

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)
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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 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 gradient recharge gradient by releasing potassium