Simulation Study on Bio-molecular Function and mechanism

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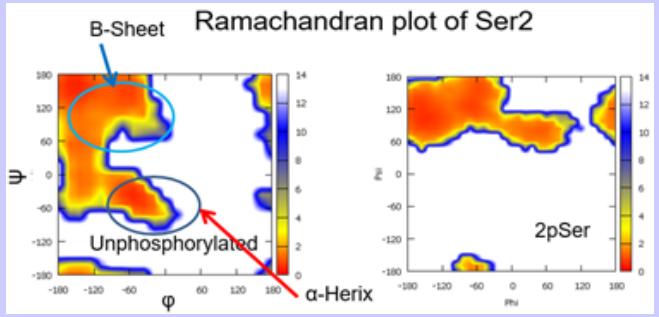
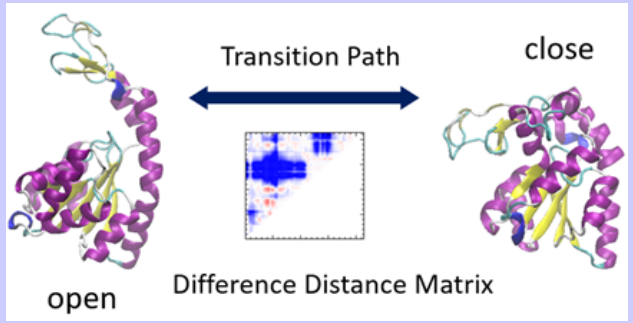
Research Area

1. Study on the function and mechanism of bio-molecules by Molecular dynamics Simulations
2. Development of novel algorithms for investigation of the free energy of Bio-molecules
3. Making use of the deep learning method for the analysis the MD simulation big data.

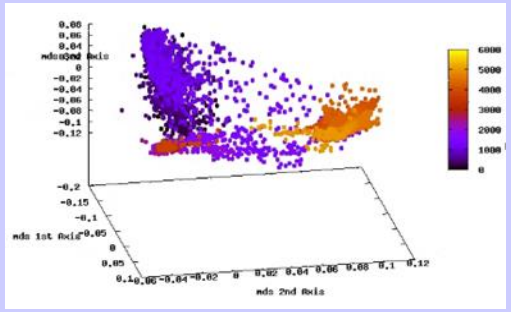
Conformation of the CTD by McMD



Large dynamic motion of Ake



Isomap analysis of CTD



Recent Activities

- **Free Energy Reconstruction from Logarithmic Mean-Force Dynamics Using Multiple Nonequilibrium Trajectories, T. Morishita , Y. Yonezawa, and A. M. Ito, J. Chem. Theory Comput., June 12, 2017**
- **A Method for Predicting Protein Conformational Pathways by Using Molecular Dynamics Simulations Guided by Difference Distance Matrices, Y. Yonezawa, Journal of Computational Chemistry, Vol. 37, Issue 13, p1139-1146, 2016**
- **Molecular Dynamics Study of the Phosphorylation Effect on the Conformational States of the C-terminal Domain of RNA Polymerase II, Yonezawa Y., J. Phys. Chem., B118 , 4471-4478, 2014**