Abstract

The most popular type of pesticide is the organophosphate (OP) family, which effectively eliminates pests owing to its acute neurotoxicity. Organophosphorus hydrolase is a bacterial enzyme that is capable of degrading a wide range of neurotoxic organophosphate nerve agents. Organophosphorus hydrolase of Kocuria sp was isolated but its protein is not having any predicted 3-Dimensional structure available in PDB (Protein databank) as elucidated by X-ray crystallography or NMR. Its structure was determined in silico by sequence homology. The gene sequence of the Organophosphorus hydrolase of Kocuria sp was known and its protein sequence was subjected to PSI-BLAST at NCBI. There was neither identical sequence available nor the nearest neighbour in the blast analysis. Then an alternative method for finding the homologous protein i.e., fold prediction method was used. The generated model was subjected to several repeated cycles of energy minimization using SPDBV software and the final model was subjected to stereo chemical evaluation. The homology modeled structure of the Organophosphorus hydrolase of Kocuria sp was docked by different OP by Molgro virtual docker and the data were presented.
- www. expasy. org/prosite

Index Terms

Computer Science  Applied Sciences

Keywords

Chloropyrifos  Organophosphorus hydrolase  SPDBV  Molegro Virtual Docker