UMSAEP Research Visit Report for Prof. Jacques Joubert and Mr Luke Zondagh

Date of Visit: April 11 – June 29, 2023

Place of Visit: Prof. Xiaoqin Zou Laboratory, Dalton Cardiovascular Research Centre, University of Missouri – Columbia

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Introduction:

Luke Zondagh conducted a research visit to Prof. Xiaoqin Zou's laboratory for approximately 2.5 months during the first semester of 2023. The purpose of his visit was to identify novel small molecules targeting two known Alzheimer's Disease (AD) targets, GSK-3β and SIRT-1. Prof. Xiaoqin Zou and her team possess extensive experience in identifying therapeutic small molecules and peptides through diverse computational techniques. During his visit, Luke employed computational and biological methods to identify potential anti-AD agents. Additionally, the visit played a pivotal role in strengthening the collaboration between Prof. Joubert's and Prof. Zou's laboratories, while also contributing to the development of the research collaborator hub involving Prof. Samuel Egieyeh and Dr. Erika Kapp.

Objectives:

1. Identify anti-AD agents targeting GSK-3β and SIRT-1 using computational and biological techniques.
2. Strengthen collaboration between Prof. Joubert's and Prof. Zou's laboratories.
3. Acquire and share advanced computational techniques with Prof. Joubert, Prof. Egieyeh, and Dr. Kapp upon returning to UWC.

Methodology:

During his approximately 2.5-month research visit at MU - Columbia, Luke conducted structure-based and template-based virtual high throughput screening. Subsequently, he employed cheminformatic techniques to evaluate compounds' potential activity against the two AD targets. The identified compounds were procured and sent to Reaction Biology, USA, for in vitro protein-based biological activity assessment. Prof. Zou and her research scientists provided invaluable assistance throughout the entire process.

Research Results:

The compounds identified through virtual screening demonstrated significant activity against GSK-3β at 20 µM. One compound has been submitted for IC50 calculations against GSK-3β.

Furthermore, two compounds exhibited activity against SIRT-1, both of which are undergoing further analysis.

Activities, Observations, and Additional Research:

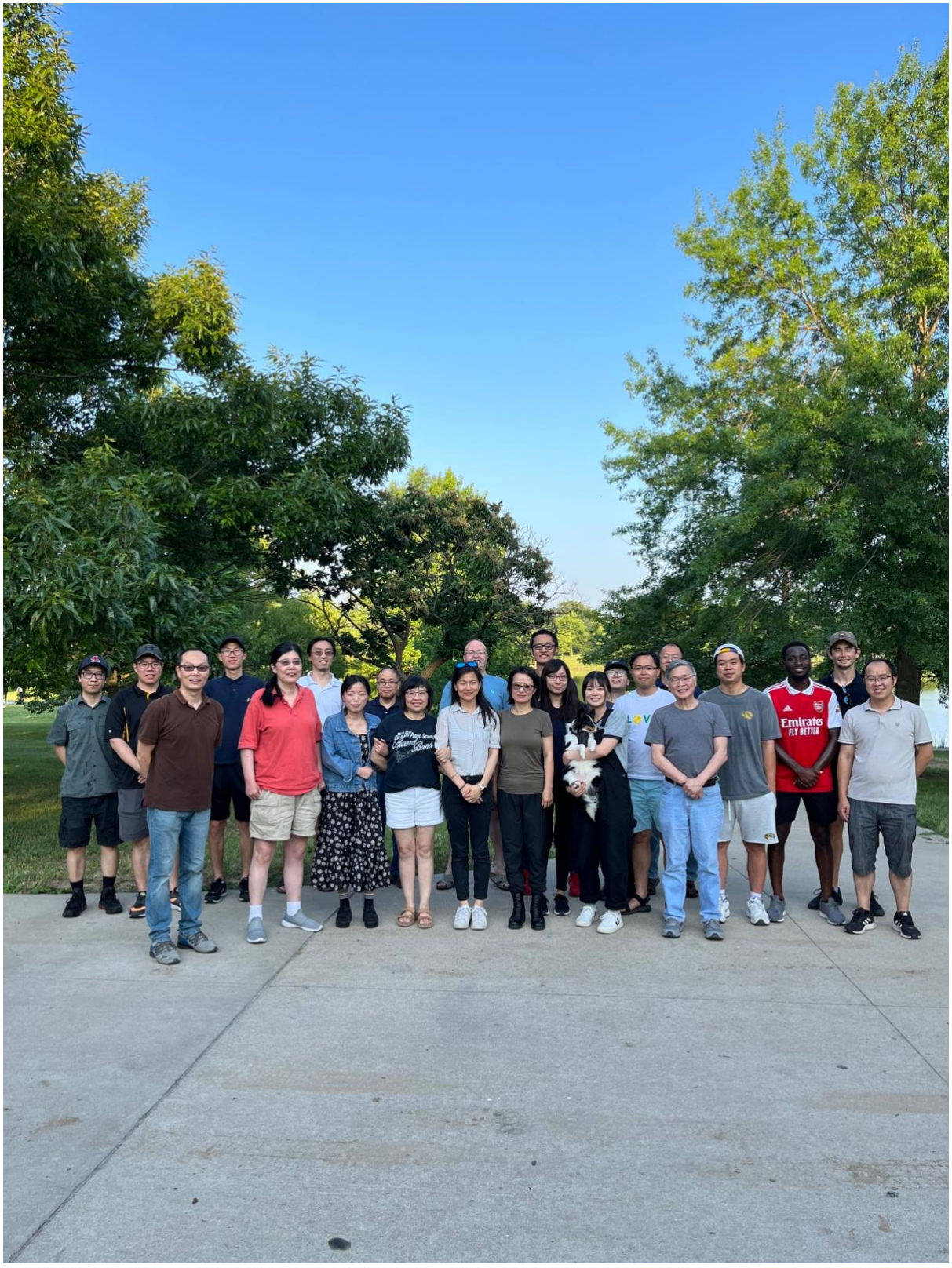
During his visit, Luke initiated a collaborative research effort with Prof. Zou's lab, aligning with his Ph.D. thesis. Leveraging Prof. Zou's expertise in computational protein-peptide techniques, they conducted protein-peptide docking and MD simulations for Luke. The resulting insights will contribute to explaining how his compounds inhibit protein-peptide complex formation. Luke developed strong connections with Prof. Zou, her research scientists, and a Ph.D. student, fostering anticipated future collaborations.

Luke resided at University Place Apartments (UPA) in Columbia, conveniently located near downtown and university facilities. The scenic MU campus and warm hospitality of the people enriched his experience. Exploring nature trails during lunch breaks further enhanced his stay.

Conclusion:

In summary, Luke Zondagh's research visit to Prof. Xiaoqin Zou's laboratory at the University of Missouri - Columbia proved highly productive and impactful. Over a span of approximately 2.5 months, Luke successfully identified potential anti-Alzheimer's Disease (AD) agents targeting GSK-3β and SIRT-1 using advanced computational and biological techniques. Collaborative efforts between Prof. Joubert's and Prof. Zou's laboratories were strengthened, contributing to the ongoing development of the research collaborator hub. Luke also formed valuable connections within Prof. Zou's lab, initiating a collaborative research initiative aligned with his Ph.D. thesis. This visit not only achieved its objectives but also facilitated knowledge exchange and future collaborations. Luke's adaptability to the new environment and his eagerness to return to Columbia reflect the positive impact of this research visit.

First Day at Dalton Cardiovascular Center. Left to right Dr. Liming Qui, Prof. Xiaoqin Zou, Dr. Xianjin Xu, Mr. Luke Zondagh, Dr. Rui Duan.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