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The molecular dynamics and energetics of ion permeation and molecular recognition

Which are the mechanisms underlying molecular recognition involved in protein complexes? How do K+ ions efficiently, yet selectively pass through potassium channels? How can designed conformational shifts control binding affinity or selectivity? Molecular dynamics simulation results will be presented to address these questions. Ubiquitin data will be presented that suggest a conformational selection mechanism that allow it to engage in a large number of different complexes, each requiring a specific conformation. Indeed, designed mutants in the ubiquitin core with an altered conformational equilibrium show a corresponding shift in binding specificity. In addition, results from computational electrophysiology simulations will be shown that show the efficient permeation of K+ ions, but not of the slightly smaller Na+ ions through the selectivity filter of potassium channels.