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Dear Colleagues,

The Department of Physical Pharmacy of the Faculty of Pharmaceutical Sciences in Sosnowiec Medical University of Silesia in Katowice is pleased to invite you to the **6th General Academic Seminar "Physicochemical Methods in Scientific Research". The patrons of this year's edition are His Magnificence Rector of the Medical University of Silesia in Katowice Mr. Professor Tomasz Szczepanski, PhD, the Mayor of Katowice Marcin Krupa and the Mayor of Sosnowiec Arkadiusz Chęcinski.**

Physicochemical methods are a crucial component in scientific research. They are an essential tool for obtaining valuable data and their analysis, through thoughtful discussion, leads to the necessary knowledge regarding the proper functioning of living organisms. **The aim of the event is to popularize science by presenting interesting scientific studies conducted using various physicochemical methods in the fields of pharmacy, biology, medicine and related sciences.**

Similarly to the previous years, the Seminar is dedicated to academics, young scientists, PhD students, master's students, members of scientific research groups, and all science enthusiasts. During the Seminar, you will be able to listen to interesting lectures by invited guests and exchange experiences and knowledge of physicochemical methods presently used in science by presenting the results of research.

We provide a friendly atmosphere among scientists from different fields, hoping that the great interest will contribute to making our Seminar a regular meeting.

On behalf of the Department of Physical Pharmacy
Faculty of Pharmaceutical Sciences in Sosnowiec
Medical University of Silesia in Katowice

KIEROWNIK
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dr hab. n. farm.
Małgorzata Maciążek-Jurczyk prof. SUM

You are cordially invited to attend!

Wydawnictwo Śląskiego Uniwersytetu Medycznego w Katowicach

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CONFERENCE PROGRAMME*

08.00 – 09.00	***Registration***
09.00 – 09.15	***Opening ceremony***
09.15 – 12.30	***Plenary Session***
09.15 – 10.00	**"Pomiary przewodnictwa elektrycznego roztworów elektrolitów jako metoda badawcza w naukach farmaceutycznych",** Katedra i Zakład Chemii Fizycznej i Biofizyki, Wydział Farmaceutyczny, Uniwersytet Medyczny im. Piastów Śląskich we Wrocławiu – *prof. dr hab. n. farm. Witold Musiał*
10.00 – 10.45	„**Spectroscopic approaches for the determination of protein structure, dynamics, and function**", Zakład Biochemii Fizycznej, Wydział Biochemii, Biofizyki i Biotechnologii, Uniwersytet Jagielloński w Krakowie – *dr hab. Andrzej Górecki, prof. UJ*
10.45 – 11.00	***Coffee break***
11.00 – 11.45	**„Structural investigation of biomacromolecules using cryoEM",** Narodowe Centrum Promieniowania Synchrotronowego SOLARIS, Uniwersytet Jagielloński w Krakowie – *dr hab. Artur P. Biela*
11.45 – 12.30	**„The role of targeted metabolomics in evaluation of potential cancer biomarkers**", Zakład Farmakodynamiki, Katedra Biofarmacji i Farmakodynamiki, Wydział Farmaceutyczny, Gdański Uniwersytet Medyczny – *dr hab. n. farm. Wiktoria Struck-Lewicka*
12.30 – 13.30	***Posters session***
13.30 – 14.30	***Coffee break, lunch break***
14.30 – 15.15	**"Nanoparticles for gene and drug delivery: applying light scattering to screening and characterization",** Waters|Wyatt Technology, Germany – *Abhigyan Sengupta*, PhD, Senior Application Specialist
15.15 – 16.35	***Oral presentations***
15.15 – 15.25	**"Development of new analytical calibration methods in the chromatographic determination of bisphenols"**, Uniwersytet Śląski w Katowicach – *dr inż. Paweł Świt*
15.25 – 15.35	**"Physicochemical methods in forensic medicine"**, Śląski Uniwersytet Medyczny w Katowicach – *dr hab. Rafał Skowronek, prof. ŚUM*
15.35 – 15.45	**"Studies on biofilm growth and total polyphenolic content of fermented beverages"**, Uniwersytet Śląski w Katowicach – *dr Joanna Orzeł*
15.45 – 15.55	**"Complementary physicochemical methods in studies on the synthesis and properties of the double metal cyanide (DMC) catalysts"**, MEXEO Wiesław Hreczuch, Kędzierzyn-Koźle – *Bartosz Młynarczyk*

15.55 – 16.05	**"Analysis of the molecular structure of o-derivatives of 7-hydroxyflavone"**, Śląski Uniwersytet Medyczny w Katowicach – *Patryk Mruczek*
16.05 – 16.15	**"Implementing non-invasive techniques for assessing plant vitality in nanoparticle applications"**, Akademia Górniczo-Hutnicza im. St. Staszica w Krakowie – *dr Aleksandra Orzechowska*
16.15 – 16.25	**"Application of single-molecule FRET to investigate the structural dynamics of the Ying Yang 1 (YY1) protein"**, Uniwersytet Jagielloński w Krakowie – *Jakub Bartuś*
16.25 – 16.35	**"MRI/ultrasound-guided transperineal biopsy: new face of prostate cancer diagnosis"**, Śląski Uniwersytet Medyczny w Katowicach – *Krzysztof Walkiewicz*
16.35 – 17.20	**Closing lecture** **"History of spectroscopy in a nutshell"**, ABL&E-Jasco Polska Sp. z o.o., Kraków – *dr inż. Mirosław Danch*
17.20 – 17.45	***Award ceremony***
17.45 – 18.00	**Cl*osing ceremony (Group photo)***

*** The Organizer reserves the right to make minor changes to the Conference program**

LIST OF ABSTRACTS

L_1 POMIARY PRZEWODNICTWA ELEKTRYCZNEGO ROZTWORÓW ELEKTROLITÓW JAKO METODA BADAWCZA W NAUKACH FARMACEUTYCZNYCH

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Początki badań przewodnictwa elektrycznego roztworów sięgają okresu, kiedy Arrhenius [1], Ostwald [2] i Kohlrausch [3] badali szczegółowo przepływ prądu elektrycznego próbując ustalić wpływ hipotetycznych jonów na właściwości wodnych roztworów kwasów, zasad i soli. Zaproponowany już wtedy związek pomiędzy stopniem dysocjacji i przewodnictwem równoważnikowym umożliwił rozwój nowoczesnych metod analitycznych opartych o teorię roztworów elektrolitów przedstawioną przez Debey'a i Hueckla, a opracowaną w oparciu o równanie Poissona–Boltzmanna [4,5]. Modyfikacje wprowadzone przez Onsagera i Fuossa zapewniły dalszy rozwój teorii roztworów elektrolitów, aczkolwiek praktyczne jej zastosowanie napotyka trudności wynikające ze zróżnicowania, ale i podobieństwa jonów składających się na elektrolit. W badaniach wykorzystane mogą być podstawowe pomiary przewodnictwa elektrycznego, które obejmują m.in. przewodnictwo właściwe, molowe i graniczne. Dobrym przykładem zastosowania konduktometrii w praktyce badań farmaceutycznych jest pomiar przewodnictwa elektrycznego, które może odzwierciedlać zmiany w stężeniu leku uwalnianego z postaci dawkowania leku, czego przykładem są badania uwalniania soli żelaza ze złożonych form leków [6] oraz do oceny preparatów polimerowych i liposomowych do miejscowego i przezskórnego podawania leków [7,8]. Przeprowadzono także w naszej jednostce badawczej pomiary przewodnictwa zaproponowane do monitorowania przebiegu procesów polimeryzacji [9] oraz oczyszczania polimerów [10].

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L_2 SPECTROSCOPIC APPROACHES FOR THE DETERMINATION OF PROTEIN STRUCTURE, DYNAMICS, AND FUNCTION

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Physicochemical methods allow the investigation of protein structures at multiple hierarchical levels, from atomic detail to supramolecular assemblies. While high-resolution methods provide detailed structural information, it is often averaged over time or limited to a selected conformation. In contrast, lower-resolution techniques are more suitable for studying structural dynamics.
This seminar will focus on two spectroscopic techniques widely used in the study of protein structure and function: circular dichroism (CD) spectroscopy and fluorescence spectroscopy.
CD spectroscopy is employed to investigate the secondary and tertiary structure of proteins, as well as structural changes related to their functional roles. Fluorescence techniques, on the other hand, allow for precise localization of protein fragments under observation. This is achieved using both intrinsic fluorophores and extrinsic fluorescent labels that selectively bind to specific amino acid residues.
Fluorescence emission spectra provide insights into the polarity of the local environment of the probe, offering a way to assess its solvent exposure. The Förster Resonance Energy Transfer (FRET) phenomenon is commonly used to determine distances between fluorophore pairs, providing valuable structural information about proteins and protein complexes. Additionally, measurements of steady-state fluorescence anisotropy, as well as time-resolved anisotropy decay, offer data on the rotational dynamics of the molecule.
All these parameters can also be used to characterize the thermodynamic and kinetic properties of protein complex formation. The seminar will cover the physical principles and selected applications of these techniques.

Keywords: protein structure and function, circular dichroism, fluorescence spectroscopy

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L_3 STRUCTURAL INVESTIGATION OF BIOMACROMOLECULES USING CRYOEM

Artur P. Biela*

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Cryo-electron microscopy (cryoEM) is an excellent tool for investigation of biomacromolecules on every level of their complexity. Nowadays, we observe huge increase in number of biomacromolecule structures solved by this technique. Here in this presentation I will show the basic principles as well as the case studies, that will allow to give a general overview of the method's capabilities. Starting from large protein complexes, like viral capsids [1], virus-like particles [2], artificial protein cages [3,4], protein complexes at work [5,6] and finishing with tiny, single tRNAs [7].

Keywords: cryoEM, SPA, protein, structure

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L_4 THE ROLE OF TARGETED METABOLOMICS IN EVALUATION OF POTENTIAL CANCER BIOMARKERS

Wiktoria Struck-Lewicka[1]*, Małgorzata Artymowicz[1], Paweł Wiczling[1]
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Targeted metabolomics is the essential strategy used to examine the utility of compounds, preliminarily selected as potential biomarkers of various diseases. These compounds, often firstly selected using untargeted studies, can then be quantitatively determined based on a developed and validated determination method as well as statistically analyzed with the use of advanced chemometrics approach.
In a present study, the nucleosides and deoxynucleosides were analyzed from urine samples in order to verify their role as potential cancer markers using targeted metabolomics approach. The nucleosides are RNA metabolites that revealed to be elevated in urine of cancerous patients compared to healthy ones. Besides, deoxynucleosides, are DNA metabolites excreted in higher concentration in oxidative stress process which also can be a trigger of cancerogenesis. In this study, urine samples were collected from bladder cancer patients (n = 90) and healthy controls (n = 171). The sample pretreatment procedure was limited to dilution and centrifugation step. Next, 11 nucleosides and deoxynucleosides were analyzed using high-performance liquid chromatography coupled with triple quadrupole mass spectrometry detection (LC-QqQ/MS) after method's validation according to FDA and EMA criteria [1]. The adopted univariate (t-test, U-Mann Whitney test) and multivariate statistical methods (OPLS-DA, logistic regression) showed good discrimination between cancer and healthy groups. As a result of univariate statistical analysis, 9 out of 11 metabolites were significantly higher ($p < 0.05$) in cancer patients with fold change in a range from 0.54 to 1.52. Besides, the sensitivity, specificity and accuracy of the logistic regression model were 60%, 89% and 79%, respectively. Although the obtained results are promising, the model should be further validated on a new independent set of samples.

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L_5

NANOPARTICLES FOR GENE AND DRUG DELIVERY: APPLYING LIGHT SCATTERING TO SCREENING AND CHARACTERIZATION

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Nanoparticles play a vital role in advancing gene and drug delivery by enabling targeted and efficient therapeutic approaches. This presentation emphasizes the importance of light scattering techniques, including dynamic light scattering (DLS) and multi-angle light scattering (MALS), in screening and characterizing nanoparticles. These methods provide detailed insights into essential properties like size, stability, molecular weight, and aggregation, which are crucial for optimizing nanoparticle formulations. By leveraging the non-invasive precision of light scattering, researchers can drive advancements in nanotechnology and biopharmaceutical development, paving the way for breakthroughs in precision medicine.

L_6 HISTORY OF SPECTROSCOPY IN A NUTSHELL

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The interaction of light and matter has been and continues to be of great interest to many scientists for centuries. The result of this interest are not only theoretical works, but also works of an applied nature. As in every technological activity of man, the key to achieving success in the spectroscopy area is the right choose of tools. The presentation will give a short history of the development of spectroscopy in the context of technical inventions (research and measurement equipment) and selected applications possible thanks to it.

Keywords: history of spectroscopy, spectrometers, quantitative and qualitative analysis

O_1

DEVELOPMENT OF NEW ANALYTICAL CALIBRATION METHODS IN THE CHROMATOGRAPHIC DETERMINATION OF BISPHENOLS

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The novel approaches combining different calibration methods were conceptually developed. The first approach is based on an integrated calibration method (ICM) supported by the H-point standard addition method (HPSAM) extended with the step-by-step dilution procedure and five measurement conditions to eliminate all types of interferences. In turn, in the second methodological approach, the basic version of the H-point standard addition method and its variants (signal increment and generalized versions) have been developed with an increased number of measurement conditions (from two to five measurement conditions). Both methodologies were experimentally verified using the example of the determination of three harmful substances from the bisphenol group (BPs) (bisphenol A (BPA), S (BPS), and F (BPF)) with the use of the high-performance liquid chromatography with diode array detection (HPLC-DAD). Fluorescence spectroscopy (FS) was used as the reference method [1]. The optimized and validated HPLC method was first applied to analyze a synthetic sample of known BPs concentrations to confirm the performance of the developed calibration methods. Then, food-related products (store receipts and canned food samples) were examined to control the effectiveness of the methodologies. The received analytical results were described by very good accuracy (RE < 5%) and precision (CV ≤ 4%). The developed methodologies also allowed for risk assessment of BPs' presence in the investigated samples. The analytical chromatographic method and the methodological approaches have been rated using two tools - the RGB Additive Color Model to Analytical Method Evaluation and the AGREE - Analytical GREEnness Metric Approach. It was proven that the method could be successfully adapted for other analytical systems and purposes (the obtained color method is White) and is environmentally friendly (Significance parameter is 0.63) [2,3].

