Prediction of the stability of proteins by computational approaches: a case report

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The prediction of the stability of a protein is a very important issue in computational biology. Indeed, missense mutations are frequently associated to a change in protein stability, leading usually to destabilization, unfolding and aggregation. However, the direct measurement of the effect of mutations on proteins' stability is often impaired by the large number of mutations that can affect a protein sequence. Therefore, predicting the impact of a mutation on this feature is of remarkable interest to infer the phenotypic effects associated to a genotypic variation. For this reason, many different predictors of the effects of mutations on protein stability have been developed during the past years, and they are available online as Web servers. In the present work, we applied several tools based on different approaches to predict the stability of three proteins involved in the different forms of the rare disease galactosemia, and we compare their different results, describing also the problems that we had to face, the solutions that we have adopted and the lessons learnt from this case study.

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