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Statistical Mechanics of Protein Multimerization and Aggregation KYLE HAGNER, SIMA SETAYESHGAR, Department of Physics, Indiana University, Bloomington, MICHAEL LYNCH, Department of Biology, Indiana University, Bloomington, PAUL HIGGS, Department of Physics and Astronomy, McMaster University, Hamilton, ON — Understanding the evolution of proteins is vital to explaining the diversification of life. As a majority of cellular proteins function not in isolation, but as part of complexes of two or more proteins, developing an understanding of how these protein- protein interactions originate and evolve is crucial. One intriguing observation is that highly-conserved proteins can exhibit different quaternary structures in different lineages, with no apparent correlation between the number of subunits in a complex and organismal complexity. In this work, we develop a theoretical model to investigate the aggregation of proteins on a cubic lattice using an hydrophobic-polar (HP) model. As most protein complexes are homomeric, composed of subunits derived from the same genetic locus, we focus on aggregates of multiple copies of the same protein as a function of concentration and the free energy of protein-protein binding. We construct a fitness landscape to investigate evolutionary trends by categorizing assemblies as monomers, isologous dimers, heterologous dimers, and higher-order assemblies, each with a corresponding impact on cellular fitness.

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