Keywords: Analytical calibration, Bisphenols, Food-related products, Interference elimination, Quality of analytical results

Acknowledgements: The research activities co-financed by the funds granted under the Research Excellence Initiative of the University of Silesia in Katowice

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O_2 PHYSICOCHEMICAL METHODS IN FORENSIC MEDICINE

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Modern forensic medicine is unable to properly perform its tasks without the use of physicochemical methods. Determining the cause of sudden death often requires conducting complex chemical-toxicological tests using advanced equipment and methods, such as LC-MS and GC-MS. Poisoning with new psychoactive substances and new drugs stimulates the development of analytical methods and allows combating crime, including illegal medicines trade and drugs of abuse trafficking. However, it should be remembered that the scope of additional tests is always decided by the client - the payer (usually the prosecutor). The presentation will discuss current problems of forensic medicine, as well as the possibilities of specialization in forensic specializations provided for laboratory diagnosticians.

Keywords: forensic medicine, forensic toxicology, autopsy, GC-MS, LC-MS

O_3 STUDIES ON BIOFILM GROWTH AND TOTAL POLYPHENOLIC CONTENT OF FERMENTED BEVERAGES

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Fruit vinegar and kombucha are two types of fermented drinks known worldwide. They are produced by the selected types of microorganisms from fruits or infusions. Thus, these beverages are recognized as beneficial for our health due to the microorganisms and polyphenols they contain. A sweetening agent is typically used in both beverages, e.g., sucrose, brown sugar or honey. A characteristic phenomenon occurs during the production of both beverages - the formation of living biofilms. In vinegar, this biofilm is known as the "mother of vinegar," while in kombucha, it is called SCOBY (Symbiotic Culture of Bacteria and Yeast). These structures comprise plant-derived cellulose and living microorganisms (yeasts and bacteria), indicating a progressing fermentation process [1].
The reported studies analysed the influence of several factors on biofilm production and changes in the polyphenolic content of beverages and biofilm itself. Two types of vinegar (apple and raspberry) and two types of kombucha (black and green tea) were produced using sucrose or honey as a sweetening agent. A standard Folin-Ciocalteu method was used to analyse the polyphenolic content of samples [2].
It was observed that the biofilm growth is independent of the type of used fruits (in the case of vinegar) and tea (in the case of kombucha). The sweetening agent type influences the mother's or SCOBY's growth, respectively. For the total polyphenolic content, opposite conclusions were drawn based on the obtained results. A higher content of polyphenols characterizes vinegar produced with honey. Conversely, adding sucrose increases the polyphenolic concentration in analysed kombucha samples.

Keywords: fermentation, polyphenols, mother of vinegar, scoby

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O_4

COMPLEMENTARY PHYSICOCHEMICAL METHODS IN STUDIES ON THE SYNTHESIS AND PROPERTIES OF THE DOUBLE METAL CYANIDE (DMC) CATALYSTS

Bartosz Młynarczyk[1]*, Arkadiusz Chruściel[1], Katarzyna Wałek-Nawratek[1]
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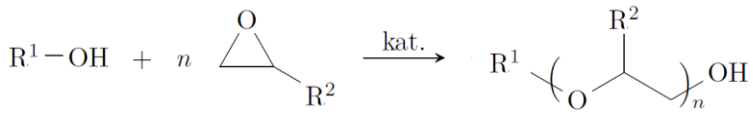
The DMC (**d**ouble **m**etal **c**yanide) catalysts are non-stoichiometric, *semi*-amorphous salts defined with the general formula $Zn_a[Co(CN)_6]_b \cdot L^1_{n_1} \cdots L^m_{n_m}$, where $L^1 \cdots L^m$ stand for ligands then *a*, *b*, n_i, are not related stoichiometrically.
The primary application of DMC catalysts lies in the ring-opening polymerization of epoxides, particularly in the synthesis of unique, narrow-fraction polypropylene glycols (1):



(1)

playing a key role in subsequent stages of polyurethane production.
The research team at MEXEO from Kędzierzyn-Koźle (Poland) — a leading global producer and supplier of DMC catalysts for over two decades — is actively engaged in advanced research on the synthesis and physicochemical properties of these materials [1-5].
The investigations involve a broad spectrum of techniques originating from various branches of physical and analytical chemistry, including state-of-the-art methods from solid-state physics.
The objective of the mentioned studies is both to optimize the manufacturing technology of DMC catalysts and to deepen the understanding of the structural factors underlying their catalytic properties. Such knowledge is crucial for the development of next-generation materials with enhanced performance and efficiency.
The complementary research methods to be referred in the presentation include structural X-ray techniques (XRD, EXAFS/XANES, XPS), thermal analysis methods (TGA, DSC, EGA/MS/FTIR), and analytical techniques for DMC (ICP-OES) and the catalysis products (HPLC/GPC, rheometry). The integration of these diverse approaches has enabled the acquisition of valuable new insights into the structure and functional properties of DMC catalysts.
The results obtained thus far represent a significant milestone in the field of DMC catalyst research and form the foundation for a new R&D project, supported by national funding.
Scheduled to launch in 2026, this project aims to develop a novel, low-emission technology for the production of DMC catalysts.

Keywords: DMC catalysts, propoxylation, polypropyleneglycols

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O_5 ANALYSIS OF THE MOLECULAR STRUCTURE OF O-DERIVATIVES OF 7-HYDROXYFLAVONE

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Flavones, significant subclass of flavonoids, are widely distributed in the plant kingdom known for their diverse biological activities, including antioxidant and anticancer properties. The chemical structure of 7-hydroxyflavone, particularly the presence and position of hydroxyl group, plays a crucial role in determining and modulating its bioactivity [1]. Studies have demonstrated that 7-hydroxyflavone exhibits moderate antioxidant activity, where the hydroxyl groups, especially -OH substituted to C7, are crucial [2]. Beyond its antioxidant potential, it has a significant impact on aromatase inhibition, which is beneficial in treating oestrogen-dependent cancers [1,3]. The clinical use of this compound may be limited due to its low bioavailability. Modification of 7-hydroxyflavone by attaching long carbon chains can increase the lipophilicity of the molecule, making it easier to penetrate cell membranes and enhancing its ability to interact with target cell receptors.
Through this approach, three derivatives were synthesized and analysed using one-dimensional ^{1}H and ^{13}C NMR (Nuclear Magnetic Resonance) spectroscopy and also two-dimensional methods such as HMBC (Heteronuclear Multiple Bond Correlation) and also HSQC (Heteronuclear Single Quantum Coherence). Combining each technique, that provides different types of information, give a comprehensive understanding of the molecular structure. This work offers valuable insights into the structure of O-derivatives of 7-hydroxyflavone as the potential anticancer agents, but further research is needed to explore its full therapeutic potential. The methods and conclusions outlined in this work provide a basis for continued exploration of these compounds and their derivatives.

Keywords: 7-hydroxyflavone, Spectroscopy, Molecular Structure

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O_6 IMPLEMENTING NON-INVASIVE TECHNIQUES FOR ASSESSING PLANT VITALITY IN NANOPARTICLE APPLICATIONS

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The assessment of the effects of nanoparticles on plant growth is becoming increasingly prevalent. Due to their unique properties, the application of nanoparticles in plant science appears very promising.
Our research included controlled laboratory studies and field experiments in which we tested the effects of titanium dioxide nanoparticles (nano-TiO_2) and silicon dioxide nanoparticles (nano-SiO_2) on plant growth, photosynthetic processes, and cellular functions.
We demonstrated that nanoparticles exhibit hormetic effects [1]. In laboratory studies using nano-TiO_2, we found that low concentrations of these nanoparticles stimulate plant growth and help alleviate negative symptoms of light stress, while higher concentrations were toxic to plants, resulting in oxidative stress symptoms [2].
We also conducted a field study to evaluate the effects of silicon dioxide nanoparticles on grapevines, performed in collaboration with Wieliczka Vineyard (https://winnicawieliczka.com). The results indicate that nano-SiO_2 stimulates photosynthetic activity in grapevines and contribute to an increase in photosynthetic pigment levels. We observed an increase in photosynthetic efficiency, an enhanced rate of carbon dioxide assimilation, and an improvement in the NDVI (normalized difference vegetation index) parameter in plants treated with foliar sprays of SiO_2 nanoparticles. These findings show a high potential for the application of SiO_2 nanoparticles in agriculture [4].

Keywords: nanoparticles, chlorophyll fluorescence, thermal imaging, photosynthetic performance

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O_7 APPLICATION OF SINGLE-MOLECULE FRET TO INVESTIGATE THE STRUCTURAL DYNAMICS OF THE YING YANG 1 (YY1) PROTEIN

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Ying Yang 1 (YY1) is a multifunctional protein that acts as a transcription factor and plays a critical role in numerous developmental processes. It consists of two main domains: a C-terminal domain containing zinc finger motifs and an intrinsically disordered N-terminal regulatory domain. Due to the unstructured nature of the N-terminal region, the molecular mechanism underlying YY1's function remains poorly understood. Elucidating this mechanism is particularly important, as it could pave the way for the development of targeted therapies for neurodevelopmental disorders associated with YY1 mutations, such as Gabriele-de Vries syndrome (GADEVS).
To address this knowledge gap, we designed a YY1 protein construct suitable for investigating its structural dynamics using fluorescence spectroscopy, with a particular focus on single-molecule Förster Resonance Energy Transfer (sm-FRET). Preliminary fluorescence spectroscopy studies revealed that YY1 adopts different tertiary structures depending on environmental conditions, such as salt concentration and the presence of zinc ions. We hypothesize that the functional mechanism of YY1 is fundamentally linked to the structural dynamics of its N-terminal region, and that environment-dependent conformational changes within this region may regulate the protein's activity. While detailed sm-FRET studies are still ongoing, our current findings offer promising insight into the molecular behavior of YY1 and represent a significant step toward fully understanding its biological role.

Keywords: Ying Yang 1, intrinsically disordered protein, small molecule-FRET

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O_8 MRI/ULTRASOUND-GUIDED TRANSPERINEAL BIOPSY: NEW FACE OF PROSTATE CANCER DIAGNOSIS

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Modern diagnostic techniques are one of the most crucial elements ensuring the detection of clinically significant prostate cancers. The fusion of magnetic resonance imaging (MRI) and ultrasound (US) in MRI/Ultrasound-Guided Transperineal Biopsy (TPB) has opened new horizons in diagnostic imaging techniques while simultaneously reducing the risk of infection. The precise localization of suspected cancerous lesions, particularly in the anterior part of the prostate, and the minimal risk of septic complications have been demonstrated in meta-analyses. Compared to traditional transrectal biopsy (TRB) techniques, TPB has shown a significantly higher sensitivity in detecting clinically significant prostate cancer (csPCA) in anatomically challenging areas (such as the apex and anterior regions of the prostate) [1-3]. This technique is highly desirable for patients under active surveillance or those undergoing a repeat biopsy after a negative first-round result [4,5].
Studies have shown that the frequency of post-procedural infections, including sepsis, is much lower with TPB than with TRB [6]. Moreover, thanks to fusion imaging, TPB ensures greater precision in sample collection, particularly from high-risk cancer areas, minimizing the number of necessary biopsy cores. This, in turn, significantly reduces the risk of overdiagnosing clinically insignificant tumors [7]. The European Association of Urology (EAU) guidelines recommend TPB as the preferred diagnostic imaging method, especially for repeat biopsies in patients under active surveillance [8].
Analyzing current scientific advancements, the future evolution of TPB will involve intensified MRI image analysis, increasing the selectivity of targeted biopsies and improving diagnostic accuracy [9]. Additionally, predictive algorithms and advanced robotic systems could optimize procedures, reducing unnecessary biopsies, improving patient comfort, and accelerating treatment—representing a significant breakthrough in prostate cancer diagnostics.

Keywords: Prostate cancer, MRI/US, TPB, transperineal biopsy, diagnostic algorithms

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P_1 DETERMINATION OF BICALUTAMIDE IN A PHARMACEUTICAL PREPARATION BY TLC-DENSITOMETRY

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Bicalutamide is non-steroidal anti-androgen that acts as an inhibitor of male sex hormones. It is usually used in tablet form in monotherapy of locally advanced prostate cancer, as well as in combination therapy with GnRH analogues (Gonadotropin-Releasing Hormones) or orchidectomy [1].
The purpose of this study was to find a new method for the determinatio of bicalutamide in a pharmaceutical formulation containing 50 mg of bicalutamide per tablet by Thin-Layer Chromatography (TLC) combined with densitometry. Chromatographic methods described so far in the literature including the Polish Pharmacopoeia are based on High-Performance Liquid Chromatography (HPLC) and the use of following mobile phases: phosphoric acid/acetonitrile/water (0.05:50:50 v/v/v) [2], phosphate buffer and acetonitrile [3,4], n-hexane and ethanol [5] or methanol and acetonitrile [6]. The most commonly used stationary phase was silica gel. In the current work, a new chromatographic conditions consisting of chromatographic plates precoated with silica gel $60F_{254}$ with a concentrating zone and coated with a mixture of silica gel 60 and kieselguhr F_{254} were applied. The plates were developed by two mobile phases such as n-hexane/propan-2-ol (32/18, v/v) and also n-hexane/ethyl acetate/glacial acetic acid (33/16/1, v/v/v). The tablets of the preparation (50 mg/tablet) were extracted with ethanol (96%), and then analyzed by using a TLC scanner at λ = 275 nm. The validation of the proposed TLC-densitometric method confirms its specificity and linearity in the studied concentration range. This method is precise and accurate. The obtained limits of detection and quantification confirm its suitability for quality control of the studied bicalutamide preparation.

Keywords: bicalutamide, chromatography, drug analysis, TLC-densitometry

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P_2 DETERMINATION OF ROSMARINIC ACID BY USING TLC WITH DENSITOMETRY

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Rosmarinic acid (RA) is one of the popular compounds from the group of phenylpropanoids. Its pharmacological action has been used for years not only in traditional medicine. It has a supportive effect, among others, in the treatment of urinary tract infections and in asthma. In addition, it also increases the secretion functions of the stomach, improves concentration and memory and reduces the inflammatory processes of the skin, which is used for skin care in cosmetics. In Poland, medical rosemary (Rosmarinus officinalis) is used as a source of rosmarinic acid. The wide use of rosmarinic acid in medicine and cosmetics makes analytical methods necessary for rapid analysis, including determination of the content of this compound in the plant raw material constituting its main source or in finished medicinal products and cosmetics.

In the present work, various chromatographic conditions were investigated for analysis, including the quantitative determination of rosmarinic acid in the form of a solution in ethanol. The chromatographic experiments carried out using thin-layer chromatography combined with densitometry indicated the possibility of both fast and effective identification of this compound and the determination of it in its samples. Using the TLC method in the reverse phase system, rosmarinic acid can be identified in the range of 1.705 to 5.1415 micrograms/band. Of all chromatographic systems used in the work, plates coated with silica gel 60P18F_{254} and acetonitrile-water mixture (25:25, v/v) were found to be the most optimal for determining the content of a given compound, which allows the lowest detectability and the limit of quantification LOQ = 1.705 micrograms/band. On the other hand, the less effective mobile phase in these studies was the one composed of 1,4-dioxane and water (25:25, v/v) with which the highest LOD and LOQ values were obtained.

