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Tamar Schlick*, 251 Mercer St., New York, NY 10012, and **Namhee Kim, Mai Zahran** and **Shereef Elmetwaly**. *Folding RNA by a Hierarchical Graph Sampling Approach*.

A current challenge in structure prediction of ribonucleic acids (RNA) is the description of global tertiary (3D) topology or helical arrangements compatible with a given RNA secondary (2D) structure. We present a hierarchical Monte Carlo sampling approach to describe RNA helical geometries by a coarse-grained sampling of 3D graphs guided by knowledge-based potentials derived from bend, twist, and radii of gyration 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. The combination of coarse-grained modeling, junction prediction, and efficient sampling leads to significant improvements over current approaches for characterizing 3D global helical arrangements in large RNAs from a given 2D structure. The remaining step of translating candidate graphs to atomic models can be approached with our ideas of graph partitioning and build-up procedures already utilized for RNA design. (Received August 25, 2014)