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POSITION DESCRIPTION

Computational Structural Biologist

Faculty/Division	DVC-Research and Enterprise
Classification Level	Professional 8
Hours & Span (Category)	G - Administrative, Clerical, Computing, Professional & Research Staff
Position number	ADMIN ONLY
Shiftwork status	NOT SHIFTWORKER
Allowances	N/A
On call arrangements	N/A
Original document creation	6 August 2024

Position Summary

A **Computational Structural Biologist** will support the collaboration between MWAC's Structural Biology Facility and Australian BioCommons as part of their national strategy to provide best-practice tools and methods for the molecular life sciences community. The position is focused on developing research infrastructure capabilities, with a particular emphasis on delivering computational structural biology tools within UNSW and at a national level. Based at UNSW, this role is to act as an intermediary between end-users that may have little skill in structural biology and/or coding, HPC infrastructure, and the broader national network of computational and informatics experts.

This role reports to the Chief Scientist of the Structural Biology Facility (UNSW), with accountabilities to Australian BioCommons, and has no direct reports.

Accountabilities

Specific accountabilities for this role include:

- Assess computational structural biology software tools and workflows (with a focus on Deep Learning types) for quality, correctness and scientific outputs.

- Deploy computational structural biology tools and workflows across institutional, state, and national compute infrastructure platforms, such as Galaxy Australia, the Nextflow Seqera platform, and command-line HPC infrastructures.

- Provide direct support and guidance to researchers and research groups in the application of computational structural biology methods with a focus on deep learning/machine learning packages, through providing subject matter expertise, delivering consultations, assisting in bespoke troubleshooting issues, and collaborating with the BioCommons training team to develop training resources.

- Actively engage with expertise at the local Mark Wainwright Analytical Centre's Structural Biology Facility (SBF) at UNSW and the national networks of BioCommons to collaboratively identify requirements, propose recommendations and develop approaches to resolve computational challenges, and integrate computational tools into workflows.

- Identify and understand user needs to ensure the deployment of functional tools that add value to the broad structural biology community, but also support the use of structural biology tools in more specific application areas across biology and medicine.

- Consult and liaise with non-structural biologists to lead and support the use of computational tools and best practices through demonstration, facilitating training sessions, providing practical assistance, designing more intuitive interfaces to the software tools, and developing documentation.

- Collaborate with user experience designers, trainers and software engineers from the Australian BioCommons network to develop and implement tools and workflows with usability and research use cases in mind, contributing to the development of documentation and training materials.

- Liaise with UNSW and BioCommons to report on progress with accountability and transparency as and when directed by the SBF's Chief Scientist and/or BioCommons A/Director of Platforms.

- Align with and actively demonstrate the [Code of Conduct and Values](#)

- Ensure hazards and risks psychosocial and physical are identified and controlled for tasks, projects, and activities that pose a health and safety risk within your area of responsibility.

Skills and Experience

- Relevant tertiary qualification with subsequent relevant experience or equivalent competence in building biomolecular models using techniques such as CryoEM, crystallography, AlphaFold, etc. with a strong understanding of model validation gained through any combination of education, training and experience. Knowledge of structural biology is highly desirable.

- Demonstrated expertise in installing, using, and troubleshooting AI and ML code packages and tools.

- Experience in supporting research groups with computational methods, including training and documentation.

- Proficiency in git and fluency in Linux/HPC environments.

- Excellent written and verbal communication skills, with a high level of attention to detail for deliverables produced.

- Proven ability to influence senior management and stakeholders as appropriate to ensure successful outcomes.

- High level of organisational, analytical, and problem-solving skills, with a demonstrated ability to consider and make informed decisions regarding experimentation issues.

- Demonstrated ability to interpret and present analytical results and contribute to scientific reports.

- Demonstrated ability to work collaboratively and productively within a team, but also to take initiative and work independently while managing competing demands.

- An understanding of and commitment to UNSW's aims, objectives and values in action, together with relevant policies and guidelines.

- Knowledge of health and safety responsibilities and commitment to attending relevant health and safety training

About this document

This Position Description outlines the objectives, desired outcomes, key responsibilities, accountabilities, required skills, experience and desired behaviours required to successfully perform the role.

This template is not intended to limit the scope or accountabilities of the position. Characteristics of the position may be altered in accordance with the changing requirements of the role.