The developed TLC procedure for the analysis of rosmarinic acid may in future be useful for its routine control in medicinal or cosmetic products.

Keywords: rosmarinic acid, TLC, densitometry, LOD, LOQ

Acknowledgements: Project No. BNW-1-067/K/4/F

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P_3

SELECTED PHYSICOCHEMICAL METHODS USED TO CHARACTERISE POLYMER-DRUG CONJUGATES

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Polymer-drug conjugates represent a significant advancement in drug delivery systems [1]. They offer numerous advantages, including enhanced drug solubility, which improves bioavailability, and prolonged circulation times, which allow for sustained therapeutic effects. These conjugates can also minimise immunogenicity, thereby reducing adverse immune responses. They also offer controlled release mechanisms that will enable gradual drug delivery to target sites, thereby reducing off-target effects. In addition, the strategic design of polymer-drug conjugates improves safety profiles by allowing lower dosage requirements and mitigating systemic toxicity. This makes them an essential component in developing more effective and patient-friendly therapies in clinical practice.
Several physicochemical methods are used to characterise polymer-drug conjugates. These include nuclear magnetic resonance (NMR) spectroscopy to determine structure, gel permeation chromatography (GPC) to determine molecular weight, differential scanning calorimetry (DSC) to analyse thermal properties and dynamic light scattering. In addition, Fourier Transform Infrared (FTIR) spectroscopy is used to identify functional groups and binding interactions, while high-performance liquid chromatography (HPLC) is often used to quantify drug loading and release profiles.
The characterisation of polymer-drug conjugates requires the extensive use of physicochemical methods. Each of these techniques allows different aspects of the conjugate's properties to be assessed, including chemical composition, structure, stability and therapeutic potential, all of which play a critical role in the development of modern targeted therapies [2].

Keywords: drug delivery, controlled release, biopolymers, polymer-drug conjugates

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P_4

DEVELOPMENT OF NEW SYNTHESIS METHOD FOR THE MANGANESE LITHIUM-ION SORBENT

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To respond to growing demand for lithium compounds which are very important as they are necessary for production of batteries[1], but also find use in treating mental disorders like depression or bipolar disorder (ChAD)[2] and show potential in helping patients with neurological illnesses like Alzheimer's and Parkison's diseases[3], new methods of obtaining them have to be developed. One of the most promising are sorption materials with a highlight on lithium-manganese oxides (LMOs)[4]. In this work, a novel method of synthesis of LMO for sorption of lithium from aqueous solution is presented. Manganese(II) salt and lithium hydroxide were milled separately and mixed with 60 % solution of hydrogen peroxide. Then precipitate was washed with deionized water, filtered, and dried. The sorbent precursor was acquired by calcinating precipitate at 125°C for 13 h and at 450°C for 6 h. The material was then activated by eluting lithium ions in acid. The influence of a variety of factors was investigated including the ratio of Lithium to Manganese, the amount of added hydrogen peroxide, time and speed of steering, temperature and type of acid elution by comparing the sorption capacity of as prepared materials.
The obtained material showed sorption capacity of up to 63.9 mg of lithium per 1 g of sorbent. This property was observed to be highly dependent on lithium content in the reaction. Future research will focus on immobilizing material to allow easy sorption from both naturally occurring and mining waste brines and seawaters. The other focus will be to further improve the properties of material primary sorption capacity and stability.

Keywords: Lithium, sorption, lithium-manganese oxides, LMOs

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P_5 THE INTERACTIONS OF SELECTED DIETARY SUPPLEMENT INGREDIENTS WITH BIOACTIVE SUBSTANCES OF *ARABICA* COFFEE INFUSIONS

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Drugs and dietary supplements often interact with each other and may also interact with food. Interactions may lead to changes in the pharmacokinetic and pharmacodynamic properties of medicinal substances and complications during pharmacotherapy. Interactions may result in changes in the time and strength of the drug or dietary supplement's action, as well as the risk of adverse effects. To avoid interactions, a time interval should be maintained between the consumption of coffee and certain medications or dietary supplements [1]. The aim of the study was to assess the interactions of dietary supplement components, such as docosahexaenoic acid (DHA) and eicosapentaenoic acid (EPA), with bioactive substances of *Arabica* coffee infusions. The aim of the study was achieved by determining the concentration of polyphenols [2] and flavonoids [3] and the total antioxidant potential [3] of *Arabica* coffee infusion and mixtures of Arabica coffee infusion with selected components of dietary supplements: DHA and EPA. The results of the antioxidant potential test showed a statistically significant reduction compared to the theoretical values (the sum of the potential values of the individual compounds) in coffee infusion with DHA or EPA addition. Moreover, the addition of EPA acid to the *Arabica* coffee infusion caused a statistically significant reduction in the concentration of polyphenols, in relation to the theoretical value. Antagonistic interactions have been observed between bioactive substances found in *Arabica* coffee infusion and DHA and EPA acids, which are components of dietary supplements. Therefore, caution should be exercised when using dietary supplements containing the tested fatty acids and not taken with coffee.

Keywords: interactions, dietary supplements, fatty acid, coffee infusion

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P_6 STRUCTURE OF 5-METHYL-9-(TRIFLUOROMETHYL)-12*H*-QUINO [3,4-*b*][1,4]BENZOTHIAZINIUM CHLORIDE

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Phenothiazine is a valid structural system commonly used in medicinal chemistry due to the revealed spectrum of biological properties. As a matter of fact, phenothiazine derivatives are an excellent example showing the impact that tiny structural changes can exert on the biological response. Practically, the analogues of phenothiazine were the first registered effective neuroleptic drug molecules. The occurrence of an aminoalkyl subgroup at the thiazine nitrogen atom, especially in case when the interval between the thiazine nitrogen atom and the nitrogen atom of the substituent was three carbons, conditioned such biological potency. Interestingly, the reduction of *N*-thiazine and *N*-substituent distance to two carbon atoms resulted in an observed change in activity from neuroleptic to antihistamine, respectively.

5-Methyl-9-trifluoromethyl-12*H*-quino[3,4-*b*][1,4]benzothiazinium chloride (**3**) was synthesized by reacting 1-methyl-4-butylthio-3-(benzoylthio)quinolinium chloride with 4-(trifluoromethyl)aniline. The structure of the resulting product was determined using ^{1}H, ^{13}C, ^{19}F NMR spectroscopy as well as HR-MS spectrometry. The spatial geometry of agent **3** and the arrangement of molecules in the crystal (unit cell) were also confirmed using X-ray diffraction. The tetracyclic quinobenzothiazinium system is fairly planar because the dihedral angle between the planes formed by the benzene ring and the quinoline system is 173.47°. In order to get insight into the electronic charge distribution of the investigated molecule the electronic structure calculations employing the Density Functional Theory (DFT) were performed. Moreover, antiproliferative activity was tested against the set of pancreatic cancer cell lines.

Keywords: phenothiazine, azaphenothiazine, anticancer agent

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P_7 APPLICATION OF ELECTRODIALYSIS WITH BIPOLAR MEMBRANE IN EPOXY RESIN SYNTHESIS

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A method was devised for the etherification of glycerol with epichlorohydrin in a sulphuric acid catalysed reaction. In the traditional approach, the catalyst would be neutralised with bases, alkalic oxides, or carbonates, and the precipitate would be filtered off. However, this procedure results in a major loss of product due to high viscosity of the post-reaction mixture. Moreover, a partial dehalogenation and oligomerisation of the product occurs, due to side reactions such as cyclisation and condensation.
In the new approach electrodialysis with bipolar membrane (BMED) was utilised to neutralise the catalyst. This method allows for strict pH control without the need of adding new reagents, and recovery of the catalyst from the post-reaction mixture. In the next step, the reaction of epoxidation was started in order to obtain epoxy resin.
The method devised is a significant element in the development of sustainable epoxy resin synthesis in mild conditions. In industry it is possible to utilise epichlorohydrin obtained in the Epicerol process from waste glycerol. Epoxy resins are widely used, especially in composite materials, which are essential materials in aviation and automotive industries.

Keywords: electrodialysis, bipolar membrane, epoxy resin, glycerol, epichlorohydrin

P_8 APPLICATION OF THIN-LAYER CHROMATOGRAPHY TO DETERMINE LIPOPHILICITY PARAMETERS OF SELECTED SUBSTANCES SHOWING ACTIVITY AGAINST THE CENTRAL NERVOUS SYSTEM

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Lipophilicity is one of the most important descriptors of bioactive molecules which has the impact on their ADMET profile [1]. Therefore the research subject was to determine the experimental values of lipophilicity parameters of selected compounds that show activity against central nervous system (CNS) such as zuclopenthixol, flupentixol, triflupromazine, trifluoperazine and fluphenazine. These compounds are popular antipsychotic drugs that block dopamine receptors located in the presynaptic and postsynaptic membrane. Trifluoperazine, triflupromazine and fluphenazine are phenothiazine derivatives whereas zuclopenthixol and flupentixol are thioxanthene derivatives. They are used to treat mental illness such as psychoses, schizophrenia, bipolar disorder, apathy and neurosis. They can be also used to control vomiting, nausea and severe hiccups [2].

Chromatographic parameters of lipophilicity (R_{MW}) of the tested compounds were determined using the Soczewiński-Wachtmeister's method [3]. The following RP-2F_{254}, RP-8F_{254} and RP-18F_{254} plates and mixtures consisting of acetone/TRIS buffer, acetonitrile/TRIS buffer and 1,4-dioxane/TRIS buffer were used. The organic modifier content changed from 40% to 90%. Cluster analysis allowed for comparison of the obtained parameters under selected chromatographic conditions.

The carried out experiments allowed to obtain the values of chromatographic parameters for all tested compounds. The analysis of the R_{MW} values indicates that the tested compounds can be arranged in the following order: zuclopenthixol < triflupromazine < fluphenazine < flupentixol < trifluoperazine. The greatest similarity was observed between the chromatographic parameters determined by using both mobile phases, acetone/TRIS buffer and 1,4-dioxane/TRIS buffer, on RP-8F_{254} and RP-18F_{254} plates. The research results confirm the usefulness of the TLC method for determining the experimental values of the lipophilicity parameter for the five tested compounds acting on the central nervous system. The chromatographic conditions proposed in this study allowed for rapid and simultaneous determination of the lipophilicity parameters of five tested compounds and can be successfully used in the design of new analogues or pharmaceutical preparations of these substances.

Keywords: lipophilicity, R_{MW}, phenazine derivatives, TLC

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P_9 MODERN SPECTROSCOPIC TECHNIQUES IN STRUCTURAL STUDIES OF NEW HETECYCLIC DERIVATIVES

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Heterocyclic compounds are widely known systems in medicinal chemistry and pharmacology. The group of these derivatives includes dipyridothiazines, which have two pyridine rings in their structure. For many years, the Department of Organic Chemistry at the Medical University of Silesia has been conducting research on this group of compounds, which show its valuable anticancer, antioxidant and immunosuppressive properties [1-3]. The main priority in these projects is the structural analysis proving the structure of new molecules, because the syntheses leading to the obtaining of molecules with a specific structure can proceed via the Smiles rearrangement or Ullman cyclization [1]. By developing research issues in the area of dipyridothiazines, a new group of 10-substituted dipyridothiazines with selected heteroaromatic rings was obtained. The determination and precise proof of the structure of these molecules was performed on the basis of NMR spectrometry, HR MS spectrometry and *in silico* computational analyses.

Keywords: heterocycles, NMR, HRMS, *in silico* calculations

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P_10 MODERN ANALYTICAL APPROACHES TO IDENTIFYING COUNTERFEIT PHARMACEUTICALS

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The phenomenon of counterfeit medicines is one of the most significant problems that global medicine is facing. It affects both developing and developed countries. It is estimated that as many as 1 in 10 medicines in the markets of poorer countries are counterfeit or substandard [1]. This is particularly dangerous because in these countries the problem affects medicines used to treat life-threatening disease, such as antimalarials, antibacterials and antivirals. In the Global North, the problem of counterfeit medicines mainly affects life-enhancing drugs such as erectile dysfunction drugs, weight loss drugs or anabolic steroids – especially when purchased online from unverified sources [2]. Therefore, it is important to introduce effective methods to detect counterfeit drugs in order to increase the safety of pharmacotherapy worldwide. This poster aims to raise awareness of the problem of counterfeit drugs and present the latest techniques for their detection and analysis.
Scientific articles were retrieved using PubMed and Google Scholar search engines using the terms "counterfeit medicines analysis" and "falsified drugs analysis". The articles considered could not be older than 8 years.
Reviewed studies indicate that the latest chemical analysis techniques, such as solid-state C^{13} NMR and Raman spectroscopy, among others, make it possible to detect a counterfeit drug both effectively and quickly, even with small amounts of sample being analyzed [3,4]. Analysis of the polymers that make up blister packaging materials, which differ in formulation or physicochemical properties from the original, also appears to be a unique approach [5]. Well-known methods such as HPLC, GC, MS are also invariably accurate [6].

Keywords: counterfeit medicines, chemical analysis, spectroscopy

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P_11 BETULIN GLYCOCONJUGATES CONTAINING A SUCCINYL LINKER AND A 1,2,3-TRIAZOLE RING-SYNTHESIS, PHYSICOCHEMICAL PROPERTIES AND EVALUATION OF PHARMACOLOGICAL POTENTIAL

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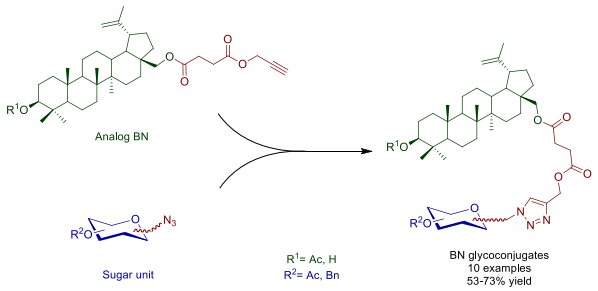
3-Lup-20(29)-ene-3β,28-diol, commonly known as betulin (BN) is a natural bioactive triterpenoid with significant synthetic and pharmacological potential [1]. Despite its anticancer, antibacterial, and anti-inflammatory properties, its therapeutic application is hindered by poor bioavailability [2]. A promising strategy to enhance its pharmacological properties is glycoconjugation, which improves solubility, selectivity and selectivity, particularly for targeted cancer therapy [3,4]. Given the high glucose demand of cancer cells [4], linking BN derivatives to sugar moieties via an *N*-heterocyclic linker using *click chemistry* represents a logical and effective strategy.



