

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