C. Symmetric Docking - SymmDock

Enveloped viruses enter cells via a membrane fusion reaction driven by conformational changes of specific viral envelope proteins.[1] The envelope glycoproteins from tick-borne encephalitis virus assemble metastable homodimers on the viral surface and due to membrane fusion it forms very stable homotrimers. The energy released during the transition from the dimers at the viral surface to the targetmembrane-inserted homotrimers is used to drive the merging of the viral and cellular membranes.

In this exercise you will solve **Target 10** of the CAPRI challenge , using SymmDock. You will need to predict the homo-trimer structure of the above envelope glycoprotein.

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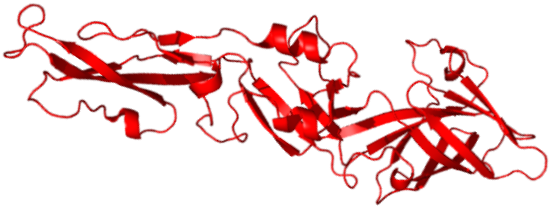
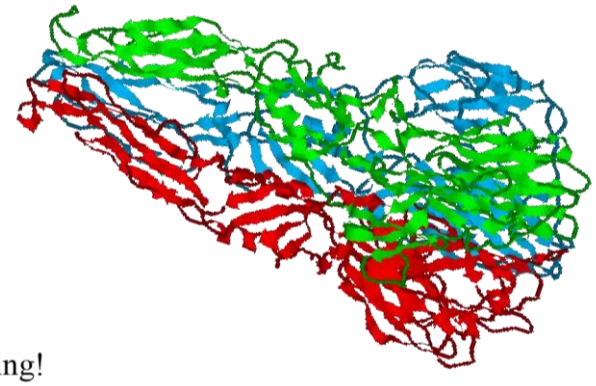


A. Submitting a SymmDock job:
   1. Look at the files in the "Ex1" subdirectory:
      1svb.pdb – The structure of the monomer in PDB format.
      NativeComplex.pdb – The structure of the correct native complex.
   2. Go to the webserver of SymmDock:
      http://bioinfo3d.cs.tau.ac.il/SymmDock/index.html
   3. Fill out the following fields in the web-server:

Unit Molecule:	Upload the *1svb.pdb* file
Symmetry Order:	3 (since we want to predict a homo-trimer)
e-mail address:	Fill out your e-mail, to which the results will be sent.

   4. Submit the form.

B. Checking the results:
   1. If SymmDock is still running go to:
      http://bioinfo3d.cs.tau.ac.il/SymmDock/runs/3_1svb.pdb_37_48_15_30_10_114/
   2. Look at the output page and examine the results.
   3. Solution number 1 is an accurate prediction of the complex.



Good luck,
and enjoy the docking!

References:
1. Bressanelli et al. (2004) EMBO J. 23(4): 728–738.
2. Janin J. (2005) Proteins. 1;60(2):170-5.

GroEL

This is an E.coli version of the GroEL. The GroEL is a Chaperonin found in many types of bacteria and is very important for the proper folding of proteins. The GroEL has a 7-fold circular symmetry so we will be predicting its structure using SymmDock.

C. Submitting a SymmDock job:

1. Look at the files in the "Ex2" subdirectory:
   1oel.pdb – The structure of the correct native complex.
2. Go to the webserver of SymmDock:
   http://bioinfo3d.cs.tau.ac.il/SymmDock/index.html
3. Fill out the following fields in the web-server:

Unit Molecule:	Write 1oel:A (to give it one chain from the symmetric complex)
Symmetry Order:	7 (since we want to predict a 7-fold circular symmetry)
e-mail address:	Fill out your e-mail, to which the results will be sent.

4. Submit the form.

D. Checking the results:

1. If SymmDock is still running go to:
   http://bioinfo3d.cs.tau.ac.il/SymmDock/runs/7_1oelA_38_0_15_2_11_114/
2. Look at the output page and examine the results.
3. Solution number 1 is an accurate prediction of the complex.
4. You can use Chimera MatchMaker, but with one chain of the solution as the reference structure, and the native complex as the structure to align.