Scheme 1. Synthetic route for obtaining glycoconjugates

We synthesized ten novel BN glycoconjugates by attaching Glu(OAc), Glu(OBn), Gal(OAc), and Gal(OBn) units at the C-28 position of betulin backbone using a succinyl linker. The compounds were obtained in good yields (53-73%). One aspect of our studies was the use of spectroscopic methods to confirm the structures of the compounds. ^{1}H and ^{13}C-NMR spectroscopy enabled precise structural characterization. The biological activity of the glycoconjugates was evaluated using MTT cytotoxicity assays, a spectrophotometric method assessing cell viability. Studies were conducted on HCT 116 (human colon cancer cell line) and MCF-7 (human breast cancer cell line), as well as NHDF-Neo (healthy human dermal fibroblasts). The results demonstrated enhanced selectivity towards MCF-7 breast cancer cells, underlining the therapeutic potential of these derivatives.
The development of glycoconjugates based on increased demand of cancer cells for glucose and overexpression of its transporters may significantly influence the progress in anticancer therapy, integrating modern chemical solutions with biological mechanisms.

Keywords: betulin, glycoconjugates, NMR spectroscopy, cytotoxicity assay

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P_12 IS DIBENZOFULVENE BETTER THAN FLUORENE? THE EFFECT OF MODIFYING THE C9 POSITION OF FLUORENE WITH N-DONOR SUBSTITUENTS ON SELECTED PHYSICOCHEMICAL PROPERTIES

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The search for chemical compounds with well-defined physicochemical properties suitable for applications in organic electronics and photovoltaics remains an active area of research. Fluorene has long been recognized as a valuable building block due to its structural versatility and ease of functionalization. In particular, dibenzofulvene (DBF) derivatives, obtained through modifications at the 9-position of fluorene, have gained significant attention due to their tunable electronic properties and broad applicability. These derivatives can be further functionalized at the 2- and 7-positions, allowing for the fine-tuning of their physicochemical characteristics to meet specific technological demands [1,2]. DBF derivatives have been widely investigated as key materials in optoelectronic devices, particularly in solar energy conversion and light-emitting applications. In dye-sensitized solar cells (DSSCs), DBFs serve as organic dyes, achieving power conversion efficiencies of up to 8% [1,2]. In perovskite solar cells (PSCs), DBFs function as hole-transporting materials (HTMs), contributing to efficiencies reaching 19–21% [1,2]. Beyond photovoltaics, DBFs have been explored as HTMs in organic light-emitting diodes (OLEDs), where their favorable charge transport properties enhance device performance [1]. Additionally, DBF-based polymers exhibit high fluorescence efficiency, excellent solubility, and notable thermal stability, making them promising candidates for polymer light-emitting diodes (PLEDs) and electrochromic materials capable of displaying a wide color range [1]. However, the complex nature of their molecular structures often complicates the assessment of how individual substituents influence their physicochemical properties.

In this study, the impact of N-donor substituents on selected physicochemical properties of six dibenzofulvene derivatives was explored and compared to the unsubstituted fluorene. Six dibenzofulvene derivatives containing selected N-donor substituents in their structure were obtained. The structures of the compounds were confirmed by NMR spectroscopic methods. The following measurements were performed: UV-Vis spectroscopy, electrochemistry and spectroelectrochemistry. The obtained findings reveal that even minor structural modifications of fluorene towards dibenzofulvene derivatives lead to significant changes in their absorption and emission properties. Notably, these modifications also enhance the electrochemical properties of the compounds, with experimentally determined values closely aligning with theoretical predictions obtained through DFT calculations.

Keywords: Fluorene derivatives, Dibenzofulvene derivatives, Knoevenagel condensation, Organic electronics, Solar cells

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P_13 ANALYTICAL METHODS USED IN RESEARCH ON BIOLOGIC DRUGS

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Biologic therapy holds a key position in managing autoimmune conditions, certain infectious diseases, and malignancies, utilizing monoclonal antibodies, recombinant proteins, along with gene and cell-based treatments [1,2]. A distinguishing factor of biologics compared to conventional therapies is the use of substances naturally produced by organisms, which can subsequently be modified to achieve the desired clinical effect [2].

This work aims to present and discuss the analytical methods currently used in research on biologics. As such, thirteen papers collected from PubMed database were reviewed using "biologics, chromatography, electrophoresis, spectroscopy, electrochemical techniques" as keywords. Among these, five were chosen for the purpose of this work. Therefore, this research reviews the most significant information about analytical methods used in research and therapy containing biological drugs.

High therapeutic potential of biologics stimulates ongoing studies focused on understanding their properties and improvement. It is especially important due to their complex structure [3]. To achieve this, chromatographic, electrophoretic, spectroscopic, and electrochemical techniques are most frequently applied [1,4]. The methods used for biopharmaceutical analysis focus mainly on evaluating molecular mass and heterogeneity, analyzing protein structure, purity, and modifications, as well as assessing biological activity and detecting potential interactions with other substances, which is crucial for determining the safety profile of a specific drug [1]. Process Analytical Technology (PAT) has a significant impact on the quality of biopharmaceuticals. It allows real-time monitoring of biologic drug manufacturing processes, allowing for the rapid detection of deviations from standards and ensuring the final product meets the required quality [3].

Keywords: biologics, chromatography, electrophoresis, spectroscopy, electrochemical techniques

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P_14 COMPARISON OF THE KINETICS OF RELEASE OF ACTIVE SUBSTANCES FROM DERENIUM PLANT EXTRACT AFTER INCORPORATION IN SELECTED HYDROGELS

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The aim of this study was to evaluate the degree of release of loganic acid, gallic acid and delphinidin 3-O-galactoside contained in a derenium extract [1] and to match the best pharmacokinetic model to the release process. Based on the study of the physicochemical properties of the studied formulations, such as pH, density, an attempt was made to select the optimal hydrogel polymer as a carrier for the derenium extract.
Hydrogels based on methyl cellulose and acrylic acid and its derivatives were prepared for the study. Potentiometric analysis of hydrogels with and without extract was performed using a pH electrode. Density and viscosity of hydrogels without extract were measured. Density was tested using a plunger and dynamic viscosity using a rotational viscometer. The release of extract from the hydrogels was tested in a paddle apparatus. Hydrogels were placed in disks from which the extract was released into phosphate buffer pH 6.8 at 37 ± 0.5°C. The release was carried out for 4 hours, and samples were taken at predetermined intervals of 2 ml, each time topping up the amount taken with fresh medium. Samples were analysed using spectrophotometric measurements. The calculated values of the released active substances were fitted to zero, first and second-order models and the Higuchi model.
The pH, density and viscosity values of the resulting hydrogels increased from methyl cellulose to acrylic acid derivatives, respectively. Addition of the extract to the hydrogels resulted in a decrease in pH. Delphinidin 3-O-galactoside was best released from the acrylic hydrogels according to the zero-order model and Higuchi's model.
The dependence of the amount and rate of derenium extract released on the pH, density and viscosity of the hydrogels was observed. The physico-chemical properties of hydrogels under study have an impact on the release of the substances they contain, which can be used in external application on the skin by adapting to the needs of patients.

Keywords: release kinetics, hydrogels, derenium extract

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P_15

THE ROLE OF TERAHERTZ SPECTROSCOPY IN BURN WOUND ASSESSMENT

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Burn injuries are complex, dynamic wounds characterized by significant tissue necrosis. Accurate assessment of their depth and healing prognosis remains a clinical challenge, as traditional diagnostic methods such as visual inspection or histopathological evaluation often fail to provide real-time, non-invasive insights into tissue viability. Early treatment of thermal injuries, either through surgical procedures or grafting, is imperative for improving healing outcomes. Thus, the need for more precise techniques for burn injury analysis remains [1,2].

This work aims to present and discuss the emerging role of teraherd (THz) imaging in assessing burn wounds, emphasizing its potential as a novel, non-invasive imaging method. As such, ten research papers collected from the PubMed database were reviewed using "teraherd radiation", "spectroscopy", "skin", and "burn wounds" as keywords. Among these, four were chosen for this work. Therefore, the focus of this literature study is to evaluate the current state of THz spectroscopy in biomedical imaging, focusing on its application in burn wound assessment.

Recent studies demonstrate that THz spectroscopy accurately and in real-time evaluates burn wound progression by detecting subtle changes in tissue hydration and structure. THz imaging operates in the far-infrared spectrum, making it highly sensitive to water content and precise in discerning healthy, damaged, and necrotic tissue [3,4]. THz spectroscopy represents a revolutionary step in diagnostics. While further research is required, its integration into routine dermatological practice could significantly enhance burn wound evaluation accuracy and treatment monitoring.

Keywords: teraherd radiation, spectroscopy, skin, burn wounds

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P_16 MAGNETIC RESONANCE SPECTROSCOPY (NMR) IN DETERMINING THE STRUCTURE OF IMPRANIL DLN

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Synthetic polymers are among the most widely produced materials, exhibiting a broad spectrum of properties that are directly related to their composition and chemical structure [1]. This group of polymers includes polyurethanes (PU), which are formed through the reaction of isocyanates with alcohols, leading to the formation of a characteristic urethane bond. The stability of this bond makes PU generally resistant to biological degradation. As a result, large amounts of PU waste persist in the environment, making them potentially hazardous compounds for living organisms [2,3].
Impranil DLN, produced by Covestro (Germany), is an anionic aliphatic polyester-polyurethane colloid used in textile coating formulations. Impranil DLN exhibits many positive features, such as commercial availability, hydrolysis stability within the pH range of 4–8, resistance to decomposition at temperatures up to 80°C, improved solubility compared to other polyurethanes, and non-cytotoxicity to most microorganisms [2]. However, the proprietary composition of Impranil DLN and inconsistency in literature regarding its structure complicates its application in assessing polyurethane biodegradation [2,4]. Therefore, the aim of our study was to characterize the structure and composition of Impranil DLN using nuclear magnetic resonance (NMR) spectroscopy.
A comprehensive structural analysis of Impranil DLN required the use of advanced NMR techniques, particularly 2D NMR methods, including both homonuclear (COSY) and heteronuclear (HSQC, CIGAR) experiments. The results obtained through NMR spectroscopy enabled us to propose the chemical structure of Impranil DLN.

Keywords: polyurethanes, Impranil DLN, polymers, NMR spectroscopy

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P_17 SPECTROSCOPIC CHARACTERISTICS OF BETULIN OXIDATION PRODUCTS

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Betulin (3-Lup-20(29)-eno-3β,28-diol, BN) is naturally occurring bioactive compound, which can be found in bark of many birch species such as *Betula pendula*, *Betula verrucosa* or *Betula pubescens* [1]. It belongs to the triterpenoid family and possesses many useful biological characteristics, including antimicrobial, antioxidative, anti-inflammatory and cytostatic properties [2]. In its structure one can distinguish five aliphatic rings and only two polar hydroxyl groups, which makes the molecule nonpolar and hydrophobic. Such properties decrease bioavailability and impair cell the penetration, limiting its use as therapeutic agent [2].
To enhance betulin's biological activity, it's molecule is subjected to various structural modifications, an example of which is oxidation [3]. The primary hydroxyl group at C-28 position can be oxidized to a formyl or carboxyl group, while the secondary hydroxyl group at C-3 position can be oxidized to a carbonyl group, giving five possible oxidation products as shown in Figure 1. The aim of this work is to present the ^{1}H and ^{13}C NMR spectroscopic characteristics of some of the compounds mentioned above.

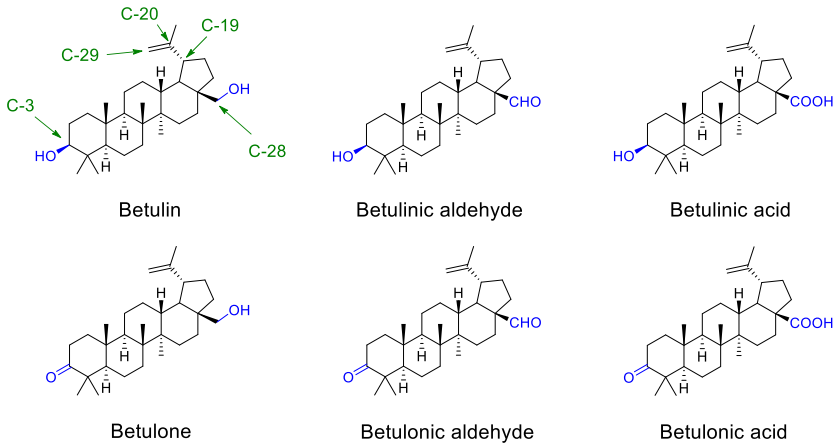

Figure 1. Structures of betulin and its oxidation products

Keywords: betulin, triterpenoids, oxidation, NMR spectroscopy

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P_18 PHYSICOCHEMICAL PARAMETERS OF NVCL POLYMERS CROSS-LINKED WITH PEGDMA OF VARYING CHAIN LENGTHS

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Poly-N-vinylcaprolactam (PNVCL) is a 'smart polymer' with a lower critical solution temperature (LCST) of 32-50°C [1]. It is biocompatible, thermoresponsive, and water-soluble. It is also stable against hydrolysis and non-toxic. Research shows PNVCL can inhibit some strains of pathogenic bacteria [2]. This makes it suitable for biomedical applications, particularly in the field of drug delivery. The physico-chemical parameters of drug carriers, such as size, charge, phase transition temperature, stability, and morphology, are crucial in the design process. The properties of thermosensitive polymers can be modified at the synthesis stage. The aim of this study was to explore how varying the length chain of the PEGDMA cross-linker affects the physicochemical properties of five synthesised PNVCL-based polymers. It will allow fundamental characterisation of the resultant particles, including their durability, binding capability for the therapeutic substance, and kinetic binding studies. This will help to select the most suitable polymer as a potential carrier for therapeutic substances. Thermosensitive polymers P1–P5 of NVCL and PEGDMAs av. Mn 750–20 000, were synthesized via surfactant-free precipitation polymerization (SFPP) using cationic initiator; 2,2′-azobis[2-methylpropionamidine] dihydrochloride (AMPA) at 70°C. The polymerization was monitored by the conductivity. An analysis was performed on all the products obtained using a range of physicochemical test methods, including ATR-FTIR, DLS, EM, SEM, TG/DTA, DSC, PXRD, SEM and TEM. In the present study, five thermosensitive spherical polymer nanoparticles were obtained and characterized by a positive zeta potential (ZP) ranging from 0.11 to 52.00 mV at 18-45°C, a hydrodynamic diameter (HD) of 21-41 nm at 18°C and a LCST in the range of 33-35°C. The nanoparticles also exhibited a propensity to aggregate. The purified polymeric dispersions exhibited a pH range of 6.4-6.7, indicating their significant potential as drug carriers in formulations intended for dermal application. Thermal analysis demonstrated the polymers' relative thermal stability up to 230°C, while PXRD studies confirmed their amorphous structure. Subsequent research plans encompass the investigation of charge density on the particle surface, the assessment of toxicity, and the execution of release studies on the model drug.

