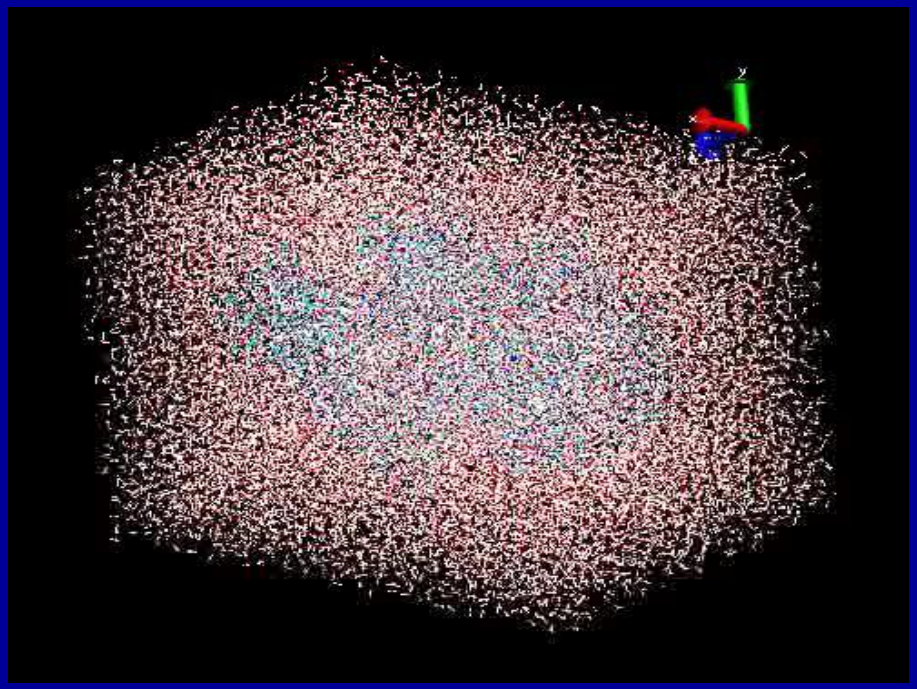
Conserved Water Sites on Active Site of Targeted Proteins for Drug Design via Molecular Dynamics Simulation

Water plays an important role in the normal functioning of proteins, and the conserved and stable water position(s) in the active site of disease-related proteins can be incorporated into the construction of the pharmacophore model and assist for drug design purpose in order to cure the disease. Cluster analysis of the waters' coordinates derived from Molecular Dynamics simulation is used to identify conserved and stable water sites for drug design purposes.



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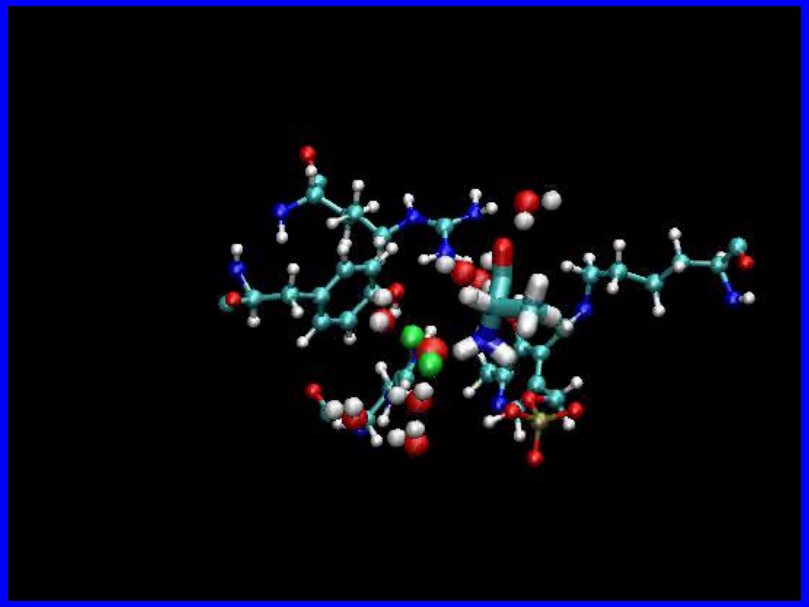
Identification of Conserved Water Sites around Protein Active Sites via MD Simulation for Drug Design



https://youtu.be/I-OBpp2F7Tk

Challenges: 1) Obtain (via Gaussian) Force Fields of uncommon molecule and/or co-factor for MD simulation (via NAMD); 2) Selection of best representative MD trajectories for data analyses; 3) Optimization of the method for the superimposition of MD trajectories.

The one hope to accomplish at 2021 SDSC-SI: Learn how to use GPU nodes for MD simulation and Bioinformatics research.