

The discovery of nucleotide cyclic motifs, the implementation of the MC-Fold and MC-Sym pipeline, and the prediction of small and large RNA 3-D structures

The ribosome post-crystallographic era and the recent enthusiasm about the involvement of small RNAs in gene regulation have greatly stimulated RNA research. In our laboratory, we developed new computational tools to systematically study RNA 3-D structures. Using these tools, we identified and formalized a new RNA structure fundamental element: the nucleotide cyclic motif (NCM). We used NCMs to develop a secondary structure prediction algorithm, MC-Fold, which naturally includes the contributions of all base pairing types. We also modified our 3-D structure algorithm, MC-Sym, to use it in combination with MC-Fold in a pipeline to predict RNA 3-D structures from sequence data. In this presentation, I will present 1) how the NCMs were discovered from a systematic analysis of a 23S rRNA crystal structure; 2) how we formalized the NCMs and how we implemented MC-Fold and MC-Sym; and, 3) how we can now use the resulting tools to predict small and large RNA 3-D structures from sequence and low-resolution experimental data.