Keywords: N-vinylcaprolactam, poly(ethylene glycol) dimethacrylates, lower critical temperature solution, electrical conductivity, dynamic light scattering

Acknowledgements: FTIR: DLS, PXRD, TG, DSC experiments were performed in the Laboratory of Elemental Analysis and Structural Research, Faculty of Pharmacy, Wroclaw Medical University

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P_19 APPLICATION OF THE UPLC-QTOF TECHNIQUE TO IDENTIFY BIOTRANSFORMATION PRODUCTS OF THE RADIOPROTECTANT – OXYBENZONE

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Radiation-protective substances found in cosmetics, plastics and varnishes pose a significant threat to biocenosis. One such substance is oxybenzone. It is toxic to marine invertebrates, including coral larvae. It was confirmed that this substance can be effectively removed from the environment using *Pleurotus djamor* fungi.
The aim of presented experiment was to identify potential biotransformation products of oxybenzone in the residue after mycelium cultivation.
The analyte was dissolved in methanol and analyzed using the UPLC-QTof technique. In the first stage, the samples were subjected to chromatographic separation and the masses of the molecular ions of the products were identified. In the second stage, the molecular ions were fragmented. Based on the precisely determined masses of molecular ions and fragment ions, the summary and structural formulas of 13 potential biotransformation products of oxybenzone were determined.

Keywords: Oxybenzone, bioremediation, degradation products, mass spectrometry

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P_20 CAN A SMALL CHANGE IN THE HETEROCYCLIC SUBSTITUENT SIGNIFICANTLY IMPACT THE PHYSICOCHEMICAL AND BIOLOGICAL PROPERTIES OF (Z)-2-(5-BENZYLIDENE-4-OXO-2-THIOXOTHIAZOLIDIN-3-YL)ACETIC ACID DERIVATIVES?

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The search for new chemical compounds with precisely defined physicochemical and biological properties has been a fundamental goal of scientific research for many years. Derivatives of rhodanine-3-acetic acid are an extremely interesting example of this type [1]. These compounds exhibit many interesting physicochemical and biological properties, thanks to which they are studied for numerous applications [1]. One of them are dye-sensitized solar cells (DSSC), in which rhodanine-3-acetic acid derivatives can act as a dye [1]. Due to their physicochemical properties, rhodanine-3-acetic acid derivatives have also been studied as fluorescent sensors for selective ion detection and fluorescent probes for bioimaging [1]. Moreover, rhodanine-3-acetic acid derivatives exhibit antibacterial, antifungal and anticancer activity [1].
In connection with the above, the study aimed to assess the effect of the heterocyclic substituent on the physicochemical and biological properties of rhodanine-3-acetic acid derivatives, and specifically three derivatives of (Z)-2-(5-benzylidene-4-oxo-2-thioxothiazolidin-3-yl)acetic acid. The considered substituents were selected so that their character changed from aliphatic to aromatic. Such small structural changes allowed us to determine the relationship between the structure of the presented compounds and their properties. It also allowed us to trace the physicochemical and biological properties of the considered compounds in the context of the (aliphatic or aromatic) nature of the substituent. In the case of derivatives with aromatic substituents (pyrrole and imidazole), the effect of an additional nitrogen atom on the considered properties was also assessed. All compounds were obtained using the Knoevenagel condensation method. Then, optical studies were performed for the obtained derivatives. Based on the optical test results, the compounds were tested as fluorescent dyes for imaging fixed and living cells.

Keywords: rhodanine-3-acetic acid Knoevenagel condensation fluorescent probes, bioimaging

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P_21 APPLICATION OF THIN LAYER CHROMATOGRAPHY IN THE ANALYSIS OF BETULIN DERIVATIVES

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Natural products are an invaluable source, widely used to search for new therapeutics [1]. Obtained, most often by extraction, compounds are used directly in their natural form or constitute the initial scaffold for obtaining semi-synthetic derivatives. Chemical modification reactions of the structure of natural compounds use the functional groups present in their molecules [2]. Introducing new substituents can have a huge effect on the biological activity of the obtained products while having little one on their behavior in chromatographic analysis. Therefore, an important issue is finding optimal chromatographic systems that enable identification and subsequent separation of the substrate and the resulting products.

The presented work aimed to find chromatographic systems that allow for the distinction of betulin and its derivatives obtained in the processes of esterification and hydrolysis [3,4]. Two stationary phases (silica gel and aluminum oxide) and eight developing systems were tested, using solvents such as chloroform, dichloromethane, ethyl acetate, acetone, petroleum ether, hexane, ethanol and methanol in various volume ratios. The chromatograms obtained were visualized by spraying with a 10% sulfuric acid solution in ethanol and then heating at 110°C. Densitometry was adopted for the analysis as well. This method is used with thin-layer chromatography for qualitative and quantitative determination. It lets transform the chromatographic spot into the chromatographic peak. It is also useful for evaluating the separation of several compounds present in the mixture.

Keywords: betulin, esterification, thin-layer chromatography

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P_22 IDENTIFICATION OF BETULIN OXIDATION PRODUCTS BASED ON TLC METHOD

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Betulin obtained from birch bark can be easily transformed into more active derivatives, which are its oxidation products such as aldehydes and carboxylic acids [1]. Various oxidizing agents are employed in this process, such as pyridinium dichlorochromate, chromium trioxide in concentrated sulfuric acid, selenium oxide, Swern's reagent and m-chloroperbenzoic acid [2]. Each of these methods results in a mixture of products, making it challenging to isolate the desired compound. Selecting the right method for product identification and separation is essential both in the reaction monitoring process and in subsequent isolation. An additional limitation is the low stability of betulin oxidation products and high reactivity. Betulin oxidation products often show higher biological activity than the parent compound and are also a starting point for the synthesis of other types of derivatives [3,4].
The goal of this study is to identify the optimal conditions for chromatographic analysis that enable the efficient identification and separation of oxidation products while keeping their structures unchanged. In this work, two stationary phases (silica gel and aluminium oxide) were considered, of which only SiO_2 met the assumed requirements. Eight eluents of different polarity were selected based on the literature data. The mobile phase components were chloroform, dichloromethane, ethyl acetate, acetone, petroleum ether, hexane, ethanol and methanol. The chromatograms were visualized by spraying them with a 10% solution of sulfuric acid in ethanol and then heating them at 110°C. Densitometric analysis was also used as a supplementary method for compound determination. This technique allows for very exact determination of the retardation coefficient value, as well as quantitative determination of the tested substance. It also allows for the detection of a very small amount of the compound due to its broad wavelength range.

Keywords: triterpene acids, oxidation, TLC method

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P_23

LIPOPHILICITY STUDY OF NIRMATRELVIR

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The increase in the incidence of bacterial and viral diseases such as Covid-19 makes there a need to systematically conduct studies using both experimental and theoretical so-called *in silico* methods, which would support the pharmacokinetic studies of various substances with antiviral and antibacterial properties, which would be useful in designing the formulation of these drugs with specific properties in action [1,2]. The parameter that is most commonly determined by the above methods is lipophilicity determined experimentally by various methods, including thin-layer chromatography in reverse phase system (RP-TLC). The studied substance is an component of valuable medicinal product used for routine treatment of Covid-19 patients. The lipophilicity studies were conducted with the use of silica gel 60RP18F_{254} precoated chromatography plates and mobile phases composed of various organic solvents such as methanol-water; acetonitrile-water and 1,4-dioxane water. The detection of the compound was carried out using copper (II) salt as visualizing agent and a TLC densitometer (λ = 200 nm). The parameters of lipophilicity (R_{MW}) obtained by the TLC method are in the range of 1.11-3.01. The closest values were obtained for the mobile phase composed of acetonitrile-water and 1,4-dioxane-water. These values are comparable to the theoretical logP (logarithmic partition coefficient value) determined using computational algorithms, including in particular WlogP and Consensus log Po/w [3].
The results obtained may be useful in the future in the design of new nirmatrelvir derivatives.

Keywords: nirmatrelvir, lipophilicity, logP, TLC, *in silico* methods

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P_24 APPLICATION OF LASER SPECKLE CONTRAST ANALYSIS (LASCA) MICROPERFUSION IMAGING FOR BURN DEPTH ASSESSMENT IN PATIENTS WITH THERMAL INJURIES

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Introduction
Accurate assessment of burn depth is crucial for determining appropriate treatment strategies and predicting wound healing outcomes. According to the European Burn Association (EBA) guidelines, the use of microperfusion imaging techniques, such as Laser Doppler Imaging (LDI) or Laser Speckle Contrast Analysis (LASCA), is recommended to enhance the precision of burn depth evaluation. Our hospital is equipped with LASCA technology, which is routinely utilized for this purpose. In addition to initial burn assessment, we frequently observe burn depth conversion, a phenomenon where partial-thickness burns may progress to full-thickness injuries over time.

Methodology
Laser Speckle Contrast Analysis (LASCA) is a non-invasive imaging technique that evaluates tissue perfusion by detecting variations in scattered laser light caused by moving red blood cells. This method provides real-time perfusion maps, aiding clinicians in distinguishing between superficial, partial-thickness, and full-thickness burns. In our study, LASCA imaging was performed on burn patients upon hospital admission and at subsequent time points to monitor perfusion dynamics and potential burn depth conversion.

Results
Preliminary data indicate that LASCA imaging enhances burn depth evaluation, particularly in cases where clinical examination alone is inconclusive. Perfusion patterns observed in LASCA images correlate well with wound healing potential and the need for surgical intervention. Additionally, LASCA imaging enables the early detection of burn conversion, allowing for timely therapeutic adjustments.

Conclusions
The incorporation of LASCA technology into routine burn assessment provides valuable insights into tissue viability and burn wound progression. This method improves diagnostic accuracy and facilitates evidence-based clinical decision-making. Further research and broader implementation of LASCA imaging could contribute to optimizing burn care and patient outcomes.

P_25

COFFEE UNDER ANALYTICAL CONTROL

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Coffee is a mixture of specific substances, the proportions of which depend on both the origin and type of coffee and the roasting method. In addition to alkaloids, coffee is a rich source of compounds with antioxidant and anti-radical properties [1,2]. The aim of this study was to combine different analytical methods for the determination of caffeine and selected compounds in coffee infusions. Spectroscopic and chromatographic methods were used. Total phenolic acids and polyphenols were determined by UV/VIS spectrophotometry, using Arnova reagent (converted to coffee acid) and Folin-Ciocalteu reagent (converted to gallic acid). High-performance reversed-phase liquid chromatography (RP18) using a mixture of 0.05% TFA in water and methanol was used to separate and determine selected compounds. NMR spectroscopy was used to confirm the presence of compounds in coffee.
Samples were prepared according to the analytical method. The corresponding weight of coffee bean samples after grinding (5-20 g) was brewed for about 15 minutes and 2 to 10 ml was taken for determination of the of the brew. The ^{1}H NMR method required dissolving the freeze-dried coffees in DMSO-d_6. Soluble coffee samples were either dissolved in 1ml of DMSO-d_6 or in 100 ml of hot water.
The caffeine content of the samples ranged from 2-5 mg/mL, Surprisingly, the caffeine content of soluble coffees may be overstated. As expected, caffeic acid and gallic acid were identified in the infusions, and the rest total phenolic acids (5-18) or polyphenols (20-35) mg/100 mL of the infusion were determined by spectrophotometric methods.
The results were similar to the literature data [3-5], which allows a comprehensive analysis of this type of matrix. At the same time, it can be hoped to propose such a topic for laboratory exercises for students.

Keywords: coffee, chromatograhy, NMR, spectrophotometry

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P_26 THIOPHENE OR 2,2'-BITHIOPHENE – WHICH SUBSTITUENT WORKS BETTER IN THE EMITTER STRUCTURE OF AN LEC CELL?

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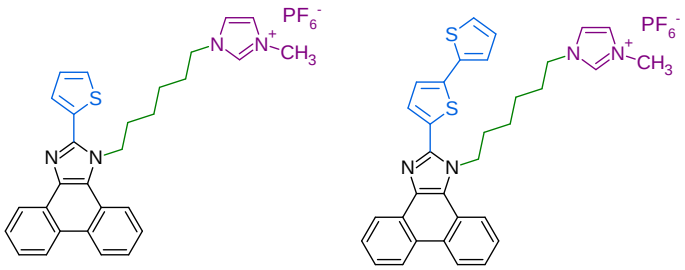
The growing number of electrical devices increases energy consumption. This creates challenges in ensuring a sufficient supply of electricity. To address this, energy-efficient devices are being developed using technologies such as light-emitting electrochemical cells (LECs). In recent years, phenanthro[9,10-d]imidazole derivatives have been studied for use as active layers in LEC cells due to their simple and cost-effective synthesis, as well as their desirable physicochemical properties [1].
The goal of this work was to synthesize and study new phenanthro[9,10-d]imidazole derivatives for potential use as emitters in LECs (see scheme). These compounds differ in the substituent at the C2 position. The derivatives were obtained through condensation and alkylation reactions. Their structures were confirmed using NMR spectroscopy. Thermal, optical, and electrochemical studies were performed. The results helped compare how different C2 substituents affect the physicochemical properties of phenanthro[9,10-d]imidazole derivatives . The study identified compounds suitable for further application research in LECs. The results contribute to the development of LEC technology. This makes LECs more attractive for use in lighting systems and electronic devices.



