Physical Chemistry for Medical Applications

European Meeting on Physical Organic Chemistry

01-05.06.2026

The European Meeting on Physical Organic Chemistry (EMPOC), known until 2018 as the *Central European School on Physical Organic Chemistry*, and before 2003 as *Szkoły Fizykochemii Organicznej* has been organized annually for over 40 years. EMPOC provides a forum for the exchange of scientific ideas, discussion of current challenges, and the development of collaborations in the field of physical organic chemistry. The Meeting also offers valuable opportunities for high-level learning for researchers at all career stages.

The theme of this year's Meeting is **"Physical Chemistry for Medical Applications."** While fundamental research remains essential, the application of physical chemistry to medicine represents one of the most dynamic and impactful directions of modern science. Recent EMPOC meetings have demonstrated that much of the presented research already shows direct or potential relevance to medicine and health care. This year's Meeting aims to bring together theoreticians and experimentalists working at the interface of physical chemistry and medical science.

EMPOC also serves as the annual meeting of the **Section of Physical Organic Chemistry of the Polish Chemical Society**. Participation is open not only to researchers directly involved in medical applications, but also to scientists from related areas such as physical chemistry, physics, and biotechnology. The interaction of complementary disciplines is key to meaningful scientific progress.

The scientific program consists of thematic sessions and includes plenary lectures, oral presentations, short oral presentations, and poster sessions with accompanying 3-minute oral pitches. EMPOC traditionally attracts a diverse audience, including senior researchers, early-career scientists, and PhD students, creating a stimulating and inclusive scientific environment.

Kazimierz Orzechowski

Physical Chemistry for Medical Applications

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Timetable

Monday, 01.06.2026

15.00	The conference office (in Wojcieszyce) is open
16.00	Conference bus departs from Chemistry Department (Joliot-Curie 14, Wrocław)
19.00	Dinner
20.00	Get together party

Tuesday, 02.06.2026

7.30-9.00	Breakfast
9.00	Opening of the conference

Chairman of the morning session Prof. Adam Proń

9.10	**Małgorzata Barańska**	Challenges in spectroscopic imaging of cells: an analytical and physical chemistry perspective
9.45	**Sylwester Mazurek**	Discriminant analysis of seminal plasma samples using FTIR-ATR spectroscopy
10.10		Coffee break
10.40	**Barbara Zupančič**	Identifying diabetes-related biochemical changes in human tissues using infrared spectroscopy
11.15	**Zbigniew Galewski**	Liquid crystals in medical science

11.40	**Amanda Bartkowiak**	SGLT-2 inhibition improves red blood cell oxygenation and elasticity: another positive effect of flozin therapy.
11.55	**Iwona Płowaś-Korus**	Osmolityes in humans - biological significance and clinical implications
12.20	**Kazimierz Orzechowski**	Dielectric methods in assessing the cleanliness of surgical margins in breast cancer
13.00		Lunch and break

Chairwoman of the afternoon session Prof. Małgorzata Barańska

15.00	**Andrzej Teisseyre**	The inhibitory effects of selected flavonoids on the activity of voltage-gated potassium channels Kv1.3
15.35	**Marta Gordel-Wójcik**	Ultrafast excited-state dynamics in trimethoxysilylazachalcone-functionalized colloidal gold nanoshells
16.00	**Justyna Krupa**	UV-induced chemistry in interstellar ice analogues: from simple molecules to complex systems
16.25	**Teobald Kupka**	Toward accurate NMR shieldings in fluoromethanes
18.00		Barbecue

Wednesday, 03.06.2026

7.30-9.00		Breakfast

Chairwoman of the morning session Prof. Halina Szatyłowicz

9.00	**Adam Proń**	Donor–acceptor macromolecular organic semiconductors as precursors of novel electronic, electrochromic, and photoelectrocatalytic materials

9.35	**Barbara Hachuła**	Rigid cage, variable nature: spectroscopic study of phase transition in adamantane-based active pharmaceutical ingredients
10.00		Coffee break
10.30	**Hansen Poul Erik**	Drugs, natural products and hydrogen bonding (online lecture)
11.05	**Rafał Szabla**	Quantifying photoinduced electron transfer in biological systems
11.40	**Michał Pocheć**	Machine learning in RNA atomistic simulations
11.55	**Dawid Dębowski**	From molecular structure to biological activity: Novel sulfonamide derivatives
12.20	**Paweł Wieczorkiewicz**	Decoding chemical resonance in π-conjugated systems with bond delocalization function (BDF)
12.35	**Barbara Lech**	Computational insights into the role of 2-thiouracil in RNA self-replication
12.50	**Kamil Wojtkowiak**	pH dependence of protoribosomal RNA conformational flexibility: MD simulation parameters benchmark and preliminary results
13.00		Lunch and break

Chairman of the afternoon session Prof. Rafał Szabla

15.00	**Piotr Cysewski**	Solubility advantage of (natural) deep eutectic solvents: insight from measurements, quantum chemistry and machine learning
15.25	**Karol Kułacz**	High temperature deintercalation of DMSO smectite
15.40	**Mirosław Jabłoński**	A thorough Systematic conformational study of an experimentally known lantern-like superphane

16.05	**Vlada Pashynska**	Nanocomposites of MoS2 with anticancer drugs for drug delivery: experimental and theoretical characterization
16.30	**Natalina Makieieva**	Towards the structure-activity correlation for selected thiosulfonates - spectroscopic studies and molecular modelling
16.45	**Patrycja Piękoś**	Meso-benzodioxole-BODIPY as pH-sensitive fluorophores
17.00		Coffee break
18.00		Dinner

Thursday, 04.06.2026

7.30-9.00	Breakfast
9.00	Walking tour/ free time
14.00	Lunch (Lunch can be extended for hikers. Advance notice required.)

Chairman of the afternoon session Prof. Andrzej Teisseyre

16.00	Poster flash presentation (3')
17.00	Poster session and coffee
19.30	Conference dinner and closing the meeting

Friday, 05.06.2026

7.30-8.30	Breakfast
9.00	The bus departs to Wrocław

Physical Chemistry for Medical Applications

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01-05.06.2026

Lectures in chronological order

Lecture 1

CHALLENGES IN SPECTROSCOPIC IMAGING OF CELLS: AN ANALYTICAL AND PHYSICAL CHEMISTRY PERSPECTIVE

A. Pieczara, K. Turczynska, B. Orzechowska, W. Korona, J. Firlej, F. Pachacz, K. Siakala, K. Brzozowski, A. Nowakowska and M. Baranska

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Spectroscopic imaging of cells by Raman and IR techniques allows for the probing of molecular structure and dynamics in living systems. However, translating these techniques into robust analytical tools presents significant challenges from both an analytical and physical chemistry perspective. Here, the key physico-chemical and methodological bottlenecks of cellular imaging are presented, including overcoming spectral congestion and water interference through selective chemical labelling with biorthogonal probes. Furthermore, the challenges of quantitative analysis at the single-cell and subcellular levels are discussed, and it is examined how to overcome diffraction and speed limitations by transitioning from spontaneous Raman to coherent techniques (Stimulated Raman Scattering, SRS) and advanced photothermal imaging (Optical Photothermal Infrared, O-PTIR) in aqueous environments. Finally, the focus is on the progression toward 4D (3D + time) imaging to monitor metabolic fluxomics, and on the application of advanced data fusion, allowing for a shift from single-biomarker identification to a holistic 'spectralomics' approach.

Acknowledgements
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Lecture 2

DISCRIMINANT ANALYSIS OF SEMINAL PLASMA SAMPLES USING FTIR-ATR SPECTROSCOPY

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Male infertility is a serious problem worldwide, affecting many couples and accounting for a significant number of pregnancy failures. The condition can have various causes, and its diagnosis and treatment require a comprehensive approach and the use of various diagnostic and therapeutic methods.
The studied material was seminal plasma (*n*=280) obtained from an infertility treatment clinic. Semen parameters, including analyses of the physical characteristics of the ejaculate and sperm quality, were determined based on the WHO guidelines. Vibrational spectra of thin dry films obtained from 1 µl portions of the material were recorded using the FTIR-ATR technique. Chemometric analysis of IR data focused on classifying samples into fertile/infertile groups and assigning them to different classes based on qualitative criteria. Principal component analysis (PCA) was performed, followed by partial least squares discriminant analysis (PLS-DA). Various techniques for variable selection and data pre-preparation were tested. PLS-DA model constructed based on 150 spectral variables indicated by the iPLS algorithm allowed for complete discrimination fertile and interfile samples, with the high parameters of the cross-validation (Acc=0.947, F1=0.974, AUC=0.952). Additionally, specific areas of the ATR spectra were correlated with plasma quality parameters, which indicates the possibility of predicting selected features based on the vibrational spectra of the material.
The obtained results indicate that spectroscopic techniques can set new standards for assessing the quality of biological material and thus support in vitro fertilization procedures.

Lecture 3

IDENTIFYING DIABETES-RELATED BIOCHEMICAL CHANGES IN HUMAN TISSUES USING INFRARED SPECTROSCOPY

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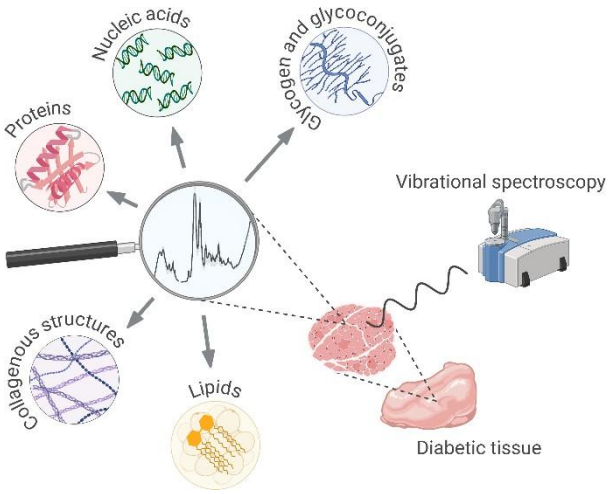
Its high and still rising global prevalence [1] makes diabetes mellitus (DM) a major metabolic disease and poses a significant public health challenge worldwide. Chronically elevated blood glucose, the defining biochemical hallmark of DM, causes metabolic abnormalities that lead to various diabetic complications. Body tissues with extensive physiological functions, such as skeletal muscle and fascia, are critically involved in these complications as they are sensitive to metabolic disruptions. Therefore, changes in their biochemical profile can provide valuable information relevant to the molecular mechanisms underlying DM and its effects.

