Uniwersytet Gdański

CHEMIA UG

MASTER Theses
OFFERED TO SECOND CYCLE STUDIES
IN CHEMISTRY
Specialisation DIGITAL CHEMISTRY

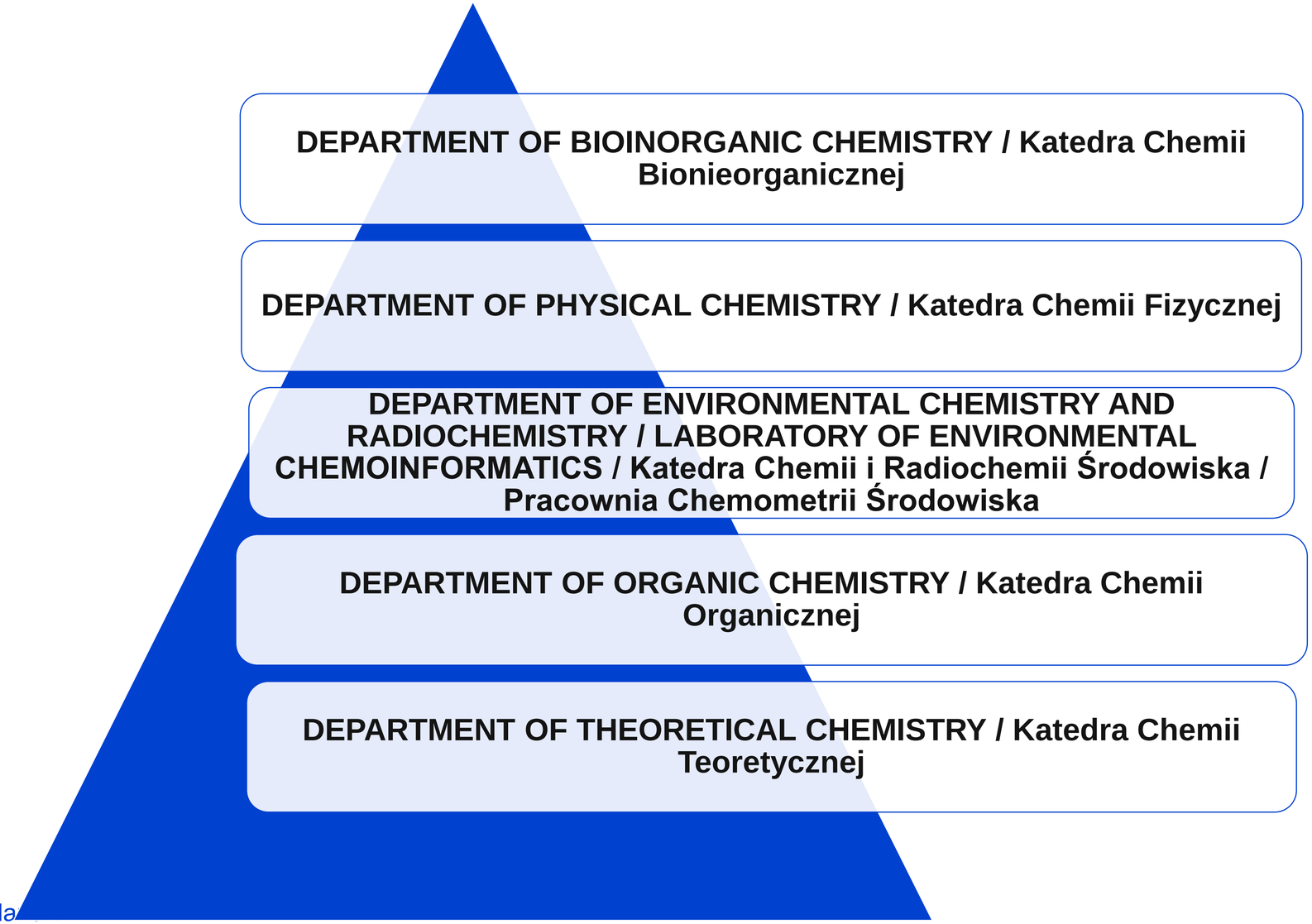
OCTOBER 2024

Faculty of Chemistry

Vice-dean for Student Affairs and Education
dr hab. Joanna Makowska, prof. UG

www.ug.edu.pl

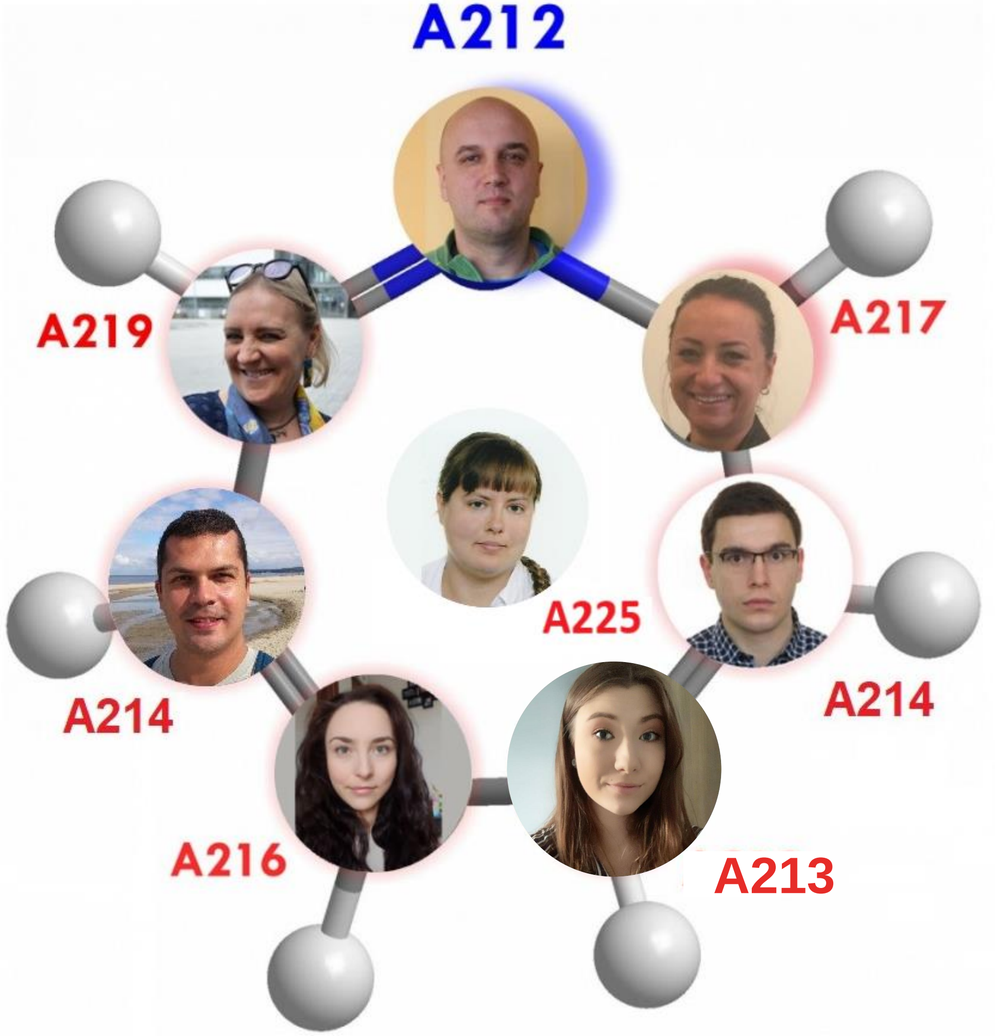
Faculty of Chemistry



Department of Bioinorganic Chemistry

MASTER'S THESIS ADVISORS

prof. dr hab. Mariusz Makowski
dr hab. Agnieszka Chylewska, prof. UG
dr hab. Aleksandra Dąbrowska, prof. UG
dr Sandra Brzeska
dr Jakub Brzeski
dr Mateusz Kowalik
dr Patrycja Wilczewska



PHD STUDENTS

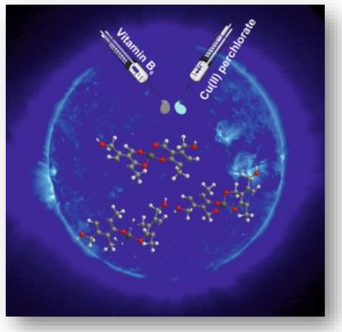
mgr Aleksandra Ciesielska
mgr Paulina Nowicka
mgr inż. Przemysław Sumczyński

Department of Bioinorganic Chemistry

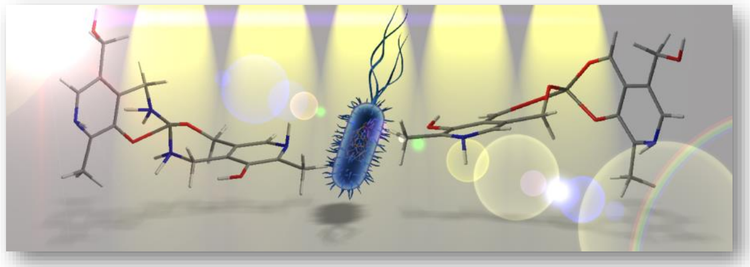
RESEARCH TOPICS

1. Research on **intermolecular interactions** of **small-molecule compounds with biomolecules** (nucleic acids, proteins, peptides, erythrocytes) using modern techniques - **biosensors**.
2. **Molecular dynamics:** studies of structures, proton transfer equilibrium reactions, determination of the properties of small- and large-molecular systems, among others by **computational methods**..
3. Design, synthesis, crystal growth and structural analysis of **bioligands** (pyrazine and pyridine derivatives, vitamins, saccharides, inorganic toxins, sulfa- and tetracycline antibiotics) and **coordination compounds** with **Ru, Cu, Fe, Ni, Cr, Co, Cd, Zn, Mn, Os** and **Ir** ions of **therapeutic or diagnostic importance**.
4. Determination of the **hydrophilic-lipophilic** nature of compounds and predicting their **solubility** in **biosystems**
5. Studies on the **equilibrium reactions** involving **acid-base** and **conformational transformations** together with the **formation of complexes** in (non-)aqueous solutions.
6. **Microbiological tests** and **cytotoxicity**.
7. **Molecular target determination.**

