MOLECULAR MODELING OF CORYNEBACTERIUM PSEUDOTUBERCULOSIS GROEL-LIKE TYPE I CHAPERONIN

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Homology molecular modeling allows one to predict the 3D structure of a protein, when experimental determination is complicated, expensive and long. It offers the possibility to further investigate the protein function, based on a theoretical model of the structure. A 60 kDa protein has been described through conceptual translation from genome sequence of *Corynebacterium pseudotuberculosis* by Estevam et al. in 2004, and it has been annotated as a chain of GroEL-like type I chaperonin from HSP60 family. Secondary structure and domain predictions have been carried out on the 541 amino acid residue long primary structure, using on-line servers (PredictProtein, PsiPred, nnPredict) and the results have associated this protein to the chaperonin family. The protein presents high sequence similarity (54% identity) with other chaperonins, including some whose three-dimensional structures have been determined by X-ray diffraction or cryo-electron microscopy. Among these structures, 6 were chosen as templates (PDB files: 1GR5, 1IOK, 1KP8, 1PCQ, 1SJP and 1WE3) in order to model the three-dimensional structure of the target chaperonin. So, the sequences of templates and target proteins were manually aligned and the resulting alignment was checked using the align_check() function of Modeller 8v2 package. This software has then been used to perform the proper modeling of the target protein and 50 models have been generated. The lowest energy structure was selected as the best model. Moreover, the model has been validated using Verify3D server and it has obtained good scores for the majority of the amino acid residues of the sequence.

Key-words: chaperonin, *Corynebacterium pseudotuberculosis*, homology molecular modeling.