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Understanding and Designing Cyclic Peptides

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ABSTRACT

Cyclic peptides (CPs) are highly sought after for several unique applications. For example, CPs can target protein surfaces with high affinity and selectivity, thereby inhibiting specific protein–protein interactions that cannot be easily targeted with other molecules. New inhibitors will enable mechanistic studies to dissect the functions of individual protein–protein interactions in the complicated cellular interactome. However, robust application of this fundamentally interesting class of molecules for these and other purposes is limited by our poor capacity to predict CP structures and the resulting inability to rationally design functional CPs. In this talk, we describe an efficient enhanced sampling method to simulate CPs, using which we aim to fill the knowledge gap of CP sequence–structure relationships, and enable rational design of CPs with desired structures.

BIO:

Professor Yu-Shan Lin received her Ph.D. in Theoretical Chemistry with Professor James Skinner at the University of Wisconsin, Madison in 2009. She did her postdoctoral work at Stanford under the direction of Professor Vijay Pande. In 2012, she joined the faculty of the Tufts University, and her research group aims to elucidate the structures and functions of biomolecules by integrating the power of advanced computations with the elegance of chemical theory. Professor Lin has received the Achievement Award from the Tufts University, and the ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry from the American Chemical Society.