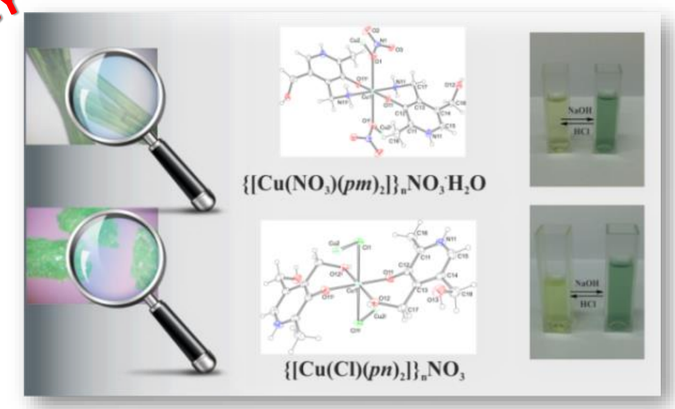
BIOTECHNOLOGY



ANALYTICS



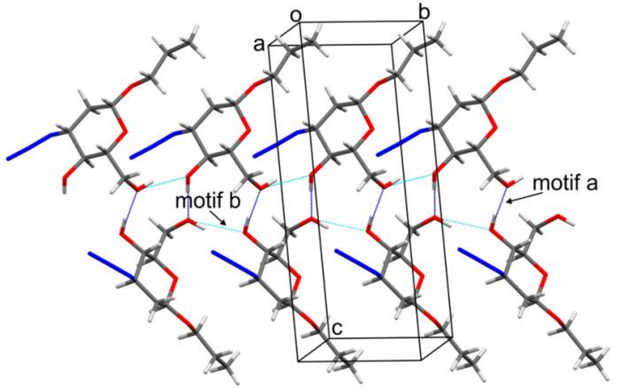
PHARAMCY



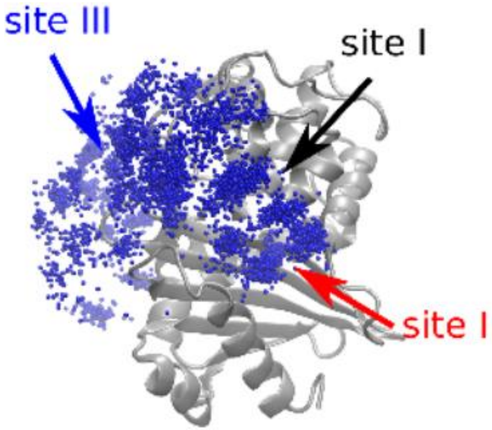
MEDICINE

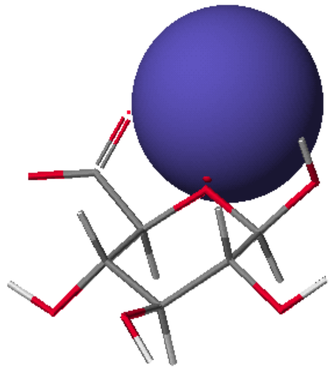
Department of Bioinorganic Chemistry

MASTER'S PROJECTS



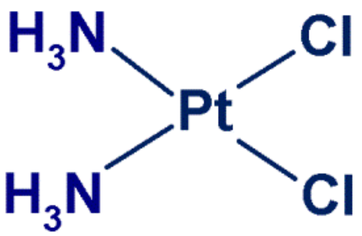
1. **Structural analyses** of compounds: spectroscopic (UV-Vis, 1H NMR, MS, ATR/IR) together with elemental analysis.
2. **Electrochemical analyses** for determination of parameters (pK_a, E_{redox}) of compounds and intermolecular interactions with biomolecules (K_b) using cyclic voltammetry.
3. **Quantitative and qualitative determination of active drug substances**, i.e. pyrazine derivatives or antibiotics, using electro-, spectro-, conductive and potentiometric methods.
4. **Conductometric, potentiometric, spectrophotometric or fluorometric titration** analyzes of aqueous and mixed-solvent systems - quantitative analyzes of composition (degree of ionization), formation of complex compounds and description of acid-base properties of the tested systems.
5. **Quantitative determination** of the interaction strength of complex connections of metal ions with biomolecules **using the flow technique**.
6. Characterization of intermolecular interactions using **theoretical tools (SAPT and QTAIM).**
7. **Quantum-chemical** description of complexation equilibria.
8. **Molecular docking** simulations of for drug development.





Department of Bioinorganic Chemistry

SPECIALIZATION LECTURE

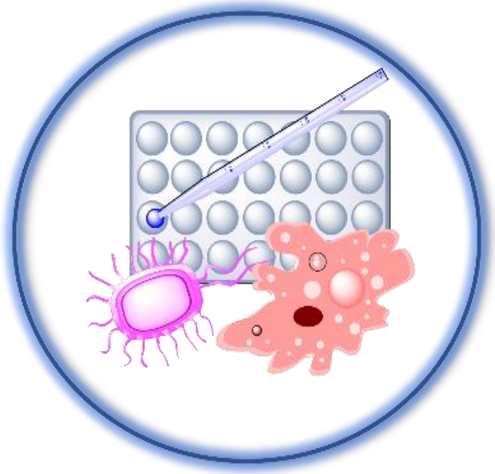


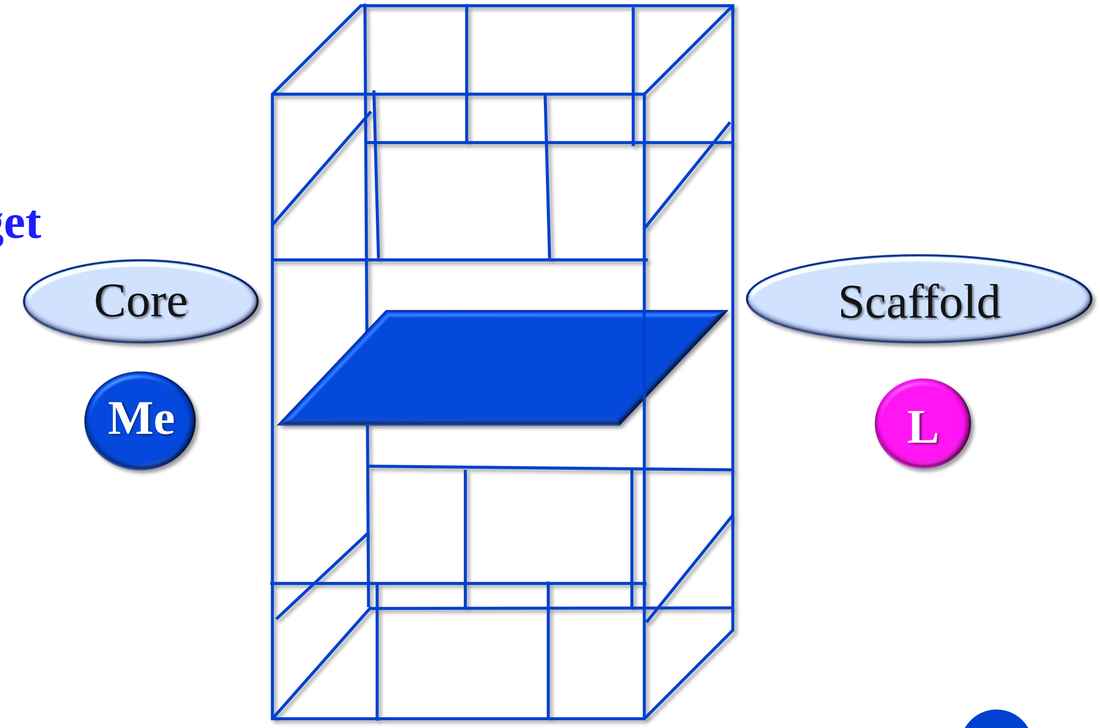
Cisplatin

Innovative metallopharmaceuticals in diagnosis and treatment

SCOPE OF THE LECTURE

- Metal pharmaceuticals – **characteristics**
- Metallopharmaceuticals – **activity**
- Metallopharmaceuticals – **properties**
- Metallopharmaceuticals – **classification**
- Metallopharmaceuticals – **examples and applications**
- Metallopharmaceuticals – **mechanism of action, molecular target**

