR are prepared to improve the physicochemical properties of CUR whilst maintaining or even enhancing the biological activity thereof.

Following this topic, the presented study showcases three separate methods of overcoming the drawbacks of curcumin. First, new derivatives of CUR were prepared by synthesizing compounds with other substituents in the benzene rings by the use of appropriate aldehydes in condensation reactions with acetylacetone. In the second approach, the CUR β-diketone group was replaced with a diazepine ring by fusing it with ethane-1,2-diamine derivatives, which would allow for the higher stability of the resulting compounds compared to CUR, as well as to modulate the activity. All the compounds obtained in these two approaches were characterized with nuclear magnetic resonance spectroscopy ^{1}*H NMR,* ^{13}*C NMR, as well as 2D techniques), UV-Vis spectrophotometry, and mass spectrometry. The third synthetic pathway used curcumin to prepare titania nanoparticles sensitized with CUR, broadening the light activation range to visible light. This was confirmed as the resulting nanomaterials were tested for their potential usefulness as photosensitizers in photodynamic therapy, most importantly mediation of reactive oxygen species generation. Additionally, the photoactive materials were characterized by thermogravimetric analysis, x-ray powder diffraction, and hydrodynamic size diameter measurements.*

The obtained results bring a promise to make CUR (or its derivatives) a potential therapeutic agent.

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TITLE

The mechanical properties of flax fibre-reinforced biocomposites influenced by plant modifier.

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ABSTRACT

The study focuses on the effects of modifying the lignocellulosic reinforcement of biocomposites. The main subject of research was the analysis of the mechanical properties of polylactide-based (PLA) biocomposites containing flax fibres that had been modified with tannic acid (TA). The research included dynamic mechanical analysis (DMA), tensile strength tests, differential scanning calorimetry (DSC) examinations, and scanning electron microscopy (SEM) analysis. The results indicate that the modified biocomposites obtained have potential applications in the packaging industry and could replace harmful materials of petrochemical origin produced on a large scale.

TITLE

New stabilizing systems dedicated for ethylene-norbornene copolymer

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ABSTRACT

One of the limitations of the use of polymeric materials is their degradation under the influence of elevated temperature, UV radiation, as well as other factors present in the environment of their operation. Therefore, almost all plastics require stabilizing systems that will prevent premature degradation of the polymer matrix during its service life. In this work, an analysis of the ultraviolet aging process of ethylene-norbornene copolymer was performed, to which stabilizing systems based on the immobilized Hostavin N 321 stabilizer on oxide carriers (silica and titanium dioxide) were introduced and examined. The samples were subjected to UV aging for 400 h. Based on the analysis of surface and mechanical properties, it was observed that the immobilization of the Hostavin N 321 stabilizer on silica and titanium oxide allowed for a longer lifetime of these polymer products and a reduction in their manufacturing costs.

TITLE

The influence of Resveratrol on models of lipid rafts

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ABSTRACT

The main goal of studies was to investigate influence of Resveratrol on lipid rafts models. Lipid rafts are specific regions in cell membrane rich in cholesterol and sphingomyelin. There is high amount of lipid rafts in cancer cells [1]. Resveratrol is a natural compound which has an influence on cardiovascular system and present anticancer activity [2,3].

The studies were obtained for different systems of lipid rafts models containing sphingomyelin (SM), 2-oleoyl-1-pallmitoyl-sn-glycero-3-phosphocholine (POPC) and cholesterol (Chol) which are the components of the cell membranes of mammals. The POPC and SM ratios were 1:1 and cholesterol content were 5, 15 and 33.3%. During the research Langmuir monolayer with Brewster Angle Microscopy technique support were applied as one of the models. The second one was liposomes [4].

Results obtained during research show a significant effect of Resveratrol on lipid raft models. It is found that the addition of this active substance leads to reduction the order of hydrophobic chains and to the changes of membrane fluidit.

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TITLE

Linear discriminant analysissupport the assignment of multidimensional NMR spectra of intrinsically disordered proteins

AUTHORS

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ABSTRACT

Nuclear magnetic resonance (NMR) spectroscopy plays an essential role in determining the structure and dynamics of proteins[1]. The standard assignment of signals in protein NMR spectra is based on the analysis of a set of results from three-dimensional experiments, which provide information on the sequential linkage (correlation) of chemical shifts of individual nuclei, e.g., 3D HNCACB[2]. The correct assignment of signals to the atomic nuclei that make up the protein's backbone is the first and, simultaneously, one of the essential steps in analyzing its structure. This is especially difficult with unfolded proteins due to slight variation in their resonance frequencies. However, in their case, in addition to the sequence assignment, it is possible to take advantage of the characteristic chemical shifts of amino acids.

We propose using statistical method- linear discriminant analysis (LDA) for the assignment of unfolded proteins of data sets with distinguished subgroups (in our case - amino acid residues). Based on the data contained in the BMRB (Biological Magnetic Resonance Data Bank) database, we have created a training set consisting of chemical shifts of 18 unfolded proteins. We noticed that four chemical shifts (Ha, Hb, Ca, and Cb) already allow precise identification of most types of amino acid residues. Then, using the obtained separation, we assigned the peaks in the experimental data set for the kinds of amino acid residues.

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TITLE

Characterization of antimicrobial peptides, especially cathelicidin LL-37

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ABSTRACT

Antimicrobial peptides (AMP) are small molecules that are part of the innate immune response of all living organisms. Different AMPs are able to fight fungi, bacteria, viruses, protozoa and even cancer cells. AMPs usually contain basic or hydrophobic amino acids in their sequence, and therefore have a net positive charge or amphiphilic.

Among all AMPs, cathelicidins and defensins were distinguished. Positively charged AMPs interact electrostatically with negatively charged phospholipids found in cell membranes. These interactions cause the formation of transitions in cell membranes [1].

Some of the known AMPs, due to their antimicrobial activity, participate in immunological processes. They reduce the inflammatory response caused by the presence of endotoxins, regulate the synthesis of pro-inflammatory factors and cytokines [2].

Catellicidins occur in humans and animals in the form of small, cationic, antimicrobial peptides. So far, only one cathelicidin hCAP 18 has been identified in the human body, which is converted to LL-37 by elastase or proteinase 3.

LL-37 is a cationic peptide with a linear, α-helical structure. The name is closely related to its primary structure as it is a 37 amino acid residue peptide. In the native structure of LL-37 with the sequence: LLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLVPRTES.

The LL-37 peptide exhibits bactericidal properties and performs immunomodulatory functions that regulate the host's response to the pathogen. It is also released during inflammation [3].

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TITLE

Optimalization of specific substrate for ADAM 17 using different fluorescence acceptors

AUTHORS

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ABSTRACT

Diabetic Nephropathy (DN), a leading cause of end-stage renal disease, is characterized by the progressive expansion of the mesangium with accumulation of extracellular matrix. Several studies support the finding that renal reactive oxygen species play a central role in injury in diabetes. The disturbance of proteolytic enzymes homeostasis is also important in the pathogenesis of DN [1].

DN is characterized by albuminuria, hypertension and progressive renal failure. The diagnosis of DN is complicated, because the shown symptoms are non-specific[2].

Several studies have demonstrated that a disintegrin and metalloproteinase 17 (ADAM 17) has been associated with pathogenesis of diabetic nephropathy. ADAM 17 is involved in proteolytic ectodomain shedding of several membrane-bound growth factors and cytokines. The expression and activity of these enzyme increase under some pathological conditions such as stroke and glioma[3].

To evaluate the activity of ADAM 17 can be used a fluorogenic substrate. The peptide fragment of substrate has been defined through the use of combinatorial chemistry. With the exceprion of cysteine all proteinogenic amino acid residues were used in the syntesis of peptide library.

Final sequence of the selected substrate: ABZ-Asn-Tyr-Met-Ala-Leu-Arg-Arg-Tyr(3-NO2)-NH2. Optimization of the fluorogenic substrate included various donor-acceptor fluorescence pairs.

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TITLE

Non-centrosymmetric Ln-MOFs (lanthanide metal-organic frameworks) as nanothermometers

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ABSTRACT

Temperature sensors make up 80% of the global sensor market, demonstrating the importance of temperature measurement. Currently, thermocouples and thermistors are the dominant technologies. However, they require thermal contact with the sample and cannot be used at the nanoscale. Luminescence thermometers offer a solution to these limitations by calculating temperature based on changes in luminescence parameters, such as intensity or bandwidth [1].

Lanthanide metal-organic frameworks (Ln-MOFs) may exhibit luminescence thermometer properties due to the presence of lanthanide ions. Additionally, MOFs are porous crystalline materials that, if their space group is non-centrosymmetric, can exhibit non-linear optical phenomena known as second harmonic generation. The intensity of this signal also depends on temperature and can be used to create a new class of nanothermometers [2].

During the presentation, we will discuss the progress made in the synthesis of new Ln-MOF materials using trimesic acid as the linker.

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TITLE

Unleashing the magic of nano - from ancient wonders to future frontiers

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ABSTRACT

There’s is plenty of room at the bottom” - it is believed that with these words of Richard Feynman in 1959 the history of nanomaterials began. The term "nanotechnologies" was introduced by Norio Taniguchi in the 70s. Nevertheless, back in the middle of the 19th century, Michael Faraday managed not only to describe the phenomenon itself, but also to prove the unusual nature of aqueous suspensions of gold nanoparticles, which he synthesized using simple methods that existed at that time [1].

"Any sufficiently advanced technology is indistinguishable from magic", and not always the development of technology is accompanied by a fundamental scientific justification. There are examples of the purposeful manufacture of nanoobjects by man, created precisely for the sake of those new physical properties that matter acquires during the transition from macro to nano, in the eras that preceded the emergence of the scientific method. These examples include the cosmetics of Ancient Egypt and Ancient Greece, ceramic dishes from Corsica island, Damascus steel, porcelain of Ancient China, ruby glass of Ancient Rome and paint for frescoes in Mexico of the 1st millennium AD. [2–4].

To date, unfortunately, we have not succeeded in developing the gray goo inspired by Feynman and proposed by Drexler, but we have already reached other frontiers of what science fiction writers could only imagine. We have found a way to build structures with atomic precision. We know how to produce a substance with new unique physical and chemical properties at the nanoscale for both inanimate and living matter. We have learned how to build crystal-like structures with nanoparticles, how to detect and describe single molecules, how to use DNA like origami, how to train viruses to be our medicine, and how to modify our cells to make them, for example, photochromic or photosynthetic [5,6].

With the help of nanotechnology, we are literally breaking the universe as we know it in many ways, bringing both incredible opportunities and unpredictable threats. There is no doubt that we are approaching a bifurcation point, and our worldview will change even more dramatically over the next decade.

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Title

Gold nanoparticles embedded in silica aerogels for catalytic applications

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Abstract

Nanotechnology is a fast-growing field of research over the last few decades. Gold nanoparticles are known for their numerous and various fields of application including medical, sensoric, and optical fields. Nanogold is also a preferred catalyst in a number of chemical reactions. However, recovery of that for further use from the reaction mixtures cannot be easily accomplished. Aerogels are suitable for forming nanocomposites with metal nanoparticles due to their structure. Immobilization of gold nanoparticles in a chemically resistant silica aerogel matrix would offer the possibility of combining the advantages of an immobilized catalyst and a highly porous and easily penetrable solid support. Unfortunately, the synthetic conditions of the sol-gel process led to rapid aggregation of the citrate-stabilized nanoparticles and the loss of catalytic activity. It has been found that organic solvents and atmospheric CO_2 *have significant effect on aggregation but cannot be entirely excluded under standard synthetic conditions. Testing several types of polymeric materials resulted in the solution, in which polyvinylpirrolidone (PVP) served as a protecting polymer which prevented the formation of the Au aggregates and allowed the preparation of nanogold-containing silica aerogels. Further studies revealed that by changing the temperature and advantageously exploiting the dimensional changes of the matrix, larger than 100 nm gold particles can be reverse-engineered into the 10-40 nm range. Catalytic activity of the as-prepared aerogels was tested by sodium hydroborate reduction of p-nitro phenol at room temperature monitored by UV-Vis spectroscopy.*

TITLE

Electrochemical determination of polyphenols in herbal infusions using carbon paste electrodes

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ABSTRACT

Carbon electrodes are commonly used in electrochemical analysis because of their wide potential range, low background current, detection capability, and low cost. Some carbon-based electrodes, such as carbon nanotube electrodes, carbon paste electrodes (CPE), and modified carbon paste electrodes, have been widely used due to the possibility of obtaining an electrochemically active surface in a simple way and at low cost [1]. Many sensors have been developed for the electrochemical determination of various bioactive compounds, including polyphenols, natural antioxidants, found in many plants, including tea. In recent years, their beneficial properties for human health have received increased scientific interest, as they have been shown to exhibit antioxidant, anti-inflammatory, anticancer, and anti-microbial activities. Several studies have shown that a diet containing polyphenols is strongly associated with a reduced risk of chronic diseases [2].

