

Job offer - postdoctoral researcher

at the International Centre for Cancer Vaccine Science, University of Gdańsk

Requirements:

- Doctoral degree obtained not earlier than 7 years before the year of employment in the project (excluding leaves related to the care and upbringing of children) in an entity other than that in which this position is to be filled, or has completed a continuous and documented postdoctoral training of at least 10 months at an institution other than the entity implementing the project, and in a country other than the country in which the doctoral degree was obtained.
- Having experience in computational structural biology methods for drug design/discovery: scaffold hopping, de novo design, fragment-based or knowledge-based inhibitor design, and high throughput *in silico* screening.
- *In silico* bioinformatics skills: molecular modeling, molecular docking, drug designing, and molecular dynamics simulations (including application of molecular mechanics and/or semiempirical methods).
- Practical skills in use of molecular modeling software such as Modeller, AutoDock, Gaussian, GROMACS, VMD, NAMD, BIOVIA Discovery Studio, MOE, AMBER, etc.
- Knowledge of Windows and Linux operating systems, as well as some basics of programming languages (e.g., Python).
- Knowledge in the field of cross-linking mass spectrometry (CLMS), proteomics, and experience of handling large datasets as well as using tools such as MAXQUANT, Perseus, etc.
- Good knowledge of the English language (written and spoken).

Responsibilities:

- Conducting research within the project.
- Applying molecular modeling and high-throughput virtual screening *in silico* methods to select promising compounds from available chemical databases, and design derivatives of active using *in silico* methods (fragment-based design) for the UPF1 gene.
- Structure-based virtual screening (SBVS) for the compound libraries retrieved from different databases to be docked into a structure of selected target binding site of the UPF1 gene.
- *In silico* filters such as absorption, distribution, metabolism, excretion, and toxicity (ADMET) shall be implemented to selected derivatives, that will be considered for synthesis and biological evaluation.
- Molecular dynamic simulations of selected protein-ligand complexes, to explore the molecular properties and conformational dynamics.
- Analyze CLMS, proteomics, or immunopeptidome datasets.
- Visualization and presentation of the obtained results during internal meetings as well as scientific conferences.
- Publishing the obtained results in scientific journals.
- Other tasks related to scientific activity under the project defined by the project manager.



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About the project:

The postdoctoral researcher will work within the project: *The impact of UPF1 ATP mimetics on the mutant immunopeptidome* led by prof. Theodore Hupp (grant agreement: UMO-2020/39/B/NZ7/02677). The project is a bilateral cooperation with the Gdańsk University of Technology, funded by NCN within the funding programme OPUS. The project will focus on understanding the mechanism and physiological functions of the NMD pathway which can have the potential for treating certain genetic diseases and cancer. Co-authors are dr inż. Umesh Kalathiya from the ICCVS, University of Gdańsk and prof. Sławomir Makowiec from the Gdańsk University of Technology. There will be an opportunity to access the Cyfronet Prometheus (~55, 000 cores) and CI TASK Tryton (~38, 000 cores) supercomputer clusters, which are consistently represented among the top 500 super computers in the world.

Work conditions:

- Employment contract for 24 months. The position is expected to start from 1 October 2022.
- Salary before tax & social insurance deductions incl. seniority bonus approx. 7.500 PLN.
- Additional yearly remuneration (so-called "13th salary") if eligible and according to binding provisions at the University.
- Work in an interdisciplinary and dynamic team.
- Presentation of scientific results during scientific conferences.
- During receiving remuneration from this project, the candidate shall not receive other remuneration from funds granted as direct costs from research projects financed within NCN competitions; and shall not receive remuneration from another employer based on an employment contract, including an employer based outside Poland.

Please note, in case of questions you are encouraged to contact **dr inż. Umesh Kalathiya** (umesh.kalathiya@ug.edu.pl) before submitting an application.

Additional information:

Please send the application in English to: iccv@ug.edu.pl quoting the reference "ATP mimetics postdoc" in the email's title **until 31 July 2022**, 23:59.

Selected candidates will be invited to an (online) interview. The candidates will be selected by a competition committee appointed by the Rector of University of Gdańsk.

Application documents:

Application documents should be prepared as one single PDF document and include:

- A full CV with list of publications.
- Copy of the PhD diploma.
- A letter of motivation explaining your general interest for this position.
- Name, affiliation, email, and phone number of two referees who can be contacted, if necessary.
- Declaration of the applicant that his work is not financed by other projects of the National Science Center.
- Please include the signed statement on the GDPR information clause for this recruitment downloaded from: <https://iccv.ug.edu.pl/work-with-us/open-positions/>