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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 increase incidence of developing Alzheimer's disease. The study was designed to predict such compounds that may helpful in designing drug 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). 6 Synthetic compounds (In clinical trials) were docked with target protein 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 show high binding affinity of -7.2 same as of natural compound S-Allyl-L-Cysteine which show high binding affinity of -7.1 but did not show hydrogen bonding with any amino acid residue. Protein-Protein interactions of apoE4 show physical and functional interaction with related proteins. Our study predict 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 has his expertise in bioinformatics approaches and passion in improving the health and wellbeing. He recently completed PhD studies from Huazhong Agricultural University, Wuhan, China and applied different bioinformatics approaches to predict the virulence factors in *Mycoplasma bovis* bacteria. Simultaneously he published review articles by applying different bioinformatics tools on proteins related to liver cirrhosis. Recently he is working on therapeutics aspects of Alzheimer's disease.

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