

Project title:

Pioneering Light-Modulated Enzymatic Catalysis: Dual Products from Azobenzodinitriles via Nitrile Hydratase

Position:

Scholarship Student

Number of positions: 1

City: Toruń

Website: <https://www.fizyka.umk.pl/en/>

Requirements:

- Knowledge of the basics of molecular modeling techniques, such as molecular dynamics and docking
- Proficiency in Linux system
- Basic programming skills
- Basic knowledge of molecular biology
- Ability to use software for protein visualization and molecular dynamics analysis (e.g., VMD)

Description of duties:

The student's aim will be to perform docking simulations of photoactive ligands (azobenzenes) in the trans and cis conformations to a non-standard biotechnological enzyme, nitrile hydratase. Analysis of the obtained docking results. Based on the best conformations from the docking, preparation of molecular dynamics (MD) simulations for various mutant variants of the nitrile hydratase (NHase) enzyme with the docked substrate and potential products. Analysis of the MD simulation results and evaluation of differences in the interactions between NHase mutant variants and the docked ligands.

Tasks:

- Preparation of photoactive ligands in trans and cis forms for docking
- Preparation of the NHase protein for docking
- Performing docking using software such as AutoDock, Schrodinger, and others
- Docking analysis and proposal of mutations
- Preparation of molecular dynamics (MD) simulations of NHase with docked trans and cis ligands
- Analysis of MD results
- Development of scripts to automate docking and molecular dynamics analysis

Competition type: Opus/

Field of science: e.g. NZ

Application deadline: 31 May 2026, 23:59

Application form: e-mail

Employment conditions:

A scholarship in the amount of PLN 1500 per month for a period of up to 12 months.

Planned period of employment: up to 12 months, up to 12 months, 1 July 2026–30 June 2027

Additional information:

The scholarship is awarded in accordance with the rules set out in the Regulations on the Award of Research Scholarships of the National Science Centre, adopted by Resolution No. 25/2024 of the Council of the National Science Centre dated 4 March 2024..

Required documents (please send these to the project manager's email address: drpepe@fizyka.umk.pl, with the subject line 'Opus 29.1'):

- Cover letter
- CV
- Copies of obtained diplomas and certificates (if any)
- Copy or scan of candidate's publications (if any)
- Information about scientific awards, scholarships and other distinctions (if any)
- Description of current research activity (if applicable)
- Consent to the processing of personal data (https://view.officeapps.live.com/op/view.aspx?src=https%3A%2F%2Fwww.umk.pl%2Fuczelnia%2Fiod%2FKonkurs_EN.docx&wdOrigin=BROWSELINK).
- Certificate of student status

Applicants will be evaluated by a selection committee appointed by the Dean of the Faculty of Physics, Astronomy and Informatics. The committee will recommend the awarding (or rejection) of the scholarship no later than 10 June 2026.

Candidates will be notified of the outcome of the competition by e-mail.

In the event of resignation of the selected candidate, the right to indicate the next candidate from the ranking list is reserved.

All documents should contain the candidate's signature or its scan.

Language of application: Polish or English.