Comparative Protein-Structure Modelling of Bacteriocins

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ABSTRACT

Structural and functional characterizations of proteins have been one of the major problems in biological studies for a long time. The conventional methods of protein structure determination of NMR and X-Ray crystallography are though more accurate but at the same time are highly time consuming and tedious to carry out. Also, the instrumentation required is not that easily available. In the absence of proper structural information, like in the case of bacteriocins, which are anti-microbial proteins or protein complexes produced by lactic acid bacteria, comparative and homology modeling can be useful in predicting the structure based on the protein sequences and there alignment with one or more already known structures. The prediction process consists of fold assignment, target–template alignment, model building, and model evaluation. The number of protein sequences that can be modeled and the accuracy of the predictions are increasing steadily because of the growth in the number of known protein structures and because of the improvements in the modeling softwares.

The present study focuses on the comparative protein-structure modelling of bacteriocins produced by five food starter cultures lactic acid bacteria. *Pediococcus acidilactici*, *Leuconostoc mesenteroids,Enterococcus mundtii,Lactobacillus plantarum* and *Lactobacillus sakei*. Which are all bacteriocins of the Class IIA subclass of these proteins and also consist of the same structural motif. The structures were all modelled using MOE software and also the accuracy was found out based on the "errat" score only those bacteriocins which have an errat score of more than 80% were considered for the further studies.

This study finds its applications in the protein structural analysis studies. Also, with the help of the motif study we can say that development of a synthetic bacteriocin can be carried out on these grounds only. This process solves the problems related to the absence of structural information of such proteins.