

Source:

1 | Preliminary Research

1.1 | Sources

<https://www.frontiersin.org/articles/10.3389/fchem.2019.00540/full>

1.2 | Notes

1.2.1 | Target Processes

1. Enzyme catalysis
2. Protein-ligand binding
3. signal transduction
4. allosteric regulation

1.2.2 | Folding Simulation Methods

1. all-atome molecular dynamics (MD)
 - Obtains all desired information regarding the kinetics and thermodynamics
- (a) Time scale bottleneck
 - very slow (supercomputers -> microseconds of simulation)
 - require microsecond to milisecond time scales
- i. optimizations
 - A. conformational sampling?
 - retains atomistic representation of the system
 - B. overcome kinetic trapping and thorough sampling of conformational space techniques
 - umbrella sampling
 - multicanonical algorithms
 - simulated tempering
 - transition path sampling
 - targeted molecular dynamics
 - replica exchange method molecular dynamics (REMD)
 - accelerated molecular dynamics (AMD)
 - see below
- ii. Accelerated molecular dynamics (AMD)