In this study, commercially available dried plants and plant infusions were analysed using CPEs. The presentation will cover the experimental methodology and results obtained, including the calibration curves, sensitivity, and detection limits achieved. Comparison of the antioxidant properties of plant extracts assessed on the basis of electrochemical studies will be provided and compared with results obtained employing spectrophotometric procedures. This work demonstrates the potential for CPE-based sensors to be used in the rapid and cost-effective determination of polyphenols in food and beverage products. The new innovative approach has potentially important implications for the food industry, as it offers a simple and cost-effective method for determining the polyphenol content of various plant extracts.

Keywords: voltammetry, paste electrode, tea extracts, polyphenols

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TITLE

Biodegradable materials based on PLA and modified with hemp extract

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ABSTRACT

Biodegradable and compostable polymers are sensitive to environmental factors such as water, light, temperature or micro-aggregates. For this reason, they need to have stabilisers in their composition in order to inhibit ageing and degradation processes. Synthetic stabilisers have traditionally been used in the polymer industry, but in recent years, in an era of environmentally friendly solutions, the use of naturally occurring compounds in plants, animals and waste materials has been on the rise. It has become increasingly popular to create composites that are entirely of natural origin. These are based on a polymer matrix of natural origin, e.g. cellulose, sugars or polymers produced indirectly from natural raw materials, such as polyalkanates (PHA), polylactide (PLA), poly(butylene succinate) (PBS) or polycaprolactone (PCL) [1,2]. An example of natural stabiliser is hemp extract, presented and investigated in this study [3-6]. It was applied to a polymer matrix of polylactide. The samples were subjected to weathering and thermo-oxidative ageing, followed by infrared spectroscopy, spectrophotometry, analysis of static and mechanical properties and analysis of the surface free energy. The results obtained confirm the validity of the assumption of an anti-ageing effect of hemp extract in the case of thermo-oxidative ageing and, very interestingly, of a catalytic effect in the case of weathering. Researching the use of this type of stabiliser in polymeric composites is a scientific novelty that no one has studied so far in polymeric materials, especially biodegradable thermoplastics. Due to the growing interest and importance of hemp and its derivatives as materials and functional substances, as well as the generation of more waste material from these products, this topic needs to be further explored.

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TITLE

Secondary bonding in the active sites of carbonic anhydrases enzymes - theoretical perspective

AUTHORS

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ABSTRACT

It was shown that the Carbonic Anhydrase (CA) IX to a large extent is responsible for the acidification of the extracellular matrix in some cancers – which influences the growth and metastasis of the tumor [1]. Due to that, finding an inhibitor for this protein family may be an important endeavor in the field of drug design. In order to facilitate such design, the detailed and comprehensive studies with regard to the interactions between CA IX inhibitors and its binding site must be employed. In fact, one of the most important types of interactions in the whole biology and chemistry are the so-called secondary bonds [2,3]. Characterized by relatively low stabilizing effect are of utmost importance for the ligand position in the binding pockets of the receptors and their mechanisms of action due to their ubiquity. It was found that the hydrogen bonds have a huge impact on the secondary and tertiary structures of proteins, as well as the secondary structures of the nucleic acids. However, the well-known non-covalent interactions in which the hydrogen atom is a bridging one, are only a part of existing vastness of various secondary bonds present in nature. The Molecular Electrostatic Potential (MEP) calculations revealed that certain atoms attached to electron-withdrawing molecular frameworks can possess the so-called σ-hole (term "σ-hole" was coined by T. Clark at the conference in Prague in 2005 and refers to the local depletion of the electron density of the bridging atom at the extension of the covalent bond with the highly electronegative entity) [4].

The strength of these interactions grow with the electronegativity of the donor atom, the polarizability of the bridging one and the basicity of the Lewis base that takes part in the interaction [5,6,7,8]. The presentation will concern the properties of above-mentioned non-covalent interactions in the context of CA enzymes family from the perspective of the theoretical chemistry.

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TITLE

In plants, we hope - the influence of phytochemicals obtained from the Black Currant fruit on the S. aureus model membrane

AUTHORS

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ABSTRACT

The main concerns faced by the cosmetic industry are preventing the microbial spoilage, ensuring the safety of the products, and prolonging their shelf-life. Cosmetic products can be contaminated by microorganisms during manufacture, packing and storage, but most importantly during the entire period of their use[1,2]. It is also important to ensure the stability of the products over a wide range of external conditions (e.g. temperature, humidity), which may change and facilitate the growth of microorganisms[1]. Microorganisms' presence in cosmetics can cause not only unpleasant discolouration or odour, but it can lead to infections, which can be very dangerous for consumers[1]. One of the most common ways of the protection of cosmetics is the use of preservatives, which might be both synthetic and natural substances inhibiting the growth of microorganisms[3]. However, although preservatives are added in low concentrations they might cause allergies and irritant contact dermatitis. Some of them, like parabens, are very controversial among scientists and consumers and it is believed that they can increase the incidence of female breast cancer and influence the development of malignant melanoma[2,3]. Nowadays there is a growing awareness among people about their health and the safety of products they use. Consumers are then expecting not only cosmetics to be innovative, effective and of high quality but also products, which are safe and free from harmful chemical compounds. This is a reason for seeking alternative cosmetic ingredients, such as natural, plant-based compounds, which are proven to be safer not only for humans but also for the environment[1].

Plants’ antimicrobial properties have been known for ages. Various plants (e.g. Allium sativum*, Thymus vulgaris, Cinnamomum) and plants metabolites (e.g. lectins, alkaloids, terpenoids, polypeptides, polyphenols) have been identified as showing antibacterial and antifungal properties[3]. Also, Black currant is known as a source of phytochemicals that exhibit antimicrobial activity. Therefore, the substances obtained from the Black Currant fruit can be used as a natural preservative while preparing cosmetics products on your own using the commercially available product PhytoCide Black Currant Powder[4]. The mechanism of the influence of natural antimicrobial substances on bacterial and mammalian cells is complex, but the most important is their ability to influence cells’ membranes’ functions and structure. To investigate the influence of PhytoCide Black Currant Powder on bacteria S. aureus cell membrane, experiments on Langmuir monolayers mimicking bacterial membranes were performed. The experiments on monolayers involved the surface pressure-area and penetration measurements. Moreover, Brewster angle microscopy studies were also performed. The obtained results enable us to discuss the mechanism of the antibacterial activity of the studied preservative.*

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Poster communications

The poster announcements were split into two sessions. These were split into two parts - a 5 minute video presentation with poster and a 2h live discussion.

TITLE

Rheological behavior of fumed silica nanoparticle suspensions in photocurable acrylate-based resins

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ABSTRACT

Photopolymerizable resins are widely applied in coating, adhesive, dentistry and 3D printing applications. Photopolymers used in the latter mainly contain monomers and oligomers which can be photopolymerized upon exposure to light forming a polymer network.[1] The light wavelength that triggers photocrosslinking is determined by the chemical structure of the employed photoinitiator.[2] Direct ink writing has recently emerged as the most versatile printing method for the broadest range of materials, however the used uncured resins must necessarily exhibit proper rheological behavior such as specific values of apparent viscosity and yield stress under shear.[3] Rheological modifiers can be incorporated into the resin in order to increase its viscosity. The suspension must exhibit thixotropic behavior, meaning that it retains its gel-like properties when stored and the dispersed particles remain stable.[4] Upon shearing, the gel becomes less viscous and is easier applied. When the shearing ends, it regains its initial structure. Such properties can be achieved with the incorporation of fumed silica. When dispersed into a fluid, fumed silica exhibits a branched structure which is able to create three-dimensional networks with nearby aggregates found in the fluid. This allows it to create strong bonds, thus giving fluids a gel-like structure. These agglomerations are only broken up when force is applied to them but will reform shortly after the mixture is allowed to rest.[5]

In this work, pyrogenic (fumed) silica was homogeneously incorporated in photocurable acrylic resins at different loadings through mechanical stirring followed by vacuum degassing in order to remove the air bubbles which were entrapped into the resins due to their high viscosity. Three commercially available, low viscous, urethane acrylate-based resins, originally designed for vat photopolymerization 3d printers, and an amorphous hydrophilic silica with a BET area of 200 m^2/g were employed in this study. Rotational shear rheometry was used to investigate the effect of fumed silica on the rheology of acrylate-based resins. The results indicate that the rheological properties of photocurable resin formulations can be effectively adjusted to the printability requirements of direct ink writing printers by the dispersion of fumed silica nanoparticles.

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TITLE

Chemical Synthesis of α-Synuclein via Solid-Phase Peptide Synthesis and Fragment Ligation.

AUTHORS

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ABSTRACT

Alpha-synuclein (α-synuclein) is a 140 amino acid protein thought to be involved in neurotransmission and vesicular trafficking.[1] However, it is also implicated in pathological processes in diseases known as synucleinopathies, such as Parkinson's disease (PD), where it typically accumulates in proteinaceous aggregates in the brain.[1,2] Given the tremendous interest in studying the physiological as well as the pathological effects of α-synuclein, we developed a robust method for the chemical synthesis of the wild type protein and of protein variants of interest, carrying either mutations or post-translational modifications. Therefore, we first prepared three peptide fragments by automated microwave-assisted solid-phase peptide synthesis (MW-SPPS) and linked them afterwards by using native chemical ligation (NCL). This synthetic pathway enabled us to successfully synthesize native α-synuclein, N-terminally acetylated α-synuclein, the α-synuclein mutants A53T, K58N and G14R, and phosphorylated α-synuclein (P-S129) with and without N-terminal acetylation for further investigations of the effects of the modifications on the protein structure and aggregation behaviour. Ultimately, our study will form the foundation for future studies of other α-synuclein variants.

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TITLE

Coloured MOFs-TiO2 Composites for Photodegradation of Pollutants

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ABSTRACT

This presentation discusses the synthesis and application of coloured metal-organic frameworks (MOFs)-TiO2 composites for environmental remediation. The heterogeneity of these materials provide a unique solution to pressing global issues like environmental pollution and depletion of fossil fuels. MOFs serve as photocatalytic centres, generating reactive electro-hydrogen pairs and trapping pollutants, thereby facilitating their degradation. The resulting coloured surfaces are versatile, finding potential uses in building decoration as pigments for gypsum/concrete mass.

In our research, we synthesized NH2-MIL-125 (Ti)- MOF1, ZIF-67 (Co)-MOF2 , NTU-9 (Ti)-MOF3 and their composites with hierarchical porcupine-shaped TiO2. We examined their photocatalytic activity and self-cleaning properties through a series of experiments, using toluene and methyl blue as model contaminants.

Our findings revealed a significant increase in the specific surface area of TiO2 after MOF modification, and the most efficient photocatalytic activity was observed in NH2MIL-125 (Ti) - TiO2 and ZIF-67 (Co) - TiO2 heterocomposites. Although the photocatalytic activity of self-cleaning surfaces was found to be lower than their powder counterparts due to the deactivation of photocatalysts by gypsum particles, these materials still hold potential as decorative elements for building facades.

In conclusion, our research paves the way for the development of effective pollutant degradation materials and offers an innovative approach to surface decoration.

