Tutorial

Folding RNA Molecules

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Sample to Insight

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Tutorial

Folding RNA Molecules

In this tutorial, you will learn how to predict the secondary structure of an RNA molecule. You will also learn how to use the powerful ways of viewing and interacting with graphical displays of the structure.

The sequence to be folded in this tutorial is a tRNA molecule with the characteristic secondary structure as shown in figure 1.

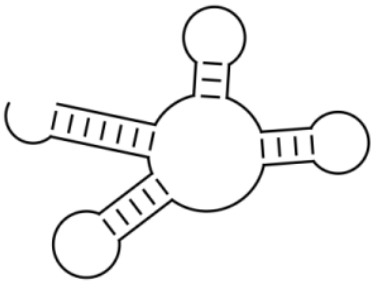

Figure 1: *Secondary structure of a tRNA molecule.*

The goal for this tutorial is to get a nice-looking graphic result of this structure.

The sequence we are working with is a mitochondrial tRNA molecule from *Drosophilia melanogaster*. The name is *AB009835*, and can be found be searching GenBank.

1. Go to:

   Download | **Search for Sequences at NCBI (**  **)**

2. Enter the name of the sequence in the Search field and click on the **Start Search** button (figure 2).

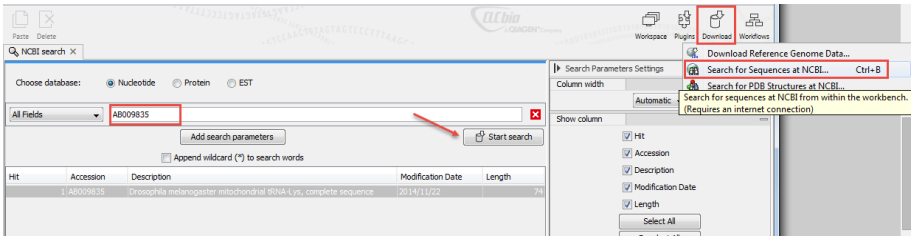

Figure 2: *Search for a sequence at NCBI.*

3. Once the sequence has been found, select it and click on the button **Download and Save** (figure 3).

4. Go to:

   Toolbox | **Classical Sequence Analysis** () | **RNA Structure** () | **Predict Secondary Structure** ()

   or use the Launch button () to find the tool.

5. Select the sequence you just downloaded and click **Next**.

6. In this dialog, choose to compute a sample of sub-optimal structure and leave the rest of the settings at their default (see figure 4).