Scheme. Synthesized phenanthro[9,10-d]-imidazole emitters with thiophene and 2,2'-bithiophene substituents at C2 position

Keywords: phenanthro[9,10-d]imidazole derivatives, electroluminescence, light emitting electrochemical cell, (LEC), light emitting devices

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P_27 SYNTHESIS OF CONJUGATES OF TETRAETHYL α-AMINOMETHYLENE-BISPHOSPHONATE WITH BIOLOGICALLY ACTIVE COMPOUNDS

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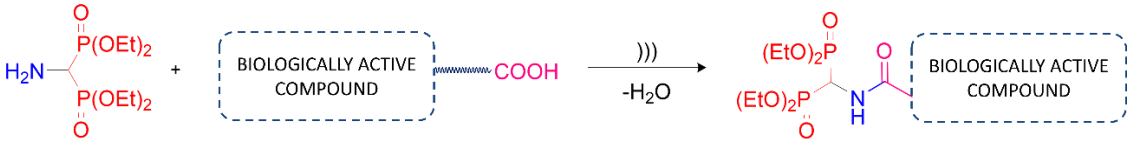
α-Aminobisphosphonates are organophosphorus compounds belonging to the group of geminal bisphosphonates that are widely used in medicine, especially in the treatment of metabolic bone diseases. The characteristic P-C-P bridge contained in their structure enables a strong binding to hydroxyapatite found in bones, which ensures their high therapeutic efficacy due to their bone resorption inhibiting properties. Furthermore, the presence of an amino group at the central carbon atom of α-aminobisphosphonates makes them attractive candidates for further structural chemical modifications to enhance their biological activity [1].
In this work, a strategy for linking α-aminomethylenebisphosphonate *via* an amide bond with selected biologically active molecules was developed. The combination of these compounds is aimed not only at increasing their bioavailability but also at giving them new pharmacological properties resulting from their additive or synergistic action [1,2].
The synthesis of conjugates was carried out based on a newly developed strategy using an ultrasound [3]. The obtained products were subjected to detailed characterization using spectroscopic methods (NMR, IR). The results confirm that the applied synthesis method is an effective and efficient approach to obtaining new conjugates of α-aminomethylenebisphosphonate with biologically active molecules. The pure products obtained can serve as a starting point for further studies on their biological activity and potential therapeutic use.



Keywords: α-aminomethylenebisphosphonate, conjugation, biologically active compounds, spectroscopic methods

Acknowledgements: This work was supported by the Excellence Initiative – Research University programme implemented at the Silesian University of Technology, years 2024–2026 (04/020/SDU/10-21-02)

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P_28

STABILITY OF NATURAL BIOACTIVE SPILANTHOL ISOLATED FROM *ACMELLA OLERACEA*

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Spilanthol (SPL, (2*E*, 6*Z*, 8*E*)-*N*-isobutyl-2,6,8-decatrienamide,) is a natural occurring compound, which is isolated mainly from *Acmella oleracea* [1]. Plant belongs to the *Asteraceae* family and contains many groups of natural substances, giving it numerous valuable biological activities. One of these groups is *N*-alkylamides, among which the main compound spilanthol is responsible for several beneficial properties such as: analgesic, antioxidant, antifungal [1]. Due to its, it recently has been used in cosmetics as an anti-wrinkle agent, as well as in dental products, particularly in toothpastes, for its pain-relieving properties [2].
The most popular form of spilanthol storage are extracts, especially ethanolic extract. Unfortunately, during the storage of the extract, the concentration of spilanthol decreases. In contact with oxygen, it can be oxidized to cyclic endoperoxide as shown in Figure 1 [3]. The aim of the presented work was to investigate the effect of storage conditions, such as solvent and temperature on the stability of spilanthol, using ^{1}H-NMR spectroscopy.

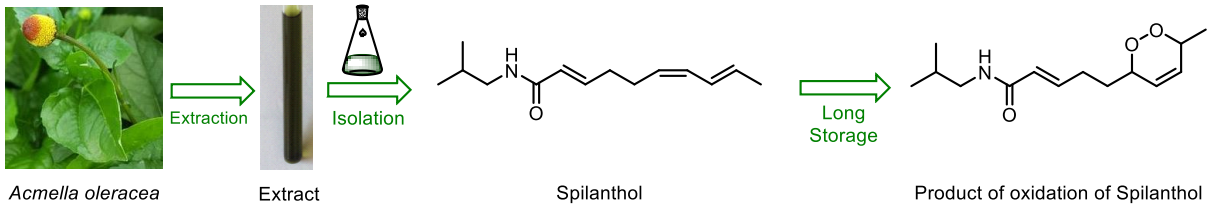

Figure 1. Isolation and stability of spilanthol

Keywords: *Acmella oleracea,* spilanthol, oxidation, NMR spectroscopy

Acknowledgements: This work was supported by the Rector's Proquality Grant, Silesian University of Technology (Poland), No. 04/020/RGJ24/1095

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P_29

SCANNING ELECTRON MICROSCOPY AS A TOOL FOR ANALYZING THE MORPHOLOGY OF SUBSTANCES

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Scanning Electron Microscopy (SEM) with Energy Dispersive Spectroscopy (EDS) analyzer is a very useful technique for imaging surface and near-surface microstructure of solid compounds. It also allows for quick qualitative and quantitative determination of the elemental composition of the compounds. Therefore, SEM can be used in the pharmaceutical field to analyze surface topography, and impurities in the examined materials.
The purpose of this study was to investigate the morphology and chemical composition of the particles of an antibacterial drug. The compound studied was norfloxacin ($C_{16}H_{18}FN_3O_3$), a drug from the fluoroquinolone group. The compound was used in the study in solid form (powder).
The study was performed in a high-resolution scanning electron microscope Supra 35 (Zeiss) with an accelerating voltage in the range of 10-20 kV and magnifications of 50–25000×. A secondary electron detector SE and a backscatter electron detector BSE were used for the study. Chemical composition analyses in micro-areas were performed using the EDS detector with Pathfinder software.
The study found that norfloxacin powder particles exhibit a regular shape, similar to a cuboid. The particle size of norfloxacin is variable, ranging from several micrometres to about 250 μm. The chemical composition tests performed using the EDS detector confirmed the presence of individual elements included in the analysed material. The results of the EDS analysis of the chemical composition demonstrate the high chemical quality of norfloxacin. The presence of aluminum may be related to the phenomenon of contamination.

Keywords: norfloxacin, scanning electron microscopy, EDS analyzer

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P_30

WHERE NANOTECH MEETS THE VINEYARD: FIELD METHODOLOGY FOR GRAPEVINE STUDIES

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This field study investigated the physiological effects of foliar-applied silica nanoparticles (nano-SiO_2) on grapevines (*Vitis vinifera* L. var. Cabernet) grown in the Wieliczka Vineyard (southern Poland), with a primary emphasis on the applied research methodology. Naturally derived nano-SiO_2 were obtained from ground quartz and applied to foliage during defined phenological stages.
Silicon uptake and accumulation were quantified via inductively coupled plasma optical emission spectrometry (ICP-OES), confirming efficient foliar absorption. Photosynthetic efficiency was monitored using a suite of physiological indicators, including net CO_2 assimilation rate (A), maximum quantum yield of PSII (Fv/Fm), and performance index (PI_{abs}), obtained through portable gas exchange systems and chlorophyll fluorescence imaging. Vegetation status was additionally assessed using NDVI values captured by portable multispectral imaging setup.
This research demonstrates the value of integrating multi-method physiological monitoring with precise elemental analysis in field settings [1]. The methodological approach outlined here provides a scalable and reproducible framework for evaluating nanomaterial-based treatments in viticulture and other perennial crops, contributing to the evidence base for sustainable agriculture [1,2].

Keywords: field study, grapevine, nanotechnology, photosynthesis, silica nanoparticles

Acknowledgements: This research was supported by the grant OPUS 24, UMO-2022/47/B/NZ9/00225 from the National Science Centre (Poland)

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P_31 AN IN VITRO ASSAY OF THE ANTITHROMBOTIC PROPERTIES OF TURMERIC, GARLIC AND GREEN COFFEE EXTRACTS

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The purpose and scope of the study: The thrombotic complication and cardiovascular diseases account for the highest percentage of death events worldwide [1]. Therefore, the search for natural substances that could reduce this risk is crucial and the compounds containing polyphenols seem to be a promising candidates [2,3]. The research involved conducting in vitro studies to determine the impact of aqueous-ethanol extracts of turmeric (*Curcuma longa*; TE), garlic (*Allium sativum*; GE) and green coffee (*Coffea Arabica*; GCE) on platelet aggregation, clot formation and stability.
Methods: All procedures were performed on the porcine blood. Platelet aggregation was measured by the turbidimetric method. The effects of these extracts on the kinetics of clot formation and stability in whole blood were evaluated by thromboelastometry. The coagulation and fibrinolysis in platelet-rich (PRP) and platelet-poor plasma (PPP) was also assessed [4]. The total polyphenol content was determined by spectrophotometric methods.
Results: All extracts inhibited platelet aggregation, in a dose dependent manner, with the strongest effect being exerted by the GE (IC_{50} = 380 μg/ml) and the weakest by the TE (IC_{50} > 1 mg/ml). The extracts caused an increase in clotting time and a decrease in clot formation parameters, measured in blood and PRP, but not in PPP. The addition of the GCE and TE increased clot susceptibility to fibrinolysis, which was not observed with the GE.
Conclusion: The use of polyphenol-rich extracts could help reduce platelet aggregation and clot formation clotting, which may potentially be beneficial in the anticoagulant therapy. Further researches are required to confirm these effects on the hemostasis system, especially in animal models or using human blood.

Keywords: clot formation, polyphenols, platelets

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P_32 THE INFLUENCE OF THE FUNCTIONAL GROUP ON THE PHYSICOCHEMICAL AND BIOLOGICAL PROPERTIES OF NEW PHENANTHRO[9,10-D]-IMIDAZOLE DERIVATIVES

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This work attempted to obtain and study new phenanthro[9,10-d]-imidazole derivatives with potential use as fluorescent probes for fluorescence imaging. The study's primary goal was to assess the effect of two functional groups (such as the formyl group and rhodanine-3-acetic acid) on selected physicochemical properties and the possibilities of practical application of the considered chemical compounds. As a result of the conducted studies, three phenanthro[9,10-d]-imidazole derivatives (PK1 – PK3) were obtained and studied for their properties and applications. PK1 was synthesized by condensation of 2,2′-bithiophene-5-carboxaldehyde, aniline, phenanthrenequinone and ammonium acetate, with a yield of 74%. Then, the obtained PK1 was subjected to a formylation reaction using N,N-dimethylformamide and phosphorus(V) oxychloride, which resulted in the synthesis of PK2, with a yield of 33%. Finally, PK2 was used for the Knoevenagel condensation reaction with rhodanine-3-acetic acid and ammonium acetate. This allowed the preparation of PK3 with a yield of 78%. Interestingly, measurements of thermal parameters showed that all of the tested derivatives (PK1 – PK3) exhibit high thermal stability above 300oC. The influence of the functional group in this aspect is insignificant. Luminescence studies were successfully carried out in five solvents. Both in absorption and emission measurements, the influence of the functional group was significant. Modifying the 2,2′-bithiophene substituent causes a significant bathochromic shift consistent with the order PK1 < PK2 < PK3. This can be attributed to an electron-withdrawing aldehyde group (–CHO) in PK2 and an electron-withdrawing heterocyclic rhodanine-3-acetic acid ring in PK3. Quantum yields were determined for all derivatives. Moreover, all compounds could stain live cells cultured in vitro. The staining efficiency was not dependent on the cell line, and we obtained correct mouse and human cell line staining. PK3 proved the most attractive among the tested compounds due to its staining potential in live cells and retention after fixation. We could also observe more than 70% viability after 24 h of exposure to 1 μg/ml PK3 and achieved a useful staining efficiency for cell imaging. PK2 staining also gave high cell viability at the concentration, which gave adequate staining efficiency. Our results showed some antibacterial and antifungal activity of the newly synthesized compounds PK1–PK3. Among them, PK3 showed the highest antimicrobial activity, especially against Gram-positive bacteria. Its activity was moderate or mild against these microorganisms.

Keywords: phenanthro[9,10-d]imidazole derivatives, rhodanine-3-acetic acid derivatives, fluorescent dyes, bioimaging, antimicrobial and antifungal activity

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P_33 COWPEA MOSAIC VIRUS AS A NANOCARRIER IN CANCER IMMUNOTHERAPY

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Nanotechnology has opened new possibilities in drug delivery through the use of different carriers, among which are organic nanoparticles such as natural and synthetic polymers or liposomes as well as inorganic nanoparticles. For nanoparticles to be clinically applicable, they must exhibit biocompatibility, biodegradability, and minimal toxicity [1]. Plant-derived virus-like nanoparticles (VNPs) have gained attention due to their high safety profile, scalability, immunogenicity, and structural uniformity. Physicochemical studies have demonstrated their effectiveness in targeted drug delivery, tumor imaging, and immunotherapy, highlighting their potential in cancer biotherapy [2].

One of the most promising candidates for a nanocarrier in cancer immunotherapy is a plant virus, Cowpea mosaic virus (CPMV). Its mechanism of action involves reprogramming the tumor microenvironment by activating and recruiting innate immune cells, such as macrophages and neutrophils, leading to the elimination of cancer cells. Additionally, CPMV functions as an adjuvant by presenting pathogen-associated molecular patterns (PAMPs) recognized by pattern recognition receptors (PRRs), including Toll-like receptors (TLRs) [3].

A review of the available literature highlights the key advantages of CPMV as a potential nanocarrier in cancer therapy. The virus exhibits tropism toward antigen-presenting cells; however, its complete biological fate in the human body remains unknown. Although there is no evidence suggesting CPMV is infectious to mammals, definitive studies confirming its full safety are still lacking [3].

In conclusion, CPMV represents a highly promising nanoplatform for cancer immunotherapy. Further research is needed to fully elucidate its safety profile and interactions within the human body, paving the way for potential clinical applications [3].

Keywords: Cowpea Mosaic Virus, virus-like nanoparticles, cancer immunotherapy, drug delivery

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P_34 THIN-LAYER CHROMATOGRAPHY AS A TOOL IN PHARMACEUTICAL RESEARCH

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Chromatography is one of the most important analytical tools used in the analysis of present in pharmaceutical and plant preparations. Its importance is growing especially in the bioactive compounds context of quality control of medicinal products and prevention of their adulteration. Thanks to its ability to be combined with various types of detection, this technique allows accurate separation, identification and quantification of compounds [1-2]. Thin-layer chromatography (TLC) is distinguished from other methods by its simplicity, accessibility and low operating costs. It enables rapid and simultaneous analysis of multiple samples, and allows detection of compounds using a variety of visualization methods - both physical (e.g., UV) and chemical [1,3-4]. It is widely used in the study of the stability of drug products, allowing the identification of degradation products under standard and stress conditions [3]. In addition, reversed-phase thin-layer chromatography (RP-TLC) is gaining increasing importance in assessing the lipophilic properties of compounds, making it possible to predict their behavior in the body, including bioavailability, distribution and elimination [5,6]. Densitometry provides a permanent record of TLC results by converting spot chromatograms into densitograms. The combination of these techniques allows efficient determination of active substances, impurities and physicochemical characteristics such as lipophilicity. TLC with densitometry and mass spectrometry is also used in the selection and evaluation of biological activity of plant material [1,2,7]. Due to its versatility, accessibility and high efficiency, TLC is an indispensable tool in modern pharmaceutical analysis and scientific research on substances of synthetic and natural origin [1,2,4].

