

UNIVERSITY OF RHODE ISLAND
Department of Chemistry
SEMINAR

3:00 P.M., Monday, October 19, 2026
Room 105 – Beapre Center

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Structure prediction of cyclic peptides
using molecular dynamics simulation and
machine learning

HOST

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Abstract

Peptides occupy a unique chemical space between small molecules and proteins. Their tunable backbone topology and amino-acid chemistry, especially through the use of non-canonical amino acids beyond the DNA-encoded twenty, enable high-affinity recognition of shallow or extended protein surfaces while offering avenues to optimize specificity, stability, membrane permeability, and other drug-like properties. Small cyclic peptides (5–15 amino acids) are of particular interest because they can balance conformational control with adaptive flexibility, enabling strong binding and, in some cases, unexpectedly favorable passive membrane permeability and oral bioavailability.

A major challenge in cyclic peptide development is the limited availability of structural information, which hinders structure-based design and makes it difficult to understand why different cyclic peptide sequences exhibit varying binding affinities, membrane permeabilities, and other properties. This lack of structural insight arises because most cyclic peptides exist as ensembles of multiple conformations in solution, making them extremely challenging to characterize experimentally using techniques such as solution NMR spectroscopy. In this talk, I will describe how molecular dynamics simulations with enhanced sampling methods can be used to obtain this critical structural information. I will also introduce StrEAMM (Structural Ensembles Achieved by Molecular dynamics and Machine learning), a framework that integrates simulation data with machine learning to rapidly generate high-quality structural predictions for cyclic peptides. This capability to efficiently predict structural ensembles will help researchers uncover the structural origins of cyclic peptide behavior and significantly accelerate the development of this promising class of molecules.