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Core-Shell Model of Folding-Unfolding Transitions (UFT) in Proteins SVETLANA AROUTIOUNIAN — There are $\sim 10^N$ conformations for a protein of length N to sort out randomly in search of lowest free energy state. Can protein folding be simple and fast? Core-shell model introduces principles, proposes mechanisms and scores residues of fast, reversible UFT in protein. According to it, during UFT the realm of intra-residual interactions leads the residue motion. The scaffold of hydrophilic residues forms external shell of unstructured, tube-like protein in unfolded state, just as the hydrophobic residues form internal scaffold – core, of the protein in folded state. As UFT proceeds, residue slides into lowest-score position permitted by its structure. Model accounts for experimentally observed features of UFT. It is based on three principles: 1) During UFT protein is *virtual* - its features or structure are inferred only statistically and with limited precision; 2) Mechanism of UFT memory is not longitudinal, but *transverse*; 3) Native design overrides specific features of residues - the alphabet of amino acids assumes an *intrinsic* score-function. Per-residue mechanism of UFT is proposed and score-function is described. Difference graphs of transitional score-function and average genome-wide abundance index show that our score-function *is* the order parameter of UFT in protein and by virtue of being it, reveals transitional key residues. It echoes the multiple-tier and funnel concepts of FEL perspective. Monte Carlo simulations of UFT in myoglobin illustrate the idea.

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