Abstract

Botulinum neurotoxin (BoNT) complexes consist of neurotoxin and neurotoxin-associated proteins. The Clostridia releases these as protein aggregate, termed as the progenitor toxins. Haeamagglutinin – 33 (HA-33) plays an essential role in the agglutination activity of the botulinum progenitor toxin; it assists in binding and translocating the progenitor toxins through the alimentary epithelial barriers. A three-dimensional homology model of HA-33 is demonstrated in this paper based upon the crystal structure of HAI1 subcomponent of botulinum type C progenitor toxin complexed with galactose. The three dimensional model was designed using MODELLER (9v11) a comparative modelling tool that built a model based on an alignment of a sequence of HA-33 based on the known structure of botulinum type C progenitor toxin complexed with N-acetylgalactosamine. The modelled structure was then evaluated using SAVES. The structural dynamics of the modelled protein was performed by elNemo and based on the scores obtained, it was found to be a reliable and accurate three dimensional structure of the Hemeagglutinin component. It gives an idea about the three dimensional structure of a protein which will would serve as a guide to a detailed understanding of its participation in the process of agglutination. This could also aid in molecular drug designing against botulism.
ences


- Yukako Fujinaga, Kaoru Inoue, Sadahiro Watanabe, Kenji Yokota, Yoshikazu Hirai, Eiko Nagamachi and Keiji Oguma (1997). The haemagglutinin of Clostridium botulinum type C progenitor toxin plays an essential role in binding of toxin to the epithelial cells of guinea pig small intestine, leading to the efficient absorption of the toxin. Microbiology. 143, 3841-3847

Index Terms

Computer Science
Applied Sciences

Keywords

Clostridium botulinum homology modelling HA-33.