TITLE

Graphene-based photocatalysts for water treatment from pharmaceuticals

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ABSTRACT

In water bodies across the world, pharmaceuticals are a rising pollutant of concern. Pharmaceuticals have been found in a variety of water sources, including surface water, groundwater, and drinking water, as a result of their extensive usage, inadequate removal during traditional wastewater treatment techniques, and persistence in the environment. Concerns have been expressed concerning possible negative impacts on aquatic ecosystems and human health as a result of the presence of these toxins in water bodies. Thus, there is an increasing demand for the creation of effective treatment processes to remove drugs from water. The creation and use of photocatalysts based on reduced graphene oxide (rGO) for the pharmacological mixture degradation are presented in this study. Using a facile hydrothermal technique, four catalysts were created by combining rGO with TiO2 and various metal oxides (CuO, NiO, and Ag2O). To examine the crystal structure and phase makeup of the produced catalysts, X-ray diffraction (XRD) was employed. In order to pinpoint the functional groups that were present in the catalysts, Fourier-transform infrared spectroscopy (FTIR) was used. To ascertain the catalysts' precise surface area and pore size distribution, Brunauer-Emmett-Teller (BET) analysis was utilized. In order to examine the shape and particle size of the produced catalysts, scanning electron microscopy (SEM) was used. By observing how a combination of medicines degraded when exposed to light, the catalysts' photocatalytic activity was assessed. This work emphasizes the potential of photocatalysts based on rGO/TiO2 for the degradation of intricate mixtures of contaminants, including pharmaceuticals. The importance of this work is in the creation of effective photocatalysts that may be used to remove developing toxins in water bodies, which can have serious effects on the environment and human health.

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TITLE

First principles studies of topological defective graphene-based superlattices with H adatoms

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ABSTRACT

In this work, we have studied graphene superlattices with an interesting topological defect called the flower-like Defect (FLD); additionally, we include patterned H adatoms. The so-called flower-like defect (FLD) forms part of the family of grain boundary loops, specifically, the rotational grain boundary family [1]. The FLD can be seen as the rotation of a 24-carbon section to the lattice, which reconfigures the covalent bonds surrounding the flower, creating pentagons and heptagons structures. It would seem that the FLD has C vacancies due to the non-hexagonal structures, but this is not true; in fact, it preserves the density of atoms and the coordination of the pristine graphene. We aim to look for a fundamental understanding of these systems' possible bandgap openings and magnetic properties. The simulations will predict the structure stability, electronic structure, energy formations, simulated scanning tunneling microscopy (STM) images, and possible magnetic properties. DFT calculations were performed with VASP using the meta-GGA functional with van der Waals dispersions r2SCAN+rvv10. The projector augmented wave (PAW) potentials described the core electrons. Additionally, an appropriate kinetic cutoff energy is required to represent the wave functions in a finite (but large enough) basis set of plane wave functions. A convergence process with a criterion of 1 meV per atom was used, obtaining a cutoff energy value of 950 eV. Similarly, a Monkhorst-Pack k-point mesh of 21x21x1 was chosen with a separation of 0.022x2π Å-1 in the reciprocal space. For all the superlattices, ionic relaxations were allowed to optimize the atoms until all the forces were less than 0.01 eV Å-1. The motivation for placing H adatoms in the FLD came to light in [2]. This work reported a significant contribution (2pz orbitals) of the edge C atoms of the FLD to the electronic structure. Then, we expected that H adatoms at the borders of the FLD would notably affect the superlattices' electronic structure. However, we discovered that this hypothesis is only partially true. The next candidate was the Moire-like H pattern reported by Balog, et al. [3], showing a significant change in the electronic structure and motivating us to study two distinct regions of this pattern separately. Ultimately, we selected three regions to analyze the effect of H adatoms in the electronic structure: the border, the inner, and the outer part of the flower, as depicted in FIG. 1. As a starting point; we chose the 6x6 graphene superlattice (FIG. 2). Within these regions, different patterned H configurations were tested for this specific superlattice, changing the sites, directions, and numbers of the H adatoms. We selected only the H configurations with a meaningful change in the band structure and higher formation energies to repeat them for other superlattices.

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TITLE

First-Principles Ultrafast Charge Carrier Dynamics of Methylammonium Lead Halide Perovskites

AUTHORS

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ABSTRACT

Methylammonium lead halide perovskite semiconductors, $MAPbX_3$ (MA = CH3NH3, X= I, Br, Cl), have become the focus of research efforts in the field of photovoltaics. Investigating processes on a nanoscale level can be achieved through real-time time-dependent density functional theory and Ehrenfest molecular dynamics. In a first-principles work based on real-time time-dependent density-functional theory, we investigate the ultrafast charge-carrier dynamics of MAPbI3. This work also includes ab initio density-functional theory (DFT) calculations on the electronic structure of using state-of-the-art functionals including HSE06 and GW approximations. Ab initio molecular dynamics calculations were also conducted to study the effect of structural fluctuations of the CH_3NH_3 substructure within the perovskite structure and its effect on the electronic structure. It was found that the $CH_3NH_3^+$ cations do not contribute to the optical absorption, but instead act as a structural filler and ensure charge neutrality of the unit cell. The ultrafast dynamics of methylammonium lead halide perovskites (X = I) were analyzed by following the evolution of the charge-carrier population using the formalism of real-time time-dependent density functional theory (TDDFT) . By impinging the system with a coherent femtosecond pulse in resonance with the HOMO →LUMO transition of the molecule and with varying intensities, it was found a pronounced intensity-dependent response, manifesting itself in high-harmonic generation, in the nonlinear behavior of the excitation energy and of the number of excited electrons, and, most interestingly, in the inversion of the photoinduced charge-transfer direction with respect to the linear regime. The nonlinear response of the system to the external perturbation leads to an inversion of the charge-transfer direction according to the intensity of the applied electric field. This behavior opens up the possibility to coherently control the sign of the interfacial electric field on the femtosecond time scale.

TITLE

Role of anion in asymmetric magnesium-catalyzed Diels-Alder reaction

AUTHORS

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ABSTRACT

II Group-metals, like magnesium, are one of the most widespread elements in the environment. Their abundance in the Earth's crust is over 108 times greater than the precious metals. For the industrial applications the important factors are the low costs of production and the higher accessibility of II group-metals' compounds. This puts the spotlight on alkaline-earth metals competing with transition elements as catalysts in organic synthesis. Features of their derivatives, like mild Lewis acidity and strong Brønsted basicity, enabled them to catalyze reactions where Lewis-acid-activation of the substrate is essential. Therefore catalysis by Earth-abundant metals can compete with noble metals catalysis and organocatalysis combining their advantages like high efficiency, being user-friendly and inexpensive and is in line with principles of green chemistry [1].

One of the most powerful tools of new carbon-carbon or carbon-heteroatom bonds formation is Diels-Alder [4+2] cycloaddition which discovery was honored with the Nobel Prize in 1950 [2]. Also its asymmetric variant enables receiving desired motifs in organic synthesis [3].

In 1992, Corey reported that chiral magnesium-bisoxazoline complex successfully – stereoselectively catalyzed reaction between 3-acryloyl-1,3-oxazolidine-2-one and cyclopentadiene [4]. But the stereoselectivity of this reaction wasn't only the result of the catalyst's structure – also the counterion of magnesium's salt mattered what proved in his computational studies Casali in 2022 [5].

As a poster presentation the relationship between the structure of substrate, catalyst, and product will be discusse.

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TITLE

Electronic structure

AUTHORS

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ABSTRACT

Since the discovery of graphene, 2D transition metal dichalcogenides (TMDs) have played an essential role in discovering new materials. The principal reason is because of their promising properties owing to their high aspect ratio, quantum size effects, and the remarkable advantage that we have to manipulate their structure by applying electric and magnetic fields in order to control some properties such as high aspect ratio, quantum size effects, and superconductivity [1]. The 2D TMD Niobium Sulfide (NbS2) is a superconductor that has received widespread attention due to its anisotropic structure and application prospects in energy and catalysis [2].

In order to know how these features can be affected when the structure interacts with other elements, one of the main purposes of this research is to add some Alkali-metals, such as Lithium (Li) and Cesium (Cs), among layers of NbS2, later named as Lithium Niobium Sulfide (LiNbS2), so that we can analyze what are the possible implications that this change can produce in our structure, especially in its bandgap. The bandgap will tell us how the electronic density distribution behaves around the Fermi level, from which we can determine the metallic, semiconductor, or insulator character. To reach this purpose, we develop further calculations using density-functional theory (DFT) within the meta generalized gradient approximation r2SCAN, including van der Waals interactions: r2SCAN+rVV10. Here, we report some important characteristics of LiNbS2 crystallographic structure, such as: cutoff energy, k-points, lattice parameters, bulk modulus, the density of states and band structure. Also, we study the LiNbS2(001) surfaces built with a vacuum slab of 15 Å with NbS2 surface terminated. Later, we expand the pristine surface to generate a topological defect to investigate the effect on the electronic structure. Reported results show that bulk NbS2 has a metallic character. However, when Lithium is added, we observe a bandgap opening. The main cause of this behavior in the fermi level could have been the high perturbation that Li atoms induce in its hexagonal lattice structure.

There are promising results that we can have by adding elements to the NbS2 structure so that the future work of this project will be to work with the remaining Alkali-metals of the periodic table (Cs, Na, K, Fr, Rb) in order to analyze what other properties we can obtain from the changes in the electronic structure of NbS2. Further analysis can be made relating to the study of their different symmetries in which we can observe how the band gap is affected [3] and by applying different hybrid functionals such as HSE06 and HSE12 in order to get more accurate results.

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TITLE

Chemical look at the planets Uranus and Neptune

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ABSTRACT

Uranus and Neptune, the ice giants of our solar system, have long been studied for their intriguing atmospheric compositions and unique characteristics. This paper presents a chemical perspective on these planets, exploring the chemical makeup of their atmospheres, including the elements and compounds present and their distribution within the planetary atmospheres. The analysis draws on data from observations[1] and theoretical modeling[2] to provide a comprehensive understanding of the chemical processes and dynamics of Uranus and Neptune. The paper also discusses the implications of these chemical findings for the broader fields of planetary science and astrobiology, including the potential for these planets to host life[3] and the role of chemical processes in shaping the evolution of our solar system.

Exploring the chemical composition of planetary atmospheres can reveal key insights into the nature and evolution of our solar system. In particular, Uranus and Neptune, the ice giants of our solar system, have long been studied for their unique atmospheric compositions. Uranus and Neptune have very similar atmospheres, composed primarily of hydrogen, helium, and methane[4]. However, their atmospheres also contain trace amounts of other compounds such as ammonia, water, and hydrogen sulfide[5]. The methane in their atmospheres gives Uranus and Neptune their distinct blue color[6]. Additionally, the atmospheres of these planets have complex temperature structures, with temperatures increasing towards the center of the planet. These temperature gradients drive complex chemical processes, including the formation of clouds and the creation of chemical compounds that may play a role in the potential for life on these planets[3,4].

While the study of Uranus and Neptune's atmospheres may not have immediate practical applications for humans on Earth, it provides valuable insights into the nature of our solar system and the potential for life beyond our planet. By understanding the chemical makeup and dynamics of these planets, we can learn more about the complex processes that shape our universe and how they may relate to our own planet and its evolution[3]. Additionally, the study of these planets may provide clues to the search for habitable exoplanets, potentially informing our understanding of the origins and distribution of life in the universe.

The chemical composition of the nuclei of Uranus and Neptune is still the subject of scientific debate and ongoing research. However, it is believed that the cores of these planets are primarily composed of rock and ice, with smaller amounts of heavier elements such as iron and nickel[7]. The high pressure and temperature within the cores of Uranus and Neptune also create a unique environment that can drive complex chemical reactions, potentially leading to the formation of new compounds and materials. Understanding the chemical makeup of the cores of Uranus and Neptune is essential for developing a comprehensive understanding of the formation and evolution of these planets and the broader processes that shape our solar system.

It is currently unknown whether there is life on Uranus or Neptune, as these planets are not considered habitable for known forms of life[3]. Both planets have extremely harsh environments, with temperatures reaching hundreds of degrees below freezing, and high levels of atmospheric pressure and radiation. Additionally, the lack of a solid surface and the presence of toxic compounds in their atmospheres make it difficult for life as we know it to exist on these planets[3]. However, there is still much to learn about the potential for life beyond Earth, and future missions and research may uncover new insights into the possibility of life on Uranus, Neptune, and other planets in our solar system and beyond.

The abstract provides a brief overview of the chemical composition of the atmospheres of Uranus and Neptune, highlighting the presence of unique molecules such as methane, hydrogen, and helium. It also discusses ongoing research into the chemical makeup of the cores of these planets, which are believed to be primarily composed of rock and ice. While there is no evidence of life on these planets, understanding their chemical nature is crucial for developing a comprehensive understanding of the formation and evolution of our solar system.