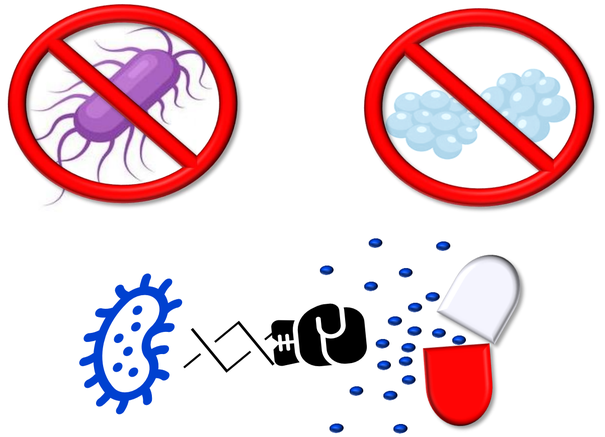




Department of Bioinorganic Chemistry

MONOGRAPHIC LECTURE

Interactions of antimicrobial compounds with metal ions

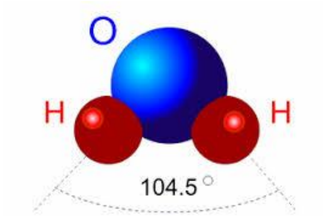


SCOPE OF THE LECTURE

- Characteristics of antimicrobial drugs;
- Antimicrobial antibiotics - classification
- Antimicrobial drugs - mechanism of action;
- Antimicrobial drugs - therapeutic index; leading structure; drug resistance; pharmacodynamics; physicochemistry of complexes;
- Antimicrobial drugs - examples

Intermolecular interactions in bioinorganic systems

SCOPE OF THE LECTURE



- Theories of chemical bonds.
- Types of intermolecular interactions.
- The molecule and its surroundings.
- Intermolecular and intramolecular hydrogen bonds.
- Low-energy intermolecular interactions in complex compounds.
- Factors affecting the strength of intermolecular interactions.
- Intermolecular interactions and physical properties.
- Theoretical and experimental evidence of the existence of hydrogen bonds.
- Elements of pharmacokinetics

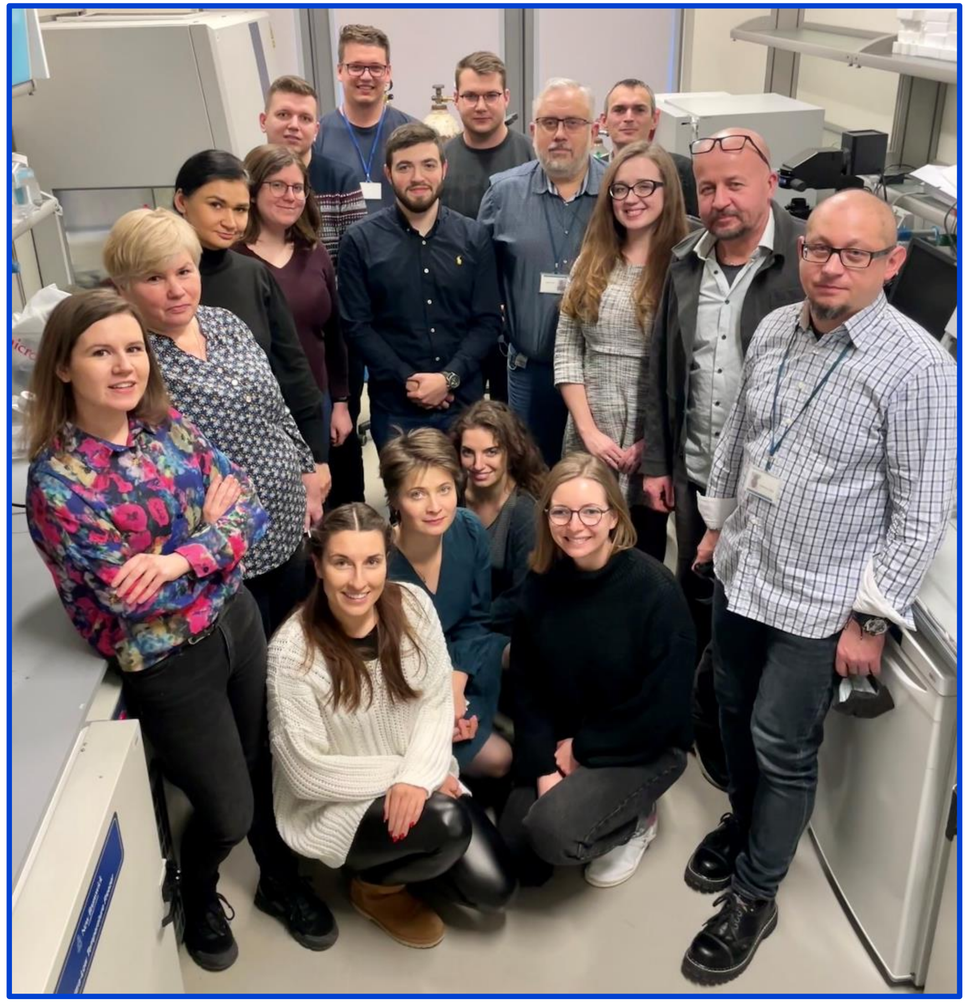
Department of Bioinorganic Chemistry

OPEN DAYS:

DATE: 17.10.2024 18.10.2024r. 10:00-14:00

CONTACT:
Jakub Brzeski (jakub.brzeski@ug.edu.pl),
Mateusz Kowalik (mateusz.kowalik@ug.edu.pl)

Department of Physical Chemistry



Head of the Department:

Prof. Janusz Rak, PhD, DSc

Staff:

Karol Krzymiński, PhD, DSc
Artur Sikorski, PhD, DSc
Piotr Storoniak, PhD, DSc
Lidia Chomicz-Mańka, PhD
Artur Mirocki, PhD
Samanta Romanowska, PhD
Beata Zadykowicz, PhD, Eng.
Magdalena Zdrowowicz-Żamojć, PhD
Beata Roszkowska

PhD students:

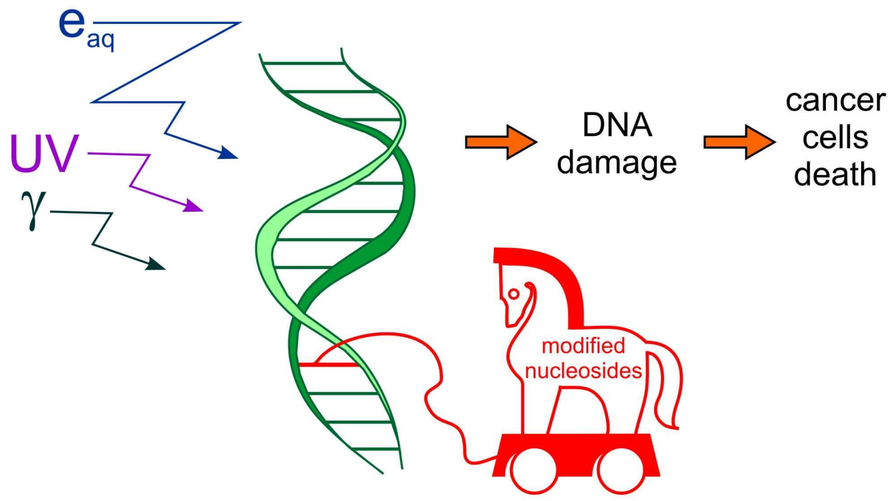
Anna Czaja, MSc
Magdalena Datta, MSc, Eng.
Vladyslav Ievtukhov, MSc
Patryk Nowak, MSc, Eng.
Paula Pryba, MSc
Małgorzata Rybczyńska, MSc
Adrian Szczyrba, MSc

