Understanding the 3D structural properties of RNAs will play a critical role in identifying their functional characteristics and designing new RNAs for RNA-based therapeutics and nanotechnology. In an attempt to achieve a better insight into RNAs, biochemical experiments have been used to produce data with positional details of atoms in RNA structures. These data have created opportunities for applying computational analysis to solve various biological problems. In this dissertation, we addressed annotation issues of base-pairing interactions in the low-resolution structure data and presented new methods to analyze RNA structural motifs. Annotating base-pairing interactions is one of the critical steps in analyzing RNA structures. However, it is challenging to annotate the interactions, especially if the data is low-resolution. We have developed a method, CompAnnotate, that utilizes the geometric information available in high-resolution homolog structures to improve the annotations in the low-resolution structures. The benchmarking results show that CompAnnotate can improve the annotation results of all existing state-of-the-art annotation methods. The improved annotation creates better opportunities to analyze the RNA structures even when the data is low-resolution. The second significant goal we achieve is providing extensive means to compare and contrast RNA structural motifs. We have developed a new method, RNAMotifContrast, which builds relational graphs among motifs based on their structural similarities. Applying this method, we have recognized and generalized the concept of motif subfamilies. From a dataset of known RNA structural motif families, we showed that subfamilies possess unique structural variations while holding standard features of a family. Finally, we have applied RNAMotifContrast to discover new families and corresponding subfamilies by clustering motifs from all non-redundant RNA structures. Overall, the outcome presented in this dissertation gives a new perspective to observe the relations among motifs more closely and provides valuable insights into RNA's diverse roles.

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The public is welcome to attend.