In our study, we examined the macromolecular composition of human skeletal muscle and deep fascia from diabetic and healthy individuals using infrared spectroscopy as an alternative to traditional histochemical assays for tissue analysis. By applying spectral decomposition, we extracted multifaceted information on the spectral profiles of the main macromolecular species from an infrared absorption spectrum [2]. This provided a comprehensive view of the biochemical composition, with the set of descriptors enabling comparison between diabetic and healthy tissue.



In skeletal muscle, the most evident effects of DM are reflected in the altered levels of myofibrillar proteins, glycogen, and lipids, while in deep fascia, DM appears to primarily affect the levels of collagenous structures and glycosaminoglycans.

Infrared spectroscopy combined with chemometric processing proved to be an efficient approach for tissue analysis, as it enabled identification of the main biomolecular species composing the tissue simultaneously from a spectrum measured in a single experiment with minimal sample preparation.

Acknowledgments

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Lecture 4

LIQUID CRYSTALS IN MEDICAL SCIENCE

M. Piwowarczyk[1] and Z. Galewski[2]

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Today's remarkably rapid development of medicine is due to the widespread use of achievements primarily in physics, chemistry, and physical chemistry. These sciences offer significant advancements by enabling a thorough understanding of processes and phenomena occurring in the human body.

One such concept, first observed 138 years ago during an attempt to determine the molecular formula for cholesterol, is the liquid crystalline phenomena. This presentation will precisely define this phenomenon based on the latest IUPAC recommendations.

Numerous applications will also be presented, with thermography being the most extensively discussed.

Lecture 5

SGLT-2 INHIBITION IMPROVES RED BLOOD CELL OXYGENATION AND ELASTICITY: ANOTHER POSITIVE EFFECT OF FLOZIN THERAPY

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Background: Sodium–glucose cotransporter 2 inhibitors (SGLT2), commonly referred to as flozins, provide cardiovascular and renal benefits in patients with heart failure (HF), which appear early after treatment initiation and may be largely driven by hemodynamic mechanisms [1,2]. However, cellular contributors to these effects remain incompletely understood. The aim of this study was to investigate the effect of empagliflozin (EMPA) on red blood cells (RBCs) functional and structural properties in patients with advanced ischemic systolic heart failure, supported by complementary in vitro experiments on isolated RBCs.
Methods: Blood samples from selected patients (Figure 1 - left) were collected before initiation of EMPA 10 mg/day (red) and after ≥3 months of therapy (green). A reference group of young healthy subjects served as controls (yellow). In parallel, in vitro experiments were performed by incubating donor-derived RBC for 7 days with EMPA or dapagliflozin (DAPA).
Results: EMPA therapy was associated with a marked reduction in RBC stiffness, with a ~60% decrease in Young's modulus compared with baseline, reaching values comparable to those observed in young healthy controls and showing reduced intercellular variability (Figure 1 - right). In vitro Raman spectroscopy demonstrated a protective effect of EMPA on hemoglobin oxygenation state after 7 days of incubation, preserving oxyHb, whereas DAPA-treated and control samples showed higher contribution of deoxyHb and other spectral features characteristic of physiological RBC aging.

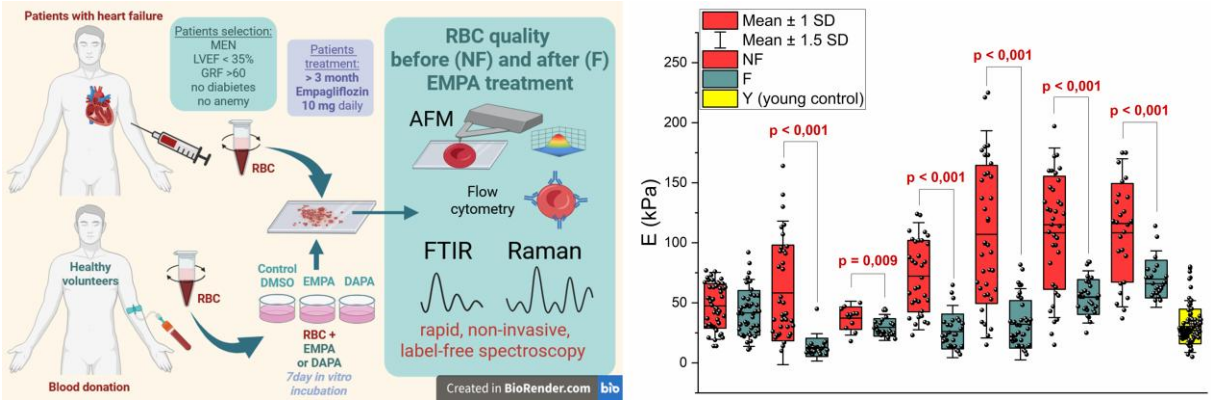

Figure 1. Scheme of the experiments: RBC isolation from patients with HF before (NF) and after (F) treatment with EMPA and in vitro incubation of isolated RBCs from donors with EMPA or DAPA.

Summary: Empagliflozin improves erythrocyte mechanical properties in patients with advanced heart failure and exerts a protective effect on hemoglobin oxygenation in vitro. These findings suggest that modulation of erythrocyte function may contribute to the early cardiovascular benefits of SGLT2 inhibitors.

Acknowledgments
This work was supported by the Polish National Science Centre (2024/08/X/NZ5/01041 and UMO-2021/41/B/NZ3/04146).

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Lecture 6

OSMOLITYES IN HUMANS – BIOLOGICAL SIGNIFICANCE AND CLINICAL IMPLICATIONS.

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Water is the medium for essentially all chemical reactions in living cells. Thus to comprehend biochemical reactions within organisms it is essential to provide deep insight into the understanding of molecular interactions and accompanying dynamics of the water-soluble molecules that can be found in the cell cytoplasm. Examples of such molecules are osmolytes, low-molecular weight compounds with an ability to maintain osmotic pressure and thereby the intracellular water balance [1]. These protective compounds accumulate in the cell cytoplasm to preserve the structure and functions of biomolecules against abiotic stresses like drought, salinity, temperature, and pressure extremes [2]. Osmolytes commonly found in nature belong to various classes of compounds, such as amino acids [3], methylamines [4], polyols [5], sugars [6], and ureas [7]. In particular, osmolytes like sorbitol, betaine, inositol, taurine, and glycerophosphocholine (GPC) can be found in the human renal medullary cells. [3] On the other hand, some osmolytes like ectoine have a protective and moisturizing effect on the skin. [8] In the case of ectoine, it was found that even under stressing environmental conditions, osmolytes are strongly hydrated and thereby preserve cell water volume [9]. Furthermore, many of these compounds remain well-hydrated even at high concentrations [10]. It appears that in aqueous solutions the presence of stabilizing osmolyte molecules near a protein preferentially causes the formation of water-protein interactions [11]. Any change in preferential binding or preferential hydration triggers osmolytes to control biochemical reactions [12].
This presentation aims to highlight the biological significance of osmolytes in humans and their clinical implications in various diseases.

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Lecture 7

DIELECTRIC METHODS IN ASSESSING THE LINECLINESS OF SURGICAL MARGINS IN BREAST CANCER

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In this talk, it will be present a method designed to verify the absence of cancerous tissue at surgical margins during breast cancer surgery - commonly referred to as the "clean margins" issue. The technique involves measuring the dielectric properties of breast tissue removed from the operative site. Significant differences between cancerous and normal breast tissue have been recognized since the 1930s. However, only recently have we resolved the challenges associated with conducting dielectric measurements in the long-wavelength (LW) range in the presence of highly conductive biological fluids such as blood and lymph.
We will present both the physical principles and clinical results supporting this method. An intraoperative breast cancer detection probe has been developed and patented, and a startup company, **Onco Scanner Ltd**, has been established to bring this innovation to clinical practice.

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Lecture 8

THE INHIBITORY EFFECTS OF SELECTED FLAVONOIDS ON THE ACTIVITY OF VOLTAGE-GATED POTASSIUM CHANNELS Kv1.3

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Voltage gated potassium channels Kv1.3 are membrane proteins, which contain a water-filled pore enabling a selective transmembrane transportation of potassium ions down their electrochemical gradient. The channels play an important role in a regulation of cell life and death. Blockage of Kv1.3 channels may putatively be beneficial in treatment of various diseases, including some cancer disorders with an up-regulation of these channels. Among many Kv1.3 channel blockers there are some naturally occurring flavonoids, chalcones and statins [1, 2].

Here we report an inhibitory effect of two flavonoids; quercetin and morin, on the activity of voltage-gated potassium channels Kv1.3 expressed in a model system of cancer cells – human lymphoblastic T cell line Jurkat. The study was performed applying the whole-cell patch-clamp technique [3].

The obtained results demonstrate that both quercetin and morin inhibited Kv1.3 channels in Jurkat T cells in the concentration range from 30 to 105 μM. The inhibitory effect of quercetin was concentration-dependent, whereas the inhibition of the channels by morin did not depend on the concentration. The inhibitory effects were reversible. The channels' inhibition was not complete, nevertheless, it was significant. Similarly to what was observed in case of other flavonoids [2], the inhibition was significantly augmented upon a co-application of quercetin with the statins: simvastatin and mevastatin. The inhibitory effect was synergistic when co-applying quercetin with simvastatin and it was additive upon a co-application with mevastatin. In case of morin, the inhibitory effect was additive upon a co-application with simvastatin and it was not additive upon a co-application with mevastatin.

The inhibition of Kv1.3 channels may putatively be involved in anti-cancer activities of both compounds, especially on cancer cells over-expressing these channels. This may putatively be beneficial in supporting chemotherapy of cancers with an over-expression of these channels, such as melanoma, pancreatic ductal adenocarcinoma (PDAC), multiple myeloma and B-type chronic lymphocytic leukemia (B-CLL) [2].

Acknowledgments

The studies on the influence of quercetin and morin on the activity of Kv1.3 channel in Jurkat T cells were supported by the Polish Ministry of Research and University Education funds for Wrocław Medical University.