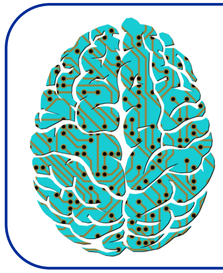
Department of Physical Chemistry

Laboratory of Biological Sensitizers

(Head of the Laboratory: prof. Janusz Rak)

- **Design and analysis of photo and radiosensitizers** for the process of DNA damage.
- Aim: **to increase the efficiency of radiotherapy or photodynamic therapy** in the anticancer treatment.
- Cooperation with Leopold Franzens Universität Innsbruck (CEUS-UNISONO grant)





Designing of new biological sensitizers

- Studies on the mechanisms of action of radiosensitizers using quantum chemical methods and machine learning
- Proposing new potential radiosensitizers
- Compounds of interest: modified nucleosides and nitroimidazolic derivatives

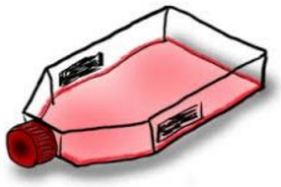
Chemical synthesis of new biological sensitizers

Stationary radiolysis experiments

- Enzymatic synthesis of DNA fragments with modified nucleosides
- Exposure of model DNA fragments to UV/X radiation
- DNA damage analysis with the use of mass spectrometry, electrophoretic and chromatographic techniques

Molecular biology

- Assessment of the cytotoxic activity of the tested compounds.
- Introducing sensitizers into the genome of human cancer cells.
- Study on the radiation-induced cellular response by flow cytometry.



Department of Physical Chemistry

Laboratory of Luminescence Research

(Head of the Laboratory: prof. Karol Krzymiński)

Synthesis and identification of new heterocyclic luminogens

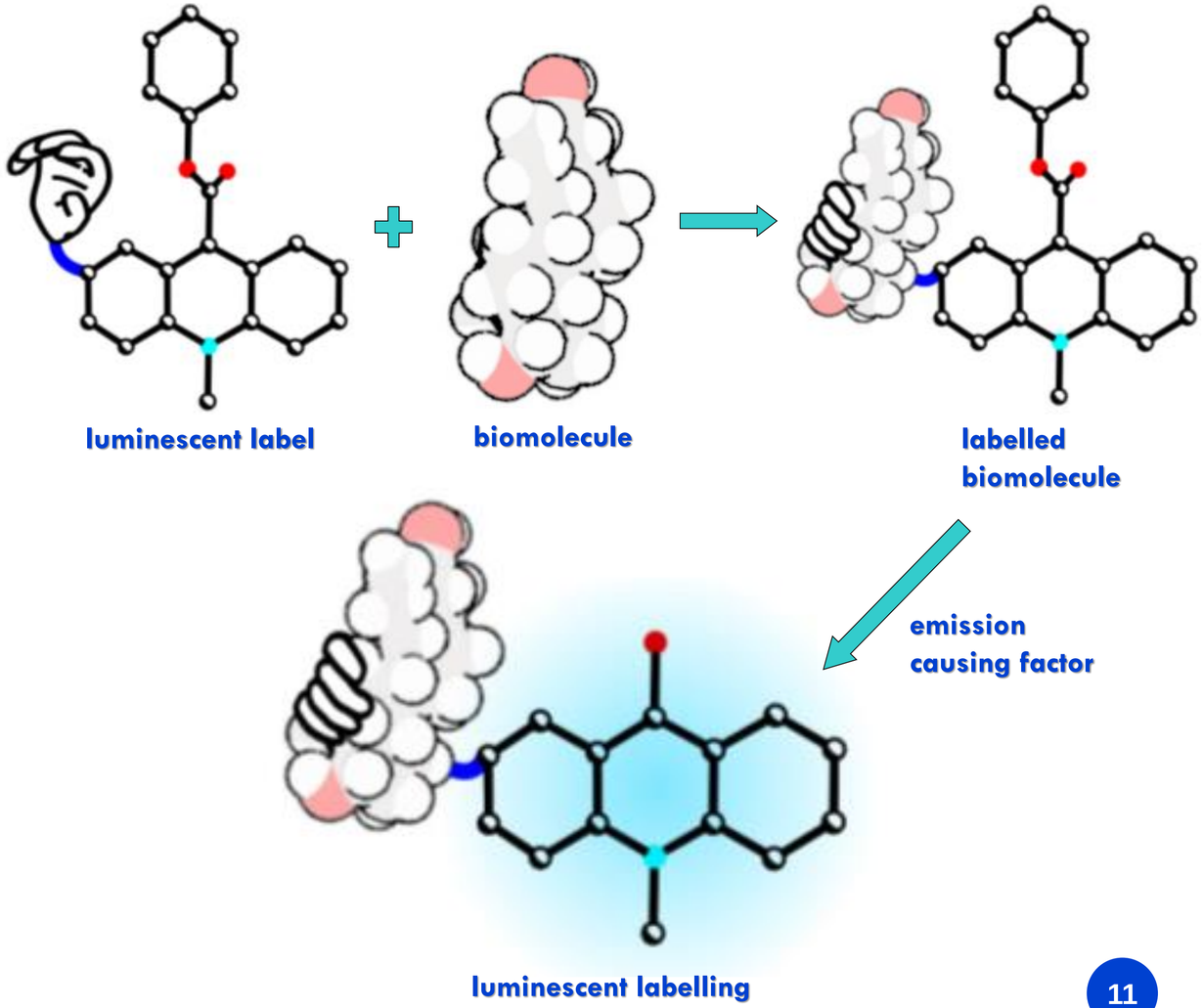
- Synthesis of heterocyclic compounds capable of emitting radiation
- Spectroscopy of heterocyclic compounds: NMR, MS, UV-VIS, IR techniques; structure-property correlation studies

Luminescence of heterocyclic compounds

- Emission spectroscopy of organic compounds (fluorescence and chemiluminescence studies)
- Chemiluminescent and fluorescent indicators and labells in luminescent immunodiagnostics
- Determination of the antioxidant capacity of biological compounds using emission techniques