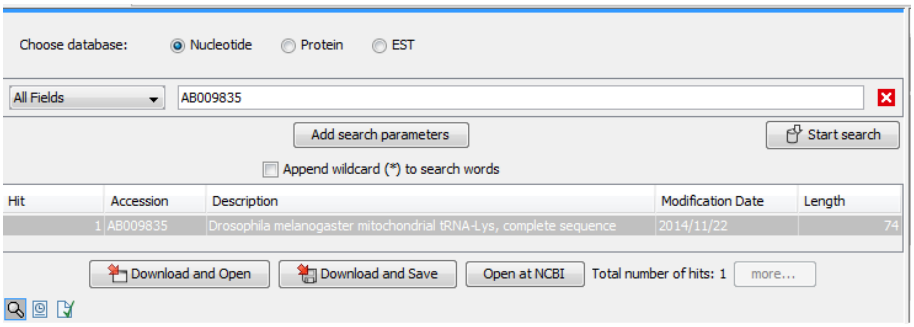

Figure 3: *Download and Save the sequence in the Navigation Area.*

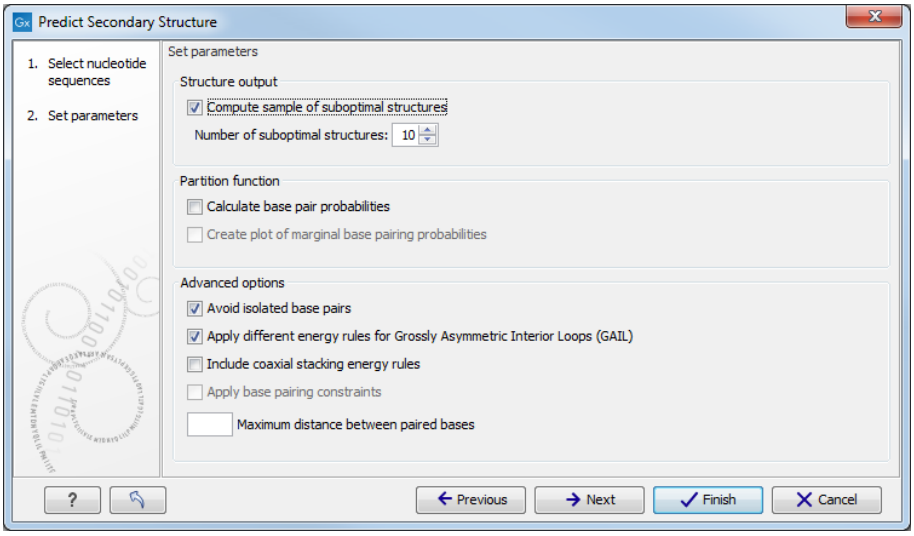

Figure 4: *Selecting to compute 10 suboptimal structures.*

7. Leave the options as default in the "Result handling" window and click on **Finish**.

You will see a linear view of the sequence with structure information for the ten structures below the sequence, and the elements of the best structure are shown as annotations above the sequence (see figure 5).

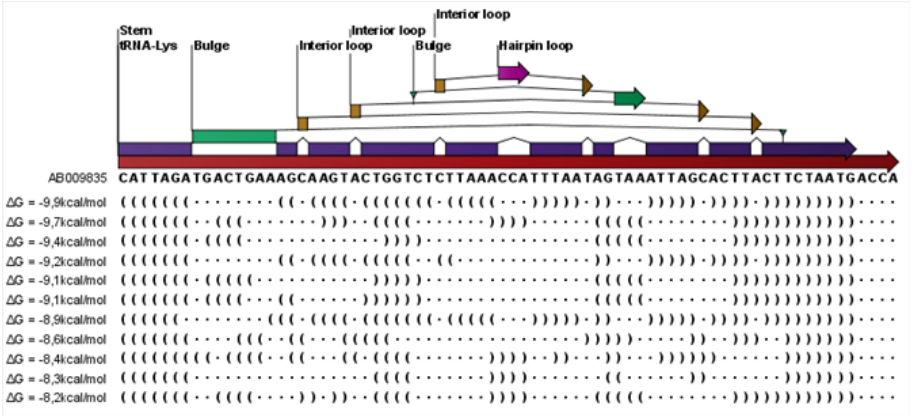

Figure 5: *The inital, linear view of the secondary structure prediction.*

For now, we are not interested in the linear view. Click the **Show Secondary Structure 2D View** ( ) button at the bottom of the view to show the secondary structure. It looks as shown in

figure 6).

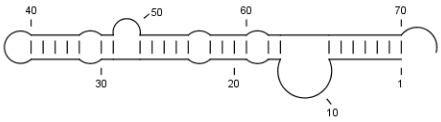

Figure 6: *The inital 2D view of the secondary structure.*

This structure does not look like the one we expected (shown in figure 1) so we will now take a look at some of the other structures (we chose to compute 10 different structures) to see if we can find the classic tRNA structure.

Open a split view of the **Show Secondary Structure Table** ( ) by holding Ctrl (or ⌘ on Mac) and the icon for **Show Secondary Structure Table** ( ).

You will now see a table displaying the ten structures. Selecting a structure in the table will display this structure in the view above. Select the second structure in the table. The views should now look like figure 7).

