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Downstream part

Phy-U : a biophysical approach of protein threading

Our Team was in charge of ‘downstream’ tasks which are 1) to thread given protein on a template and 2) score this threading according standard calculations. We decided to adopt a biophysical approach of this work. First, the threading was executed on the protein C-α chain and backbone, which was then completed into a full-atom representation and finally turned into coarse-grain model. The design of the score function was based on Lennard-Jones, DOPE and Coulomb scores and variants. The data we used were provided by Team 10. The first interest of our work is to give a meaningful score of a given threading by using this prosaic approach. Another advantage is the multiplicity of views onto this task, using no less than three protein modelling and five scores. Aside, our approach suffers from many assumptions which prevents it from being biologically interpretable. Also, this work can only give an overview of this method.

First results were rendering quite a balanced result: in proportions, half of the predictions seems to be correct as false and true associations are almost mixed. On the four score we implemented, only three are used in our optimal score function, based on Van der Waals interactions and statistical potential (*cf. Figure shown below: Enrichment curves of our different score functions*).

The results provided us another enlightenment on our work: it confirmed that our tool had a high False Discovery Rate. Also, it is clear that this tool is not to consider for integration studies: it is assumed we only simulate a single protein with no interaction with its environment. However, other knowledges have been discovered that could be integrated to our tool and thus improve its performance.