Computational studies

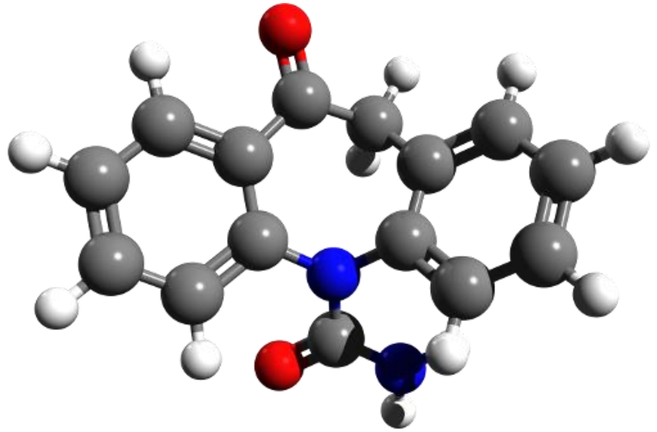
- Studies on the structure and mechanism of luminescent reactions
- Design of new fluorescent and chemiluminescent luminogens



Department of Physical Chemistry

Laboratory of Crystal Chemistry

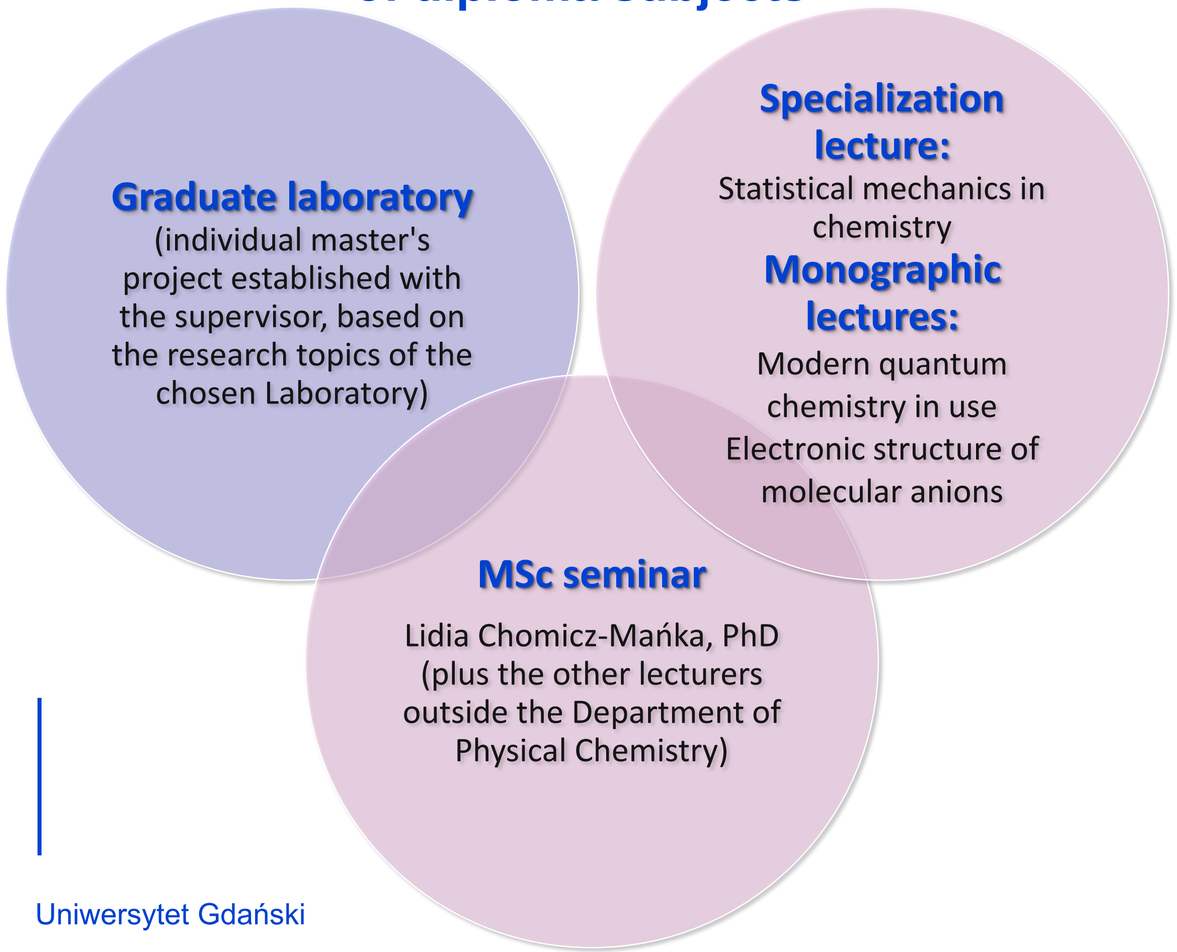
(Head of the Laboratory: prof. Artur Sikorski)



- Crystallographic studies of multi-component crystals (salts, cocrystals, solvates) containing biologically active compounds.
- Polymorphism of pharmaceutical substances.
- Analysis of intermolecular interactions in crystals.

Department of Physical Chemistry

Method of implementing a block of diploma subjects



Exemplary topics of master's theses

Laboratory of Biological Sensitizers

- **Electron-induced proton transfer in an aqueous solution of electrophilic nucleosides.**
- **8-substituted purine nucleoside derivatives as potential radiosensitizer.**
- **QM/MM studies on the phosphorylation of modified pyrimidine nucleosides by thymidine kinase 1.**
- **Rational design of oxygen mimetic radiosensitizers based on DFT modeling.**

Luminescence Research Laboratory

- **Computational study on the mechanism of chemiluminescence and energy transfer using acridinium salts.**

Crystal Chemistry Laboratory

- **Statistical analysis of structural data using the CSD crystallographic database.**

Department of Physical Chemistry

OPEN DAYS:

DATE: **October 17th and 25th, 2024**

CONTACT PERSON: **Lidia Chomicz-Mańka, B318 office**
e-mail: lidia.chomicz-manka@ug.edu.pl

WE INVITE YOU TO INDIVIDUAL MEETINGS WITH HEADS OF THE LABORATORIES OR PROJECT SUPERVISORS AND CONTACT US BY E-MAIL

Head of the Department and coordinator of enrollment:
Prof. Janusz Rak, B319 office
e-mail: janusz.rak@ug.edu.pl

Department of Environmental Chemistry and Radiochemistry

- Laboratory of Environmental Analytics and Radiochemistry
- **Laboratory of Environmental Chemoinformatics**
- Laboratory of Toxicology and Radiological Protection.