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[2] Hazy Blue Worlds: A Holistic Aerosol Model for Uranus and Neptune, Including Dark Spots - Irwin - 2022 - Journal of Geophysical Research: Planets - Wiley Online Library

[3] In Depth | Neptune – NASA Solar System Exploration / In Depth | Uranus – NASA Solar System Exploration

[4] Diagram of the Atmospheres of Uranus and Neptune | ESA/Hubble (esahubble.org)

[5] Top 5 elements in the atmosphere of Neptune (usra.edu)

[6] Gemini North Telescope Helps Explain Why Uranus and Neptune Are Different Colors | NOIRLab

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TITLE

The Influence Of Silicon Compounds On The Composition Of Biopolymer Gel

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ABSTRACT

In recent times, raw materials from renewable sources have a huge impact on the creation of innovative polymer materials, whose decomposition products will be absorbed by the natural environment after the use of such material. Smart specialization and sustainable economic development is based on spreading the slogan "green chemistry" and striving to limit the use of harmful chemicals as well as entire processes leading to the final production of a given material.

Despite many studies carried out on the creation of packaging material with biodegradable properties, synthetic polymers of the polyolefin type are still the core and the polymer matrix to produce films or packaging; PP polypropylenes, PE polyethylenes, aromatic PC polycarbonates, etc. The growing number of plastics produced both on the European and global market, reaching almost 280 million tonnes [1], prompts reflection on the global pollution of natural ecosystems. In order to counteract this, intensive research should be undertaken on the production of biodegradable and composted packaging [3]. For this purpose, natural raw materials or their derivatives are used; modified starches, chitosans, chitins, chemically, physically, and enzymatically modified celluloses, protein hydrolysates, etc.

The composition of biodegradable polymer developed by me with improved mechanical properties and stable thermal properties, strengthened by the introduction of silicon compounds for presubstitutes, can be used to produce, for example, foil or material for biodegradable packaging.

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TITLE

Reactive dye removal from aqueous solutions by poly(ε-caprolactone)-co-poly(2-hydroxyethyl methacrylate) adsorbent

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ABSTRACT

Water contamination with numerous anthropogenic pollutants is one of the major environmental problems that humanity is currently facing. Textile industry effluents are regarded as a major source of natural water bodies' chemical pollution. It is estimated that 280,000 tonnes of various chemically diverse synthetic dyes are released annually into the aquatic environment as untreated or partially-treated colored industrial wastewaters.[1] Apart from causing aesthetic deterioration of water bodies, these noxious compounds also have diverse negative effects on almost all forms of life due to their toxic, mutagenic and carcinogenic effects.[2] Among the available wastewater decolorization methods, adsorption is the most popular one due to its high efficiency, inexpensiveness, operational simplicity, large-scale applicability and lack of by-product formation, while polymers constitute the most widely studied class of dye adsorbent materials.[3] In this work, we report the synthesis of poly(ε-caprolactone)-co-poly(2-hydroxyethyl methacrylate) (PCL-co-PHEMA) and its characterization by Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). Copolymer's adsorption performance towards toxic anthraquinone-based dye Remazol Brilliant Blue R (RBBR), also known as Reactive blue 19, was evaluated by batch adsorption experiments. The effect of solution pH, contact time, temperature and initial dye concentration on the adsorption of RBBR was determined. The final dye concentration was determined by spectrophotometry at a wavelength of 593nm. The successful synthesis of PCL-co-PHEMA was confirmed by FTIR, while SEM revealed a smooth surface with some cracks and a moderate overall porosity. The optimum solution pH value of the adsorption process was found to be alkaline. The kinetic data were fitted to pseudo-first-order, pseudo-second-order and pseudo-third order models. The equilibrium adsorption data at temperatures of 25oC, 45oC and 65oC were fitted to the Langmuir and Freundlich adsorption isotherm models. The results indicate that PCL-co-PHEMA can be effectively employed for removal of RBBR from aqueous solutions.

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TITLE

Nano-QSPCR Mix models for sustainable design of efficient TiO2-based multicomponent nanomaterials: one step before synthesis

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ABSTRACT

The well-organized doped - or modified- TiO2-based nanotubes (NTs) have been widely designed as highly promising photocatalysts for degradation of pollutants, H2 production, or photoconversion of CO2. The main limitation in designing sustainable and advanced TiO2-based materials is thousands of possible combinations of structural features and a lack of systematic knowledge about the relationship between experimental conditions, structure modification, and the efficiency of newly designed TiO2 nanotubes. Because of the high cost and time-consuming experimental study, it is irrational to synthesize and test all possible structures to find the most optimal combination. Thus, in our research, for the first time, we applied machine learning (ML) methods combined with a high throughput screening methodology to study the quantitative relationship between the experimental condition, structure modification, and the efficiency of newly designed well-organized TiO2 nanotubes. The data-driven approach has been utilized based on a developed library of available literature data of ordered TiO2 NTs synthesized in thin layers synthesized by anodic oxidation of titanium foil that is highly active under vis or UV-Vis light. Then, by employing Hierarchical Clustering analysis (HCA) and Principle Component Analysis (PCA), we grouped and examined the structural similarity of 144 different TiO2-based NTs. Then, we have developed a predictive Quantitative Structure-Property Relationship model (QSPR) for the photocatalytic activity of investigated TiO2-based nanotubes NTs. Finally, through proposed supervised learning methods and developed predictive models, we have determined how to manipulate structural features and experimental conditions to reduce cost and speed up the process of efficient product design at the earliest possible stage. The proposed data-driven approach may be extended to optimize the design process of another type of advanced multicomponent nanomaterials in line with the sustainability-by-design strategy.

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TITLE

IL@MOF composites and derived carbons for CO_2 separation

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ABSTRACT

Carbon dioxide (CO2) is the gas species that is mostly contributing to global warming and, consequently, to climate change. The emissions of this gas must be mitigated so that further consequences for life on the planet can be averted. With this purpose in mind, different CO2 capture/separation technologies can be used. Specifically, both gas adsorption and absorption have an environmentally friendly character and have been proposed to mitigate CO2 emissions.

Regarding which materials to use for these technologies, Metal-Organic Frameworks (MOFs) and Ionic Liquids (MOFs) can contribute to the capture/separation of CO2 as, besides their physical and chemical properties, they have shown good sorbent properties like high CO2 sorption capacity and/or be highly selective toward this gas [1,2]. In the last decade, hybrid materials combining ILs and MOFs were proposed to obtain IL@MOF composites. Through synergistic effects, it is expected that sorbent properties are further improved [3]. In parallel, both MOFs and ILs can also be precursors of porous carbon materials at very high temperatures under an inert atmosphere [4,5]. Carbonization of IL@MOF composites has been scarcely reported in the literature for CO2 capture/separation.

In this work, different IL@MOF materials were produced. ILs with different structures were chosen and impregnated into MOF ZIF-8, at a constant IL molar loading, to study the anion and cation effects. Using a standard static gravimetric method [6], gas sorption-desorption measurements of CO2, CH4 and N2 were performed at 303 K, between 0-10 bar. The cationic and anionic structures were tailored so that synergistic effects could be promoted to improve sorbent properties such as gas sorption capacity and selectivity performance between 0-1 bar [7]. Also in this work, three distinct cyano-based ILs were impregnated into MOF ZIF-8 with different IL loadings. The produced composites were carbonized at 1073 K to study the anionic and loadings effects along with the N content, to determine how they impact adsorbent properties of the produced IL@MOF-derived carbons [8].

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TITLE

Characteristic of Cathepsin S using combinatorial chemistry methods

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ABSTRACT

Cathepsin S is a lysosomal cysteine protease that is mainly expressed in antigen-presenting cells (i.e., macrophages, B lymphocytes, and dendritic cells) [1]. The enzyme is best known for its critical function in the proteolytic cleavage of invariant chain chaperones, thereby controlling antigen presentation to CD4+ T cells by major histocompatibility complex (MHC) class II molecules or to NK1.1+ T cells via CD1 molecules. Cathepsin S also appears to be involved in direct processing of exogenous antigens for presentation by MHC class II to CD4+ T cells or in cross-presentation by MHC class I molecules to CD8+ T cells [2].

In this presentation, the synthesis and selection of internal quenched substrates for cathepsin S using combinatorial chemistry approach will be described. The general formula of the peptide library for "non-prime" (based on the Schechter-Berger notation) positions is presented below:

ABZ-X4-X3-X2-Arg-ANB-NH2
ANB-NH2 – amide of 5-amino-2-nitrobenzoic acid
ABZ – 5-aminobenzoic acid
X2, X3, X4 – coded amino acids exept for Cys.

In the next step of our research the peptide resulting from above described studies was incorporated into internal quenched library with general formula: ABZ-Lys-Met-Phe-Arg-X1'-X2'-X3'-Tyr(3-NO2)-NH2 where in position X1', X2', X3' set of proteinogenic amino acid exept Cys were presented. The libraries were synthesized manually on a solid support with the use of "split and mix" method and Fmoc/tBu protocol. For deconvolution iterative method in solution was used.

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TITLE

Computational studies of the metal-organic framework $Cu_2(CO_2)_4$ + H2ABDC-X (X=F, Cl, Br): stability, electronic structure, and defects

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ABSTRACT

Metal-organic frameworks (MOFs) are promising materials that have been widely studied due to their interesting morphological properties, such as high specific surface area and high porosity. Important properties of MOFs are based on various combinations of metal nodes and organic linkers. This feature increases research interest in applications related to solar energy harvesting, absorption, catalysis, separation, and sensing [1]. In a world where technology develops according to society's needs, these materials provide an opportunity for research and development in areas of interest, such as energy resources and the decomposition of greenhouse gasses. In order to study a promising metal-organic framework for photovoltaic applications, some researchers collect information from the reported bandgap and make a comparison with metal ion variation and/or organic/conjugation linker. The UiO66 zirconium-based MOF was one of the promising materials among those reviewed, with an average bandgap of 2.20-3.10eV [1]. Then, we propose a modification of the metallic node to the zirconium-based MOF UiO-66 with Cerium and Titanium to obtain suitable material for photovoltaic and/or photocatalytic applications; in this study, we also investigate the effect of structural defects on the electronic properties. Investigations on MOF report the close dependence between the ligand center and the transfer through the metal-linker interaction when determining the bandgap [1]. This bandgap is the crucial parameter and establishes the light-harvesting window, which according to the Shockley-Queisser limit, Eg must be between 1-2eV [2] to be a material with potential applications in photovoltaics. We performed ab initio density-functional theory calculations with r2SCAN and HSE06 functionals; we analyzed the stability of the structures using machine learning and molecular dynamics. The calculations yield properties of MOFs with volumes of 2054.99 and 2512.27 Å3 and compressibility modulus of 0.3644 and 0.2984 GPa for UiO66-Ti and UiO66-Ce, respectively. Bandgap values were also obtained: 3.72 eV for UiO66-Ti and 2.78 eV for UiO66-Ce. These

computed values indicate the high specific surface area and their mechanical softness. In addition, when analyzing the density and partial density of states, the dependence on the metal-linker transfer is evident since, in the valence band, the main contribution comes from carbon and oxygen, elements that make up the linker, while in the conduction band, the main character comes from metal; either Ti or Ce. These studies also consider UiO66 with a mixture of Ce and Ti in the same MOF and structures with defects on the organic linker. The results are discussed in light of the available experimental data.

