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Coarse-grained Simulations of Protein-Protein Association: Energy Landscape on a Globe SICHUN YANG, Case Western Reserve University — Understanding how proteins interact and associate into large functional complexes is critical in revealing the molecular basis of virtually every biological process in a living cell. Here, a theoretical simulation pipeline using coarse-grained (CG) models with an efficient sampling method is presented from the studies of protein-protein association. A concept of "energy globe" is introduced and implemented via the projection of simulation data onto a three-dimensional globe specifying protein-protein orientations and interacting energies. This energy-globe approach has the key advantage of locating and identifying multiple stable conformations that are physically accessible on the energy landscape. Tests on several well-studied protein-protein complexes show that the crystal-like conformation is favorable on the energy landscape even if the landscape is relatively rugged with metastable conformations. Recent applications to CG simulations of nuclear hormone receptors, whose experimental structure are still lacking, have predicted multiple favorable conformations on their corresponding landscapes, thereby providing insight into the cross-talk mechanisms of functional domains in the hormone signaling.

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