**USING MODELLER**

http://www.salilab.org/modeller/

My modeller key (you need it for some websites): MODELIRANJE

STEP 1:

Create a “modeller” folder

Copy in the template files (targetname.ali, targetname.py)

STEP 2:

a) Target prep - get protein sequence in fasta frormat from uniprot

- BLASTp against protein databank to find template

b) Template prep - find template in pdb

- download template sequence in fasta format

- download pdb file

STEP 3:

Use the 2 FASTA files to do a pairwise sequence alignment using Emboss Matcher

<http://www.ebi.ac.uk/Tools/psa/emboss_matcher/>

Download the alignment file

STEP 4:

Prepare the modeller files (BE CAREFUL!)

1. The py file – 4 edits required (change filename to the target name, and 3 in text edits)
2. The ali file – 7 edits required (change filename to the target name, and 6 in file edits)

STEP 5:

CD to folder containing files (modeller rmust be run from within this folder)

Command: “mod9.19 xxx.py” (replace the xxx with the .py filename)

Possible problems:

- Mismatched sequences → open the log file to find mismatch → edit .ali file

- Unequal length sequences → same fix

STEP 6:

Open log file → scroll to “ >> Summary of successfully...”

Best model has lowest “molpdf” (Property Density Function - measure of energy state)

In the modeller folder, rename that model to “bestmodel.pdb”

Visualise the model using Pymol

STEP 7:

ramachandron plot <http://mordred.bioc.cam.ac.uk/~rapper/rampage.php>

errat <http://servicesn.mbi.ucla.edu/ERRAT/>

verify3d <http://servicesn.mbi.ucla.edu/Verify3d/>