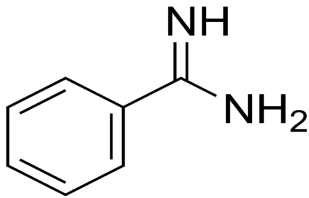


Analysis of the interaction between Ancrod and benzamidine

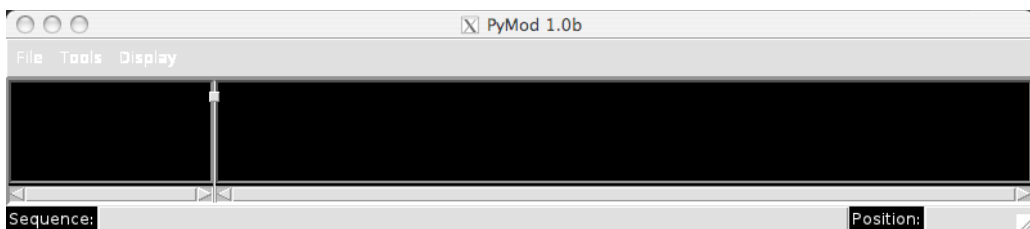
Using the three-dimensional model, obtained by sequence homology, of the serine protein Ancrod (present in snake venom *A. contortrix*), we will study the interaction between this protein and benzamidine, its competitive inhibitor:



BENZAMIDINA

1. MACROMOLECOLE: Connect to Pubmed, and download the FASTA sequence of the protein with GI code: 461512 (Snake venom serine protease from *A. contortrix*).

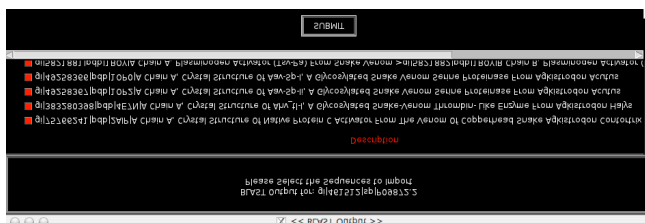
Launch the PyMol program, and from the "Plugins" menu, select "PyMod 1.0". A new window will appear (a second window will ask you to create a new directory, click on OK):



From the "File" menu of this window, import the previously saved sequence (File->sequence-> add from file)

Left click the sequence name (which turns green), then select "PSI-Blast" from the "Tools" menu. In the window that appears, click on Submit, and wait for the results.

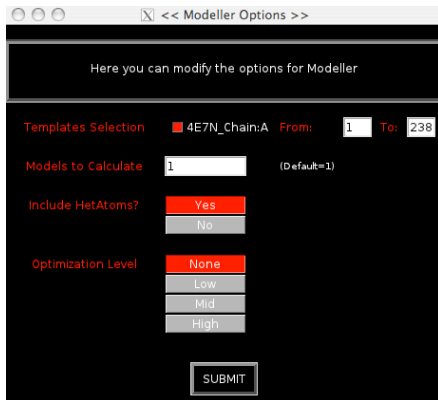
Among the possible templates to use for modeling, select the pdb 4E7N code, checking the red box next to the relevant code, and press submit:



In the window with the PyMod sequences, a red square with the sign "+" will appear. Click on the square. The protein sequence with code 4E7N will appear. Select it (left button on the name, it turns green), then pressing the right button select "Extract sequence". Then select it again and right click on "Get PDB File"

Select both sequences, and click on ClustalW from the Tools menu. In the window that appears, click on Submit. Note that the two sequences have been aligned.

Now select only the sequence to be modeled, and click on Modeler from the Tools menu. In the window that appears, select the template by checking the red square. Under "Include HetAtoms, select" NO ". Finally, click on Submit. After a few minutes, the Ancred model will appear on the main PyMOL window.



Save your model: "File -> Save Molecule" from PyMOL menu.