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

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)

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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