12th International Conference on

Alzheimer's Disease & Dementia

October 29-31, 2018 | Valencia, Spain

In silico identification of novel ApoE4 inhibitor for Alzheimer's disease therapy

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ApoE4 is a major genetic risk factor due to its increased incidence of developing Alzheimer's disease. The study was designed to predict such compounds that may help in designing drugs to suppress the over activity of ApoE4 protein. 22 natural compounds (marine, microorganism and plant derivative) were used as inhibitors and docked with ApoE4 (PDB id 1B68). Six synthetic compounds (in clinical trials) were docked with target proteins to compare and analyze the docking results with natural compounds. Compounds S-allyl-L-cysteine, epicatechin gallate and fulvic acid show high binding affinity i.e., -7.1, -7 and -7, respectively. Epicatechin gallate shows hydrogen bond with Gln156 and Asp35 and fulvic acid shows hydrogen bonding with Glu27. In case of synthetic compounds, tideglusib did not show hydrogen bonding with any amino acid residue of ApoE4 but showed high binding affinity of -7.2, same as that of natural compound S-allyl-L-cysteine which showed high binding affinity of -7.1 but did not show hydrogen bonding with any amino acid residue. Protein-protein interactions of ApoE4 showed physical and functional interaction with related proteins. Our study predicted a compound epicatechin gallate on the basis of binding affinity and hydrogen bonding with amino acid residue as a potential lead compound which may be used as an inhibitor.

Biography

Muhammad Asif Rasheed recently completed PhD studies from Huazhong Agricultural University, Wuhan, China. He has his expertise in Bioinformatics and passion in improving health and wellbeing. He applied different bioinformatics approaches to predict the virulence factors in *Mycoplasma bovis* bacteria. He simultaneously published review articles by applying different bioinformatics tools on proteins related to liver cirrhosis. Currently, he is working on therapeutic aspects of Alzheimer's disease.

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Journal of Alzheimers Disease & Parkinsonism
ISSN: 2161-0460

Dementia 2018
October 29-31, 2018

Volume 8

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