FoldRNA

Program for RNA secondary structure prediction based on dynamic programming (Nussinov and Jackonson, 1978, Zuker, 2005). For energy calculation nearest neighbor energy rules are used.

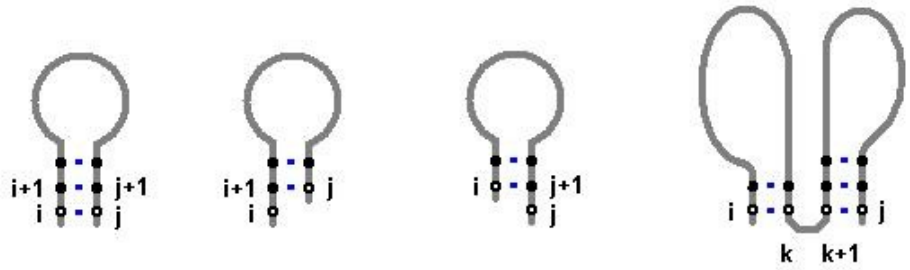
FoldRNA uses energy parameters similar to mfold.

FoldRNA uses energy parameters mainly from:
Turner D.H. and Sugimoto N. (1988) RNA structure prediction Ann.Rev.Biophys.Biophys.Chem. 17, pp. 167-92; Table 1

METHOD DESCRIPTION:

FoldRNA predicts optimal and suboptimal secondary structures of RNA using dynamic algorithm for energy minimization.

Solution of a long sequence is decomposed into solutions of smaller problems:
Let's define E(i,j) = minimum energy for subchain starting at i and ending at j, and a(i,j) = energy of pair i,j.
If values E(i,j) are calculated for line which is maximally close to main diagonal of matrix LxL, where L = sequence length. (min. hairpin loop should have size not less than 3 nt), then we can find step by step this values for lines next after this, using the following recursion scheme (4 possible cases):



1 2 3 4

```
1) i,j is paired,      E(i,j) = E(i+1,j-1) + a(i,j)
2) i is unpaired,      E(i,j) = E(i+1,j  )
3) j is are unpaired,  E(i,j) = E(i  ,j-1)
4) bifurcation         E(i,j) = E(i,k) + E(k+1,j)
```

```
Recursion (iteration over length):

E(i,j)=min{
            E(i+1,j),

            E(i,j-1),

            E(i+1,j-1)+a(i,j),

            min  ( E(i,k) + E(k+1,j) )
           i<k<j

          }
```

When all matrix is filled, the programs searches for lowest value of E(i,j), and then restores by the matrix corresponding secondary structure and sends it to output.
Program is provided with viewer.

Output example:

```
Program RNAfold (Softberry Inc.) version 3.0
Sequence_name: "At-MIR156a_Stem" Length: 183

::: structure # 1 :::
Energy: -82.9 kkal/mol 75% in helices

        10        20        30        40        50        60
gugaaugaaagaguugggacaagagaaacgcaaagaaacugacagaagagagugagcaca
((((..((.((((((((((((((((((.....((((..((((((((((((((((((.
        70        80        90       100       110       120
caaaggcaauuugcauaucauugcacuugcuucucuugcgugcucacugcucuuucuguc
(((.((((((..((((......)))).)))))....))).)))))))).))).)))))))
       130       140       150       160       170       180
agauuccggugcugaucucuuuggccugucuucguucucuaugucucaaucucucucuau
)).....(((.(((((.....))))))))))))..)))))).)))))))).)))).))..)
       190
cac
)))

GCG format:
    1 g       0    2  183    1
    2 u       1    3  182    2
    3 g       2    4  181    3
    4 a       3    5  180    4
    5 a       4    6    0    5
    6 u       5    7    0    6
    7 g       6    8  177    7
    8 a       7    9  176    8
    9 a       8   10    0    9
   10 a       9   11  174   10
   11 g      10   12  173   11
   12 a      11   13  172   12
   13 g      12   14  171   13
   14 u      13   15  169   14
   15 u      14   16  168   15
   16 g      15   17  167   16
   17 g      16   18  166   17
....
```