Technique	Pros	Cons	CPU Complexity
Molecular dynamics (MD)	Continuous actions	Expensive; short time span	10 picoseconds = weeks for 50,000 atoms
Targeted MD (TMD)	Connection between two states; useful for ruling ut steric clashes	Not necessarily physical	Same as MD for each step
Continuum salvation	Mean-force potential approximates environment and reduces model's cost; useful information on ionic atmosphere and intermolecular associations	Approximate	Technique-dependent; can be as expensive as MD, but number of variables is reduced
Brownian dynamics (BD)	Large-scale and long-time motion	Approximate hydrodynamics; limited to systems with small relative inertia	Days for long DNA (1000s of base pairs)
Monte Carlo (MC)	Large-scale sampling; useful statistics	Move definitions are difficult	Hours of a million configurations
Minimization	Valuable equilibrium information; experimental constraints can be incorporated	No dynamic information	Minutes to hours for biomolecules
Stochastic Path Approach	Filtering of high-frequency motion; approximate long-time trajectories	Expensive (global optimization of entire trajectory)	1 picosecond approximate trajectory (1000 simulated annealing steps) = 1 day on 100 processors for 25,000 atoms
Normal mode analysis	Fast with interesting statistics, but potential unrealistic; may have large memory requirements	No dynamic information	Seconds to minutes to hours depending on problem and implementation