Practical course 6
Synthesis of the practical courses

You will use during this TP some tools used in the previous TP's. A report about this TP6 is asked and must be sent to dgilis@ulb.ac.be, in PDF format, before December 21 2018 at midnight. The mark of the report will be decreased by one point per day of delay. You must include in your report the results, a discussion and an analysis of these results. The report must be 6 pages long maximum. This report is individual and plagiarism will be sanctioned by a mark of 0. This report will contribute for 20% of the global mark of the course.

A] Monellin and brazzein are sweet-tasting proteins (see http://pdb101.rcsb.org/motm/199). Their PDB code are 3MON and 2BRZ, respectively.

1) Analyze the quality of the experimental structure of monellin. The PDB file of monellin contains four dimers (chains AB, CD, EF and GH). Select one of the dimer for the task A.2, on the basis of their experimental quality. Justify your selection.
2) Superimpose the 3D structure of brazzein to the two chains of monellin selected in section A.1. Analyze the results in detail (statistical significance of the superimpositions, value of the rmsd's, analyse of the superimpositions, analyze of the superimposed regions, …). Remark: keep in mind that it is possible to superimpose a structure to all the chains of another structure individually or as a whole.

B] You will work in this section on the nitrogen regulatory protein P-II from *Porphyra purpurea* (Uniprot code P51254; http://www.uniprot.org).

1) Model the 3D structure of this protein by comparative modelling and analyze the quality of your model. Which tool and template did you use?
2) Predict the secondary structure of this protein. Which tool(s) did you use and why? What are your results: give the limits of the predicted alpha helices and beta strands? Discuss the results.
3) The STRIDE server (http://webclu.bio.wzw.tum.de/cgi-bin/stride/stridecgi.py) has been developed to assign (not predict) secondary structures from a PDB file (experimental or modelled structure). Use this tool to assign the secondary structure of the models obtained in section B.1. Compare the limits of the secondary structure of your 3D model to the secondary structure prediction of section B.2 and discuss your result.