Chapter 3: Computational Methodology

3.1 Introduction

* Talk about the importance of computation through my time in grad school, catching up, and how there are good tools to do so
* Reference papers that seem to do a good job mixing in computation with the biology simplifying for learners
* Emphasize the importance of computation due to high-throughput data analysis and AI

3.2 Structure prediction tools

* Rosetta -> Alphafold -> all the new methods that are still coming up
  + Maybe give each method a subsection so it’s easy to find

3.3 Molecular software library

* Protein design code and how it came about
  + Analysis of the membrane protein pdbs (cite where I got them from and memprotDB)
  + Utilize it’s structure prediction tools to determine geometries suitable for protein design
  + Energetics terms that have been made accessible and how to add to the field
  + talk about my “energy” terms that I developed
    - sequence entropy and baseline monomer energy (similar to Rosetta and another paper)
* Paired with code that reads in pdb structures and does local structure repacks
  + Optimized by decreasing the repack distances in accordance with the monte carlo, making a very refined repack (similar to Rosetta)
* Talk about ways to improve the molecular software library and/or to transition some of these scripts to something more usable like Rosetta/Alphafold/how to make this easy to use
  + Creating a webserver was a pipe dream I had but never got the skill to do it
* How to utilize the information from this paper to make the code better at design

3.4 Analysis

* Python scripts built for ease of use and how to use them all detailed here, probably with images
  + ngsReconstruction
  + runAllAnalysis
  + toxgreenAnalyzer

3.5 Conclusion