Homology Modeling and Docking Studies on stem cell derived protein BDNF of Alzheimer's disease

Priyanka kashyap J, Suganya, RadhaMahendran*
Department of Bioinformatics, Vels University, Chennai- 600 117, India.
Corresponding author email: mahen.radha@gmail.com

From National Conference on Natural Products as therapeutics, Medical Microbiology, Nanobiology and System biology: Current Scenario & Emerging Trends, 'NATCON-2014'.
Post Graduate & Research Departments of Biochemistry, Microbiology, Biotechnology and Bioinformatics, Mohamed Sathak College of Arts & Science, Sholinganallur, Chennai-600119, India.
18-19 September 2014.

American J of Bio-pharm Biochem and Life Sci 2014 September, Vol. 4 (Suppl 1): P 20

ABSTRACT

Alzheimer's disease (AD) is the most important neurodegenerative disorder that affects brain neurons by forming plaques and tangles. Till today neither vaccine nor effective drugs were identified to cure the disease and in the last few years, research is going on stem cell to find out better treatment for treating AD patients. From the research on "neural stem cell" it was recognized that the protein "neurotrophin" enhances the level of neurotrophin in brain which will be fruitful in treating AD. The protein neutrophins possess four factors (NGF, BDNF, NT3, NT4), among them BDNF (brain derived neurotrophic factor) plays an important role in enhancing the process of "neurogenesis". The objective of the present work is to evaluate the effect of protein (BDNF) and drug (ligand) interaction. The protein BDNF was modeled for docking studies. From the literature survey, the eight drugs which induce BDNF were identified and its structure was retrieved. Docking results were analyzed and the drugs were ranked according to its binding interaction with protein. Among the 8 drugs, FTY720-P exhibits the highest binding energy -9.72442kcal\mol by having best hydrogen bond interactions with active site residues of the protein. In future this study can be further implemented to *in* vitro analysis for the drug designing which play a central role in lowering the effect of AD.

Published: September 2014.