

Computer Simulation of Conformational Equilibria Using Fluctuation Theory

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The computer simulation of conformational equilibria is a major goal in computational biophysics. Here, we use molecular dynamics simulation, coupled with the fluctuation theory (FT) of solutions, to help understand and rationalize the effects of temperature, pressure, and solution composition on the conformational equilibria of small solutes. Expressions describing the effects due to changes in T, P, and N for infinitely dilute solutes will be provided, and illustrated using several examples of biophysical interest. It is argued that the current approach avoids the need for traditional (subjective) definitions of protein volume and compressibility, for example.