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Lecture 9

ULTRAFAST EXCITED-STATE DYNAMICS IN TRIMETHOXYSILYLAZACHALCONE-FUNCTIONALIZED COLLOIDAL GOLD NANOSHELLS

M. Gordel-Wójcik,[1,2,5] M.A. Thottappali,[2] M. Pietrzak,[3] E.F. Petrusevich,[4] J. Vohlídal,[5] J. Pfleger[2] and B. Jędrzejewska[3]

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A synthetic approach toward trimethoxysilylated azachalcones donor-acceptor (D-A) chromophores characterized by pronounced intramolecular charge-transfer behavior is presented. Comprehensive spectroscopic analysis, supported by theoretical calculations, reveals their distinct optoelectronic properties and confirms their suitability for advanced functional applications. To further exploit these properties, the chromophores were covalently immobilized onto plasmonic gold nanoshells (NSs), yielding hybrid nanostructures designed to facilitate efficient molecule-plasmon interactions.

Femtosecond transient absorption measurements indicate substantial alterations in the excited-state dynamics upon nanoshell functionalization. In comparison to the free chromophores, all resolved lifetime components exhibit pronounced extension, increasing from 700 fs, 1.93 ps, and 5.64 ps to 3.7 ps, 430.5 ps, and 15 ns, respectively. This effect is attributed to localized surface plasmon resonance (LSPR), which enhances the local electromagnetic field, enables hot-electron transfer to the chromophore's lowest unoccupied molecular orbital (LUMO), and suppresses non-radiative relaxation pathways through restricted molecular motion and strong interfacial electronic coupling. In addition, plasmon-induced photothermal effects contribute to the overall excited-state behavior, providing an additional pathway for energy dissipation and influencing relaxation dynamics at longer timescales.

The findings demonstrate the capacity of plasmonically coupled hybrid systems to modulate excited-state processes in a controlled manner. Such systems are promising for applications in photonic devices, optical sensing, and light-responsive biomedical technologies, including photodynamic therapy and bioimaging, where extended excited-state lifetimes and coupled thermal effects can enhance performance and functionality.

Acknowledgments:
This work was supported by the project No. UMO-2021/43/D/ST5/02249, SONATA 17, funded by National Science Center Poland (NCN).

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Lecture 10

UV-INDUCED CHEMISTRY IN INTERSTELLAR ICE ANALOGUES: FROM SIMPLE MOLECULES TO COMPLEX STRUCTURES

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Understanding UV-driven chemistry in extreme environments is essential for modeling molecular evolution in planetary atmospheres and interstellar space. In particular, interstellar ices on dust grains provide unique conditions where low temperatures and radiation fields enable formation of complex molecules from simple precursors.

Here, we present a combined experimental and theoretical study of UV-induced photochemistry of small molecules isolated in low-temperature matrices. Matrix isolation FTIR spectroscopy, supported by quantum chemical calculations, allows direct observation of photochemical transformations and transient species under well-defined conditions.

Upon UV irradiation, precursor molecules undergo efficient decomposition and isomerization, leading to formation of reactive radicals and stable photoproducts. These species are confined within matrix cages, where ultrafast recombination and secondary reactions result in stabilization of weakly bound molecular complexes. We demonstrate that such cage effects play a decisive role in directing reaction pathways.

A key finding of this work is the strong dependence of photochemical mechanisms on the matrix environment. Comparative studies reveal that inert and weakly interacting matrices promote different reaction channels, influencing radical mobility, cage escape, and complex formation efficiency. These effects provide insight into how chemical reactivity is modulated under astrochemically relevant conditions.

The presented results highlight the importance of combining spectroscopy and theory to unravel elementary photochemical steps. They provide a molecular-level perspective on radical-driven chemistry, energy dissipation, and complex stabilization processes occurring in interstellar ice analogues.

Acknowledgments

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Lecture 11

TOWARD ACCURATE NMR SHIELDINGS IN FLUOROMETHANES

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The latest results on testing Locally Dense Basis sets approach on fluorine containing small molecules using high level coupled cluster method, CCSD(T), as well as Hartree-Fock, combined with a family of Dunning type basis sets, aug-cc-pVXZ, where X = D, T, Q, 5 and 6, are reported. All geometry optimalizations and GIAO CCSD(T) NMR shieldings were conducted using CFOUR ver. 2.1 program.
A comparison of nuclear shieldings in CF4, CF3H, CF2H2, CFH3 and CH4, obtained with 28 density functionals and aug-cc-pVTZ basis set with respect to CCSD(T)/aug-cc-pVTZ values is shown. The individual differences in performance of the studied density functionals are discussed.

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Lecture 12

DONOR–ACCEPTOR MACROMOLECULAR ORGANIC SEMICONDUCTORS AS PRECURSORS OF NOVEL ELECTRONIC, ELECTROCHROMIC, AND PHOTOELECTROCATALYTIC MATERIALS

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Alternating donor–acceptor copolymers can be obtained via condensation polymerization of appropriately functionalized acceptor (A) and donor (D) monomers or through electrochemical polymerization of compounds that generatethe polymer repeat unit [1]. The presentation will discuss -(DAD)-type copolymers containing dithienopyrrole or carbazole donor (D) units and benzothiadiazole, diketopyrrolopyrrole, thiadiazole, tetrazine, or naphthalene diimide acceptor (A) units. Methods of their synthesis, as well as their electrochemical and spectroelectrochemical properties (UV–vis–NIR, EPR, Raman spectroscopy), will be discussed in detail.
These polymers are characterized by very low bandgaps. This feature, combined with the reversibility of their redox processes—both in oxidation and reduction modes—results in highly interesting electrochromic properties [2,3], including electrochromism in the near-infrared region, a phenomenon highly desirable from a technological standpoint. Pre- or post-polymerization functionalization with hydrophilic substituents enables their application as active layers in organic ambipolar electrochemical transistors (OECTs) operating in aqueous electrolytes [4], which is also a valuable yet rarely observed feature among organic semiconductors. Finally, donor–acceptor polymer films can serve as photocathodes in visible-light-driven photoelectrocatalytic reduction of oxygen to hydrogen peroxide [5].

Acknowledgments
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Lecture 13

RIGID CAGE, VARIABLE NATURE: SPECTROSCOPIC STUDY OF PHASE TRANSITIONS IN ADAMANTANE-BASED ACTIVE PHARMACEUTICAL INGREDIENTS

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Adamantane is a tricyclic saturated hydrocarbon characterized by high symmetry and a rigid structure, which makes it a fundamental building block for numerous compounds of significant pharmacological and materials science importance [1–3]. Its derivatives, including amantadine, memantine, and rimantadine, exhibit antiviral and neuroprotective effects and are used to treat diseases such as Parkinson's disease, Alzheimer's disease, and multiple sclerosis [1,3]. Numerous experimental studies have also shown that adamantane and its derivatives can form plastic crystalline phases (plastic crystals). This feature—where long-range translational order coexists with rotational freedom of molecular units—makes these compounds particularly attractive for research aimed at developing advanced functional materials. This presentation reports the results of spectroscopic investigations on two adamantane-based compounds: 1-adamantylamine (amantadine; AMA) and 3,5-dimethyl-1-adamantylamine (memantine; MEM). Temperature-dependent infrared and Raman measurements enabled the detection of plastic crystalline phases, as evidenced by changes in the profiles of absorption bands associated with the C–H vibrations of the adamantane ring and H-bonded functional groups. Both compounds exhibited distinct phase transitions: MEM transformed from a liquid state into a plastic crystalline phase (I, II), while AMA exhibited transitions among several plastic phases (I, II, III, IV) [3]. For MEM, these transformations were reversible; the substance returned to its original commercial liquid form after a cooling–heating cycle, whereas AMA did not revert to its initial commercial state [3]. Moreover, for MEM, high-pressure studies (from ambient conditions to ~5 GPa) were performed using a diamond anvil cell (DAC) and Raman spectroscopy. The results indicated that compression maintains a liquid-like state and leads to a weakening or redistribution of H-bonding interactions. Thus, our studies have shown that MEM adapts differently to the given thermodynamic conditions: while cooling triggers a phase transition into a plastic crystal, high pressure effectively inhibits this transition, allowing MEM to retain its liquid-like spectral character through local structural changes within the adamantane skeleton (manifested by the variations in C-C bond lengths) and modifications in H-bond geometry.

Acknowledgments

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Lecture 14

DRUGS, NATURAL PRODUCTS and HYDROGEN BONDING

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The talk will concentrate on intramolecular hydrogen bonding and tautomerism in relation to drugs and natural products that are or have potential to become drugs. The tools will be isotope effects on chemical shifts and DFT calculations. In Figure 1 is shown the purpurin anion, which may show both multiple hydrogen bonding and tautomerism.

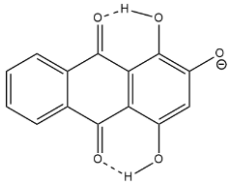

Figure 1. Purpurin anion

Another case of multiple hydrogen bonding is that of rifampicin. Tautomerism is also found in piroxicam. A recent example is that of 25CN-NBOH, a selective serotonin 2A receptor.
Usnic acid and derivatives thereof will illustrate how natural products can be the starting products for new drugs.
A number of new natural products with possible medical use will also be discussed.
The last and surprising example will be that of humic acid.

Lecture 15

QUANTIFYING PHOTOINDUCED ELECTRON TRANSFER IN BIOLOGICAL SYSTEMS

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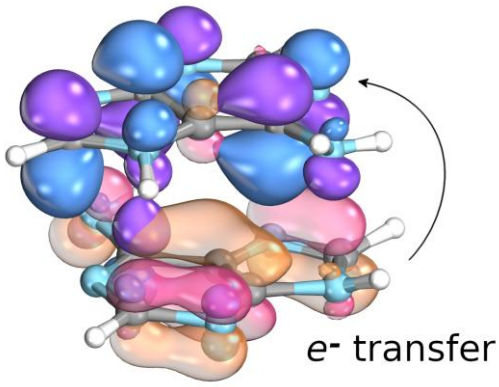
Photoinduced electron transfer (PET) is one of the most common consequences of the absorption of UV light by nucleic acids. It leads to the population of long-lived excited charge transfer (CT) states, which often involve several stacked nucleobases in a DNA strand. Recently, we also demonstrated that PET is the key step in the synthesis of RNA and DNA nucleosides under the conditions of early Earth [1,2]. In this talk, I will demonstrate that the efficiency of PET in DNA is strongly dependent on structural factors such as nucleobase stacking overlap [3]. I will also show that the efficiency of PET can be strongly influenced by chalcogen bonding interactions, the role of which has not been considered in photochemistry until recently [1,2,4]. My talk will be focused on our recent discoveries of productive photoredox reactions and on the mechanistic description of nonenzymatic self-repair of RNA and DNA, which can be used for predicting photoreactivity in related systems [5,6]. Finally, I will demonstrate how to accurately predict photoinduced electron transfer timescales, based on nonadiabatic transition state theory [7].



