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Stochastic Protein Multimerization, Cooperativity and Fitness KYLE HAGNER, SIMA SETAYESHGAR, Department of Physics, Indiana University, Bloomington, MICHAEL LYNCH, Department of Biology, Indiana University, Bloomington — Many proteins assemble into multimeric structures that can vary greatly among phylogenetic lineages. As protein-protein interactions (PPI) require productive encounters among subunits, these structural variations are related in part to variation in cellular protein abundance. The protein abundance in turn depends on the intrinsic rates of production and decay of mRNA and protein molecules, as well as rates of cell growth and division. We present a stochastic model for prediction of the multimeric state of a protein as a function of these processes and the free energy associated with binding interfaces. We demonstrate favorable agreement between the model and a wide class of proteins using E. coli proteome data. As such, this platform, which links protein abundance, PPI and quaternary structure in growing and dividing cells can be extended to evolutionary models for the emergence and diversification of multimeric proteins. We investigate cooperativity - a ubiquitous functional property of multimeric proteins - as a possible selective force driving multimerization, demonstrating a reduction in the cost of protein production relative to the overall proteome energy budget that can be tied to fitness.

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