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Namhee Kim*, kimnamhee@gmail.com, and **Tamar Schlick**. *Mathematical RNA Biology: Graph Theory Approaches for RNA Structure Modeling and Prediction*.

Ribonucleic Acid (RNA) molecules become a prominent subject in modern biology due to recent discovery of their essential cellular roles. Understanding the mechanisms behind RNA's biological roles requires RNA tertiary (3D) structural knowledge. The modular and hierarchical RNA structures offer a solid ground for mathematical approaches, such as graph theory, to model and predict RNA 3D structures. Here, I present a hierarchical graph sampling approach to describe and predict RNA topologies by a coarse-grained sampling of 3D graphs guided by knowledge-based potentials derived from bend, twist, and compactness measures based on known structures. Sampling RNA graphs accelerates the global search for candidate RNA topologies, and the scoring potentials help select good candidates using a clustering approach. I also present recent applications of graph partitioning algorithms to discover the modularity of RNA networks and develop systematic design strategies for new RNA structures. (Received September 16, 2014)