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Discovery of novel leads as dual acting inhibitors of acetylcholinesterase using pharmacophore modeling, docking consensus and 3D-QSAR studies for Alzheimer's disease

Elvis A. F. Martis, Rakesh C. Chandarana, Premlata K. Ambre, Raghuvir R. S. Pissurlenkar and Evans C. Coutinho
Molecular Simulations Group, Department of Pharmaceutical Chemistry, Bombay College of Pharmacy, India

Alzheimer's disease (AD) is the most debilitating and chronic irreversible neurological condition, characterized by dementia and cognitive impairment due to the depletion of acetylcholine in the nervous system. The existing experimental data obtained from animal studies and other neurological studies are all indicative that, the main cause of dementia is the decrease of the integrity of the cholinergic inputs, which is believed to be due to its rapid hydrolysis of acetylcholine in the synaptic clefts by acetylcholinesterase (AChE).The limited number of drugs available for the treatment of AD, and many recent studies which have provided ample evidences of the molecular mechanisms of the progression of the disease has been our driving force for designing novel agents for treatment of AD. The structural insights provided by many studies of our target enzyme, AChE, in recent times have boosted our confidence of designing more potent and safer agents to tackle the disease more efficiently.

The objective was to identify hit candidates with probable AChE inhibitors by a process of virtual screening the public databases based on pharmacophore hypothesis (positive ionizable group, two hydrogen bond acceptors, and two aromatic rings). The relevant hypothesis was built using the known inhibitors of AChE as templates to investigate the pharmacophoric elements that represent the critical receptor-ligand interactions. The identified hits were predicted for activity by the 3D-QSAR models i.e. CoRIA {Comparative Residue Interaction Analysis} and later short listed for in vitro testing. The most potent predicted compounds were procured from Enamine and tested by the Ellman's colorimetric method. The inhibitory concentration for the most active candidates was 1.7, 21.14, and 35.4 μM.

Biography

Elvis A. F. Martis is currently pursuing his Master of Pharmaceutical Sciences with specialization in Pharmaceutical Chemistry from University of Mumbai. He is currently working on various in silico methods to develop potent therapeutic agents for Alzheimer's disease. He has authored 11 papers which include four Research articles, six Review articles and one book chapter.

elvis_bcp@elvismartis.in

Evaluation of antioxidant and anticancer potential and identification of polyphenols by RP-HPLC in Michelia champaca flowers

V. Nagavani and T. Raghava Rao
Department of Biochemistry, Andhra University, India

There is a growing interest in the food industry and in preventive health care for the Development and evaluation of natural antioxidants from medicinal plant materials. In the present work, flowers of M. champaca plants used in ayurveda and traditional purposes in India were screened for their enzymatic, non-enzymatic antioxidants with antioxidant potentials in aqueous, ethanol and methanol extracts and cytotoxic activity. The Folin-Ciocalteu procedure was used to assess the total phenolic concentrations of the extracts as Gallic acid equivalents. A modified reverse phase high pressure liquid chromatography (RP-HPLC) was used to obtain chromatographic profiles of the phenolic compounds in the medicinal plants. The predominant phenolic compounds detected in different extracts of the flowers were catechin, quercetin, caffeic acid and p-coumaric acid. Results indicated that high levels of phytochemicals such as phenols, flavonoids, tannins as well as antioxidant potential and cytotoxicity were found to be more in the methanol extracts of M. champaca dry flowers. It is very interesting that the levels of enzymatic antioxidants were found to be high in the aqueous extracts of M. champaca fresh flowers.

Keywords: Medicinal plants, Antioxidant activity, Total phenolics, RP-HPLC, Enzymatic and nonenzymatic antioxidants and cytotoxic activity.

vani.biochemistry.2009@gmail.com