Acknowledgments
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Lecture 16

MACHINE LEARNING IN RNA ATOMISTIC SIMULATIONS

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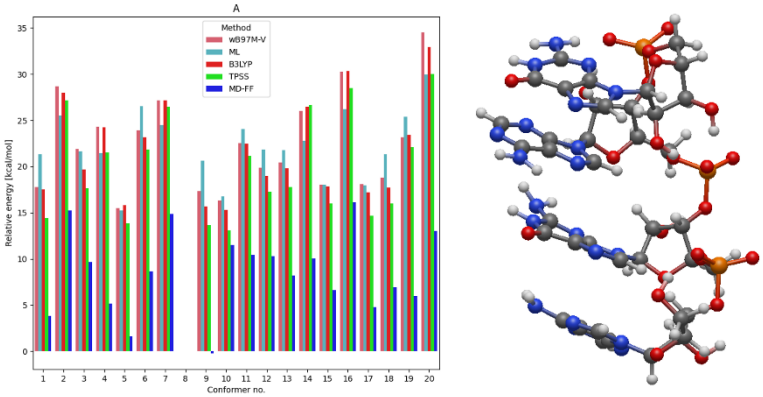
In the past 10 years Artificial Intelligence (AI) and Machine Learning (ML) have become technologies widely used not only in day-to-day lives but have gained significance in science. From predicting trends in data to building complex models, they have become the mainstay in many data-driven fields [1]. Here, the preliminary results of atomistic simulations of RNA and its building blocks using the ML approach are presented. The nucleic acids are one of the hardest groups of compounds to model using computational chemistry – their functional systems are large, with plethora of intricate interactions and challenging structural features, such as the charged backbone.



SpookyNet [2], the physics-informed, message passing neural network has been used as the architecture of choice. It has been trained on the data set consisting of almost 0.5 million diverse data points. The network and hyperparameters have been fine-tuned to achieve the best possible fidelity. Models have then been tested in different scenarios against the reference method (DFT, ωB97M-V functional), as well as some other typically used approaches, such as classic force fields (MD-FF) and DFT (B3LYP, TPSS).
The models have achieved accuracy surpassing the dedicated RNA MD-FF and TPSS in predicting the relative conformational energies of nucleosides and Watson-Crick nucleoside pairs, in most cases approaching the B3LYP level of accuracy. This level of accuracy for the single-point calculations has been achieved in times orders of magnitude faster than even the fastest DFT level of theory, retaining almost linear scaling with the system size. The model ensembles have been tested in optimization tasks for AGAG oligomer for both RNA and DNA, with self-written implementation of implicit solvation model, showing RMSD (Å) below 0.7 and proving that the models are transferable to different nucleic acids without additional training.

Acknowledgments
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Authors would like to gratefully acknowledge Wrocław Center for Networking and Supercomputing for providing computational resources.

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Lecture 17

FROM MOLECULAR STRUCTURE TO BIOLOGICAL ACTIVITY: NOVEL SULFONAMIDE DERIVATIVES

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Sulfonamides remain a fundamental class of compounds in medicinal chemistry, serving as versatile scaffolds for the design of diverse biologically active agents [1]. Beyond their classical antibacterial applications, sulfonamide derivatives have shown growing promise in the treatment of cancer, as well as metabolic and neurodegenerative diseases [2,3]. In particular, primary sulfonamides have attracted considerable attention as inhibitors of tumor-associated carbonic anhydrase isoforms, especially CA IX and CA XII.
In this study, two distinct classes of sulfonamide-based compounds were examined. The first class comprises derivatives bearing aryl moieties that vary in the size and degree of aromatic conjugation [4]. Owing to their planar and rigid structures, hydrophobic character and extended π-electron systems, these molecules are expected to engage in π–π stacking interactions with DNA base pairs, suggesting a plausible intercalative binding mode and potential anticancer activity.
The second class consists of coordination complexes derived from a newly synthesized phenanthroline-based sulfonamide ligand, used to generate Rh(III) and Ir(III) complexes. Comprehensive physicochemical characterization was performed, including the determination of partition coefficients (logP), which are relevant to membrane permeability and biological activity. Interactions with DNA and inhibition of carbonic anhydrase were investigated, enabling evaluation of both binding modes and kinetics.
Preliminary in vitro cytotoxicity studies (IC_{50}) showed that one of the Rh(III) complexes exhibits greater selectivity for cancer cells than the other compounds tested, supporting its relevance for further investigation. The results indicate that both investigated sulfonamide-based groups may represent promising multifunctional systems capable of interacting with DNA and inhibiting cancer-associated enzymes.

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Lecture 18

DECODING CHEMICAL RESONANCE IN Π-CONJUGATED SYSTEMS WITH BOND DELOCALIZATION FUNCTION (BDF)

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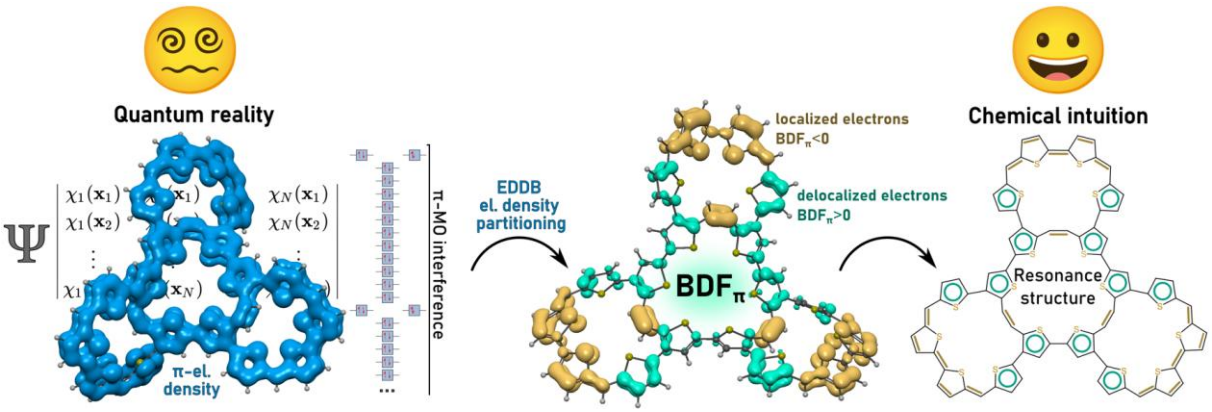
Understanding the electronic structure of π-conjugated systems remains a central challenge in contemporary chemistry, given their importance in materials science, molecular electronics, photophysics, and catalysis. Here we introduce a wavefunction-based analytical protocol — the π-Bond Delocalization Function (BDF_π) — which maps the spatial organization of localized and delocalized π-bonding directly from the ground-state one-electron density matrix [1,2]. Rather than relying on predefined resonance models or orbital localization schemes, the method extracts bonding topology from the complete occupied π-orbital space.

BDF_π provides, in a single intuitive graphical representation, a clear distinction between regions where electrons are predominantly delocalized and where electrons remain localized in specific bonds or lone pairs. This representation parallels the conceptual language of resonance theory familiar to all chemists, while retaining the rigor and quantitative foundation of molecular-orbital-theory-based analysis. Conceptually, BDF_π provides a measure of the net effect of the superposition of all resonance structures, enabling identification of the most significant contributors.

In this presentation, we will outline the theoretical foundations of BDF_π and demonstrate its application to representative poly-and macrocyclic π-conjugated systems. The results will be discussed in the context of existing experimental observations and theoretical results, in order to provide a fresh perspective on how the π-electronic structure is determined by the topology of the π-system.



Acknowledgments

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Lecture 19

COMPUTATIONAL INSIGHTS INTO THE ROLE OF 2-THIOURACIL IN RNA SELF-REPLICATION

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Precise replication of nucleic acids is crucial for maintaining genetic integrity, since the misincorporation of nucleotides can result in mutations and, in some cases, cancer. [1–2] In modern eukaryotic cells, specialized protein systems detect mismatches and either remove incorrectly added nucleotides or rebuild the affected DNA strand. Such sophisticated repair machinery, however, did not exist under prebiotic conditions, implying that alternative processes must have operated to limit mutation frequencies.[3–4] Nonenzymatic RNA primer extension is associated with an error rate of approximately 17%, primarily caused by formation of the guanosine–uracil wobble pair.[5] Modified nucleotides, including inosine and 2-thiouridine, have been proposed as candidates capable of producing more stable and selective base pairing.[6–7] Replacing uracil with 2-thiouracil enhances replication efficiency while having little effect on the addition of following nucleotides. Notably, 2-thiouracil is also able to generate a strong self-pairing interaction (tU:tU), which contributes to stabilization of double-stranded RNA.[8] At the same time, this tU:tU pair strongly inhibits further strand elongation, causing primer extension to stall once tU is incorporated opposite another tU.
Molecular dynamics simulations and DFT calculations allow investigation of the influence of 2-thiouracil on nonenzymatic RNA self-replication at the molecular level. Clustering algorithms reveal characteristic binding behaviors and indicate how efficiently activated mononucleotides interact within the reactive site. Meanwhile, DFT-derived binding energies suggest that reaction efficiency cannot be predicted solely from the interaction pattern of an individual base pair. Instead, the conformational stability of the activated mononucleotide and the structure of double stranded helix are a key factors governing the efficiency of the process, rather than binding energy alone.

Acknowledgments
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Lecture 20

PH DEPENDENCE OF PROTORIBOSOMAL RNA CONFORMATIONAL FLEXIBILITY: MD SIMULATION PARAMETERS BENCHMARK AND PRELIMINARY RESULTS

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Protoribosome is one of the oldest, sequentially and structurally well-conserved fragment of contemporary ribosome, which preceded the emergence of last universal common ancestor [1, 2]. Protoribosome is a captivating system to study the microscopic phenomena associated with dimerization, coacervate formation and translation processes [3]. Typically, it consists of protoribosomal RNA (prRNA) and short peptides that bind with various strength and specificity. According to the recent studies, non-enzymatic replication of prRNA presumably needed freeze-thaw cycles that could facilitate the RNA strands detachment and liquid-liquid phase separation via pH oscillations [4]. Recent experiments from Sutherland laboratory may support that hypothesis - it was shown that low pH environment significantly decreases short RNA duplexes melting temperatures and prevents the phosphodiester bonds cleavage or depurination in the presence of the magnesium ions [5]. To our knowledge, the microscopic nature of this phenomenon is not known. To address the role of pH on the prRNA conformational stability, we setup, executed, and analysed a series of molecular dynamics (MD) simulations. In this talk I will discuss how specific MD parameters improve sampling. Furthermore, I will show our preliminary results of the the protonated 130 nt-long prRNA and explain, what effect low pH has on prRNA structural integrity and conformational flexibility. Our results provide a solid baseline for further investigations of pH-dependence of protoribosome molecular details in the prebiotic context.

