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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 role in the increased incidence of developing Alzheimer's disease. The study was designed to predict such compounds that may be helpful 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 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; 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 the 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 show physical and functional interaction with related proteins. Our study predicts 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.

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