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Friday, November 1, 2024

12:00-1:00 pm

**Biotechnology Center Auditorium
or via Zoom**

<https://uwmadison.zoom.us/j/97615509019>

Predicting and Discovering Protein Dynamics

Abstract: The functions of biomolecules are often based in their ability to convert between multiple conformations. Recent advances in deep learning for predicting and designing single structures of proteins mean that the next frontier lies in how well we can characterize, model, and predict protein dynamics. In the first part of my talk, I will describe a simple adaptation of AlphaFold to predict multiple conformations. Combining the resulting “AF-Cluster” method and NMR dynamics experiments allowed us to learn more about the complete conformational landscape of KaiB, and how the slow interconversion that biology necessitates for circadian rhythms is encoded in its sequence. However, a major bottleneck for the field of predicting dynamics has been a lack of standardized datasets of experimental measurements of the timescales of protein motions, and especially those on a micro-millisecond timescale where many biologically-relevant processes occur. In the second part of my talk, I will describe the development of large-scale benchmarks of dynamics from across multiple types of NMR experiments, and initial insights if it might already be possible to predict the presence of biologically-relevant motions.



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