

Project 4.2. Computer simulations of partially disordered proteins (theoretical)

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Unit: ON5

WWW: <https://sites.google.com/view/bartosz-rozycki-biomembranes>

Background:

Among the current challenges for molecular biophysics are partially disordered proteins (PDPs), i.e. such macromolecules that contain both folded protein domains and intrinsically disordered polypeptide segments. To determine molecular conformations of PDPs it is usually necessary to combine data from several complementary experiments. An important example of PDPs is oxysterol-binding protein (OSBP)-related protein 8 (ORP8). The biological function of ORP8 is to transport lipids between the place of their synthesis (i.e. endoplasmic reticulum) and the plasma membrane, which contributes to maintaining the proper lipid composition of cellular membranes. However, the molecular mechanisms that allow ORP8 to perform its biological functions remain unexplained.

Aim:

The PhD student will use numerical methods to study molecular conformations of PDPs – both in aqueous solutions and at lipid membranes. In particular, he/she will use Monte Carlo simulations and ensemble refinement methods to integrate data from X-ray crystallography, small angle X-ray scattering (SAXS) and Förster resonance energy transfer (FRET) experiments to determine molecular conformations of the ORP8 protein. The ultimate goal of the project is to obtain a detail molecular model of lipid transport between membranes by the ORP8 protein. This project will be carried out in close collaboration with the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Science.

Requirements:

- MSc in physics or chemistry or a related branch of science, or an equivalent degree that qualifies one for PhD studies in physics in the country of issue,
- Good knowledge of statistical mechanics and of numerical methods in physics or chemistry,
- Interest in molecular biophysics. Communicativeness and good command of spoken and written English,
- Diligence at work and consistency in achieving results,
- Additionally, programming skills within the Linux environment (including scripting languages) as well as prior experience in application of numerical methods (such as molecular dynamics simulations) in physics or chemistry will be considered strong assets.

Funding:

Scholarship of 5000 PLN per month, before subtracting obligatory employer and employee social security contributions (~15%), for the first 30 months (grant funding). Afterwards, in months 31-48, standard Polish PhD scholarship (currently about 3240 PLN per month net).

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