

# Predicting New Protein Conformations from Molecular Dynamics Simulation Conformational Landscapes and Machine Learning

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## Abstract

Molecular dynamics (MD) simulations are a popular method of studying protein structure and function, but are unable to reliably sample all relevant conformational space in reasonable computational timescales. A range of enhanced sampling methods are available that can improve conformational sampling, but these do not offer a complete solution. We present here a proof-of-principle method of combining MD simulation with machine learning to explore protein conformational space. An autoencoder is used to map snapshots from MD simulations onto the conformational landscape defined by a 2D-RMSD matrix, and we show that we can predict, with useful accuracy, conformations that are not present in the training data. This method offers a new approach to the prediction of new low energy/physically realistic structures of conformationally dynamic proteins and allows an alternative approach to enhanced sampling of MD simulations.

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