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Automated building of three-dimensional RNA structures[1] YUNJIE ZHAO, Department of Physics, Huazhong University of Science & Technology; Department of Physics, George Washington University, ZHOU GONG, YANGYU HUANG, YI XIAO, Department of Physics, Huazhong University of Science & Technology, CHEN ZENG, Department of Physics, George Washington University — RNAs have been found to be involved in many biological processes. Difficulties of experimental determination of tertiary structures of RNA limit our understanding of their biological functions. Therefore, some computational methods of building tertiary structures of RNA have been proposed. However, current algorithms of RNA tertiary structure prediction give satisfactory accuracy only for RNA of small size and simple topology, and most are not fully automatic. Here, we present an automated and efficient program, 3dRNA. Since the organization of RNA structure is largely defined by topological constraints in the secondary structure as well as the tertiary contacts, we build the RNA tertiary structure from the smallest secondary elements (SSEs) by using a two-step procedure. We first assemble the SSEs into hairpins or duplexes and then into complete structure since the tertiary structures of hairpins and duplexes usually can be built with a high accuracy. In a benchmark test with known structures, 3dRNA can give predictions with reasonable accuracy for RNAs of larger size and complex topology.

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