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), protien 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 thourough 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)

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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 cristolography
        - 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