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McGenus: A Monte Carlo algorithm to predict RNA secondary structures with pseudoknots

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We present McGenus, an algorithm to predict RNA secondary structures with pseudoknots. The method is based on a classification of RNA structures according to their topological genus. McGenus can treat sequences of up to 1000 bases and performs an advanced stochastic search of their minimum free energy structure allowing for non trivial pseudoknot topologies. Specifically, McGenus employs a multiple Markov chain scheme for minimizing a general scoring function which includes not only free energy contributions for pair stacking, loop penalties, etc. but also a phenomenological penalty for the genus of the pairing graph. The good performance of the stochastic search strategy was successfully validated against TT2NE which uses the same free energy parametrization and performs exhaustive or partially exhaustive structure search, albeit for much shorter sequences (up to 200 bases). Next, the method was applied to other RNA sets, including an extensive tmRNA database, yielding results that are competitive with existing algorithms. Finally, it is shown that McGenus highlights possible limitations in the free energy scoring function. The algorithm is available as a web-server at this http URL

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