

## HALRIC Research Internship Programme

### Internship Proposal

**Project Title:** Exploring Molecular Flexibility: Integrative BioSAXS and Molecular Dynamics Simulations for Dynamic Protein Systems

**Name of Institution/Country:** Lund University, Sweden

**Name of internship provider:** Professor Marie Skepö, Postdoc Nabanita Mandal, PhD-students Oskar Svensson and Xiaopian Tian

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**Proposed timeframe:** The internship offers **three positions**, each with a duration of 4-6 months, providing a comprehensive learning experience.

**Application deadline:**

June 2025, start September 2025 or upon agreement

**Administrative contact person at the organisation:**

**Scientific research questions:** This project investigates how Intrinsically Disordered Proteins (IDPs) and Multi-Domain Proteins (MDPs) adopt structural ensembles in solution. It integrates BioSAXS and Molecular Dynamics (MD) simulations to refine models and explore the functional implications of their conformational flexibility.

**Experimental approach:** The project combines BioSAXS experiments to obtain structural data and validate protein conformations with advanced data analysis to compare experimental and simulated results, extracting valuable biophysical insights. This integrative approach enhances understanding of protein disorder.

**Tasks of the intern:** The intern will gain hands-on experience in BioSAXS data acquisition, MD simulations, computational modelling, and scientific communication. This opportunity provides expertise in structural biology methodologies and contributes to molecular research.

**General information about the work group, the university and the region:** At Lund University, our research group explores the static and dynamic properties of IDPs using simulations and scattering experiments. We aim to bridge simulations and experiments while advancing scattering data analysis techniques. Lund, a leading research hub, offers a vibrant academic environment in southern Sweden.

**Eligibility and qualification of the applicant.** We are looking for **three** motivated MA/BA student in biophysics, structural biology, computational biology, or related fields, with a plus for knowledge in MD simulations or programming, and strong analytical skills.