Henry Mitchell Scholarship Report

Research Visit at University of the Western Cape

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Introduction

As a doctoral student in Physics with a focus on protein-ligand interactions for therapeutic discovery, I was privileged to conduct a two-month research visit at Professor Joubert's Drug Design Laboratory at University of the Western Cape (UWC). The primary aim was to identify compounds capable of activating the SIRT1 enzyme using both experimental and computational approaches. SIRT1 is a critical enzyme involved in cellular regulation, aging, and metabolism. Enhancing molecular docking methodologies aims to increase the efficiency and accuracy of identifying promising SIRT1 activating compounds for therapeutic applications. This report provides an overview of the objectives, methodologies, findings, and future implications of this research endeavor. The visit also played a key role in strengthening the collaboration between Prof. Joubert's and Prof. Zou's laboratories.

Objectives

1. To establish and validate SIRT1 Assay in the laboratory.
2. To enhance the molecular docking capabilities for SIRT1 within the Drug Design Laboratory.

Methodology

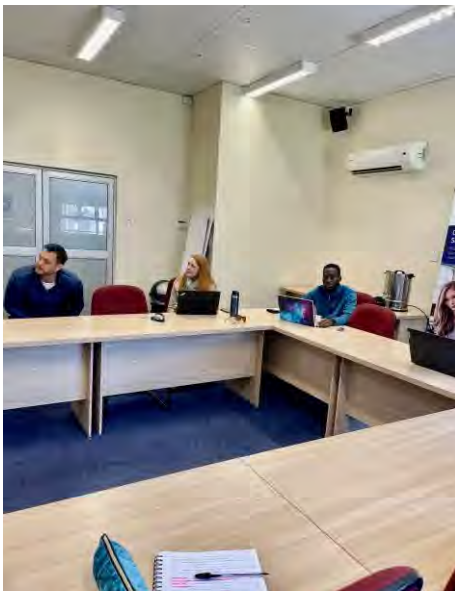
During the two-month research period, under Prof. Joubert's supervision, I conducted extensive structure-based virtual screening using two distinct molecular docking protocols, Glide and Auto Dock Vina, to gain insights into their binding mechanisms at SIRT1's active site. Compounds were selected from virtual screening based on their binding affinity and interactions with key SIRT1 residues, ensuring a focus on potential activators. Unfortunately, logistical delays in South Africa affected the timely setup of the SIRT1 assay. Anli, a master's student in Prof. Joubert's group, will perform the assay once all necessary consumables arrive to validate our computational predictions. Compounds identified through virtual screening will also be sent to Reaction Biology in the United States for in vitro assessment of their biological activity against the SIRT1 enzyme.

Conclusion and Future Work

This research visit established a strong foundation for advancing SIRT1 docking methodologies in Prof. Joubert's lab, setting the stage for future drug discovery research collaborations between Prof. Joubert's and Prof. Zou's labs. Upon completion of the assays, biological activity data will guide compound optimization, refining computational models and streamlining the discovery process for potential SIRT1 activators. This collaboration and the resulting data will contribute significantly to the Drug Design Laboratory's research capabilities and our collective understanding of SIRT1 activators.

Exploration of Cape Town

Beyond research, I had the chance to explore Cape Town's incredible natural beauty and cultural landmarks. Highlights included hiking in the stunning Table Mountain National Park, experiencing the lively V&A Waterfront, touring the historic Robben Island, and visiting the scenic Cape Point. Each experience allowed me to appreciate the rich natural and cultural heritage of South Africa.

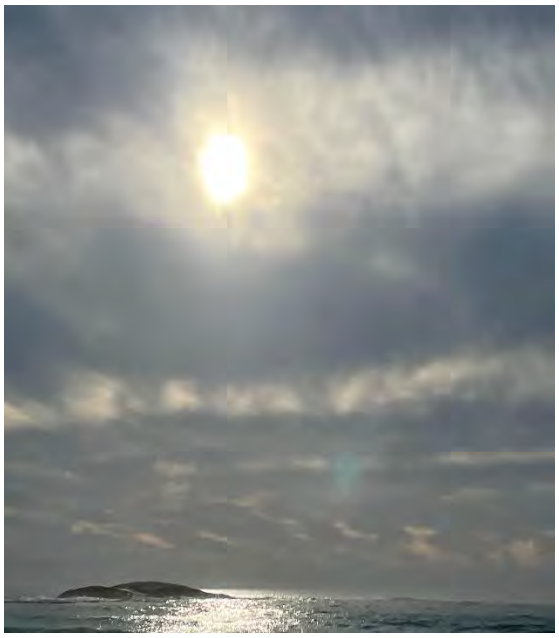


Participating in Prof. Joubert's group meeting

Table Mountain National Park

V&A Water Front

Visit to Robben Island



Cape Point

Sunset at Camp's Bay beach

Acknowledgement

I am sincerely grateful to the Henry Mitchell Scholarship Committee for this invaluable opportunity to expand my research horizons. My heartfelt thanks to Prof. Uphoff for his unwavering support, which made this trip smooth and memorable. I am also deeply appreciative of Prof. Joubert for his insightful guidance throughout my research visit, and finally, I extend my gratitude to my supervisor, Prof. Xiaoqin Zou, for her belief in me and my work.