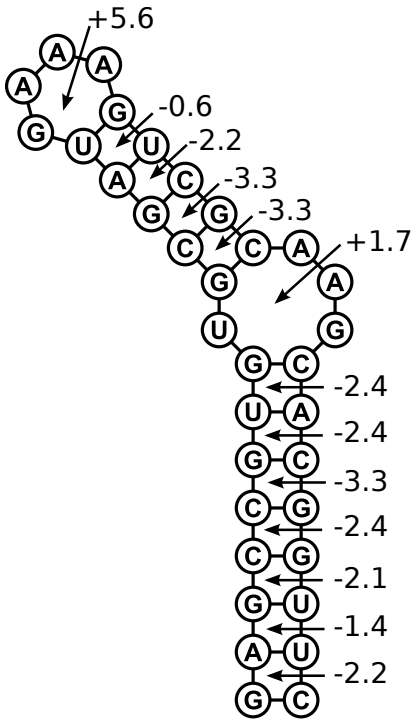
Solution: Energy Based RNA Secondary Structure Prediction

1 Nearest Neighbor Energy Parameters

Solution for 1.b:



Stacked base pair energy: $\Delta G_{base-stack} = -25.6$ kcal/mol
Loop energy: $\Delta G_{loop} = 7.3$ kcal/mol
Gibbs free energy: $\Delta G = \Delta G_{base-stack} + \Delta G_{loop} = -18.3$ kcal/mol

2 MFE folding recurrences

Solution:

table	term	explanation
C_{ij}	$\min_{i<u<j} M_{i+1,u} + M^1_{u+1,j-1} + a$	Adds multi-loop free energy contributions to closed structure free energy where the multi-loop is closed by (i,j) and defined by $M_{i+1,u} + M^1_{u+1,j-1}$; u defines the size of the first part of the multi-loop; a is a penalty for adding a multi-loop.
M_{ij}	$\min_{i<u<j} (u-i+1)c + C_{u+1,j} + b$	The first part of the multi-loop is defined by unpaired region $x[i..u]$ and a component enclosed by $(u+1,j)$; $(u-i+1)$ is the length of the unpaired region, for each unpaired base a penalty energy c is added; b is an energy contribution for adding a component to a multi-loop
M_{ij}	$\min_{i<u<j} M_{i,u} + C_{u+1,j} + b$	Adds a component, i.e. enclosed structure to the multi-loop which is subsequence $x[u+1..j]$; u determines where the component starts, thus the size of the component; b is a energy contribution for adding a component to a multi-loop
M_{ij}	$M_{i,j-1} + c$	Extends mutli-loop by an unpaired base; c is a penalty energy for unpaired bases.
M^1_{ij}	$M^1_{i,j-1} + c$	The final part of the multi-loop is extended by an unpaired base; c is a penalty energy for adding an unpaired base
M^1_{ij}	$C_{ij} + b$	The final part of the multi-loop is defined by the closed structure C_{ij}, i.e. component closed by (i,j); b is an energy contribution for adding a component to a multi-loop

Table 1: Multi-loop energy model - explanation.