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Statistical Mechanics of RNA Structure Prediction

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RNA structure is hierarchical and therefore the secondary structure, the set of the canonical base pairs, can be predicted independently of the 3D structure. For decades, these predictions were based on predicting the lowest free energy structure, that with the highest probability of forming. In these calculations, free energy change is predicted using an empirical, nearest neighbor model.

The accuracy of secondary structure prediction can be significantly improved by determining the probabilities of formation of structures using partition functions. In this talk, I will show that structures composed of base pairs with high pairing probability are more accurate, on average, than lowest free energy structures. I will also show that probabilistic predictions of secondary structure can be used to improve the design of short interfering RNA (siRNA), which are widely used in science and medicine to silence expression of specific genes.

David Mathews is a professor of Biochemistry & Biophysics at the University of Rochester Medical Center in New York State. He attended both medical school and graduate school at the University of Rochester, where he received his Ph.D. in Chemistry. His thesis work was with Doug Turner on determining the set of free energy change nearest neighbor parameters for RNA folding, developing methods to constrain folding based on wet lab experiments, and predicting a secondary structure common to two sequences. He did a post-doc with David Case at the Scripps Research Institute, San Diego, California, to work on all-atom modeling of RNA. He founded his lab in 2004 and currently studies the computational biology of RNA, including improving methods for secondary structure prediction, identifying novel ncRNAs in genomes, and all-atom modeling of RNA