Keywords: thin-layer chromatography, densitometry, bioactive compounds

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P_35

OPTIMIZATION OF THE CHIP-EXO METHOD AS A TOOL FOR ANALYZING FUNCTIONAL DIFFERENCES BETWEEN THE HOMOLOGOUS TRANSCRIPTION FACTORS YY1 AND YY2

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Chromatin immunoprecipitation combined with lambda exonuclease digestion (ChIP-exo) enables genome-wide identification of protein–DNA interaction sites with single-nucleotide resolution. This study focuses on the transcription factors YY1 and YY2, which, despite high sequence similarity – particularly within their DNA-binding domains – display distinct *in vivo* binding profiles, suggesting divergent regulatory functions.

The aim of this work was to optimize the ChIP-exo protocol in HEK293 cells transfected with plasmids encoding Strep-tagged YY1 or YY2, in order to generate high-quality sequencing libraries for precise mapping of their binding sites. Chromatin was fragmented using micrococcal nuclease and compared to fragmentation with a nuclear lysis buffer. The nuclease-based approach proved more effective, especially with extended incubation, and eliminated the need for additional sonication. Immunoprecipitation and purification using a commercial kit yielded better results compared to buffers from the reference protocol by M.J. Rossi et al. [1].

The optimized workflow enables efficient, high-resolution identification of YY1 and YY2 binding sites. These results provide a solid foundation for high-throughput sequencing and downstream bioinformatic analyses, which may uncover distinct genomic targets of each protein. This approach may ultimately support the investigation of transcriptional networks underlying development and disease.

Keywords: ChIP-exo, YY1, YY2

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P_36 MOLECULAR DYNAMICS INVESTIGATION OF DEBYE RELAXATION ORIGIN IN 3-PHENYLPROPANAL

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While structural relaxations in low-molecular-weight glass-forming liquids are well explored for cooperative molecular motion, the origin of secondary (especially Debye-type) relaxations remains elusive, particularly in weakly associating systems like 3-phenyl-1-propanal. Using broadband dielectric spectroscopy (BDS), X-ray diffraction (XRD), and molecular dynamics (MD) simulations, we uncover an unexpected Debye process, distinct from conventional H-bonding mechanisms [1,2]. Contrary to expectations, the weak H-bond driving this relaxation is mediated not by the aldehyde proton but by the α-hydrogen, which cooperates with π-stacking interactions. These findings challenge the existing paradigms in molecular dynamics of the mentioned systems. Fourier Transform Infrared Spectroscopy (FTIR) supports the involvement of the aldehyde groups in the associations. While conducting the comparative analysis with the corresponding alcohol, we found the existence of an additional shoulder in the XRD spectrum, which is more prominent for aldehydes than alcohols. In the dielectric loss spectra, the Debye process is well separated and has a low amplitude. This reveals that the spectral differences in 3-phenyl-1-propanal arise from a delicate balance between competing intermolecular interactions: hydrogen bonding versus π-π stacking. This discovery resolves a long-standing ambiguity in the literature regarding Debye processes in weakly H-bonding liquids and provides new design principles for optimizing optoelectronic materials and pharmaceutical formulations. By elucidating the delicate balance between H-bonding and π-stacking, our work opens avenues for tailoring charge transport and amorphous stability in functional organic materials.

Keywords: 3-phenyl-propanal, Molecular Dynamics, Debye relaxation, H-bonding

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P_37 INNOVATIVE CARRIERS FOR PLASTOCHROMANOL-8 IN EMULSION FORMULATIONS FOR UV PROTECTION

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Plastochromanol-8 (PC-8), a tocopherol-related compound with potent antioxidant and photoprotective properties, has recently gained interest as a promising ingredient for topical applications, particularly in UV protection. This study focuses on the development and physicochemical characterization of emulsion-based delivery systems containing PC-8, utilizing two types of nanocarriers: liposomes and niosomes.

The formulations were evaluated in terms of stability under UV exposure. Additionally, in vitro assays assessed the antioxidant capacity and UV-absorbing potential of PC-8 when embedded in different carrier systems. Preliminary results demonstrate that both liposomal and niosomal emulsions effectively encapsulate PC-8, though they exhibit distinct stability and release profiles [1].

This research contributes to the ongoing development of innovative cosmetic and dermatological formulations aimed at enhancing skin protection through the use of natural, bioactive compounds delivered via advanced nanocarrier systems. Further biological testing is underway to assess efficacy on skin models.

Keywords: antioxidants, liposomes, niosomes, oil-in-water emulsion, plastochromanol, UV

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P_38 INFLUENCE OF CYCLOADDITION OF 1,3-BUTADIYNES ON CIS-DIBENZOPERYLENEDIIMIDE'S OPTICAL AND ELECTROCHEMICAL PROPERTIES

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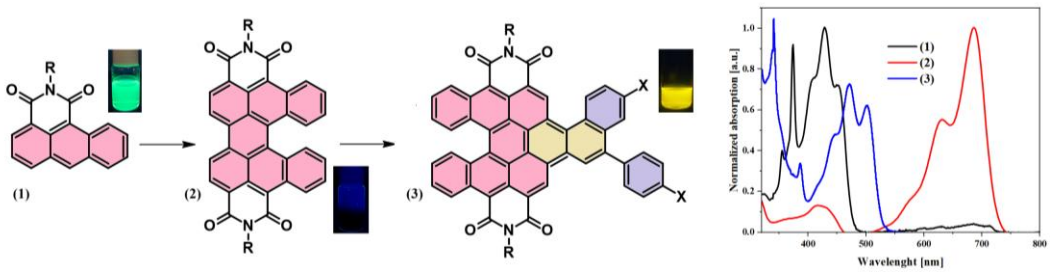
Graphene and molecular nanographenes (MNGs) play a significant role in modern technologies, including dyes-industry, pharmacy, catalysis, energy storage, organic electronics. It's possible, due to their unique properties, namely, thermal, emission, chemical and electrochemical as well as electron mobility. From organic chemistry's point of view, molecular nanographene is a polycyclic aromatic hydrocarbon (PAH) or heteroaromatic system consisting of at least 5 conjugated, aromatic rings [1,2]. Currently, almost only the "bottom-up" method, which involves the expansion of smaller structures into MNGs, in a controlled manner, as far as their size, shape, type and position of heteroatoms and functional groups [3-5]. The synthetic tool often used to expand the pi-electron structure is the Diels-Alder cycloaddition, especially the cycloaddition in the PAH cavity (e.g. perylene, perylenebisimide) [2,6].

The choice of the starting structure is essential in the way leading to the designed final MNGs. The research began with synthesizing a nanographene precursor, i.e. cis-dibenzoperylenebisimide (cis-DBPDI), using classical (but in an innovative version [7]) chemical synthesis and an entirely innovative electrochemical method (anthracene as a starting compound). Importantly, cis-DBPDI was subjected to further functionalization, i.e. pi-expansion according to the APEX strategy, via cycloaddition of 1,3-butadiynes to its cavity (bay region). Several pi-expanded derivatives, entirely new ones, were obtained; DFT calculations of frontier orbitals were performed and parameters characterizing the structures, such as NMR and HRMS, were determined. The obtained derivatives were subjected to physicochemical measurements, such as UV-Vis spectroscopy, photoluminescence and electrochemistry. So far, the results of these measurements have shown that the obtained MNGs possess unique physicochemical properties due to their electronic structure and distorted or/and chiral structure.



R- 2-ethylhexyl; **X** = H, Br, I, t-Bu, ...; **X** = I for **(3)**

Figure 1. MNGs: synthesis, products example **(3)**, absorption, pi-expansion versus colour changing (from 1 to 3)

Keywords: bisimide, Diels-Alder cycloaddition, 1,3-butadiynes

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P_39 POLY(VINYLPYRROLIDONE) WITH VARIOUS TOPOLOGIES AS EFFECTIVE POLYMER MATRICES FOR TUNING THE DESIRED PROPERTIES OF LIQUID CRYSTALLINE DRUGS

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Active pharmaceutical ingredients (APIs) with a liquid crystal structure constitute an extremely interesting group of compounds due to their dual nature – they have properties of both liquid and solid. Unfortunately, most of them belong to the class of compounds that are very poorly soluble in water. Therefore, researchers are constantly looking for methods to effectively differentiate their molecular order, allowing for tuning of physicochemical properties depending on the needs. One of the methods to improve the properties of active substances is to create amorphous mixtures with various excipients. In this aspect, a frequently used group of compounds are polymeric materials, among which poly(vinylpyrrolidone) (PVP) stands out in particular – a non-toxic and biocompatible polymer, currently widely used in the pharmaceutical industry. Unfortunately, scientists only consider the effect of molecular weights (M_n) of commercially available PVPs on improving the bioavailability of drugs, while the literature completely overlooks such important aspects as dispersibility (Đ), topology or microstructure of polymers. In response to an interesting research gap, the conducted studies aimed to determine the influence of the PVP polymer architecture on the molecular ordering of the model active substance – itraconazole (ITZ) and its solubility. Hence, synthetic pathways were developed to obtain PVP homopolymers with different topologies and strictly controlled macrostructural parameters (M_n, Đ). Then, the synthesized, innovative polymers with a linear (*lin*PVP) and star-shaped (*star*PVP) architecture were used to create binary mixtures with ITZ, which were further subjected to detailed characterization using various techniques: differential scanning calorimetry, X-ray diffraction and broadband dielectric spectroscopy. Interestingly, already at the stage of preparing binary mixtures, an extremely intriguing relationship was observed, i.e. greater miscibility of *star*PVP with API compared to *lin*PVP. Calorimetric studies showed that even a small addition of the polymer matrix effectively suppresses the liquid crystalline order of ITZ. Importantly, only *star*PVP macromolecules have the ability to completely destroy mesophases and obtain a fully amorphous material. Further structural and dielectric experiments confirmed the results obtained from thermal analysis, and long-term diffraction studies showed the highest stability of the ITZ-*star*PVP system and no tendency to rebuild the liquid crystal structure. In addition, solubility studies showed a significant improvement in API solubility in all tested binary systems compared to the pure drug, with the strongest increase in solubility noted for ITZ-*star*PVP mixtures. This study reveals that by selecting only the appropriate polymer matrix and its amount, it is relatively easy to change the molecular order of liquid crystal drugs, and thus modulate their properties depending on the needs.

Keywords: polyvinylpyrrolidone, topology, drug, binary mixtures, bioavailability

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P_40 APPLICATION OF EPR SPECTROSCOPY TO THE ANALYSIS OF COSMETIC AND PHARMACEUTICAL PREPARATIONS

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Electron paramagnetic resonance (EPR) spectroscopy is a physical method used to study paramagnetic substances in a magnetic field by absorption of microwave radiation [1,2]. The aim of this review work is to present cosmetic and pharmaceutical application of EPR spectroscopy. The analysis of EPR spectra of free radicals is carried out in order to obtain information about molecules containing unpaired electrons that are formed in chemical reactions, photolysis, thermolysis, and radiolysis [3]. The cosmetic and pharmaceutical preparations should be stored in conditions in which free radicals are not formed. Spectroscopic analysis of preparations allows for determining the optimal conditions for their storage [2].
g-Factor allows the type of free radical to be determined [1]. Amplitude and integral intensity of EPR lines depend on the number of free radicals in the tested preparations [1,2]. The changes of the parameters of EPR lines with increasing of microwave power provides information about relaxation processes [1,2].
EPR method and the model DPPH (1,1-diphenyl-2-picrylhydrazyl) free radicals are used to examine antioxidant properties of the substances [4]. Interactions of antioxidants with DPPH free radicals reduce the EPR signals of DPPH. In this work the examples of EPR examination of antioxidant preparations with free radicals are presents. The special attention was paid to antioxidant plant cosmetic and pharmaceutical preparations [5]. The influence of the composition of the complex plant raw material on the quenching of free radicals by their extracts was discussed.

Keywords: EPR spectroscopy, free radicals, antioxidants, cosmetic and pharmaceutical preparations

Acknowledgements: This work was supported by Medical University of Silesia in Katowice (Poland).

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P_41

THE ROLE OF WETTABILITY IN THE RATES OF EQUILIBRATION OF HYDROGEN-BONDED OLIGOMER PMMS UNDER CONFINEMENT

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The behavior of soft materials under nanospatial confinement have been the subject of intensive research for decades. It is well established that spatial restriction can significantly alter key physical parameters—such as viscosity, diffusion coefficients, relaxation dynamics, and phase transition temperatures. These effects depend not only on the nature (soft or hard) and degree of confinement or finite size effects but also on interfacial interactions (tuned via physical or chemical substrate modifications e.g., adjusting surface energy, roughness, or hydrophilicity). In the case of thin supported polymer films, numerous studies have shown that confinement-induced alterations can be fully or partially reversed by annealing, which leads to the recovery of bulk-like behavior. Polymers such as polystyrene, polyvinyl acetate, and poly(methyl methacrylate) have demonstrated the ability to recover solid-substance rheological characteristics after prolonged thermal treatment. The mechanisms behind this recovery involve free volume equilibration and the formation of irreversibly adsorbed interfacial layers.

While the annealing behaviour of thin-supported polymer films is relatively well understood, considerably less is known about the behaviour of polymers confined within mesoporous matrices. We addressed this gap, and we investigated the thermal equilibration of poly(mercapto-propyl-methylsiloxane) (PMMS) infiltrated into mesoporous anodic alumina (AAO) and silica (SiO_2) matrices with pore diameters ranging from 8 to 120 nm. Using broadband dielectric spectroscopy (BDS) combined with differential scanning calorimetry (DSC) and temperature-dependent contact angle (θ) measurements, we explored the influence of confinement and thermal history on polymer dynamics.

Our results indicate that the dielectric relaxation times of confined PMMS diverge from bulk behaviour near the glass transition temperature (T_g). Isothermal BDS measurements revealed that equilibrium rate constants increased as temperature decreased, showing only weak sensitivity to cooling rate or sample history. In contrast, the activation energy of the equilibration process (E_a) was strongly dependent on both pore-diameter and matrix composition. This variation correlates with temperature-dependent changes in PMMS wettability, suggesting that adsorption-desorption dynamics at the polymer–pore interface are significantly disrupted at lower temperatures. These findings provide new insight into how interfacial interactions and confinement geometry influence the thermal equilibration of confined polymers—knowledge that is crucial for the rational design of advanced nanostructured materials.

