

**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
  - catalyzing reactions with actions
2. Protein-ligand binding
  - neurotransmitters (dopamine), protein is dopamine receptor how does the ligand bind the proper site to open the channel?
3. signal transduction
  - bind to other protein to trigger chain of actions
    - release calcium from intercellular stores
4. allosteric regulation

#### 1.2.2 | Folding Simulation Methods

1. all-atom 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
2. Accelerated molecular dynamics (AMD)
  -

## 1.3 | Meetings

### 1.3.1 | 12 oct 2020

- computational prediction modeling
  - trying to predict the crystal structure
    - why?
      - to analyze would this fit?
      - does it work with this target
- solving the structure
  - xray cristologyraphy
    - gold standard
    - now got the structure
      - what does that mean?
      - can we simulate how it interacts?
      - can you then do modeling on that to see if drug molecules work? are useful
- look at some concrete examples?
- tell a biological story alongside with computational relevance piece

#### 1. protien synthase

not as much simulation stuff

#### 2. neurotransmitters

dopamine sodium rushes in, electrochemical and concentration gradient recharge gradient by releasing potassium

##### (a) nerst equation

electrochemical gradient as battery

##### (b) goldman-katz equation

- applied to neuro
- ions?