

Combinatorial Optimization Applications in Computational Biology.

Many computational biology problems can be represented as combinatorial optimization problems. The resulting complex optimization problems can then be tackled by effective and scalable local search and hybrid search techniques. In this talk I will describe two of such applications: protein folding and RNA energy barrier. A well-studied model for protein folding is the HP model whose goal is to maximize the number of HH contacts (hydrophobic-hydrophobic) I will present an efficient implementation of Large Neighborhood Search (LNS) for the protein folding problem under the HP-model in the Face Centered Cubic Lattice (FCC). The RNA energy barrier is the problem of finding a path between two different RNA structures (for the same sequence) in which the structure of highest energy is minimal. I will present an efficient technique inspired by tabu search to find the path of lowest energy for bistable RNA switches