Acknowledgments
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Lecture 21

SOLUBILITY ADVANTAGE OF (NATURAL) DEEP EUTECTIC SOLVENTS: INSIGHT FROM MEASUREMENTS, QUANTUM CHEMISTRY AND MACHINE LEARNING.

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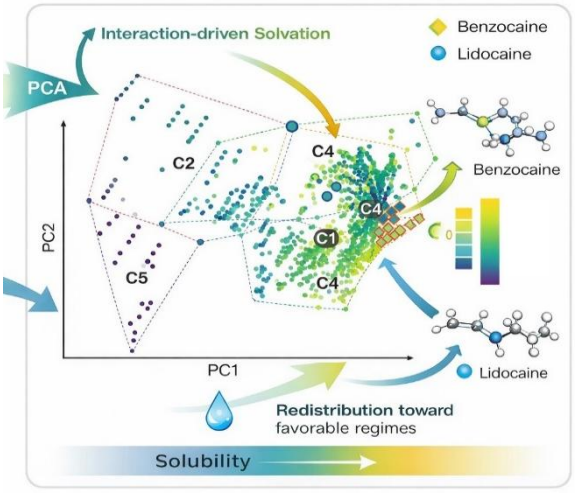
Deep eutectic solvents (DESs), particularly natural DESs (NADES), have emerged as highly effective media for enhancing the solubility of poorly water-soluble active pharmaceutical ingredients (APIs). However, rationalizing and predicting their solubility advantage remains challenging due to strong intermolecular associations, non-ideal thermodynamics, and compositional complexity. In this contribution, an integrated framework combining experimental measurements, quantum-chemical modeling (COSMO-RS), and machine learning to systematically unravel the origins of the solubility advantage in DES systems is presented. Our new experimental data are combined with literature datasets to construct large, chemically diverse solubility databases suitable for machine learning [1-5].



At the molecular level, COSMO-RS-derived interaction energies reveal that DESs are highly associated liquids dominated by hetero-complexes and dimers, where solute-containing species govern solubility maxima and depend sensitively on solvent composition. These insights are further generalized through a data-driven thermodynamic taxonomy, which reduces complex descriptor spaces into physically interpretable axes and identifies two principal solubilization mechanisms: interaction-driven and destabilization-driven regimes [1-3].
To move beyond qualitative understanding, we develop machine learning models using the DOOIT2 frameworks, enabling accurate and parsimonious prediction of API solubility across DES and conventional solvent systems. The results demonstrate that ML can significantly outperform physics-based models in chemically diverse systems, while offering limited gains in homogeneous domains, thereby defining clear applicability boundaries [4].
This work establishes a unified, mechanism-informed strategy for DES-based formulation design, bridging experimental data, molecular theory, and data-driven modeling. The proposed approach replaces empirical screening with predictive, interpretable tools, enabling more efficient exploitation of DESs and NADES as solubility-enhancing media and mechanism-aware design of DES/NADES formulations for pharmaceutical applications [5].

Acknowledgments
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Lecture 22

HIGH TEMPERATURE DEINTERCALATION OF DMSO SMECTITE

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Clay minerals have a wide range of applications in industry, agriculture, medicine, and cosmetology. They constitute a natural, layered substrate that can be modified to produce nanocomposites used for aquatic environmental remediation as adsorbents of heavy metals and organic dyes, as well as for air purification [1]. These minerals are also used as additives to improve the thermal and mechanical properties of polymers and concrete. In addition, they are widely applied as insulation materials, thermal protective coatings, catalysts, and hybrid materials with antibacterial and antifungal properties, as well as carriers for biologically active substances [2]. In systems such as smectite intercalated with biologically active substances, the guest molecules are stabilized in the interlayer spaces of the mineral layers (host). In the intercalation process, a wide variety of molecules can theoretically be incorporated into the interlayer spaces of smectites [3,4]. However, the stability of such hybrid systems, as well as the stability of the guest molecules themselves, remains a crucial issue [5]. It is therefore important to understand how the presence of guest molecules influences both the overall stability of the resulting hybrid material and the kinetics and mechanisms governing the release of the intercalated molecules. The talk will focus on a detailed discussion of the deintercalation process in the NNT–DMSO system (nontronite with intercalated DMSO). Particular attention will be given to the shrinking effect, which is a gradual decrease in the interplanar distance (d_{001}) induced by the deintercalation process, as well as to the decomposition of DMSO that occurs as the material is heated to higher temperatures.

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Lecture 23

A THOROUGH SYSTEMATIC CONFORMATIONAL STUDY OF AN EXPERIMENTALLY KNOWN LANTERN-LIKE SUPERPHANE

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Superphanes [1], belonging to the large group of cyclophanes [2], are an exceptionally interesting group of organic compounds due to their aesthetic beauty, but above all because of their unique encapsulation and adsorption properties. Recently, it has been shown that pinwheel superphanes can trap a variety of simple molecules and ions [3-4], including water dimer [3]. In the latter case, the superphane (**SP**) was characterized by having 4 of the 12 imine nitrogen atoms pointing towards the center of the cage (one pair each at the top and bottom; Figure 1). However, this conformation (2i-2i) does not have to be the most energetically stable.
Hereby, we present the results of our in-depth conformational studies of **SP** [5]. It is shown that the relative energies of the lowest-energy conformers within a given type increase with the number of imine nitrogen atoms pointing inward the **SP** cage (N_{in}). Thus, the conformer with all outward-pointing N atoms is the most energetically stable. The most energetically stable conformers of the types with $N_{in} \leq 2$ have a pinwheel structure, whereas those of types with $N_{in} \geq 6$, on the contrary, feature rosette-like structures (Figure 2). Both DFT-based and GFN2-xTB-based minima searches are performed. Both these methods locate the same minima, and the energies correlate fairly well. The latter method, however, gives smaller energetic differences between conformers (Figure 2), and dispersion effects are more pronounced. Molecular dynamics simulations show that periods of low potential energy are related mainly to conformers with low N_{in}, close to 4. The influence of dispersion, electrostatic interactions, and angular stresses on the structural motifs of **SP** conformers and their energies is also investigated. We propose several possibilities for the experimental (based on IR spectra) determination of the conformational type of the **SP** superphane (i.e., determination of the putative number N_{in}).

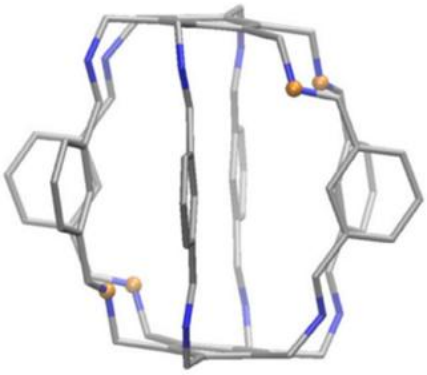

Figure 1.

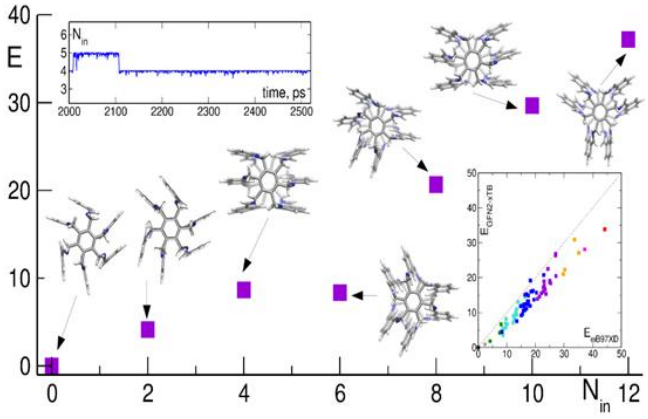

Figure 2.

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Lecture 24

NANOCOMPOSITES OF MoS_2 WITH ANTICANCER DRUGS FOR DRUG DELIVERY: EXPERIMENTAL AND THEORETICAL CHARACTERIZATION

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The development of effective nanostructured drug delivery systems remains a significant challenge in contemporary applied nanoscience and related scientific fields. Among the emerging solutions, two-dimensional MoS_2-based nanomaterials have gained substantial attention as versatile platforms for anticancer drug delivery. This interest is driven by the unique structural and physicochemical properties of MoS_2, including its remarkable photothermal conversion efficiency in the near-infrared (NIR) spectrum range. This characteristic enables a synergistic combination of chemotherapy and photothermal tumor therapy. Although several promising MoS_2-based systems for anticancer drug delivery have already been developed, more in-depth research is needed to better understand the interactions between drug molecules and their nanocarriers. The physical and chemical interactions within drug delivery nanoassemblies can significantly affect the stability of drug molecules and the processes of controlled loading and release of drugs. Our recent combined experimental and quantum-chemical modeling study on nanosystems containing MoS_2 nanosheets and anticancer agent 6-thiopurine or 2-thioadenine revealed the possibility of chemical transformations of the molecules of these anticancer thioderivatives of purine nucleobases within the nanocomposites that can influence the drug's therapeutic activity [1].

The current study provides experimental and computational insights into the interactions between the components of nanocomposite of MoS_2 with widely used anticancer agent doxorubicin (DOX). For experimental characterization, laser desorption/ionization mass spectrometry was employed, using the methodology established in the prior research [1]. Nanocomposite samples for experimental measurements were prepared by ultrasonic treatment of aqueous suspensions of MoS_2 and DOX, followed by the nanoparticles precipitation. Analysis of the resulting mass spectra revealed distinct signals of ions characteristic for DOX, including the intact drug molecule characteristic signal. Such spectral data testify to both the effective loading of the drug molecules onto MoS_2 nanosheets and the preservation of DOX's chemotherapeutic properties within the nanocomposite.

