Dissecting the relationship between protein structure and sequence variation[1] AMIR SHAHMORADI, CLAUS WILKE, Univ of Texas, Austin, WILKE LAB TEAM — Over the past decade several independent works have shown that some structural properties of proteins are capable of predicting protein evolution. The strength and significance of these structure-sequence relations, however, appear to vary widely among different proteins, with absolute correlation strengths ranging from 0.1 to 0.8. Here we present the results from a comprehensive search for the potential biophysical and structural determinants of protein evolution by studying more than 200 structural and evolutionary properties in a dataset of 209 monomeric enzymes. We discuss the main protein characteristics responsible for the general patterns of protein evolution, and identify sequence divergence as the main determinant of the strengths of virtually all structure-evolution relationships, explaining $\sim 10-30\%$ of observed variation in sequence-structure relations. In addition to sequence divergence, we identify several protein structural properties that are moderately but significantly coupled with the strength of sequence-structure relations. In particular, proteins with more homogeneous back-bone hydrogen bond energies, large fractions of helical secondary structures and low fraction of beta sheets tend to have the strongest sequence-structure relation.

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