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Free Energy Landscape - Settlements of Key Residues. SVETLANA AROUTIOUNIAN, Dillard University — FEL perspective in studies of protein folding transitions reflects notion that since there are $\sim 10^N$ conformations to scan in search of lowest free energy state, random search is beyond biological timescale. Protein folding must follow certain fel pathways and folding kinetics of evolutionary selected proteins dominates kinetic traps. Good model for functional robustness of natural proteins - coarse-grained model protein is not very accurate but affords bringing simulations closer to biological realm; Go-like potential secures the fel funnel shape; biochemical contacts signify the funnel bottleneck. Boltzmann-weighted ensemble of protein conformations and histogram method are used to obtain from MC sampling of protein conformational space the approximate probability distribution. The fel is F($rmsd$) = -1/$\beta\bullet$Ln[Hist($rmsd$)], β=k$_B$T and $rmsd$ is root-mean-square-deviation from native conformation. The sperm whale myoglobin has rich dynamic behavior, is small and large - on computational scale, has a symmetry in architecture and unusual sextet of residue pairs. Main idea: there is a mathematical relation between protein fel and a key residues set providing stability to folding transition. Is the set evolutionary conserved also for functional reasons? Hypothesis: primary sequence determines the key residues positions conserved as stabilizers and the fel is the battlefield for the folding stability. Preliminary results: primary sequence - not the architecture, is the rule settler, indeed.

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