Title: Trajectory of Information Entropy During Peptide Folding

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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 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. We use molecular dynamics, MD, simulation software from Schrodinger to create atom positional data trajectories over the evolution of (LK)7 from its extended to α-helical forms. Using Python and the SciPy ecosystem we create atom adjacency matrices of each frame of the trajectory and weight these matrices by the atoms’ respective counts of valence electrons. We then calculate and plot the information entropy and energy based on these valence electron adjacency matrices over the evolution of (LK)7. Moving forward we will also create trajectories using different data from the same MD simulation. One of these trajectories will involve weighting of atom adjacency matrices by electrons in orbitals not limited to the valence shell. Another will include the atom positional data of water molecules in the system. The last trajectory will use both modifications. Using these trajectories, we plan 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.