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Abstract

Olanzapine mesoporus non structured lipid carrier: Charecterarization and physiologically based pharmacokinetic modelling

Dr. B.C. ROY COLLEGE OF PHARMACY & ALLIED HEALTH SCIENCES, India

Abstract:

Protein fibrillation is referred to the formation of numerous linear agglomerates of protein formed often due to misfolding into insoluble fibrils, known as amyloidic proteins. Pathogenic amyloids forms fibrous deposits as plaques around cells which can disrupt the healthy functioning of tissues and organs. It is associated with a plethora of diseases such as diabetes mellitus, Alzheimers disease, Parkinsons' disease, neurodegenerative disorders of any kind and many others.

Amyloid-ś protein precursor (AśPP) is a hydrophobic self-aggregating peptide consisting of 39 to 42 amino acid residues. AśPP is sequentially processed by ś- and ś-secretases to release amyloid-ś (Aś). The ś-site amyloid precursor protein cleaving enzyme 1 (BACE1) is an important regulator for the production of amyloid plaques. The proteolytic cleavage of the amyloid precursor protein (APP), by BACE1, produces an insoluble amyloid-ś (Aś) fragment which has the ability to aggregate and form fibril.

Curcumin interferes with the oligomer formation by destabilizing Asp23-Lys 28 salt bridge of amyloid-ś protein. Curcumin and Ferulic acid share common phenolic structure that is responsible for fibril destabilization. In silico drug design is performed using BACE1 and Amyloid-ś protein pdb files. Curcumin modifications are carried out by isoters addition and top 5 compounds out of 55 library compounds are selected which shows best results in both the protein. Docking scores of Molecule 3,4,8 show docking score like -8.0, -7.3, -7.2 similar to standard like that of curcumin having docking score of -8.1. Replacing ketone by alcohol groups and modification using electron donating groups shows promising result. Further de novo ligand design by ELEA 3D generates novel compound library of curcumin that may be a promising lead for inhibiting protein fibrillation which is further screened for its toxicological potential in silico to emerge with potential leads with reduced toxicity.

Biography:

Dr. Souvik Basak has completed his PhD at the age of 32 years from Nanyanag Technological University, Singapore and currently working as Associate Professor at Dr. B.C. Roy College of Pharmacy & Allied Health Sciences, Durgapur, WB, India. He is He is also currently associated as Scientific consultant with industries like Innoscience Research Sdn Bhd, Malaysia and SHRM Biotechnologies Pvt Ltd., India. He has published more than 25 papers in reputed journals and has been serving as an reviewer and editorial board member of journals of repute. He has received sevral national and international journals in his career.

Publication of speakers:

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