Abstract

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


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**Index Terms**

Computer Science

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**Keywords**

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