Biophysical Chemistry I, Fall 2010

Homework Assignment #5, due Nov. 9

1. Go to *http://mfold.bioinfo.rpi.edu/.* This page is maintained by Michael Zuker, who was a key developer of algorithms to estimate secondary structure for RNA. Follow the "Applications" link to "RNA Folding". (You are encouraged to read the paper linked at the top of the page (which has some instructions), but you don't need to absorb everything in that paper.) Use the server in "immediate mode" to estimate the structure and folding free energy of the sequence "GCCGUUCGCGGC". Report the predicted structure and the estimated folding free energy. (Hint: there are lots of file formats available; I suggest you follow the link called "Structure 1".)

2. Now let's try something harder: go to *http://rose.man.poznan.pl/5SData/* for a database of information about 5S RNA. If you click on "3D" you can see an xray structure and secondary structure for the 5S RNA for *H. marismortui*. Find its sequence (the "sequences" tab; you can use sequence labeled "Haloarcula marismortui 1") and copy and paste that into the mfold server. You should see several low energy structures, but look at just the first three for the purposes of this homework assignment. (Hint: look for "View individual structures" and click on the "pdf" link to get a nice visualization.) Put these pdf figures into your homework, and briefly discuss how well the server did, concerning the following three points:

   (a) How well did it predict the helices (stems) that are actually present in the xray structure?

   (b) Qualitatively, how similar or different are the first three structures compared to each other?

   (c) How different are the predicted folding free energies for these three structures? Do you think the differences are significant, given the uncertainties in both the secondary structure and in the method by which these numbers are obtained?