Abstract

Botulinum neurotoxin (BoNT) complexes consist of neurotoxin and neurotoxin-associated proteins. The Clostridia releases these as protein aggregate, termed as the progenitor toxins. Hemagglutinin – 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 HA1 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.
References

Insilico Studies on HA 33 Subunit of Haemagglutinin of Clostridium botulinum – Construction of Three Dimensional Model and Validation


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