Building G, 3rd floor

Laboratory of Environmental Chemoinformatics

Prof. dr hab. Tomasz Puzyn
Profesor, Kierownik zespołu | Full Professor, Group Leader

tel. 58 523 52 48
tomasz.puzyn@ug.edu.pl

Katedra Chemii i Radiochemii Środowiska
Pracownia Chemoinformatyki Środowiska
Laboratory of Environmental Chemoinformatics

Research area

Machine Learning (ML),
Artificial Intelligence (AI)

Experiment
- ☒ Cost
- ☒ Time
- ☒ Laboratory animals

Computational methods
- ☑ Cheap
- ☑ Fast
- ☑ Without animals testing

Laboratory of Environmental Chemoinformatics

Prof. dr hab. Tomasz Puzyn

- OECD expert in QSAR methods,
- Author of over 170 scientific publications,
- Editor of 5 books,
- Speaker of over 30 invited lectures at international conferences,
- Collaborates with over 30 research teams on 5 continents,
- Winner of prestigious domestic and foreign awards,
- President of QSAR Lab Sp. z o. o.

Dr hab. Agnieszka Gajewicz-Skrętna

- Passionate about the development of computer methods,
- Author of over 60 scientific publications,
- Manager of national and international scientific projects,
- Winner of national and international scientific awards

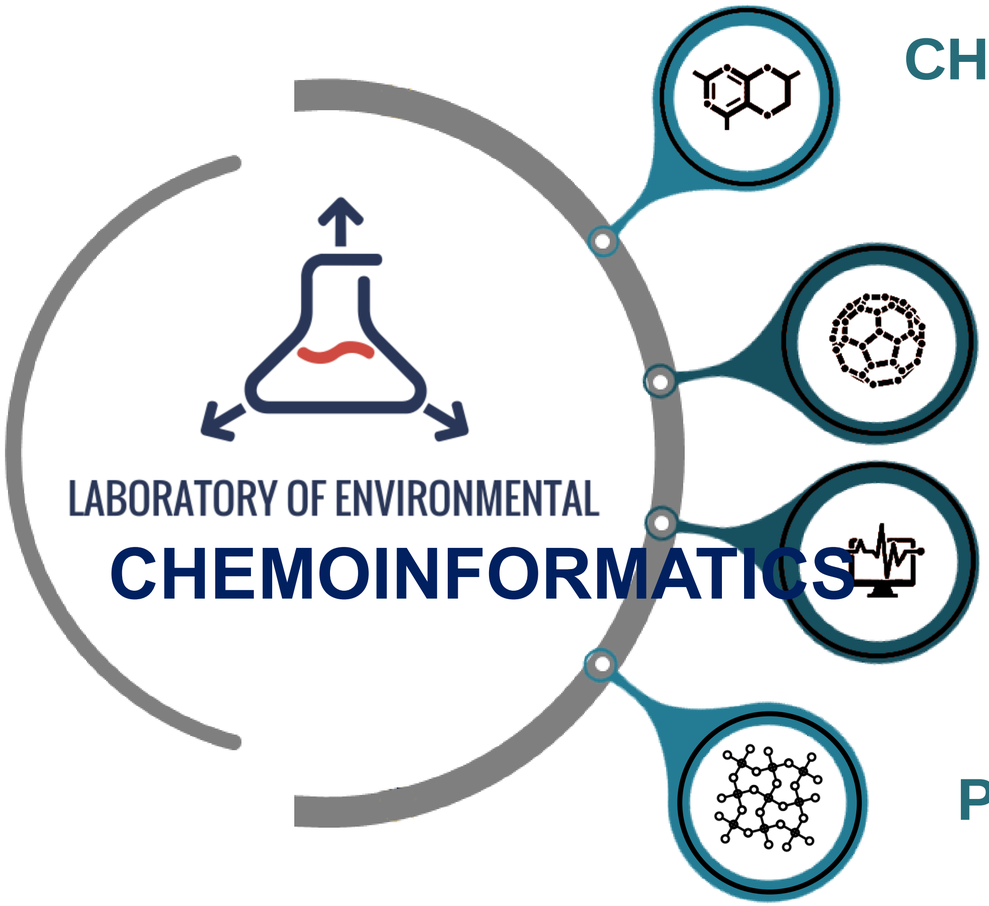
Dr inż. Karolina Jagiełło

- Specialist in statistics and chemometrics,
- Author of over 40 scientific publications,
- Coordinator of international projects at QSAR Lab Sp. z o. o.

Dr Alicja Mikołajczyk

- Expert in the design of functional materials in silico,
- Author of over 40 scientific publications,
- Coordinator of international projects at QSAR Lab Sp. z o. o.,
- Winner of national and international scientific
- awards

Areas of application of our AI/ML-based models



CHEMICAL INDUSTRY

NANOTECHNOLOGY

NANOMEDICINE
AND NANODIAGNOSTICS

PHARMACY

Research topics

- modeling of material properties at the electronic, atomic and mesoscopic levels,
- assessing (eco)toxicity and the end state of materials in the environment,
- understanding the role of the structural properties of materials in inducing responses at the ‘-omic’ level (e. transcriptomic, proteomic, metabolomic etc.),fundamental causes of adverse effects observed under the proposed Adverse Outcome Pathways (AOP),
- explaining the role of biophysicochemical interactions in the mechanism of material toxicity,
- active participation in adapting risk assessment guidelines to the specificity of (nano) materials in the regulatory context.

Department of Organic Chemistry

Laboratory of Carbohydrate Chemistry (Pracownia Chemii Cukrów)

Laboratory offer for Digital Chemistry MSc candidates:
By constructing appropriate models and using computer simulations (mainly using molecular dynamics), specific interactions between biomolecules can be identified and described.