Keywords: polymers, annealing experiments, confinement, dielectric spectroscopy, wettability

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P_42

INDISTINGUISHABLE OR NOT? A COMPREHENSIVE STUDIES OF FLURBIPROFEN ENANTIOMERS AND THEIR RACEMIC MIXTURE

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Introduction: Recently, chiral compounds—specifically enantiomers (*R*- and *S*- isomers) and their racemic mixtures—have attracted growing interest across diverse scientific disciplines, including chemistry, physics, and pharmaceutical sciences. Although enantiomers often share similar physicochemical properties, they can exhibit striking differences in their biological activity, toxicity, and pharmacokinetics. A prime focus within this area is the class of 2-arylpropionic acids, commonly known as profens (e.g., ibuprofen (IBP), ketoprofen (KTP), and flurbiprofen (FLP)). These compounds rank among the most widely used active pharmaceutical ingredients (APIs) due to their potent anti-inflammatory, analgesic, and antipyretic effects. The presence of a carboxylic group capable of forming hydrogen bonds near the chiral center plays a key role in influencing molecular organization, self-assembly behavior, and more. As a result, profens continue to be intensively studied from physical, chemical, and pharmaceutical viewpoints.

Objectives: We aimed to determine whether pure enantiomers of FLP and the racemic mixture differ in their molecular organization in both the crystalline and supercooled liquid states—and, if such differences exist, to understand their implications. Additionally, the study sought to assess if the atomic structure, thermal behavior, and molecular dynamics (under ambient and high-pressure conditions) of pure *R*- and *S*-FLP are comparable to those of the *RS*-FLP.

Materials and methods: *R*-, *S*- and *RS*-FLP were analyzed by using differential scanning calorimetry (DSC), X-ray diffraction (XRD), Fourier transform infrared (FTIR), broadband dielectric spectroscopy (BDS), molecular dynamics (MD) simulations and density functional theory (DFT) calculations.

Results: Based on the analysis of collected X-ray diffraction patterns, thermograms, infrared spectra, and dielectric measurements, it was initially concluded that the enantiomers of FLP exhibit physicochemical properties closely resembling those of the racemic mixture. However, a more in-depth analysis of the high-pressure data revealed unexpected variations in the activation volume among *R*-, *S*-, and *RS*-FLP. Subsequent MD studies attributed this peculiarity to a higher prevalence of small molecular aggregates—such as dimers, trimers, and tetramers—in the pure enantiomers. Further, complementary DFT calculations identified highly specific and remarkably strong fluorine–π (F–π) interactions, which appear to govern the local molecular arrangement in both the supercooled liquid and crystalline phases of the investigated compounds. The presented data contribute to a better understanding of the correlation among the structure, intermolecular interactions, and physical properties of the enantiomers and racemates.

Keywords: flurbiprofen, chirality, enantiomers, broadband dielectric spectroscopy, high-pressure studies

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P_43 CANNABIDIOL (CBD) AND CANNABIGEROL (CBG) - POTENTIAL NEW DRUGS: CHEMICAL REACTIVITY AND BIOAVAILABILITY *P.O. IN SILICO*

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Cannabidiol (CBD) and cannabigerol (CBG) are cannabinoids with a broad spectrum of biological activity, exhibiting antioxidant and anti-inflammatory properties [1,2]. More and more studies indicate their potential use in the treatment of inflammatory diseases, in which oxidative stress plays a key role. Excess free radicals lead to cellular damage and homeostasis disorders, contributing to the development of neurodegenerative, autoimmune and metabolic diseases [1]. The mechanisms of action of CBD and CBG, including modulation of oxidative and inflammatory pathways, may constitute the basis for new therapeutic strategies aimed at reducing oxidative stress and chronic inflammation [3].
The aim of this study was to analyse the electrochemical properties of CBD and CBG molecules, as well as their pharmacokinetic and bioavailability parameters. Pharmacokinetic parameters such as gastrointestinal absorption, blood-brain barrier permeability, and drug-likeness were determined in silico using the pkCSM and SwissADME programs.
Our results indicate that CBD and CBG exhibit similar properties; however, CBG may have greater central nervous system (CNS) effects, while CBD appears to have better blood-brain barrier penetration. Both molecules comply with Lipinski's rule and demonstrate favourable pharmacokinetic properties.
This conclusions alure to further research on these molecules pharmaceutical potential in various diseases therapy.

Keywords: CBD, CBG, Lipinski's rule, bioavailability

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P_44 CELUGEL IN PHARMACEUTICAL FORMULATIONS – THE IMPACT OF COMPOSITION ON PHYSICOCHEMICAL PROPERTIES

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The purpose and scope of the study

Celugel is the first hydrogel-based pharmaceutical compounding vehicle registered in Poland. It consists of water (~80%), glycerol, and hydroxyethylcellulose as the gelling agent. Due to its favorable properties—ease of application, absence of an oily residue, and strong mucoadhesive characteristics—Celugel shows potential for intranasal drug delivery. Loratadine is an FDA-approved, long-acting second-generation antihistamine used in the treatment of allergic rhinitis. Although available in various pharmaceutical forms, no intranasal gel formulations containing loratadine have been registered to date. The aim of this study was to evaluate the impact of Celugel-based formulation composition on the physicochemical properties and pharmaceutical availability of loratadine intended for nasal application.

Main methods used in the study

The investigation included measurements of pH and osmotic pressure of the prepared gels. Possible interactions between the formulation components were examined using Fourier-transform infrared (FTIR) spectroscopy. Additionally, the pharmaceutical bioavailability of loratadine from the Celugel-based gel was assessed through in vitro testing simulating nasal cavity conditions.

Main results

The results confirmed that Celugel is a suitable compounding base for intranasal preparations in terms of physicochemical stability and compatibility of components. However, the pharmaceutical availability of loratadine from the tested gel formulation was found to be very low.

State the main conclusions and potential results for further work or practical applications

Although Celugel demonstrates promise as a vehicle for nasal drug delivery, the low bioavailability of loratadine highlights the need for further formulation development. Future studies should focus on optimizing the composition of the hydrogel base to enhance drug permeability and efficacy in alleviating symptoms of allergic rhinitis.

Keywords: Celugel, loratadine, hydrogel, hydroxyethylcellulose, intranasal gels

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P_45 DETERMINATION OF PHYSICAL PARAMETERS OF LIQUIDS AND THEIR IMPORTANCE IN MEDICINAL THERAPY

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The properties of liquids are described by physical laws [1-2]. The aim of this review work is to present the main physical parameters of liquids and indicate the ways of their determining. Density, surface tension, viscosity, hydrostatic pressure and dynamic pressure, were selected for analysis. The special attention was paid to the properties of water. The therapeutical application of water was discussed.
Density of liquids can be determined using a pycnometer and a hydrometer [1-4]. The immersion of a body in a liquid depends on its density [2-4]. Depth immersion decreases with increasing of density of liquid [3]. A body floats partially immersed in a liquid when its density is less than the density of the liquid. A body floats completely immersed in a liquid when its density is equal to the density of the liquid. A body with a density greater than the density of the liquid sinks. Surface tension is measured by the use of stalagmometer [1-4]. Surface tension acts tangentially to the surface of the liquid and tends to make this surface as small as possible. The surface tension coefficient of a liquid depends on the type of liquid and temperature. Ubbelohde'a viscometer and Stokes method are used to determine the viscosity coefficient [2-4]. Viscosity coefficient depends on type of liquid and depends on temperature. At higher temperature the lower values of the viscosity coefficient are observed. Viscosity is important factor during kinesitherapy bath [5-6]. Hydrostatic pressure increases with increasing of the liquid column height [2-4]. Dynamic pressure dynamic pressure increases with the increase in the speed of the liquid stream [2-4]. During hydrotherapy, the body is exposed to buoyancy, viscous force, hydrostatic and dynamic pressure [5-6]. Water therapy treatments affect the circulatory system, respiratory and nervous system, muscle and kidney function, digestive tract and metabolism [5-6].

Keywords: liquids, density, surface tension, viscosity, medicinal therapy

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P_46 HIGH PRESSURE STUDY OF THE PHARMACEUTICAL – RITONAVIR

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In this work, we performed thermal, molecular dynamic, structural order, and H-bond pattern measurements on the active pharmaceutical ingredient – ritonavir. Using dielectric spectroscopy (BDS) to molecular dynamics study of this compound in the supercooled liquid state revealed some peculiar phenomenon such as the narrowing of the main, structural α-relaxation peak in high temperature and pressure conditions. Moreover, during the compression of liquid ritonavir into the glassy state, in dielectric spectra we observed a new secondary relaxation process.
To explain these unusual behaviors of ritonavir, calorimetric (DSC), structural (XRD), and infrared (FT-IR) measurements on the pressure-densified glass, along with ordinary glass samples as references have been performed.
Interestingly, for densified ritonavir glass we observed double glass transitions and significant variations in the structural organization of molecules and H-bonding pattern. These changes are accompanied by a decrease in medium-range order at the expense of the short-range order and greater heterogeneity of H-bonds in pressurized glass compared to the reference glass. What is more, the varying local structure of investigated pharmaceutical at high pressure induced an additional polarization and appearance of extra local mobility not observed at p = 0.1 MPa. These combined data clearly demonstrated a change in the H-bonding pattern and local organization of molecules in the compressed ritonavir, which contributes to the narrowing of the structural process at varying thermodynamic conditions.
We are convinced that the data obtained for the H-bonded pressure-densified glass can be very useful in better understanding the behavior of associated liquids at elevated pressure.

Keywords: ritonavir, high pressure, densified glass

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P_47 PRELIMINARY SPECTROSCOPIC STUDIES OF THE INTERACTIONS BETWEEN 10-(2-(N-PIPERIDINYL)ETHYL)OXY-5-METHYL-12(H)-QUINO[3,4-B][1,4]BENZOTHIAZINIUM CHLORIDE (SALT7) AND DNA

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Cancer is the leading cause of death worldwide and its treatment is a challenge for modern medicine. The development of new anticancer drugs requires a comprehensive understanding of their mechanism of action and interactions with human proteins.
10-(2-(N-Piperidinyl)ethyl)oxy-5-methyl-12(H)-quino[3,4-b][1,4]benzothiazinium chloride (Salt7) is a newly synthesized substance with promising anticancer activity. Its antiproliferative activity was tested against Colorectal adenocarcinoma Cell Line (C-32), human astrocytoma cell line (SNB-19) and M D Anderson - Metastatic Breast Cell Line (MDA-MB-231) using cisplatin as a references substances. The IC_{50} values were reached 1.2 ± 0.7 μM, 1.2±0.7 μM and 3.0 ± 0.9 μM, respectively.
Deoxyribonucleic acid (DNA) is a molecule of biological importance. DNA is involved in processes of replication, transcription and translation, therefore plays a key role in cell development. The ability of small organic molecules to bind to DNA can interfere with processes responsible for cell survival and proliferation, inhibit or modify cellular DNA function as well as induce cell death. It can allow to alleviate or control the disease. DNA is therefore an important target for pharmacological research.
The main aim of the study was to verify whether Salt7 can form a complex with calf thymus DNA (ctDNA). Spectroscopic techniques were used for this purpose.
The spectroscopic analysis conducted showed that Salt7 can form a weak complex (K_a = (2.48 ± 0.84) $\cdot 10^3$ M^{-1}) in the ground state with ctDNA via groove binding. In addition, it was observed that Salt7 could modify the ctDNA structure, therefore affect the processes of ctDNA replication, transcription and translation but it requires further confirmation.
The results obtained do not provide a definitive explanation of Salt7 mechanism of action on ctDNA, but nevertheless encourage further studies involving other research techniques and proteins responsible for cancer cell death.

Keywords: spectroscopic studies, deoxyribonucleic acid, 10-(2-(N-Piperidinyl)ethyl)oxy-5-methyl-12(H)-quino[3,4-b][1,4]benzothiazinium chloride

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P_48 THE ROLE OF EXOSOMES IN DRUG TRANSPORT

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Exosomes, small extracellular vesicles (sEVs), are natural nanocarriers that have long been the subject of scientific investigation. One of their most promising functions, increasingly studied in recent years, is their potential as drug delivery vehicles. Due to their nanoscale size (30–150 nm), biological origin, and ability to cross the blood-brain barrier, sEVs can efficiently transport chemotherapeutic agents without triggering an immune response [1,2].

This review aims to present current findings on the chemical and transport-related properties of exosomes, with particular attention given to their isolation, loading, and surface modification methods. Their application as drug carriers is especially relevant in oncology, such as in the treatment of gliomas and in neurology, for instance, in Alzheimer's disease [3].

This work summarises recent scientific literature and highlights the growing potential of exosomes in the development of precision medicine.

Keywords: exosomes (sEV), drug delivery, targeted therapy, blood-brain barrier, nanocarriers

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P_49

HYDROLATES AND ESSENTIAL OILS AS COSMETIC RAW MATERIALS WITH ANTIOXIDANT ACTIVITY

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Hydrolates and essential oils are natural products of distillation, which have antioxidant activities. They are extracted from specific parts of plants, based on their therapeutic properties. Both hydrolates and essential oils contain chemical components, which help to reduce the impact of oxidative stress. It makes them useful in supporting human skin, even affected by diseases. Therefore, they are popular ingredients of the cosmetic and dermatological products [1,2]. The aim of this work was to analyse the existing data on hydrolates and essential oils, especially used as antioxidants.

Hydrolates (hydrosols) are useful in treatment of skin diseases [1,3]. They are products of hydrodistillation, so they can be applied directly on the face [3]. In these aqueous-based components there are water soluble aromatic compounds (i.e. volatile organic compounds) from essential oil and various antioxidants, such as flavonoids [1,3]. This chemicals can donate electrons to radicals, neutralize reactive oxygen species (ROS) and in this way reduce the potential damage [3,4]. The hydrolates with the highest antioxidant activity against the DPPH radical include: Damascus rose, chamomile, linden tree, tea tree and rosemary products [3]. The high antioxidant activity also have *Hyssopus officinalis*, *Marrubium vulgare, Lavandula officinalis* and *Thymus vulgaris* hydrolates. Some hydrosols (i.e. *Thymus capitatus* and *Nepeta cataria*) have also antimicrobial and antifungal properties [1].

Essential oils also contain the chemical components that alone or in synergy show the antioxidant activity [2,5]. They include even up to several hundred chemical compounds, mainly terpenes, but also allyl- and propenylphenols [2]. The essential oils with the highest antioxidant activity against the ABTS cation radical are, for example, jasmine, common yarrow, thyme red, nutmeg, myrrh, clove bud and cinnamon leaf [5]. The essential oils` high free radical scavenging capacity is very promising not only in dermatology, but also in food preservation [2].

Hydrolates and essential oils should be the object of future studies due to their valuable properties.

Keywords: hydrolates, essential oils, antioxidant

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