Identifications and prediction of protein flexibilities in amino-acid solutions

Madhurima Jana

Department of Chemistry

National Institute of Technology Rourkela, India, Odisha 769008

Email: janam@nitrkl.ac.in

The use of amino acids as osmolytes or excipients in protein formulation is known.[1] Different amino acids as additives in solution play a diverse role in the protein stabilization process due to the heterogeneity in the side chain functional group. In this presentation, emphasis will be given to identifying the temperature-dependent conformational behavior of small model proteins in the basic and aromatic amino acid solutions, compared to their native folded structure using atomistic molecular dynamics simulations.[2-5] Further, I shall briefly discuss the evolutionary prediction accuracy of three neural network-based models in calculating the molecular simulation generated time series of native contacts of the protein, which is one of the most vital parameters in order to define the resemblance of a protein conformation with its native state.[6]

References:

1. T. Arakawa, K. Tsumoto, Y. Kita, B. Chang, and D. Ejima, *Amino Acids* **2007**, 33, 587
2. S. Santra, M. Jana *J. Chem. Inf. Model*. **2020**, 60, 3105−3119.
3. S. Santra, S. Dhurua, M. Jana *J. Chem. Phys*. **2021**, 154, 084901.
4. S. Santra, M. Jana *J. Comput. Biophys. Chem*. **2022**, 21, 391–404.
5. S. Santra, M. Jana *J. Phys. Chem B* **2022**, 126, 1462−1476.
6. S. Santra, M. Jana *Computational Biology and Chemistry* **2022**, 97, 107625.