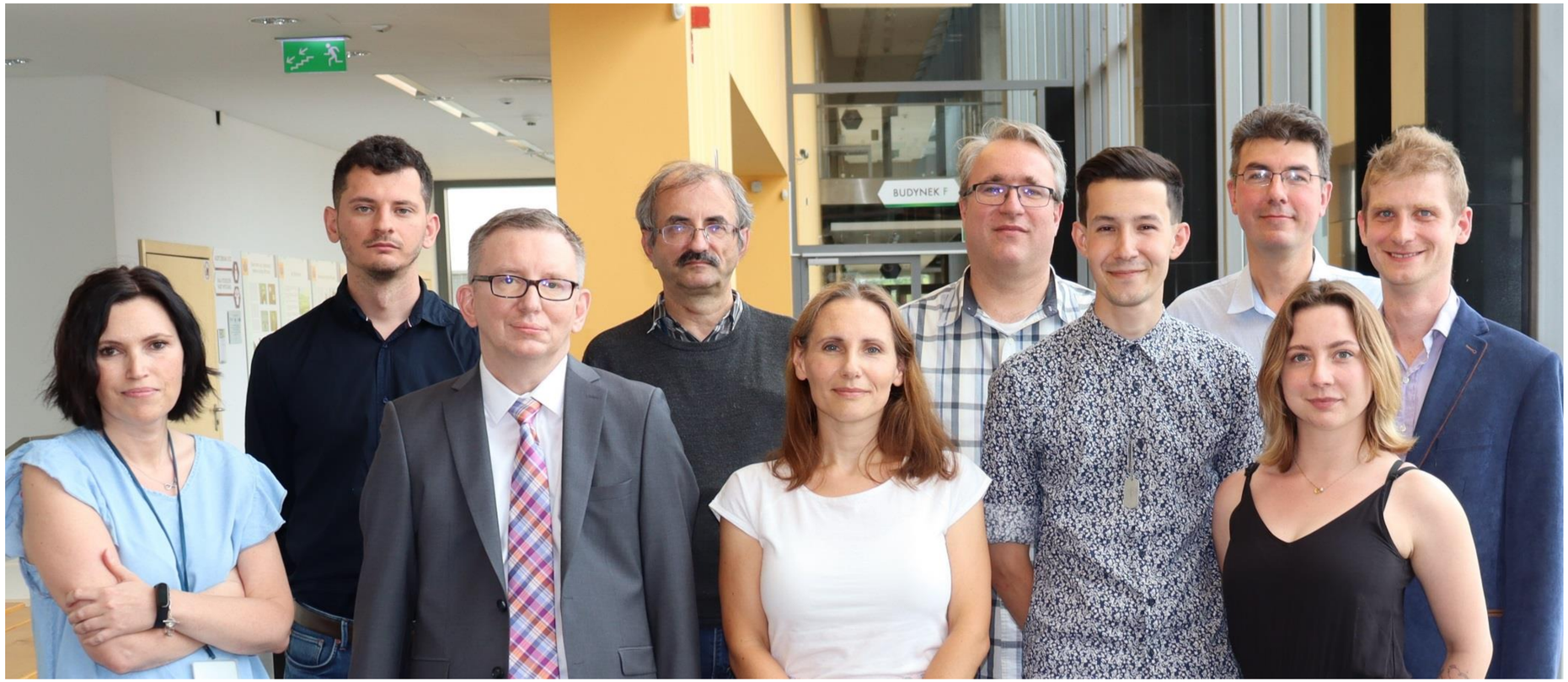
Required skills and knowledge:
- theoretical chemistry
- numerical methods – basic 😉
- high-level interpreted programming language or shell scripting

Topics of master's theses:
Ionic liquids and their dynamics.

Molecular dynamics studies on biomolecular, sugar derived systems.

CONTACT PERSON: Rafal Slusarz, rafal.slusarz@ug.edu.pl, room B11.

Department of Theoretical Chemistry



Prof. Piotr Skurski
Prof. Adam Liwo
Prof. Iwona Anusiewicz
Prof. Cezary Czaplewski

Dr hab. Adam Sieradzan, prof. UG
Dr hab. Artur Giełdoń, prof. UG
Dr hab. Sergey Samsonov

Dr Magdalena Ślusarz
Dr Sylwia Freza
Dr Marcin Czapla
Dr Margrethe Gaardlos

Department of Theoretical Chemistry

Laboratory of Quantum Chemistry

- designing novel valence- and non-valence-bound molecular anions; investigating their electronic and thermodynamic stability
- designing molecules exhibiting desired properties (tailor-made molecules), including strong oxidizing agents, superacid having desired acid strength, ionic liquids characterized by desired viscosity and electric conductivity)
- utilizing various mineral acids and superacids as catalysts
- investigating reaction mechanisms (catalyzed and non-catalyzed reactions, processes involving anions and other radical systems)
- verifying thermodynamic stability of synthons used in retrosynthesis

Laboratory of Molecular Modeling

- designing a physics-based Unified Coarse-Grained Model of biological macromolecules
- prediction of three-dimensional structures of proteins and nucleic acids
- simulations of the kinetics, dynamics, thermodynamics, and free-energy landscapes of proteins and nucleic acids
- investigations of receptor-ligand interactions by molecular docking
- NMR-assisted studies of the coonformations of biologically-active peptides
- simulations of the role of local and electrostatic interactions in shaping protein structure

Laboratory of Polymer Simulations

- modeling of protein-protein, protein-peptide, and protein-small ligand interactions
- simulations of grafting thin layers of parylen (poly-(p-xylylene))-family polymers
- theoretical prediction of physicochemical properties of ionic liquids
- modeling of the changes of ionic-liquid properties in the presence of ferromagnetic nanoparticles

Department of Theoretical Chemistry

Proposed Topics of Master's dissertations:

Laboratory of Quantum Chemistry

- Designing novel strong oxidizers based on superhalogen systems
- Theoretical prediction of the strength of Lewis-Brønsted superacids
- Verification of electronic and thermodynamic stability of synthons
- Mechanisms of chemical reactions catalyzed by superacids

Laboratory of Molecular Modeling

- Testing of the new linear algorithm of molecular dynamics simulations with the coarse-grained UNRES model
- Optimization of the UNRES force field by maximum-likelihood method
- Development of algorithms for biomolecular simulations
- Modeling of the interactions of G-protein-coupled receptors with selected ligands

Laboratory of Polymer Simulations

- Protein folding simulations with the UNRES force field and Markov state model
- Simulations of large-scale conformational changes important for protein functions
- Comparison of large protein assembly simulations using MARTINI and UNRES coarse-grained models
- Implementation of FIRE minimization algorithm in UNRES package

Department of Theoretical Chemistry

Registration	**Sylwia Freza** email: sylwia.freza@ug.edu.pl
Maximum number of candidates	**15 students**

Department of Theoretical Chemistry

Open days:

Date: October 11th and October 22th

Contact person: Dr. hab. Sylwia Freza