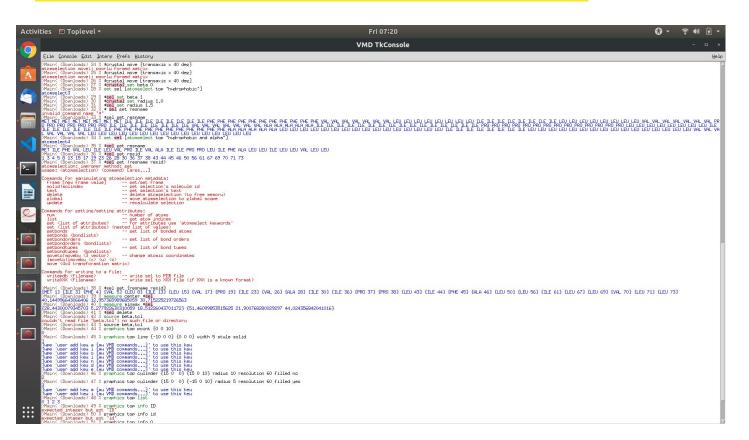
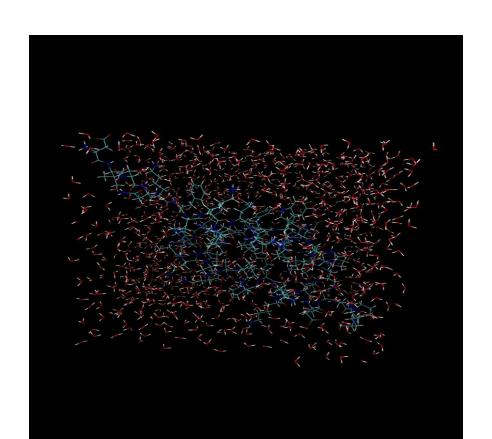
# Progress so far

- Went through a journal to understand some basic steps and terminologies to perform a simulation.
- Setup NAMD and VMD and went through their respective tutorials.
- Explored the msi2namd tool.

### Read VMD tutorial related to TCL scripting



## Performed SMD for SpA protein in water box



### **Progress so far**

 There were a few papers that we were asked to read but were unable to access.

https://iopscience.iop.org/article/10.1088/1748-6041/10/3/032001/meta

And

https://advances.sciencemag.org/content/2/11/e1600998

Was asked to recreate the simulation environment by reading the following:
<a href="https://www.researchgate.net/publication/346428290">https://www.researchgate.net/publication/346428290</a> Adhesin Protein Interaction of Staphylococcus Aureus Bacteria with Various Biomaterial Surfaces but couldn't do it as I wasn't able to access the full paper.

#### THANK YOU