At the next stage of the study, quantum chemical modeling using the DFT/M06-2X method was conducted to explore the structural and energetic characteristics of DOX interactions with MoS_2 nanosheets. The calculations indicated that DOX molecules can form stable noncovalent stacked complexes with the MoS_2 nanoparticles as well as covalent bonds with the edges of the nanosheets. These findings underscore the potential of MoS_2-based platforms for multifunctional drug delivery applications, offering valuable insights into strategies for achieving effective control over drug loading and release mechanisms.

Acknowledgements
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Lecture 25

TOWARDS THE STRUCTURE-ACTIVITY CORRELATION FOR SELECTED THIOSULFONATES – SPECTROSCOPIC STUDIES AND MOLECULAR MODELLING

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Antimicrobial resistance (AMR) has become one of the key healthcare problems in recent years [1]. It provides the necessity to analyse the antibiotics market on drugs` effectiveness and to develop new medicines. Thiosulfonates are one of the promising potential antibiotics, but the scientific literature demonstrates limited information on their structure-activity relationships [1,2]. To expand the available data, three derivatives were studied: 4-aminobenzene-1-sulfonothioate (1), S-ethyl 4-acetamidobenzene-1-sulfonothioate (2), and S-methyl 4-acetamidobenzene-1-sulfonothioate (3). The crystal and molecular structures of 1-3 thiosulfonates were studied experimentally at 100 K. Theoretical analysis, using density functional theory (DFT) on their molecular structure and vibrational IR, Raman, as well as NMR parameters were provided. Electronic properties of all studied compounds were explored using predicted geometric and magnetic aromaticity indexes, as well as substituent push-pull effects. Compounds 1-3 antibacterial properties were studied on two model bacteria strains: Gram-positive *Staphylococcus aureus* ATTC 6538P and Gram-negative *Escherichia coli* ATTC 8739. A general mechanism of thiosulfonates 1−3 biochemical actions was proposed according to the literature data [1,2]. Its feasibility was analysed using DFT theoretical studies. The obtained results provide a deeper insight into compounds 1-3 molecular structure and IR/Raman and NMR spectroscopic and chemical reactivity properties. A direct correlation between some NBO parameters and the S-S bond energy in compounds 1−3 with their activity against both studied bacterial strains was observed.

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Lecture 26

MESO-BENZODIOXOLE-BODIPY AS PH – SENSITIVE FLUOROPHORES

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BODIPY dyes constitute a well-established class of fluorophores distinguished by their strong absorption, high fluorescence quantum yield and remarkable photostability, which make them versatile platforms for the development of responsive fluorescent systems.
This work focuses on the structure–property relationships in four BODIPY dyes bearing different functional groups capable of modulating the electronic structure and protonation behaviour of the chromophore (*Fig.1*) including Schiff bases or Serotonin.[1-5]

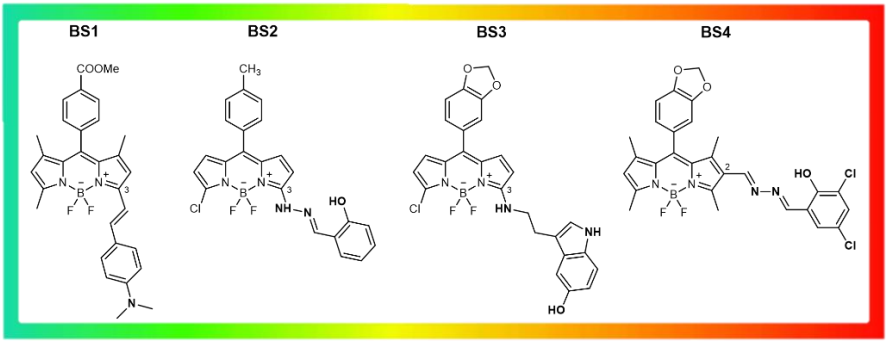

*Fig. 1 Chemical structures of selected BODIPY fluorophores (**BS1–BS4**).*

All dyes were synthesized and fully characterized by NMR spectroscopy and mass spectrometry (MS). Their photophysical properties were investigated using UV-Vis absorption and fluorescence spectroscopy in solvents of varying polarity and across different pH.
To support the experimental results, DFT and TD-DFT calculations were performed, providing insight into the electronic structure, conformational preferences, and non-covalent interactions. The combined experimental and theoretical studies show that rational modification of the BODIPY dyes enables one to tune their photochemical response and sensitivity to pH.
An insightful study reveals that the BODIPY dyes exhibit pronounced solvatochromic and halochromic behaviour. Moreover, substitution at 4,4-difluoro-4-bora-3a,4a-diaza-*s*-indacene core with the proton-responsive groups makes the BODIPY dye a potential pH-sensor. These findings highlight the potential of the investigated systems as adaptable fluorescent probes for applications in biologically relevant environments.

Acknowledgments
The authors gratefully acknowledge the Wrocław Centre for Networking and Supercomputing (WCSS) for computational facilities

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Physical Chemistry for Medical Applications

European Meeting on Physical Organic Chemistry

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Posters in alphabetical order

Poster 1

DIAGNOSING RHEUMATIC DISEASES USING VIBRATIONAL SPECTROSCOPY AND NMR-BASED METABOLOMICS

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Rheumatic diseases are a subclass of autoimmune diseases that affect multiple systems in the human body, causing severe pain and suffering in those affected. Correctly diagnosing these conditions is challenging, as rheumatic diseases share similar clinical symptoms but lack specific markers and tests for rapid differentiation. This is the case, for example, with rheumatoid arthritis (RA) and psoriatic arthritis (PsA) [1]. In our research aimed at rapidly distinguishing patients with RA from those with PsA, we utilize spectroscopic diagnostic techniques based on the construction of discriminative mathematical models derived from the vibrational spectra of body fluids. Nuclear magnetic resonance (NMR) spectroscopy can be used as a complementary tool to study the metabolome of patients, providing new information that can be correlated with the variance in the vibrational spectral dataset.

FT-Raman and near infrared (NIR) spectra of lyophilized blood sera of RA and PsA patients as well as healthy controls were collected. ^{1}H NMR spectra of deproteinized samples in phosphate buffer were also acquired. Discriminant models were constructed with the use of partial least squares discriminant analysis (PLS-DA) and counter propagation artificial neural networks (CPANN). Optimization of classifiers involved selecting specific spectral ranges and applying an appropriate data processing procedure, which produced models with the highest predictive abilities. Quality parameters such as sensitivity, specificity and overall accuracy (OA) were used to assess the performance of classifiers. Several models achieved accuracy levels above 90%. By including selected biochemical parameters of blood serum into the spectral dataset, so-called 'hybrid' models were created which operated on higher level than their predecessors, achieving OA of 94% for PLS-DA classifiers [2]. Obtained results demonstrate that vibrational spectra of body fluids are a valuable source of data for construction of classifiers which enable differentiation between clinically similar diseases. The developed analytical protocols can be used as a potential tool in population-based screening studies of rheumatic diseases.

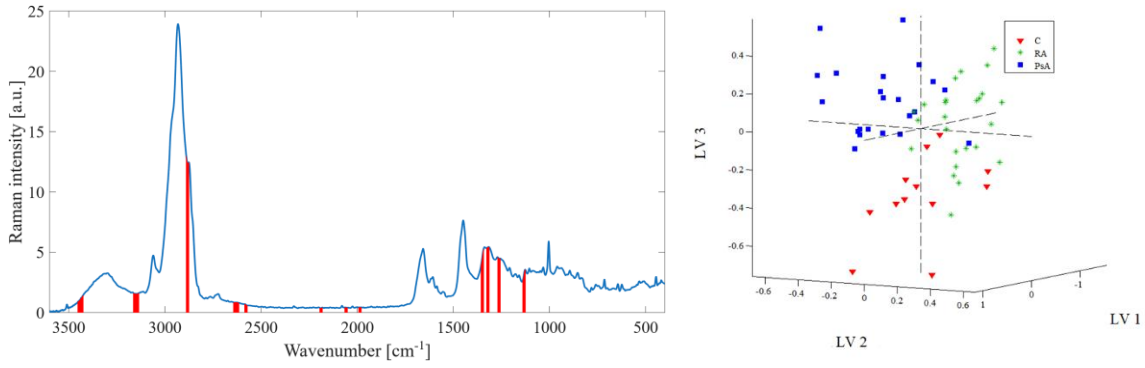

Fig. 1.: Raman spectrum of lyophilized blood serum with regions selected for analysis (right); scores plot for PLS-DA classifier based on Raman spectra (left).

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Poster 2

DIELECTRIC PROPERTIES OF REVERSE MICELLES FORMED BY NONIONIC SURFACTANTS

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The relationship between composition, microstructure, and physicochemical properties of nonionic surfactant systems was investigated using model microemulsions based on Tween-type surfactants. Particular attention was paid to the formation of reverse micelles and their dielectric behavior.

Phase behavior was analyzed using ternary phase diagrams, while the microstructure of the systems was characterized by polarized optical microscopy (POM) and dynamic light scattering (DLS). Additional measurements of density and viscosity provided complementary information on the structural organization of the systems.

The applicability of the critical packing parameter (CPP) and hydrophilic-lipophilic balance (HLB) [1] for predicting aggregation behavior was evaluated. While both parameters proved useful at a qualitative level, their limitations became evident in multicomponent systems. Tween 20, characterized by a high HLB value, favored the formation of normal micelles in the Tween 20/cyclohexane/water system, whereas reverse micelles were formed only in the Tween 80/Span 80/decane/water system.

Dielectric spectroscopy [2] revealed a strong dependence of system properties on composition, particularly water content. In the Tween 20/cyclohexane/water system, within the isotropic region – where reverse micelle formation could be expected - significant low-frequency dispersion was observed, associated with electrode polarization and indicating the presence of effective charge transport pathways. This suggests that the system behaves as a homogeneous isotropic solution rather than a typical reverse micellar structure. In contrast, the reverse micellar system based on Tween 80/Span 80 exhibited reduced conductivity and weaker electrode polarization, indicating better isolation of the aqueous phase within micelles.

Nonlinear changes in dielectric permittivity (ε') and dielectric loss (ε") with increasing water content were observed, reflecting structural reorganization of the aggregates. Three distinct regimes were identified, corresponding to morphological transitions, stable micellar structures, and increased contribution of the polar phase to the dielectric response. The observed behavior indicates that water plays a key role in controlling micellar size, interactions, and charge transport mechanisms.