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Title

Study of Modification Process of Oxyethylated Nonylphenolformaldehyde Resins by IR spectroscopy

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Abstract

Modification process of oxyethylated nonylphenolformaldehyde resins (ONPFR) by nitrogen-containing compounds was studied on the example of imidazolinamines synthesized on the basis of natural petroleum acids and polyethylenepolyamines in various molar ratios [1]. The modification process was studied by IR spectroscopy. The spectra of imidazolinamine-modified ONPFR were recorded on LUMOS IR-Fourier spectrometer from BRUKER in the wave frequency range of 600-4000 cm^{-1} *and shown in Fig. 1.*

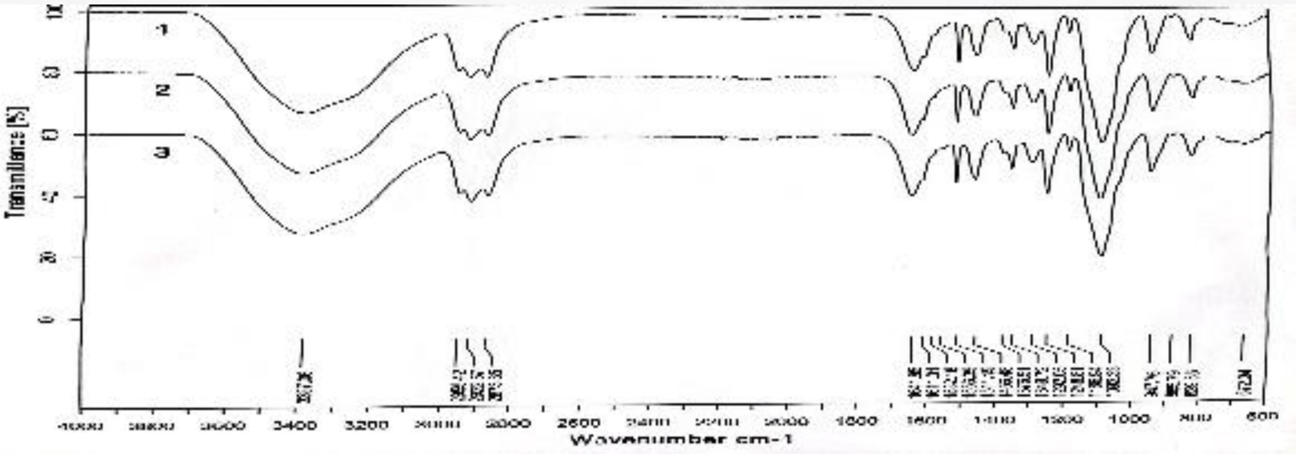

Fig. 1.IR spectra ONPFR modified by imidazolines on the basis of NPA and PEPA in a molar ratio of 1-1:1; 2-2:1; 3-3:1

The spectra of imidazolinamine-modified different compositions of ONPFR are identical with slight shifts. Consider the example of ONPFR modified by imidazolinamine in a molar ratio of 3:1 (Fig. 1). The spectrum showed: deformation vibrations at 1376, 1456 cm^{-1} and valence vibrations at 2872, 2923, 2955 cm $^{-1}$ of CH bond of CH_2 groups; deformation vibrations of N-H bond at 1556 cm^{-1}; valence vibrations of C-N bond at 1186 cm^{-1}; valence vibrations of C=N bond at 1641 cm^{-1}; deformation vibrations of C-H bond of benzene ring at 829 cm^{-1}; valence vibrations of C-C bond of benzene ring at 1611 cm^{-1}; valence vibrations of O-H bonds at 3395 cm^{-1} and valence vibrations of C-O-C bonds of ether at 1248 cm^{-1}. Thus, infrared spectroscopy analyses proved modification process of ONPFR by imidazolinamines of various molar compositions.

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TITLE

Comparison of the usefulness of JC-1 and MTO for mitochondrial membrane potential measurement in Chlamydomonas reinhardtii cells

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ABSTRACT

Phytoplankton is an important element of the food chains in aquatic ecosystems. The eukaryotic microalgae, like other oxygenic organisms, for cell respiration use electron transport chain that takes place in mitochondria – the organelles important because of their multi-functional role in metabolism, energy production, ion transport and distribution, and redox homeostasis. In investigations of mitochondria activity, mitochondrial membrane potential (MMP) is often examined, since MMP together with the proton gradient form the transmembrane potential of hydrogen ions which is inevitable to make ATP. Since MMP reflects performance of the mitochondria, it is believed to be a good marker of disorder of electron transport system and cell's energetic state.

Because of such an important role of MMP in biological assays, there are different fluorescent dyes for measuring the MMP value: TMRM, TMRE, Rhodamine 123, DiOC6(3), Mito Tracker™ Orange (MTO), and JC-1. Among them, JC-1 is often called "the gold standard" for MMP analysis, while MTO is believed to offer more complex and informative mitochondrial analysis.

JC-1 is successfully used in phycological studies, including our research of Chlamydomonas reinhardtii cells. In contrast, MTO-based analysis of mitochondrial mass and activity is effectively performed in humans' and animals' cells but has rarely been used in phycology. Since a contradictory statements about MTO usefulness for algal mitochondria staining can be found in literature, we decided to compare its suitability for in vivo MMP measurement in Chlamydomonas reinhardtii cells, with JC-1-based method. In our study we used population of cells synchronized by alternating light and dark periods, which allowed us to check the efficiency of mitochondria staining at different stages of algal cell development. Cells were sampled at 0h, 3h, 6h and 9h after the start of the light period of cell cycle. The MMP was measured after cells incubation (20 min for JC-1 and 45 min for MtO) at 30°C with the appropriate fluorochrome on black 98-wells plates. The waves of excitation were 488 nm and 551 nm, for JC-1 and MTO respectively and waves of emission: 538 and 596 nm for JC-1, and 576 nm for MTO.

Our results showed that MTO allows to detect changes in MMP already in young developing cells (3rd hour of the cell cycle), while in the case of the JC-1, changes in MMP became visible in fully developed cells, after 9 hours of the cell cycle. Thus, MTO turned out to be more sensitive to early changes in mitochondrial activity. The possible reason for such high sensitivity may lie in the mechanism of MTO action. MTO, after entering the cells, is oxidized and selectively binds to peptide groups of the components of the mitochondrial membrane. In opposite, JC-1 responds to significant changes in selectivity of mitochondrial membrane (mainly caused by damage of membrane's structure) thus, probably, cannot detect subtle changes that occur during cells development.

Due to the described differences, we recommend using MTO for algal tests, especially when subtle MMP changes are expected.

This work was partially supported by the National Science Centre Poland [grant UMO-2021/41/N/NZ8/00124].

TITLE

Impact of beach recreation on mercury pollution of coastal zone sediments of the southern Baltic Sea

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ABSTRACT

Mercury is a potent neurotoxin considered to be one of the most dangerous contaminants. Chemical form of mercury plays an important part in its toxicity and exposure of living organisms. It also influences the transport of mercury within and between environmental compartments. Among large number of forms existing in the environment, bioaccumulative and biomagnifying organic mercury compounds, such as methylmercury, pose the greatest risk.

The research was conducted in the Puck Bay located in the Polish part of the southern Baltic Sea. Study material was collected during four campaigns at the end of each season: June 2020 (spring), September 2020 (summer), December 2020 (fall), and March 2021 (winter). Samples of surface sediments (top 10 cm) were collected using a van Veen grab at three stations with varying degrees of recreational use (no activity, moderate activity, intense activity).

Total mercury (Hg[sub]TOT[/sub]), as well as labile (Hg_{LAB1A}, Hg_{LAB1B}, Hg_{LAB2}) and stable fractions (HgS, Hg_{RES}) of Hg, were analyzed by AAS method on DMA-80 (Milestone) [1, 2]. Methylmercury (MeHg) concentration was analysed using AFS-GC technique on MERX-M (Brooks Rand) after previous extraction and ethylation [3]. Additionally, an analysis of physical features of sediments were performed: granulometric composition and the content of organic matter (LOI in 550 °C). The results indicated that concentrations of HgTOT in sediments at stations used recreationally were higher than at the reference station. The highest concentrations were measured in the area where motor boats and jet skis are used, while in the area dominated by sustainable water activities (kitesurfing, stand up paddling). This includes also the concentration of bioavailable labile fraction (HgLAB1B) and the most toxic form of Hg, MeHg. This poses a threat to marine organisms, especially benthic flora and fauna, as well as humans consuming fish and other seafood.

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Sediment contamination was particularly noticeable after the summer season, when recreational activity was most intense. Summer season activity also influenced the increase in water dynamics, as reflected in the granulometric composition of the sediments. This affects the process occurring at the sediment-water interface, and may enhance the remobilization of dangerous pollutants to the water column accumulated in sediments over the years.

This research was supported by the National Science Center grant (2018/31/N/ST10/00214) conducted at the University of Gdańsk.

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TITLE

Photosynthetic parameters as markers of the toxicity of nabumetone and flufenamic acid to Chlamydomonas reinhardtii

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ABSTRACT

Pharmaceuticals are currently common pollutants in the aquatic environment. Among them, the most numerous and diverse group are non-steroidal anti-inflammatory drugs (NSAIDs), for example, flufenamic acid (FFA) and nabumetone (NBT) used in the present study. Knowledge about their potential toxicity to non-target organisms, especially higher plants and algae, is still insufficient.

Photosynthesis is a biochemical process characteristic for "green" organisms. This process enables them to produce energy and all the necessary organic compounds. Thus, one of the most important ecotoxicological problems is to investigate the possible adverse effects of environmental pollutants on plants' photosynthetic efficiency. Among the model organisms that are used in such investigations are planktonic algae. In this work, the green alga Chlamydomonas reinhardtii was chosen as a suitable model for studying the toxic effects of NSAIDs on photosynthesis.

The main objective of this work was to investigate the phytotoxicity of FFA and NBT used at the EC50 concentration toward C. reinhardtii by analyzing the parameters related to photosynthesis. The research hypothesis assumed that both pharmaceuticals, differing in chemical structure, would cause different effects on the functioning of the photosynthetic apparatus. The hypothesis was verified by determining the content of photosynthetic pigments as well as analyzing selected parameters of chlorophyll a fluorescence in vivo (OJIP test).

It was found that both tested drugs significantly increased the content of chlorophyll a and b in C. reinhardtii cells, however, greater stimulation was caused by NBT. The content of carotenoids, whose increased synthesis is observed in response to abiotic stress, almost doubled in drugs-treated cells, as compared to control. The analysis of the fluorescence induction curve clearly indicated the changes in the course of photosynthesis in drugs-treated cells. As a result of NBT action, electron transport between photosystem II (PS II) and photosystem I (PS I) changed. The reduction of the plastoquinone pool significantly increased. Presumably, plastoquinone could not be re-oxidized, as evidenced by the higher values of fluorescence between the J-step and I-step of the fluorescence curve. In opposite, electron transport was not affected by FFA, but a decrease in the fraction of active reaction centers of PS II was observed. A detailed comparison of the quantum efficiencies obtained during the OJIP test confirmed the presence of differences in the mechanisms of action of the tested compounds.

In summary, NBT and FFA clearly alter the functioning of photosystems in [i] C. reinhardtii [/i] cells, although their action differs significantly. This study strengthens the existing evidence that NSAIDs pose a serious threat to photosynthetic aquatic organisms, and the mechanisms of their toxic effects should be thoroughly investigated.

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TITLE

Liquid-Phase Oxidation of Higher Fatty Acids Isolated from Corn Oil

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ABSTRACT

In organic chemistry and technology, oxidation processes are the transformations of substances under the action of oxidizing agents. There are two types of oxidation: oxidation without breaking the carbon chain and destructive oxidation proceeding with the splitting of carbon bonds. Molecular oxygen is used in most types of oxidation reactions in the form of air or technical oxygen. Under normal conditions, the C-C bond of organic substances is quite stable, and the nucleation of chains with the breaking of this bond usually does not occur. Therefore, chain nucleation is possible with the participation of oxygen and initiating additives with an attack on the weakest π-C-C and C-H bonds. Ions of a number of metals (manganese, cobalt, chromium, vanadium, molybdenum) catalyze oxidation processes with fairly high yields. In this work, we studied the process of oxidation of a mixture of fatty acids isolated from corn oil in the presence of a chromium naphthenate catalyst. The oxidation of a mixture of higher fatty acids isolated from corn oil is based on a liquid-phase free radical oxidation process under the action of atmospheric oxygen. Higher fatty acids subject to oxidation isolated from corn oil were studied by IR spectroscopy on a BRUKER ALPHA IR-Fourier spectrometer in the wave frequency range of 600-4000 cm $^{-1}$.

