

Summer Research UCSB April to August 2022

Last Summer I was lucky enough to undertake research with the Shell lab in the University of California Santa Barbara. This lab applies molecular dynamics simulations to fields such as protein assembly, water physics and industrial formulation design. I worked with a PhD candidate on a project where we studied the effect tau proteins have on neurodegenerative diseases.

Tau is a protein that lines important structures called microtubules in the brain. In certain neurodegenerative diseases tau dissociates from the microtubules and forms into clumps of specific folded structures. These folded structures are specific to different neurodegenerative diseases. For example, Alzheimer's patients will have different folds of tau in their brain compared to patients with corticobasal degeneration. To analyse tau protein simulation data was gathered for a small section of the Alzheimer's fragment in which a 'clamping' effect was observed to happen. The linker chain for this fragment was then modified and this was the independent variable in experimentation. Simulations were run for different linkers and under different salt conditions.

My work involved using molecular dynamics analysis and statistical analysis tools to generate measurable data such as solvent accessible surface area and residue minimum distances (smallest distance between individual amino acids in the chain). This data was then used to identify the best distinguishing features between the different linkers. Highlighting these features led us to understand that the clamping effect is primarily due to hydrophobic interactions between two amino acids in the fragment. My work culminated in a 30-minute technical presentation to lab managers and supervising professors. Some of the figures I generated are currently being compiled into a paper on hydrophobicity which will aid the understanding of tau protein's role in neurodegenerative disease which hopefully will eventually lead to better therapeutics for diseases such as Alzheimer's.

This Summer was the best one of my life! As well as engaging with faculty in the research lab I made many new friends and visited plenty of amazing places. My best friend Eoin and my sister Lucy came out to visit me at two different points, so we visited San Francisco, Sequoia National Park, Los Angeles and Big Sur as well as go on numerous climbing, surfing, and camping trips at the weekends.

To conclude I would like to thank several people for making this Summer happen. Drs Jessica Whelan and Eoin Syron, thank you for helping me through the process of finding a suitable research placement. My thanks to Professor Scott Shell of UCSB for facilitating my visa extension which allowed me to stay for the Summer. A huge thank you to Sam Lobo for taking me on as a researcher, for mentoring me in so many ways. As well as technical skills, Sam taught me the importance of being curious in all aspects of life, a trait vital to any researcher. Finally, I would like to thank Kate and Martin McAdam for making this whole experience possible. The skills I have learned and the people that I have met are invaluable to me and I am extremely grateful to have been given this opportunity. It was my pleasure to represent the UCD community in the fifth best Chemical Engineering programme in the US. Thank you for your kindness in supporting me, the students before me and the students who will come after me.

Go raibh míle maith agaibh.



In Sequoia National Park with my sister



At the summit of Alta Peak in Sequoia