The nonlinear dielectric effect (NDE) [3] was found to be positive in nonionic reverse micellar systems and was primarily attributed to field-induced structural changes and anisotropy of the aggregates, representing a mechanism distinct from that observed in ionic reverse micelles, where charge transport and migration of charged species play a dominant role [4]. The magnitude of the effect increased with water content, confirming the importance of structural factors in determining the dielectric response of nonionic systems.

The results demonstrate that, although simple parameters such as CPP and HLB are useful for preliminary system design, the actual behavior of nonionic micellar systems is governed by complex structural and dynamic processes, including aggregate reorganization and interactions between confined water and surfactant molecules.

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Poster 3

Β-SITOSTEROL-INDUCED MEMBRANE RIGIDIFICATION IN MODEL LIPID BILAYERS: AN FT-IR STUDY

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The physicochemical properties of lipid membranes are strongly influenced by the presence of sterols, which modulate membrane fluidity, packing, and phase behavior. Phytosterols, including β-sitosterol [1], are of particular interest due to their biological activity and potential applications in liposomal drug delivery systems [2,3]. However, the effect of β-sitosterol on lipid bilayers differing in surface charge and conformational order remains insufficiently understood.

This study investigates the influence of β-sitosterol on the conformational organization of lipid membranes composed of dipalmitoylphosphatidylcholine (DPPC) [4], dipalmitoylphosphatidylcholine/dipalmitoyl-phosphatidylglycerol [5] (DPPC/DPPG), and egg phosphatidylcholine (eggPC) [6]. Liposomes containing β-sitosterol at different molar ratios (8.5:1.5, 8:2, and 7:3) were analyzed using Fourier-transform infrared (FT-IR) spectroscopy in the temperature range of 15–60 °C. Structural changes in the hydrocarbon chains were evaluated based on the $\nu_{as}(CH_2)$ and $\nu_s(CH_2)$ stretching vibrations, while Principal Component Analysis (PCA) was applied to support the interpretation of thermotropic properties.

The results demonstrated that β-sitosterol induces conformational ordering of lipid bilayers by increasing the proportion of *trans* conformers within the hydrocarbon chains [7,8]. In DPPC systems, the strongest rigidifying effect was observed at the lowest β-sitosterol concentration, particularly at elevated temperatures, indicating reduced membrane fluidity and decreased cooperativity of the main phase transition. In negatively charged DPPC/DPPG membranes, the effect of β-sitosterol was significantly weaker, suggesting that membrane surface charge limits sterol-induced ordering. In contrast, eggPC membranes, characterized by a higher initial content of *gauche* conformers, exhibited pronounced sensitivity to β-sitosterol, particularly at low temperatures, where significant membrane rigidification was observed.

Overall, the results indicate that both membrane charge and the initial conformational disorder of lipid hydrocarbon chains strongly affect the interaction of β-sitosterol with lipid bilayers. The observed membrane-stiffening effect suggests that DPPC- and eggPC-based liposomes may represent promising carriers for β-sitosterol delivery and other bioactive compounds.

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Poster 4

SPECTROSCOPY-BASED IMAGE OF HEALTHY HUMAN ERYTHROCYTES

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Erythrocytes are specialized cells with a characteristic biconcave shape, whose function is to transport oxygen and carbon dioxide via hemoglobin - a protein containing four globin subunits with heme groups, each with an iron atom [1,2]. Red blood cells exhibit significant biochemical and structural changes used to assess health status [3].

Raman spectroscopy is widely used in biochemical and medical research, including the analysis of erythrocyte structure and function [4]. When combined with optical microscopy Raman microspectroscopy enables the analysis of cellular molecular composition at the level of individual structures [5]. This technique allows for the identification of key erythrocyte components, such as heme porphyrin groups, providing information on the organization and properties of the macromolecules that make up blood cells.

The aim of the study was to develop a spectroscopic profile of erythrocytes taking into account gender and age. Raman spectra of erythrocytes obtained from study participants—sixteen women and twelve men—were analyzed, and principal component analysis (PCA) was then applied to identify differences between the modeled groups. The results indicate the possibility of distinguishing erythrocytes based on sex and age using their spectroscopic characteristics, which confirms the potential of Raman microspectroscopy as a tool to support diagnostics and biomedical research.

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Poster 5

FROM DISORDER TO STABILITY: PEG MODULATION OF PHYTOSTEROL-CONTAINING DPPC MEMBRANES

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Understanding the factors that govern the stability and organization of lipid membranes is essential for the development of advanced drug delivery systems. Liposomes, as biomimetic models of biological membranes, are widely applied in pharmaceutical and nutraceutical fields; however, their performance strongly depends on the physicochemical properties of the lipid bilayer. The incorporation of phytosterols can modulate membrane fluidity and stability, but may also disrupt lipid packing and reduce the cooperativity of phase transitions. In this context, PEGylation has emerged as an effective strategy to enhance colloidal stability and prolong circulation time of liposomal carriers, although its role in phytosterol-containing systems remains insufficiently understood.

This study investigates the effect of PEGylation on the structural and thermotropic properties of dipalmitoylphosphatidylcholine (DPPC) lipid bilayers containing phytosterols and their fatty acid esters. Liposomes were prepared using the thin-film hydration method with DPPC as a model system, supplemented with stigmasterol and its derivatives (myristate, oleate, and palmitate), in the presence or absence of DSPE-PEG(2000). Membrane organization was analyzed using Fourier-transform infrared (FT-IR) spectroscopy over a temperature range of 10–60 °C, supported by principal component analysis (PCA), while transmission electron microscopy (TEM) provided insight into vesicle morphology.

The results show that phytosterols increase conformational disorder and reduce the cooperativity of the main phase transition. In contrast, PEGylation enhances membrane stability, leading to smoother phase transitions, higher transition temperatures (Tm), and increased lipid chain mobility. Spectroscopic data and PCA indicate improved structural homogeneity in PEGylated systems, while TEM images confirm more uniform and flexible vesicle morphology. Overall, PEGylation mitigates the destabilizing effects of phytosterols, promoting the formation of more stable and functional lipid bilayers, highlighting their potential as advanced nanocarriers.

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Poster 6

POLYPHENOL-MEDIATED MODULATION OF LYSOZYME–MEMBRANE INTERACTIONS UNDER PHYSIOLOGICAL IONIC CONDITIONS

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Protein–membrane interactions play a critical role in both physiological processes and the early stages of protein misfolding and aggregation. In particular, membrane charge and ionic conditions strongly influence protein conformational stability, while small bioactive molecules may modulate these effects. In this study, we investigate how selected polyphenols affect lysozyme (LSZ) behavior in negatively charged lipid membranes under physiological ionic conditions.

Model membrane systems were prepared as large unilamellar vesicles (LUVs) composed of zwitterionic DPPC and anionic DPPG (1:1 molar ratio). The presence of NaCl at physiological concentration was used to mimic ionic environments relevant to biological systems. Temperature-resolved Fourier-transform infrared (FT-IR) spectroscopy, combined with principal component analysis (PCA), was applied to monitor structural changes in both lipid bilayers and LSZ, with particular emphasis on the amide I region and CH_2 stretching vibrations.

The results show that physiological ionic conditions promote destabilization of negatively charged membranes, leading to vesicle fusion, lipid loss, and significant conformational rearrangements in LSZ. These changes follow a characteristic β → α → β transition pattern, suggesting the formation of intermediate states associated with early-stage misfolding and aggregation. Morphological observations support a mechanism involving progressive membrane disruption and lipid-mediated protein aggregation.

The introduction of polyphenols (resveratrol, quercetin, and caffeic acid) alters this behavior. PCA analysis reveals reduced structural heterogeneity and a shift toward more stabilized protein–membrane systems. These effects are accompanied by increased membrane order and partial suppression of LSZ-induced bilayer disruption, indicating that polyphenols can modulate both membrane properties and protein conformational dynamics.

Overall, this study demonstrates that polyphenols can mitigate ion-induced destabilization of lipid membranes and influence the conformational landscape of proteins at membrane interfaces. The combined FT-IR–PCA approach provides detailed molecular insight into these processes and offers a framework for understanding and controlling early misfolding events in biologically relevant environments.

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Poster 7

MOLECULAR DYNAMICS ANALYSIS OF THE EFFECT OF MG^{2+} ON NONENZYMATIC SELF-REPLICATION OF RNA

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The nonenzymatic self-replication of RNA is a key concept in origin-of-life research. Central to the RNA World hypothesis is that the nonenzymatic, template-directed extension of RNA primers must have occurred efficiently prior to the emergence of enzymes. While it is well-established that divalent metal ions such as Mg^{2+} play an essential catalytic role in promoting phosphodiester bond formation [1], the exact molecular mechanism by which they facilitate this process remains under investigation. In this study, we present a detailed computational study of the structural and catalytic dynamics of RNA primer extension using imidazole-activated nucleotides, the reactive electrophilic species in template-directed copying [2,3]. Using Molecular Dynamics (MD) simulations, we explored the specific coordination of the reaction site. Our results indicate that Mg^{2+} ions contribute to preorganization of the primer–template complex by stabilizing reactive conformations. In addition, we show that pyrimidine thiolation enhances Watson–Crick fidelity and structural readiness, acting synergistically with Mg^{2+} to promote nucleophilic attack. By deciphering these molecular interactions, this work highlights the essential roles of metal catalysis and chemical diversity in early evolution. These findings offer insights into the role of metal ions and deepen our understanding of RNA's potential for self-replication in prebiotic environments.

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Poster 8

DECODING MOLECULAR MECHANISM OF NIR-INDUCED THERMAL PROTECTION

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The outermost layer of skin, the stratum corneum (SC), serves as a vital biological barrier protecting the organism from external physical, chemical, and mechanical factors. This layer's integrity depends on the "bricks and mortar" organization, in which protein-rich corneocytes are embedded in a complex lipid matrix consisting of ceramides, cholesterol, and free fatty acids. Temperature and Near-Infrared (NIR) radiation induce significant molecular modifications in these components. While high temperatures usually lead to irreversible protein denaturation and lipid disorder, NIR radiation is widely used in biomedical engineering and phototherapy due to its deep penetration and potential for photobiomodulation [1].

The porcine skin was used as a model for healthy human tissue. The temperature-induced changes (from 20 to 90°C) were monitored by Attenuated Total Reflectance Infrared (ATR-IR) spectroscopy. To study the effect of NIR radiation, samples were exposed to the light (700–2000 nm) for 15 minutes. The spectral analysis focused on the Amide I band, which is a highly sensitive marker for the secondary structure of proteins. Lipid phase transition temperatures were determined by two independent methods: the first derivative of the Boltzmann function and the method of tangent lines applied to sigmoidal temperature-dependent band shifts.