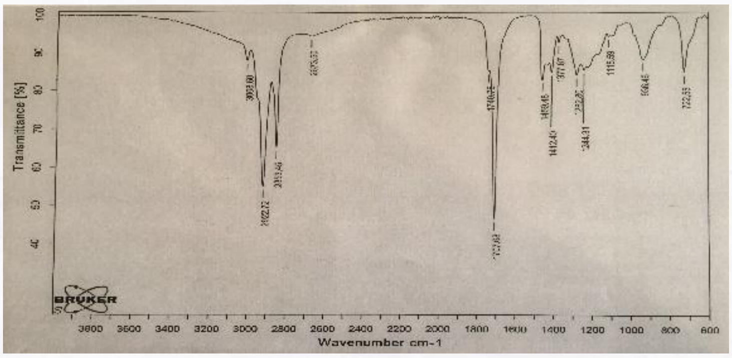

Fig. 1. IR spectrum of oxidized higher fatty acids isolated from corn oil

On the IR spectrum of a mixture of oxidized acids isolated from corn oil (Fig. 1), there were observed: deformation vibrations at 1377, 1412, 1459 cm^{-1} and valence vibrations at 2853, 2922 cm^{-1} of C-H bonds of CH_3 and CH_2 groups, deformation vibrations at 936 cm $^{-1}$ of O-H bond of acid, valence at 1707 cm^{-1} vibrations of the C=O bond, valence vibrations of the COOH group at 2673 cm^{-1}, valence vibrations of the C=C bond at 3008 cm^{-1}, and the formation of a new peak was also observed at 1740 cm^{-1} indicating the formation of new components and thus confirming the passage of the oxidation process.

TITLE

Multicomponent composite for the alendronate delivery and osteoporosis treatment

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ABSTRACT

Osteoporosis is one of the most widespread disease that affects skeletal system, which could be developed due to the genetic, metabolic, hormonal, and immune system imbalances, as well as the lifestyle and medications – especially steroid drugs[1]. Bisphosphonates are one of the most commonly used drugs for treating and preventing osteoporosis. Although they are considered the gold standard in treatment, they can have serious side effects, mainly related to their oral administration (inflammation and ulcers of the esophagus, indigestion, and stomach pain). In addition, they are poorly absorbed from the gastrointestinal tract - their bioavailability is about 0.6-1%[2]. Therefore, to address these issues, multicomponent composite was designed, that could not only be used as a drug delivery system, but also, by itself, improve the bone regeneration. Mesoporous silica, decorated with hydroxyapatite was used as an alendronate carrier. These drug-loaded particles were suspended in hydrogel matrix[3] composed of collagen, chitosan and modified chondroitin sulfate and crosslinked with genipin solution. It was demonstrated, that the prepared hybrid composite was not only injectable, but also allowed for more ***sustained drug release****, with decreased burst effect. Additionally, particle-dependent changes in swellability, wettability and degradability were demonstrated. Higher particle concentration allowed for the preparation of materials with* ***improved mechanical properties****.* ***The antibacterial activity*** *was assessed against Staphylococcus aureus and Escherichia coli in in vitro experiment. Hybrid systems were bioactive, as they supported apatite formation, and they were biocompatible with MG-63 cells, as they not only supported their proliferation but also their differentiation.* ***Therapeutic potential*** *was also established with model osteoclast cell lines, as the composites hindered their proliferation [4][5].*

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TITLE

Chemical composition of extra virgin olive oil

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ABSTRACT

The main component of the chemical composition of olive oil is the saponification fraction (98-99% by volume of oil). The saponification fraction consists of acylglycerols, saturated fatty acids, monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA). The unsaponifying fraction (1-2%) contains antioxidants, volatile compounds, hydrocarbons and sterols [1]. The following types of olive oils are distinguished: extra virgin olive oil, refined olive oil and lampante olive oil [2]. Extra virgin olive oil is distinguished by the content of health-promoting antioxidant chemicals such as α-tocopherol, squalene, β-sitosterol and polyphenols. The fatty acid profile of extra virgin oil consists of the following fatty acids: oleic acid (55–83%), palmitic acid (7.5–20%), linoleic acid (3.5–21%) and stearic acid (0.5–5%) [3].

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TITLE

Modification of the surface of core-shell nanostructures with amino, and thiol groups and determination of the number of deposition

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ABSTRACT

The research objective of the work was the synthesis and later modification of a nanocomposite composed of a gold core and a silica shell. The project was based on a one-step and one-pot synthesis using: nanoparticle precursors, including tetrachlorosilane acid and tetraethoxysilane, a reducing agent needed to reduce nanogold, in this case hydrazine, and additional compounds including surfactants such as hexadecyltrimethylammonium bromide. Further modification of the nanomaterial is possible due to the presence of silanol groups on the surface of the core-shells. The modification consisted in adding an amine and a thiol group, the undoubted advantage of the entire procedure is the gaining even more applications of the composite. After the modification process, the deposition number was determined, which provided information on how many active amine and thiol groups were present in the synthesized preparation. For the calculation, the method of determining the amino acids anchored to the resin, protected by a fluorenylmethoxycarbonyl (Fmoc) group, was used. Spectrophotometric measurements and reasonable calculations were performed which show that less Fmoc deposition was obtained for the thiol group than for the amino group.

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TITLE

Low-phonon titanate-germanate glass co-doped with Er3+/Yb3+ ions for near-infrared luminescence application.

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ABSTRACT

Since 1987 and after many years of further research, no viable alternative has been found which could widely replace erbium-doped fiber amplifier EDFA, due to its emission at 1550 nm originating from the 4I13/2 → 4I15/2 transition of erbium [1]. Most of the research work has been performed on silica glasses. The major drawback of silica glass due to its strong Si-O-Si covalent bonds. A lower concentration of trivalent erbium ions results in a narrow profile, which limits broadband near-infrared transmission. On the other hand, the high doping concentration easily leads to the formation of clusters, which results in luminescence quenching due to the ion-ion energy transfer. Moreover, the silica-based EDFA system shows narrow full width at half maximum (FWHM), which limits data transmission capacity. A. Polman [2] observed the main band at 1.535 um of erbium ions in pure silica glass, where the spectral width of the main peak was around 11 nm! The barium gallo-germanate glass system offers an alternative to overcome the drawback of silicate, tellurite, and fluoride matrix. This ternary system combines the attributes of a broad region of glass forming ability, excellent stability with respect to crystallization, infrared transparency, transmission beyond 5 micrometers, and high rare-earth solubility (5 mol.%) [3]. One of the most perspective options to improve the properties of glasses is titanium dioxide [4]. It is assumed that titanium dioxide can significantly broaden and enhance the luminescence bands of rare earth ions. However, the effect of titanium dioxide on barium gallo-germanate glasses co-doped with rare earth ions have not been often examined and their spectroscopic properties are less documented in the literature. In this presentation, we will address the properties of barium gallo-germanate glasses co-doped with Er3+/Yb3+ in the presence of titanium dioxide for photonics applications. This innovative approach has been expanded to explain the issue of varying Er2O3/Yb2O3 content on luminescence on characteristic emission bandwidth at around 1530 nm. In the first step, glass samples were prepared by the traditional melt quenching method using precursor metal oxides of high purity.

The excitation energy transfers are resonantly very fast from the 2F5/2 (Yb3+-sensitizers) to the 4I11/2 (Er3+-activator) due to a small energy mismatch between the interacting excited levels. For this reason, characterization was started by emission spectra measured in the wavelength range from 1400 nm to 1700 nm under excitation by a 980 nm line of ytterbium ions. With increasing the Er2O3/Yb2O3 molar ratio the near-infrared emission intensities of the band centered at 1530 nm increase, and the full width at half maximum (FWHM) increases from 24 to 33 nm. At the same time, when the concentration of TiO2 increases from 0 up to 30 mol% observed the significantly broadened and enhanced the main laser transition. In this case, the FWHM parameter increases from 42 to 63 nm. The luminescence decays for glasses were measured and analyzed in detail. The preliminary studies conducted are promising from a scientific and application point of view.

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TITLE

Biodegradation of diclofenac by green alga Chlamydomonas reinhardtii

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ABSTRACT

Introduction. Pharmaceuticals, including non-steroidal anti-inflammatory drugs (NSAIDs), are often found in the environment at relatively low concentrations, but in some cases can pose a significant threat to non-target organisms, so the removal of NSAIDs from natural water bodies and wastewater is a priority. Diclofenac (DCF) is one of the most studied NSAIDs. In recent years, algae have been shown to have a high capacity for bioremediation (biosorption, bioaccumulation and/or biodegradation). Based on the above, the aim of our work was to investigate the remediation potential of a unicellular alga C. reinhardtii in relation to DCF.

Materials and methods. The algal culture was exposed to DCF at a concentration of 32.7 mg/L, corresponding to the EC10/24 for 4 days. Using appropriate extraction and HPLC/DAD-ESI-HRMS analysis and a qualitative and semi-quantitative assessment of biotransformation products in algal biomass and culture medium was carried out. Also, the diclofenac removal from the nutrient medium was studied.

Results. Based on the levels and temporal profiles of individual DCF transformation products, the main pathways of DCF metabolism in C. reinhardtii were suggested. In the quantitative terms, the most pronounced metabolites found in biomass were compounds with m/z 250, 278 and 310.04, the level of which increases with increasing exposure time. The structure of these metabolites indicates that they are formed by decarboxylation, amidation and methylation, respectively. In addition, a high level of the transformation product with m/z 312 associated with hydroxylation by monooxygenase was observed in the culture medium. The formation of some metabolites is expected to involve such processes as O-acetylation, glucuronidation, dehydrogenation, oxidation, ring-opening reactions (carbon-carbon bond cleavage) and C–N cleavage.

Conclusions. A wide range of DCF transformation products was found, wherein in C. reinhardtii, many of the proposed metabolic pathways are similar to those in animals, bacteria and in higher plants, some of the pathways have not been previously described. At the same time, despite the large number of metabolites found, semi-quantitative analysis showed that the decrease in the level of diclofenac cannot be fully explained by the transformation into the suspected products, this may be explained by the fact that diclofenac was partly metabolized further into compounds with a lower mass, therefore difficult to detect using HPLC/DAD-ESI-HRMS, or completely metabolized by C. reinhardtii (final mineralization to CO2, NH3, H2O, and chlorine). Additionally, certain amount of diclofenac intermediates could remain in the non-extractable cell fraction and this aspect needs further study. An important area of research may also be the potential toxicity of the identified metabolites to aquatic organisms.

TITLE

A new derivative of a sulfonamide antibiotic – synthesis and its ability towards complexing of osmium(III) ions – chemical, technological and economic aspects

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ABSTRACT

The primary objective of this research was to devise a method for the synthesis, isolation, and determination of the chemical structure of a novel compound, 4-amino-N-(3-methoxyphenyl) benzenesulfonamide ***(AM-3-OMe-SĄ)****. Additionally, the study aimed to investigate its coordination abilities towards osmium(III) ions. To achieve this, a two-step synthesis was employed, which resulted in a 79% yield of the product. The compound's purity was verified using elemental analysis and various chromatographic techniques, including thin-layer chromatography (TLC) and liquid chromatography with ultraviolet detection (LC-UV).*

To identify and determine the chemical structure of AM-3-OMe-SA, several spectroscopic methods were employed, such as proton nuclear magnetic resonance (1H NMR), infrared (IR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, and mass spectrometry (MS). Through the complexometric titration method, it was confirmed that the synthesized AM-3-OMe-SA, referred to as the ligand, possesses two nitrogen donor atoms.

The study also focused on determining the stability constants of the osmium complex compound [OsIIIL2]3+. The logarithm of the stability constant (logK) for the title compound with osmium(III) ion was calculated to be 6.2 and 6.32, respectively. Furthermore, the research explored various modes of coordination for osmium(III) ions with the ligand.

In conclusion, this work successfully developed a method for synthesizing, isolating, and determining the chemical structure of the novel compound 4-amino-N-(3-methoxyphenyl)benzenesulfonamide (AM-3-OMe-SA). The compound's coordination abilities towards osmium(III) ions were also investigated, and the stability constants of the osmium complex compound [OsIIIL2]3+ were determined. This research provides valuable insight into the potential applications of AM-3-OMe-SA in coordination chemistry involving osmium(III) ions

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Keywords: antibiotics; synthesis and complexing properties of sulfonamides with osmium(III); stability constants.

