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-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)
    -

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?