

Exercise 1.

Predict the secondary structure for the given sequences using Jnet, PSIPRED or PREDICTPROTEIN servers

<http://www.compbio.dundee.ac.uk/jpred/>

<http://bioinf.cs.ucl.ac.uk/psipred/> (This takes a long time)

<http://ppopen.rostlab.org/>

a)

```
>sp|O15105|SMAD7_HUMAN Mothers against decapentaplegic homolog 7 OS=Homo sapiens
MFRTKRSALVRRLWRSRAPGGEEDEEGAGGGGGGGELRGEGATDSRAHGAGGGGPGRAGCC
LGKAVRGAKGHHHPHPAAGAGAAGGAEADLKALTHSVLKKLKERQLELLLQAVESRGGTRT
ACLLLPGRLLDCRLGPGAPAGAQAQPPSSYSLLPLLLCKVFRWPDRLRHSSEVKRLCCCESYGKIN
PELVCCNPHHLSRLCELESPPPPYSRYPMDFLKPTADCPDAVPSSAETGGTNYLAPGGLSDSPLL
LEPGDRSHWCVVAYWEEKTRVGRLYCVQEPSLDIFYDLPQGNFCLGQLNSDNKSQLVQKVR
SKIGCGIQLTREVDGVWVYNRSSYPIFIKSATLDNPDSRTLLVHKVFPGFSAKAFDYEKAYSLQR
PNDHEFMQQPWTGFTVQISFVKGWGQCYTRQFISSPCWLEVIFNSR
```

b)

```
>teszt
```

```
QLTQKNKSADGLVFNVTQDMINKSTKPYRGHRFTKENVRILESWFAKNIENPYLDTKGLENL
MKNTSLSRIQIKNWVSNRRRKEKT
```

Ignore the known structure.

Now look at the protein structure with the PDB code 1mmn.

Focus on the C and D chains.

Remove all chains except C and D.

Split the two chains and superimpose them

Turn on the command line:

Favourites

Command Line

In the lower field type:

Split

Now you can superimpose them

Tools

Structure Comparion

Matchmaker

Choose one chain as the reference and align the other one.

Apply

How similar are the two structures? Where do they differ?

What is the predicted secondary structure where you can see the difference?

Exercise 2.

Find coiled coil regions the following sequence:

>SEQUENCE

WSLLEQLGLAGADLAAPGVQQQLELERERLRREIRKELKLKEGAENLRRATDDLGRSLGPVEL
LLRGSSRRLDLLHQQLQELHAHV

using the server

http://www.ch.embnet.org/software/COILS_form.html

How many did you find? How long are they?

Change the weighting of the hydrophobic residues. How do the results change?

What are the secondary structure predictions for these regions?

Exercise 3.

Try to decide if these proteins have transmembrane regions and if they do, what is their topology?

>1

MCSRGWDSCLALELLLLPLSLLVTSIQGHLVHMTVVSGSNVTLNISESLPENYKQLTWFYTFDQ
KIVEWDSRKSKEYFESKFKGRVRLDPQSGALYISKVQKEDNSTYIMRVLKKTGNEQEWKIKLQV
LDPVPKPKVIKIEKIEDMDDNCYLKLSCVIPGESVNYTWYGDKRPFKELQNSVLETTLMPHNYS
RCYTCQVSNSVSSKNGTVCLSPCTLARSFGVEWIASWLVTVPPTILGLLLT

Use the HMMTOP methods:

<http://www.enzim.hu/hmmtop>

and DAS-Tmfilter method

<http://mendel.imp.ac.at/sat/DAS/DAS.html>

Search for signal sequences using SignalP:

<http://www.cbs.dtu.dk/services/SignalP/>

Remove the signal sequence and run HMMTOP again. How did the result change?

Exercise 4.

>2

MLSVAARSGPFAPVLSATSRGVAGALRPLVQAAVPATSESPVLDLKRSVLCRESLRGQAAGRPL
VASVSLNVPASVRYSHTDIKVPDFSDYRRPEVLDSTKSSKESSEARKGFSYLV TATTTVG VAYAA
KNVVSQFVSSMSASADVLAMSKIEIKLSDIPEGKNMAFKWRGKPLFVRHRTKKEIDQEAAVEV
SQLRDPQHDLERVKKPEWVILIGVCTHLGCVPIANAGDFGGYYCPCHGSHYDASGRIRKGPAP
LNLEVPSYEFTSDDMVIVG

Carry out prediction using the TMHMM method

<http://www.cbs.dtu.dk/services/TMHMM/>

Also using the Phobius prediction method:

<http://phobius.sbc.su.se/>

Examine the protein with the Scampi prediction method as well:

<http://scampi.cbr.su.se/>

Find the protein in the Uniprot database:

e.g.:

<http://www.uniprot.org/blast/>

Find the section about the subcellular location :

Subcellular location

Check crossreferences to PDB.

Select one structure and find it the PDBTM database. Does the structural assignment agree with the predictions?

Exercise 5.

Check out the abstract of this paper

PMID: 21835165

What do you think of the suggested interaction?

Hint: Check the localization of the two proteins (Q9UBP4 and P63172).

Use Wolf-Psort (<http://psort.hgc.jp/form2.html>) and TargetP <http://www.cbs.dtu.dk/services/TargetP/> prediction methods and check the Uniport annotation and the <http://compartments.jensenlab.org/Search> server.