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TITLE

The efficiency of photosynthesis in green algae Chlamydomonas reinhardtii cells treated with selected non-steroidal anti-inflammatory drugs

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ABSTRACT

Human activity contributes to environmental pollution with many biologically active substances. One of the main classes of pollution are pharmaceuticals, like non-steroidal anti-inflammatory drugs (NSAIDs), which production and consumption are constantly increasing. NSAIDs have been detected in various types of water bodies including seas, lakes, rivers, and groundwater. However, little is known about their impact on higher plants and algae that play a key role in aquatic ecosystems.

In this research, the hypothesis that NSAIDs interfere with photosynthesis in green algae cells has been verified. As a model organism Chlamydomonas reinhardtii was chosen. C. reinhardtii CC-1690 (wild type) purchased from Chlamydomonas Resource Center (USA), was cultured in liquid mineral medium (HSM) at 30º C under continuous fluorescent light ≈125 µmol photons/m^2 *s*$^{-1}$ *and bubbled with sterilized air with 2.5% (v/v)* CO_2*. The cells were exposed to selected NSAIDs: diclofenac (DCF), flufenamic acid (FFA), indomethacin (IMC), nabumetone (NBT), or naproxen (NPX) at concentrations of 65.6 mg/L which is equal to* EC_{25} *of DCF, determined in our previous studies. Samples for the analysis of oxygen evolution andchlorophyll "a" fluorescence in vivo (OJIP-test) were taken 6 hours after NSAIDs application. The obtained results indicate that individual substances, belonging to the same group of non-steroidal anti-inflammatory drugs, can exhibit different levels of phytotoxicity and cause different effects on Chlamydomonas reinhardtii photosynthetic apparatus. NPX and IMC at used concentrations did not disturb photosynthesis. In FFA- and DCF-treated cells inhibition of photosynthetic oxygen evolution was observed. Analysis of chlorophyll "a" fluorescence in vivo in those cells revealed a decrease in "photosynthetic vitality" (performance index, PI) caused mainly by diminishing the fraction of active reaction centers of photosystem II (RCM) and an increase in non-photochemical energy dissipation (φD0). What is interesting, neither FFA nor DCF affected electron transport efficiency between photosystem II and photosystem I.*

The strongest phytotoxic effect was caused by NBT. Its toxicity manifested in drastic inhibition of oxygen evolution, a significant decrease in the fraction of active reaction centers of photosystem II (RCM), lowering of quantum yield of primary photochemistry (φP0), and inhibition of electron transport (Ψ0; φE0, φR0). As a result, a significant decrease in photosynthetic vitality and an increase in non-photochemical energy dissipation (φD0) were seen

It is worth bearing in mind that pharmaceuticals may have a toxic effect on non-target organisms, which was proved by the presented studies. In addition, the amount of pharmaceuticals and other pollutants in the environment is constantly increasing, therefore knowledge of the actual contribution of these pollutants and the mechanisms of their toxic action is essential for the proper assessment of the risks they pose to the environment.

The work was supported by National Science Centre Poland, UMO-2016/23/B/NZ9/00963.

TITLE

Novel chitosan-based aerogels for oil absorption

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ABSTRACT

Several researchers are concerned about water treatment. Oil spills pose a significant hazard to both the environment and humans, so they must be addressed. Chemical dispersions, oil booms, skimmers, and in-situ burning are all potential oil spill clean-up remedies. Still, the aforementioned approaches have significant limitations that have caused problems throughout the years. Consequently, the current study recommends the usage of aerogels derived from bio-polymers, to absorb only the oil. Given the advantages of in-situ absorption, effective oil recovery, and low energy consumption, absorption with porous materials is recommended. Our aerogels are non-toxic, biodegradable, and lightweight. For their synthesis, chitosan (CS), poly(vinyl alcohol) (PVA), graphene oxide (GO) and reduced graphene oxide (rGO) aqueous solutions were used in different ratios, with glutaraldehyde being the cross-linking agent. Aerogels were obtained through the freeze-drying method. Novel CS/PVA/GO and CS/PVA/rGO were fabricated. FTIR and XRD analysis confirmed the synthesis.

TITLE

Polymerase chain reaction

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ABSTRACT

Polymerase chain reaction (PCR) is a groundbreaking method developed by Kary Mullis. PCR allows for an amplification of a small DNA fragment. With this reaction it is now possible to amplify a small sample of DNA in a short amount of time, hence there are many uses of the polymerase chain reaction in, for example, medical diagnostics. [1]

The reaction is carried out in cycles and in each cycle is formed in three steps. In the first step the DNA is heated up to 94 degrees Celsius, which causes DNA strands to separate. In the next step the temperature is decreased to around 50-60 degrees Celsius and two oligonucleotide fragments called primers bind to the opposite strands of the DNA. In the last step, the temperature is increased up to 72 degrees Celsius, and then thermostable [i]Taq[/i] polymerase can synthesize the new DNA strand. Then, the newly created DNA strands act as templates for another cycle. Usually the reaction is stopped after 30-40 cycles, resulting in millions of newly synthesized DNA fragments. [1] [2]

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TITLE

Novel polymer compositions for drug delievery system.

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ABSTRACT

The great challenge of modern medicine is the synthesis of an effective drug, but its controlled, safe and effective delivery to the target is equally important. The development and production of novel polymeric drug delivery systems (DDSs) has been growing rapidly in recent years. So far, a number of articles have been published describing the potential use of various polymer compositions as drug carriers. Important aspects in improving the application of polymers for the DDS are their mechanical properties, biodegradability and bioavailability. The technology of drug delivery systems using polymers is developing dynamically, various modifications and strategies are proposed. Techniques such as pH-sensitive polymers, modifications with nanoparticles, polymeric micelles and many others can be mentioned here. This poster highlights various types of novel polymeric drug delievery systems, their advantages and disadvantages, preparation methods and drug release mechanisms. Examples of novel polymers used for DDS will also be discussed.

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TITLE

Ab initio studies of Electronic and Phononic Properties of XGeTe3 Monolayers (X = Cr, Mn): A Comparative Study of Ferromagnetic and Antiferromagnetic Phases

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ABSTRACT

In order to know how these features can be affected when the structure interacts with other elements, one of the main purposes of this research is to add some Alkali-metals, such as Lithium (Li) and Cesium (Cs), among layers of NbS2, later named as Lithium Niobium Sulfide (LiNbS2), so that we can analyze what are the possible implications that this change can produce in our structure, especially in its bandgap. The bandgap will tell us how the electronic density distribution behaves around the Fermi level, from which we can determine the metallic, semiconductor, or insulator character. To reach this purpose, we develop further calculations using density-functional theory (DFT) within the meta generalized gradient approximation r2SCAN, including van der Waals interactions: r2SCAN+rVV10. Here, we report some important characteristics of LiNbS2 crystallographic structure, such as: cutoff energy, k-points, lattice parameters, bulk modulus, the density of states and band structure. Also, we study the LiNbS2(001) surfaces built with a vacuum slab of 15 Å with NbS2 surface terminated. Later, we expand the pristine surface to generate a topological defect to investigate the effect on the electronic structure. Reported results show that bulk NbS2 has a metallic character. However, when Lithium is added, we observe a bandgap opening. The main cause of this behavior in the fermi level could have been the high perturbation that Li atoms induce in its hexagonal lattice structure.

There are promising results that we can have by adding elements to the NbS2 structure so that the future work of this project will be to work with the remaining Alkali-metals of the periodic table (Cs, Na, K, Fr, Rb) in order to analyze what other properties we can obtain from the changes in the electronic structure of NbS2. Further analysis can be made relating to the study of their different symmetries in which we can observe how the band gap is affected [3] and by applying different hybrid functionals such as HSE06 and HSE12 in order to get more accurate results.

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TITLE

Synthesis and characterization of N-arylsubstituted spiroxaziridines

AUTHORS

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ABSTRACT

At the end of the 1950s, chemists began working on a new group of heterocyclic compounds, which in later years was given the name oxaziridines. Oxaziridines consist of the three-membered ring with oxygen and nitrogen. The oxaziridinering is characterized by a very strong angular tension, it explains a high reactivity of these compounds. Due to the high ring stress, no configuration inversion occurs on the nitrogen atom. This causes this atom to become the center of chirality, which in turn translates into the possibility of separating both its enantiomers [1].

There are many methods for the synthesis of oxaziridines. Most of them rely on the oxidation of the corresponding imines using peroxyacids. The first published oxaziridination reactions were carried out using peracetic acid [2]. Currently, m-chloroperoxybenzoic acid (m-CPBA) is used for this purpose [3]. It is relatively stable compared to other peracids and is also very soluble in many organic solvents. Other oxidants, such as peracetic acid, are less stable and therefore more difficult to obtain commercially or have to be manufactured in situ.

In ourwork, we focused on the synthesis of N-arylsubstituted spiroxaziridines obtained by oxidation of imines derived from cyclic ketones. These reactions were carried out using [i]m[/i]-CPBA.

The obtained compounds will form the basis of substrates in studies on the photochemicalrearrangement of oxaziridines into lactams.

There are many methods for the synthesis of oxaziridines using m-CPBA available in the literature, but in practice attempts to replicate these results often fail due to insufficient description of the syntheses performed.

Therefore, it seems advisable to refine this method to obtain a reliable and reproducible procedure for the synthesis of this group of compounds.

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[3] K.S. Williamson, D.J. Michaelis, T.P. Yoon, [i]Chem. Rev. 2014, 114, 8016−8036.

TITLE

Hyaluronic acid in skin care

AUTHORS

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ABSTRACT

This abstract explores the properties of hyaluronic acid (HA) in the context of face care. HA is a naturally occurring molecule in the body, particularly abundant in the skin, that is well-known for its ability to retain moisture. In face care, HA is an essential ingredient as it helps to hydrate the skin, reducing the appearance of fine lines and wrinkles. Additionally, HA has a soothing effect on the skin, making it ideal for use on sensitive skin types. Furthermore, its lightweight nature makes it easily absorbed, suitable for all skin types. Lastly, HA has been shown to stimulate the production of collagen, thus enhancing the skin's overall health and appearance. Understanding the properties of HA can aid in selecting the right skincare products for optimal results. [1], [2], [3]

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[3] B. Bravo, P. Correia, J. E. Gonçalves Junior, B. Sant'Anna, D. Kerob (2022) Benefits of topical hyaluronic acid for skin quality and signs of skin aging: From literature review to clinical evidence. Dermatologic Therapy/Volume 35, Issue 12/e15903.

TITLE

Superior properties of mRNA capped with N2 modified dinucleotide tetraphosphate cap analogs

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ABSTRACT

The presence of a 5'-end cap structure that includes a 7-methylguanosine molecule connected to the first nucleoside through a 5'-5' triphosphate bridge is crucial for maintaining the stability and functionality of mRNA. This unique structure can be recognized by specific cap-binding proteins and is involved in several processes, such as maturation, export from the nucleus, initiation of translation, and degradation of mRNA. mRNA-based vaccines have gained attention due to their ability to provide material without the risk of genomic integration, and the ease with which mRNA can be engineered to introduce modifications that enhance translational efficiency or stability. Here, we describe the continuation of our previously published research with the use of a wider range of cap analogs. We focus on the use of N2 modified tetraphosphate dinucleotide cap analogs in mRNA transcripts. The presented N2-guanine modifications within the cap structure ensure proper attachment of the dinucleotide to the transcripts in the IVT reaction, guarantees their incorporation only in the correct orientation, and enables highly efficient translation of mRNA in the in vitro translation system. Additionally, the mRNA stability is increased by modifications in the phosphate chain of the cap structure that make mRNA resistant to decapping enzymes, thus increasing the lifetime of mRNA in the cell..

