

Exercise in protein structure predictions

Submit your answers to a.p.goultiaev@liacs.leidenuniv.nl before 29.04.2019, 23:59.

Email subject: CMB2019 exercises.

It is sufficient to describe what has been done and to give answers to the questions.

Please don't send large files in the attachments.

The answers given as URL's will not be considered.

Using the protein structure homology modeling server SWISS-MODEL (<https://swissmodel.expasy.org>), predict the structures of Xrn1 enzymes of humans and yellow fever mosquitoes (accession numbers NP_061874 and EAT39382, respectively). For the sake of simplicity, for each of the proteins use only one of the templates found by SWISS-MODEL, namely the best in the default sorting according to the value of GMQE, Global Model Quality Estimation.

Which parts of the two proteins are modeled? In each of the models, identify the largest region of lower-quality prediction (coloured red in model-template alignment according to QMEAN local scores). What kind of secondary structures are predicted in these regions, α -helices, β -strands or loops? Do these regions contain insertions or deletions in modeled proteins as compared to the template?

Note: It is advised to watch SWISS-MODEL reporting on the steps of template searching during the program run: it gives more clear picture of how homology modeling works. It is also interesting to explore the obtained model, e.g. identifying some amino acids in both protein structure and amino acid sequence.