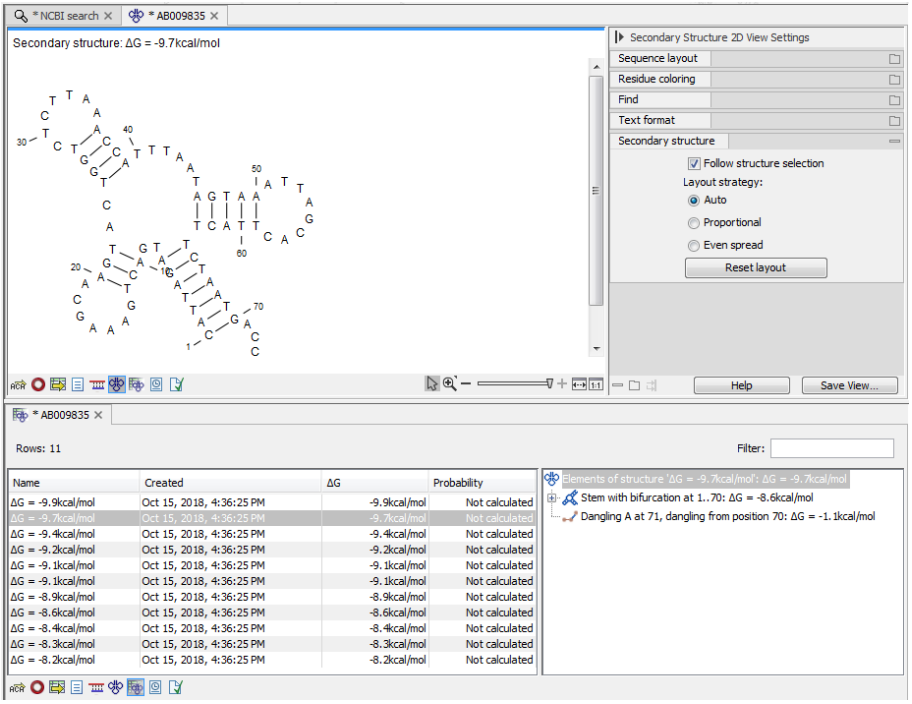

Figure 7: *A split view showing the scondary structure table at the bottom and the Secondary structure 2D view at the top. (You might need to Zoom out to see the structure).*

The secondary structure now looks very similar to figure 1. By adjusting the layout, we can make it look exactly the same: in the Side Panel of the 2D view, under **Secondary Structure**, choose the **Proportional** layout strategy. You will now see that the appearance of structure changes.

Next, zoom in on the structure to see the residues (with the Fit Width ( ) button for example).

If you wish to make some manual corrections of the layout of the structure, you will need the **Pan** ( ) mode. To select it, right click on the magnifier ( ) and select the Pan mode by clicking on the hand icon ( ) (figure 8).

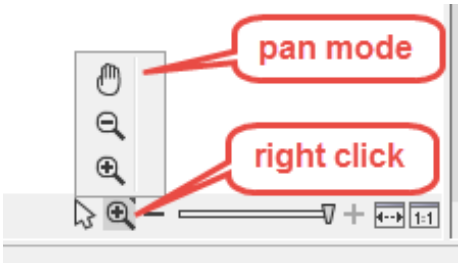

Figure 8: *Right click on the magnifier to display the pan mode option.*

Now you can place the hand cursor on the opening of a stem, and a visual indication of the anchor point for turning the substructure will be shown (see figure 9).

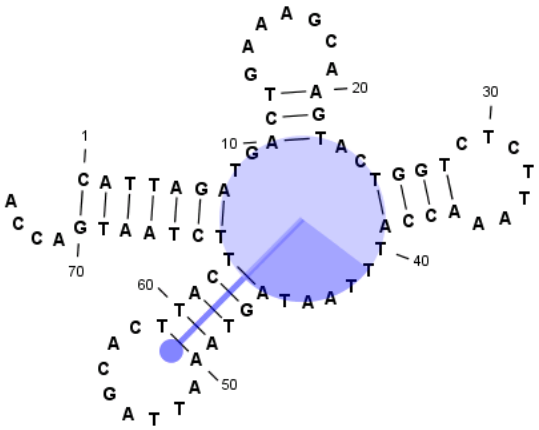

Figure 9: *The blue circle represents the anchor point for rotating the substructure.*

Click and drag to rotate the part of the structure represented by the line going from the anchor point. In order to keep the bases in a relatively sequential arrangement, there is a restriction on how much the substructure can be rotated. The highlighted part of the circle represents the angle where rotating is allowed.

In figure 10, the structure shown in figure 9 has been modified by dragging with the mouse.

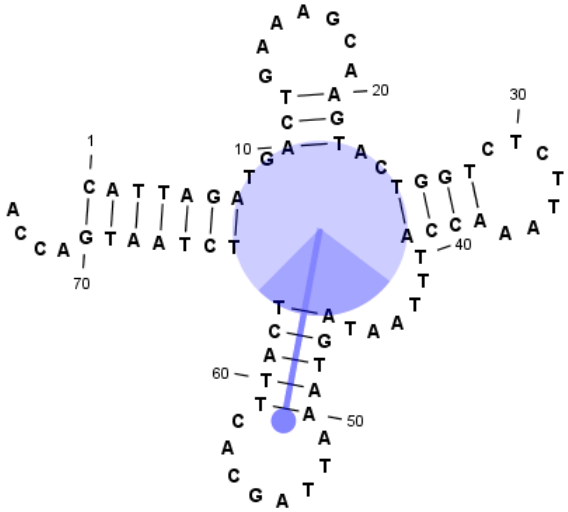

Figure 10: *The structure has now been rotated.*

The view can of course be printed ( ) or exported as graphics ( ).