TITLE

Cycloalkylation reactions of para-chlorophenol and methylenecyclene in the presence of zeolite-containing seokar-2 catalyst

AUTHORS

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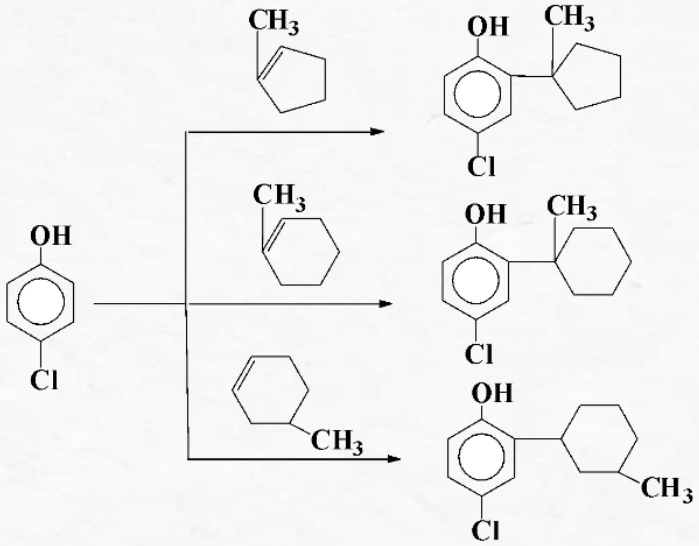
ABSTRACT

The paper deals with the study of cycloalkylation reactions of para-chlorophenol and cyclic hydrocarbons of various structures in the presence of zeolite-containing Seokar-2 catalyst. [1-3]



Effect of kinetic factors (temperature, reaction time, molar ratios of primary components, catalyst amount) on the yield of the obtained products - 2-methylcycloalkyl-4-chlorophenols and the selectivity of the reaction was studied for determining effective conditions for catalytic cycloalkylation reactions of para-chlorophenol and methylcyclenes in the presence of Seokar-2 catalyst.

Cycloalkylation reactions of para-chlorophenol were studied at 80-140°C in 2-6 hours, in the molar ratios of para-chlorophenol to cyclene from 2:1 to 1:2, the catalyst amount was 5-20% (according to the taken para-chlorophenol). As a result of determining the factors affecting the direction, yield and selectivity of the reaction, the optimal conditions for each cycloalkylation reaction were found: temperature 110-125°C, reaction time 5-6 hours, molar ratio of para-chlorophenol to methylcyclene 1:1, catalyst amount 12-15% (taken according to para-chlorophenol). Under these conditions, the yield of the target products was 69.4-74.5%, and selectivity was 88.6-90.3% according to the para-chlorophenol

Physico-chemical properties of the synthesized 2-methylcycloalkyl-4-chlorophenols were determined, and the chemical structures were confirmed by spectroscopic methods.

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TITLE

Analysis of fatty acid uptake in human cancer cells by Raman Spectroscopy.

AUTHORS

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ABSTRACT

Continuous adaptation of cellular metabolism to changing environmental conditions, including intensification of β-oxidation of fatty acids, is the main survival mechanism of cancer cells [1]. Therefore, tracking fatty acid uptake and metabolism is a crucial aspect of understanding carcinogenesis processes and its invasiveness. Raman microscopy is a powerful method for studying lipid content and distribution at the subcellular level [2]. On the basis of Raman spectrum, and using multivariate statistical and chemometric approaches it is possible to investigate metabolic changes induced by exogenous stimuli. Raman imaging was used to monitor changes in the molecular composition of a single promyeoloblastic cell as a result of saturated fatty acid exposure. The objective was to monitor the process of uptake of fatty acids and better understand their metabolism in human cancer cells.

Measurements were made using a confocal microscope coupled with a WITec Alpha3000 R Raman spectrometer. Multivariate analysis of spectroscopic data collected from promyeoloblasts (HL-60 cell line) incubated with palmitic acid and deuterated palmitic acid was performed using principal component analysis (PCA). PCA reduces dimensionality while simultaneously preserving the greatest variance. Herein, PCA on the collected Raman data allowed us to highlight the differences between cells incubated with selected fatty acids and control cells.

The profile of Raman spectra of HL-60 cells incubated with fatty acids in comparison to the spectra of the control cells showed an increase in lipidity of cells. PCA indicated spectroscopic markers that discriminate the spectra of the control and treated cells. Obtained results revealed that bands originating from C-H lipid stretching vibrations characterize cells incubated with fatty acids. In the case of cells treated with deuterated fatty acids, the analysis of the bands at ca. 2100 cm^{-1}*, originating from C-D group vibrations, allowed us to track uptake and distribution of the exogenous fatty acid. Since these bands are located in the so-called 'spectral silent region', free of Raman signals from biomolecules, they can be easily used as unique markers to determine the monitoring of the uptake process, distribution, and metabolism at the subcellular level.*

The „Label-free and rapid optical imaging, detection and sorting of leukemia cells" project is carried out within the Team-Net programme of the Foundation for Polish Science co-financed by the EU. This work was partially funded within the budget of the "Excellence Initiative - Research University" program at the Jagiellonian University in Krakow ("Young Laboratories" Program (Edition 2), "Real-time analysis of metabolism of live cancer cells by means of stimulated Raman spectroscopy").

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TITLE

Synthesis of a N2 modified cap analogs using "click" reaction and their biological properties as components of mRNA

AUTHORS

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ABSTRACT

Recently, thanks to COVID-19 pandemic, mRNA vaccines have gained huge popularity. Their advantage over DNA vaccines is that they are safer and there is no risk of genomic integration. Additionally, delivery of such therapeutics is less problematic and they can be easily obtained using an in vitro transcription reaction (IVT). The most important element of the mRNA present at the 5' end that is responsible for its functionality and vitality is the unique structure known as a "cap". It consists of 7-methylguanosine linked via a 5'-5' triphosphate bridge to the first transcribed nucleoside. The cap is involved in many processes, including maturation, nuclear export, translation initiation, and turnover. In the context of mRNA vaccines, the most important functions are the enhancement of translation initiation and protection against 5'-to-3' exonucleolytic degradation. The former can be achieved by introducing cap analogs with high affinity to the eukaryotic translation initiation factor 4E (eIF4E). Within this work we describe the continuation of our previously published research with the use a wider range of cap analogs. In this case, we are focusing at the length of the added linker at the N2 position and its influence on biological properties.

TITLE

All That Glitter Isn't Gold

AUTHORS

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ABSTRACT

Microplastics are the most widespread form of solid waste worldwide and pose a significant biological and ecological threat to aquatic ecosystems, also to humans. Glitter is an example of microplastics commonly found in our homes, especially in cosmetics.

In response to this demand for "eco-friendly" glitter, there is a rapidly growing market for alternative glitters with many new brands entering the marketplace. Biodegradable glitters are cellulose products which - to obtain the appropriate visual effect - are covered with thin layers of aluminum and plastic. It turns out that although they mostly consist of biodegradable cellulose, they are not neutral to the environment due to the coating. Moreover, natural or synthetic fluorphlogopite mica are also used as alternative glitters in cosmetics as shimmers. Unfortunately, none of the alternatives is completely safe for either the marine world or for humans.

On December 18, 2015, Congress amended the Federal Food, Drug and Cosmetic Act (FD&C Act) by passing the Microbead-Free Waters Act of 2015. The new law defines the term "plastic microbead" as any solid plastic particle that is 5 millimeters or less in size, and intended to be used to exfoliate or cleanse any part of the body. It means that all glitter is forbidden for use in cosmetic products.

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[2] https://www.fda.gov/cosmetics/cosmetics-laws-regulations/microbead-free-waters-act-faqs

TITLE

Antibody-Drug Conjugates - how can we use cancer cells antigens overexpression in our favour for targeted cancer therapy

AUTHORS

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ABSTRACT

Antibody-Drug Conjugates (ADCs) are an emerging class of targeted cancer therapeutics that combine the specificity of monoclonal antibodies with the potent cytotoxicity of small-molecule drugs. ADCs have the potential to overcome the limitations of conventional chemotherapy by delivering toxic payloads directly to cancer cells while sparing healthy cells, thereby improving therapeutic outcomes and minimizing side effects[1,2].A good ADC possesses several key characteristics that contribute to its effectiveness.These essential attributes include: specifity, potent cytotoxic payload, stable linker, low immunogenicity, efficient internalization and low off-target toxicity. This innovative strategy aims to surpass conventional chemotherapy limitations by selectively delivering toxic payloads to cancer cells, sparing healthy cells, ultimately improving therapeutic outcomes and minimizing side effects. Nevertheless, the development of ADCs faces numerous challenges, such as optimizing pharmacokinetics, ensuring site-specific payload release, achieving homogeneous drug distribution within tumors, mitigating undesired side effects, and overcoming drug resistance. Additionally, the complexities of treating various types of cancer and understanding their unique microenvironments further complicate the development process. However all these challenges are being addressed as numerous companies eagerly try to create an ideal antibody-drug conjugate, currently having over 100 compounds only in clinical trials[3].

In my poster I will try to elucidate what ADC are, what key components characterize an ideal conjugate and what opportuninites and challenges lie in front of us with such a technology.

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TITLE

Computational studies of the metal-organic framework Cu$_2$(CO$_2$)$_4$ + H2ABDC-X (X=F, Cl, Br): stability, electronic structure, and defects

AUTHORS

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ABSTRACT

In the light of new technologies to fight climate change, MOFs are proven to be quite useful. Metal-organic frameworks (MOFs) are porous materials formed by linking organic units with metal clusters as nodes (SBU). Large porosity and surface area values make them a good candidate for any application where storage is involved (e.g., drug delivery, water harvesting, hydrogen and methane storage, carbon dioxide capture, and catalysis applications.) In this work, we have presented spin-density functional theory calculations (spin-DFT) to study the electronic properties of three different MOFs based on copper SBU and functionalized linker ABDC-X, X = F, Cl, Br (cf. Fig 3.7 from ref [1])–each considering four magnetic phases– to assess photocatalytic applications. Electronic relaxation with meta-GGA functionals (r[sup]2[/sup]SCAN+rVV10) yielded an antiferromagnetic phase (AFM2) as the optimal state. All AFM2 structures (i.e. MOF-X-AFM2) show band gap energies inside the visible spectra, E_g= 2.5 - 2.7 eV showing good photoabsorption capabilities. Atomic partial density of states (atomic-pDOS) calculated with hybrid functional HSE06 displays ligand-to-metal (LMCT) and ligand-to-ligand (LLCT) charge transfer band gap excitations are present in all stable MOFs, which creates charge-separated states essential for photocatalysis. Aligned band edge positions (according to Butler et.al. [2]) against redox potentials of water splitting and CO$_2$ reduction enabled MOF photocatalysis activity evaluation. Our findings encourage the application of MOF-ABDC for photocatalytic water splitting and CO$_2$ reduction. Future research will focus on ABDC functionalization with I, NH$_2$, NO$_2$, and defects that could present even better electronic properties.

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TITLE

Extraction of Valuable Bioactive Compounds from Plants with Deep Eutectic Solvents

AUTHORS

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ABSTRACT

Modern chemistry pays attention to apply more ecological, green technologies, due to increasing environment pollution. Also using natural, bioactive compounds of plant origin in pharmaceutical, cosmetic and food industries is getting more popular. Considering these two aspects, an efficient and ecological isolation method of chemicals with biological activity is a needed alternative for traditional extraction with organic solvents. Recent literature presents deep eutectic solvents (DESs) as new chemicals with many possible applications, including extraction. Their structure is based on non-covalent interactions, mainly hydrogen bonds, that occur between hydrogen bond acceptor (HBA) and donor (HBD). These components are often natural, e.g. choline chloride, betaine, proline, citric acid, lactic acid. DESs have properties, which makes them „green" chemicals – they have low vapor pressure and toxicity, and can be biodegradable[1,2]. Also many of them are more effective extraction media compared to traditional solvents, such as ethanol, chloroform, methanol. Examples of plants, rich in bioactive components useful in industry, is pot marigold ([i]Calendula officinalis[/i] L.) and yarrow ([i]Achillea[/i] L.). It is possible to isolate a wide range of chemicals from these plants – saponins, carotenoids, phenolics, flavonoids. These groups of compounds are determining the important properties of plant extracts, e.g. anti-inflammatory, anticancer, antiviral[3,4]. Due to their promising properties and common occurrence in Poland, pot marigold and yarrow were chosen as material for our research.

The aim of this work was to apply chosen DESs as extraction media for flavonoids and phenolic compounds from plants. The impact of extraction temperature, water content and solvent type was examined. Also the qualitative analysis of extracts was done. According to achieved results, DESs extracts of pot marigold and yarrow are rich in phenolics and flavonoids, especially rutin, caffeic acid and chlorogenic acid. As the most effective DES, solvent based on choline chloride and lactic acid was chosen. Because of high viscosity of DES, water addition to reaction vessel improves mass transport. The highest yield of extracted compounds was achieved when water content ranged from 10 to 20% (v/v).

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CONCLUDING INFORMATION

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Contents of abstracts: conference speakers

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