The study evidenced that NIR radiation exerts a protective effect on SC components against thermal degradation. As shown, NIR exposure shifted the temperature of the first lipid phase transition (orthorhombic-to-hexagonal) from 40 °C to 46 °C, suggesting more stable lipid ordering. This shift indicates that the radiation facilitates a more stable orthorhombic packing of lipid alkyl chains. This stabilization increases the permeability of the SC, potentially improving its barrier function. While the first transition showed a significant temperature shift, the second one (hexagonal-to-disordered) near 70 °C remains nearly invariable, suggesting that the protective effect of NIR radiation is more evident during the initial stages of thermal disordering.

As shown, the α-helix structure in irradiated samples was stable up to 57 °C, whereas untreated samples showed significant unfolding and earlier denaturation. Besides, the temperature at which structurally bound water was destroyed increased from 79 °C in intact skin to 87 °C in NIR-exposed samples. These findings indicate that NIR radiation facilitates partial dehydration and strengthens hydrophobic interactions, making the SC more resistant to thermal stress [2,3].

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Poster 9

BENCHMARKING DISPERSION-CORRECTED DFT METHODS FOR THE EVALUATION OF STRUCTURAL AND ENERGETIC PROPERTIES OF SELECTED PHARMACEUTICAL COMPOUNDS

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Developing new drugs is a challenging task, and using computational techniques can make it more efficient [1, 2]. One of these techniques is density functional theory (DFT), which is widely used in condensed matter physics. The reliability of results depends on the exchange-correlation approximation used. Popular approximations such as local density or generalized gradient approximations (LDA and GGA respectively) are not suitable for studying molecular systems because they do not include long-range van der Waals interactions. However, there is a possibility to include these interactions through an atom-pairwise dispersion correction added a posteriori to the DFT total energy. Here, we benchmarked several dispersion correction schemes to study selected nonsteroidal anti-inflammatory drugs. In particular we focused on two polymorphs of acetylsalicylic acid (aspirin). While there are some reports about DFT studies of aspirin [3, 4], in our comparative study we focused on previously unused approximations, e.g. the density-dependent energy correction method or meta-GGA SCAN functional with Grimme D3 approach. The best agreement for the structural properties was found for the Tkatchenko-Scheffler and many-body dispersion methods. Relative errors were less than 0.5%, compared to up to 7% for GGA. In addition, the meta-GGA SCAN functional without dispersion correction leads to a relative error of less than 1%. Interestingly, including Grimme-D3(BJ) in the SCAN functional led to worse results compared to the uncorrected one. Finally, all approximations, except the many-body dispersion scheme, incorrectly predict the form II of aspirin as the lowest energy form.

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Poster 10

ANALYSIS OF FOLLICULAR FLUID SAMPLES BY FT-IR AND NMR SPECTROSCOPY

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Infertility is defined as inability to conceive after a year of regular, unprotected sexual intercourse, with approximately 1 in 6 people globally experiencing it in their lifetime [1,2]. However, the diagnostic process is lengthy and often requires several invasive procedures. For this reason, alternative protocols are being investigated, such as identifying infertility markers in biological fluids by spectroscopy [3].

This study focused on the analysis of follicular fluid of infertile and fertile women by FT-IR and NMR spectroscopy and identifying differences in their spectra, which in conjunction with medical data could be used in sample classification. The IR spectra were recorded using the ATR technique by applying 1 µl of liquid sample onto the ATR crystal and drying it under a steady nitrogen flow for 10 minutes before collecting the data. In the case of NMR measurements, 30 µl of sample was mixed with phosphate buffer in deuterated water and 1D-NOESY sequence was applied.

The data was then analyzed by PCA and PLS-DA with medical diagnostic information used for class assignment. Clear clustering of data points was observed, suggesting the presence of minute differences between the composition of follicular fluid in fertile and infertile women. This is supported by PLS-DA loadings showing the largest contributions to class separation as signals in the amide I and II band region and 3600-2800 cm^{-1} region which is comparable to the calculated difference spectrum between the mean spectra of both sample classes (Figure 1).

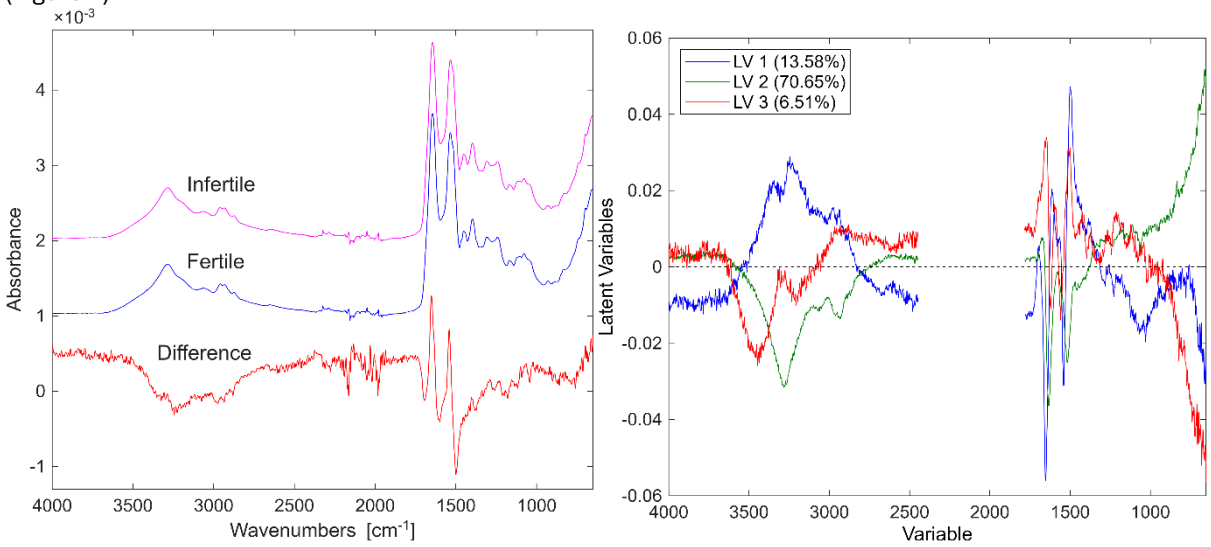

Figure 1: Left: Mean spectra of fertile and infertile women and their difference. Right: PLS-DA variable/loading plot

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Poster 11

CHEMICAL BRAIN FINGERPRINT OF A RAT WITH ASD-INDUCED DYSFUNCTION

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Autism spectrum disorder (ASD) is a neurodevelopmental disorder caused by genetic and environmental factors. This disorder develops in fetuses and very young children. ASD-related changes have been observed in brain structures such as the midbrain, hippocampus, and temporal and occipital lobes [1]. Individuals diagnosed with ASD have difficulties with communication, social interactions, and repetitive behavioral patterns. Nevertheless, the severity and frequency of symptoms may vary from person to person [2]. Currently, the diagnosis of ASD is based on behavioral assessment rather than changes in brain structure. Previous studies on the evaluation of brain tissue from rats with induced ASD have utilized electrophysiological techniques [3], NMR, or HPLC [4]. No reports have been found in the literature regarding the use of Raman spectroscopy to study brain tissue from rats with induced autism spectrum disorder. Raman spectroscopy is a non-invasive technique widely used in biomedicine [5]. Analysis of lipid composition and concentration in brain tissue may undergo significant changes in diseased tissues, making Raman spectroscopy an alternative diagnostic tool for determining, for example, the type and stage of a brain tumor or a neurodegenerative disease [6].

The aim of this study was to identify structural changes in brain tissue in an animal model with induced ASD using Raman spectroscopy.

The study used brain tissue from Sprague-Dawley rats with induced ASD and a control group. The prepared brain tissue was analyzed using a Raman spectroscopy. The measurements were performed on unfixed brain tissue. The Raman spectra for both study groups turned out to be very similar. Therefore, to analyze the obtained results, they were subjected to principal component analysis (PCA) to recognize dissimilarities between the spectra modeled by individuals with induced – ASD and the control group. The analysis was performed using Unscrambler X software. Differences between the spectra were identified and discussed.

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Poster 12

ASSOCIATION OF MENTHOL IN NON-POLAR SOLVENTS

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Alcohols form associates via hydrogen bonding. These associates can be open (dipolar) or cyclic (non-polar). The possibility of forming both types of associates is related to the structure and conformation of the alcohol. A strong external electric field is expected to favor the formation of dipolar species [1,2].

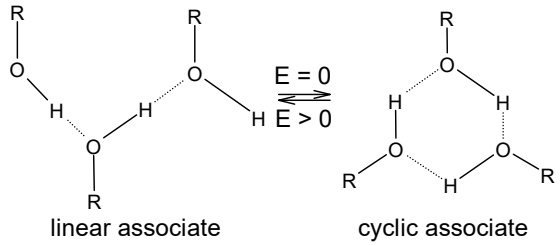

Figure 1. Formation of associations in alcohols.

The influence of a strong electric field can be investigated using the non-linear dielectric effect (NDE) technique. The NDE experiment is based on measuring the difference between the electric permittivity obtained at a strong electric field (ε'_E) and at a weak electric field ($\varepsilon'_{E\to 0}$):

$$\Delta\varepsilon_{NDE} = \varepsilon'_E - \varepsilon'_{E\to 0}.$$

According to the Debye–Langevin theory, in dipolar liquids the NDE increment should be negative and proportional to the square of the electric field strength. Nevertheless, a positive NDE increment has been observed in certain liquids, including nitrobenzene, 1,2-dichloroethane, and higher alcohols. This "anomalous" behavior is attributed either to conformational changes, as in the case of 1,2-dichloroethane, or to rearrangement of intermolecular complexes, as in the case of nitrobenzene and alcohols. This effect is a valuable property used to investigate structural questions [1–3].

This paper examines menthol solutions in non-polar solvents: p-xylene and 1,4-dioxane. A positive NDE increment is observed within a certain concentration range of the solutions. Conformational changes are unlikely to account for this effect; instead, we attribute it to an electric-field-induced shift from cyclic to linear structures. IR measurements confirm the formation of different menthol associates. The possibility of forming low-polar associates has been demonstrated by crystallographic studies of menthol, which reveal the formation of a "three-leaf clover" motif in the unit cell.

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