

Pągielska Marta

Computational Chemistry |
Molecular Modelling |
Machine Learning | PhD Candidate

CONTACT

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RESEARCH INTERESTS

Molecular Modelling
Protein-Glycosaminoglycan Interactions
Machine Learning
Computational Structural Biology

ABOUT ME

PhD candidate in computational chemistry working at the intersection of molecular modelling, data analysis and AI/ML. Experienced in molecular dynamics, predictive modelling, descriptor-based analysis, Markov State Models and Python-based scientific workflows. Leader of AI/data-driven student projects.

EDUCATION

University of Gdansk

PhD in **Computational Chemistry**
2025-present

M. Sc. in **Mathematical Modeling and Data Analysis**
2023-2025

B. Sc. in **Bioinformatics**
2020-2023

RESEARCH EXPERIENCE AND ACHIEVEMENTS

Work experience

September 2022-

GAG computational group
Department of Theoretical Chemistry
University of Gdansk

working on deciphering the sulfation code of glycosaminoglycans and developing a web-based database of cathepsin-glycosaminoglycan interactions

Publications

Pągielska, Marta, and Sergey A. Samsonov. "Molecular dynamics-based comparative analysis of chondroitin and dermatan sulfates." *Biomolecules* 13.2 (2023): 247.

Pągielska, Marta, and Sergey A. Samsonov. "The Amazing World of Glycosaminoglycans through the Eyes of a Theoretician." Glycoforum 27(6), A25 (2024)

Research Grants

NCN OPUS Research Grant – Research Team Member
“Modeling of glycosaminoglycan-induced formation of protein structure”

Principal Investigator – Young Researchers Research Grant (BMN)
University of Gdańsk
Research project investigating the molecular dynamics and allosteric mechanisms of cathepsin–glycosaminoglycan interactions using molecular dynamics simulations, Markov state models (MSMs), and residue interaction network analysis.

Scientific Internships

One-week scientific internship at the Biochemistry Department of the University of Lyon under Prof. Sylvie Ricard-Blum, as part of the NAWA project (June 2023).

Conferences

- Oral presentation on "**PapayaDB: A Web-Based Database of Cathepsin-GAG in silico Interactions**" at the **32nd International Carbohydrate Symposium**, July 2026, Bratyslava, **Slovakia**
- Poster presentation on "**Rational design of Tanshinone Derivatives Targeting the Exosite of Cathepsin K**" at the 2026 **ISQBP President's Meeting**, June 2026, Cluj-Napoka, **Romania**
- Poster presentation on "**Over 5000 Simulations Later: Finding Allostery in the Database of Cathepsin-GAG Interactions**" at the **10th Polish-Korean Conference on Protein Folding: Theoretical and Experimental Approaches**, September 2025, Gdańsk, **Poland**
- Oral and poster presentation on "**Developing a Comprehensive Database of Cathepsin-GAG in silico Interactions**" at the **22nd European Carbohydrate Symposium**, July 2025, Gdańsk, **Poland**
- Oral presentation and co-organizing of workshops on "**Hands-on Modeling of Cathepsin-Glycosaminoglycan Interactions**", October 2024 , Tours, **France**
- Oral and poster presentation on "**Chondrotin and Dermatan Sulfates: How Small Differences Lead to Huge Consequences**" at the **German Biophysics Society Meeting**, September 2024, Leipzig, **Germany**
- Poster presentation on "**Exploring Protease Regulation: A Comprehensive Database of Cathepsin-GAG in silico Interactions**" at the 2024 **ISQBP President's Meeting**, May 2024, Athens, **Greece**
- Oral presentation on "**Bridging Scales in Biomolecular Research" at the CECAM Workshop "Frontiers of Coarse-Grained Models**", April 2024, Lyon, **France**.
- Poster presentation on "**Cracking the Glycosaminoglycan Sulfation Code**" at the **8th Polish-Korean Conference on Protein Folding**, September 2023. Jastrzębia Góra, **Poland**.

ADDITIONAL INFORMATION

Scholarships

Four-time recipient of the Rector's Scholarship at the University of Gdańsk, awarded for academic excellence and scientific achievements during undergraduate and graduate studies.

Languages

English - C1
Polish - native

Interests

cooking, baking, arts&crafts, travel, orienteering, dance

LEADERSHIP AND TEACHING EXPERIENCE

DeepDive - AI Science Club
Former Chair, currently mentoring members, coordinating educational initiatives, and supporting the development of student-led projects.

deepdiveug.com

Scientific Committee Member – Polish Artificial Intelligence Olympiad (OAI)
Designing, reviewing, and refining competition tasks, preparing and processing datasets, and delivering educational lectures on artificial intelligence and machine learning.

Certified Bielik Squadron Trainer
Conducting hands-on workshops on the Polish large language model Bielik, retrieval-augmented generation (RAG), and AI agent development, including practical applications of Google Cloud technologies.

Programming and AI/ML Teacher
Creator and lead instructor of an original programming courses in Python and bootcamps in AI/ML.

COMPETENCES

Programming languages

Python, R, Bash scripting

Data analysis

Supervised/unsupervised learning, neural networks, statistical analysis, image processing

Molecular Dynamics and Computational tools

AMBER, UNRES, AutoDock, VMD, Pymol

Web Development and Database Management

Backend and Frontend Development

OTHER PROJECTS

DepressionControlApp
Team leader and developer of application designed to support mental health through digital tools.

getdca.com

Analytical Software for Brewery
Team leader and developer of ERP system with analytical module for AleBrowar Sp. z o.o. (in dev)

Thesis Reviewers System for University
Team leader and developer of a thesis reviewer matching system for Faculty of Economics at the University of Gdańsk