**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
   - very slow (supercomputers -> microseconds of simulation)