STATISTICAL THERMODYNAMICS FOR RNA STRUCTURES WITH SIMPLE TERTIARY CONTACTS AND PSEUDOKNOTS

Zoia Kopeikin

Dr. Shi-Jie Chen, Dissertation Supervisor

ABSTRACT

In this thesis, we develop statistical mechanical models for the folding of simple RNA tertiary structures. The focus is on the calculation of the tertiary structure conformational entropy. The key idea of the method is to account for the excluded volume correlations between different structural subunits by focusing on the interfacial regions. Tests against exhaustive computer lattice enumerations for chain conformations on a two-dimensional square lattice show that the model is accurate and reliable.

The theory enables predictions for the free energy landscapes and conformational transitions for simple RNA tertiary folds and pseudoknots. Further applications to the force-induced unfolding of RNA H-pseudoknots allow us to obtain the sequence-specific native structures, folding stabilities, pathways and folding cooperativities from the force-dependent free energy landscapes and the force-extension curves.

Though the model is based on a two-dimensional lattice chain representation, the general principles developed in the model are directly applicable to the conformations at the atomic level.