Title: Trajectory of Information Entropy During Peptide Folding

Coauthors: David Corbo,1,2 Tatum Hennig,1,3,4 Siddharth Rath1,5,6

Mentor: Mehmet Sarikaya1,5,6,7,8

Affiliations:

1. Genetically Engineered Materials Science and Engineering Center
2. University of Washington College of Engineering
3. Atmospheric Chemistry
4. Applied Mathematics
5. Materials Science and Engineering
6. Molecular Engineering and Science Institute
7. Chemical Engineering
8. Oral Health Sciences

Abstract:

Some peptides are known to form stable secondary structures due to their occupation of lower energy states. These folded peptides theoretically have a greater information entropy contained in the electrons upon folding, but this has not been experimentally proven. One such peptide, (LK)7, which reliably folds into an α-helix, is used as a case study here to prove that uncertainty in electron energy values increases upon formation of stable secondary structures. To do this I learned how to use the molecular dynamics simulation software Schrodinger to create atom positional data trajectories over the evolution of (LK)7 from its extended to α-helical forms. From there I used Python and the SciPy ecosystem to create atom adjacency matrices of each frame of the trajectory. I then weighted these matrices by the atoms’ respective counts of valence electrons. Currently I am writing the code to calculate and plot the information entropy and energy based on these valence electron adjacency matrices over the evolution of (LK)7. Moving forward I will also create trajectories using different data from the same molecular dynamics simulation. One will be the weighting of atom adjacency matrices by electrons in orbitals not limited to the valence shell. Another will be including the atom positional data of water molecules in the system. The last trajectory will use both modifications. Using these trajectories, we hope to experimentally prove that electron information entropy generally increases upon the folding of a peptide to a stable secondary structure. Supported by the DMREF Program of NSF through the MGI platform under DMR# 1629071, 1848911, and 1922020.