

Post-Doctoral Research Assistant in Structural Bioinformatics

"Design of new protein structures with precisely defined features using parametric models"

Applications are invited for a 3-year full-time post-doctoral position in the Centre of New Technologies, University of Warsaw, Poland. The position has been recently funded by the Polish National Science Center. The project will be conducted in collaboration with Dr. Birte Hernandez Alvarez (<http://www.eb.tuebingen.mpg.de/research/departments/protein-evolution/birte-hernandez-alvarez.html>) from the Protein Evolution Department of Max Planck Institute in Tuebingen, Germany, who is specialized in protein structure determination, particularly of regular and repetitive structures. As part of the project, frequent travel to the collaborating partners is expected. Additional funds are available to attend relevant workshops and international conferences.

Project description

The aim of the project is to set up a bioinformatics pipeline for designing new protein structures with the use of parameterization, a procedure that allows representing protein backbones with mathematical equations. The best-known protein structure class that has been fully parameterized is α -helical coiled coils, encompassing very regular structures in which canonical α helices are wound around each other to form bundles. There are a vast number of studies in which parameterization has been used to support analysis of the sequence-structure-function relationship in α -helical coiled-coil domains of various proteins (e.g., involved in bacterial signal transduction). We propose that other protein structures could be also parameterized, and thus manipulated and studied in a similar fashion to α -helical coiled coils. To investigate this hypothesis, we will study two protein classes: π -helical coiled coils, hypothetical structures that have never been observed in nature, and β -helices, widespread regular structural motifs that occur in many functionally unrelated proteins. The key aspect of the project will be experimental validation (crystallography/NMR) of novel structures designed with the aid of the parametric models. The successful candidate will work on development of parametric models for one of the two aforementioned protein classes, *in silico* design simulations, and deciphering structure-sequence relationships. Individual ideas and side-projects are also welcomed.

Assessment

The successful applicants will have a PhD in a subject of relevance to the position and a strong publication records in peer-reviewed journals. Qualifications and skills required:

- Experience in UNIX/Linux as well as in any established scripting language (preferably Python)
- Good writing and oral communication skills in English, and competence in scientific writing. Knowledge of Polish is not a requirement.
- Previous experience with protein modeling or design, usage of a computational cluster, and managing and analyzing large datasets.
- Experience related to some of the following; Rosetta modeling software; molecular dynamics packages (AMBER, NAMD etc.); sequence analysis, comparative genomics, or machine learning techniques.

The main emphasis will be placed on personal suitability and on good communication and interpersonal skills as well as on the ability to work independently and as part of a team.

Applicants should send a curriculum vitae, including a list of publications, a cover letter, and contact details of 2 references to Dr. Stanisław Dunin-Horkawicz (s.dunin-horkawicz@cent.uw.edu.pl). Informal enquiries are welcome. The closing date for the receipt of applications is **30 April 2016**. The planned start date: **1 June 2016 or as soon as possible afterwards**.

The University of Warsaw is committed to equality and diversity, and encourages applications from all sections of the community.