PHYTOCHEMICAL SCREENING AND INSILICO APPROACH FOR IDENTIFICATION OF ANTI STRESS ACTIVITY OF COMPOUNDS FROM MEDICINAL PLANTS

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Abstract. Ayurvedha and Herbal medicine are two important forms of alternative medicine that are widely available. Medicinal plants have disease curing properties and this is due to the compounds presents in the extracts. This work is mainly concerned with the identification of the therapeutic properties of Indian medicinal plant extracts. So we identified the compounds of different medicinal plants like Celastrus paniculatus, Withania somnifera, Convolvulus pluricaulis, Rauvoifia Serpentina etc which are used as medicine for Stress in Ayurvedha from previous literature. Using chemsketch software these compounds were designed and screened for antistress property. The proteins responsible for stress in Homo sapiens were collected using Protein databank (PDB). Then the compounds were docked to the Calcium channel active site in order find better inhibitor. Among 33 compounds 10 compounds showed best docking results. ADMET studies were performed using Molinspiration and OSIRIS server.

Key words: Anti stress, Docking, ADME studies, Calcium Channels

1Introduction

Biology primarily attempts to explain major concepts of stress in a stimulus-response manner, much like a how a psychobiological sensory system operates. The central nervous system (brain and spinal cord) plays a crucial role in the body's stress-related mechanisms. Whether these mechanisms ought to be interpreted as the body's response to a stressor or embody the act of stress itself is part of the ambiguity in defining what exactly stress is. Nevertheless, the central nervous system works closely with the body's endocrine system to regulate these mechanisms. One branch of the central nervous system, the sympathetic nervous system, becomes primarily active during a stress response, regulating many of the body's physiological functions in ways that ought to make an organism more adaptive to its environment.

2 METHODOLOGY

2.1. Selection of Stress expressed proteins, from NCBI and Swiss prot and searched for structures using BLAST. The best model was selected from Pdb. Then the selected protein calcium channel was modified by removing unnecessary chains. Then the required chain was selected for SPDBV software. Then for the selected chain **a**ctive site was identified.

2.2. Active site Identification

Active site of angiotensin, calcium channel and cholesterol inhibitor were identified using CASTp server.

2.3. Docking method

GOLD (Genetic Optimization of Ligand Docking) a genetic algorithm (GA) based software, mainly utilizes an evolutionary strategy involving 3 genetic operators; cross overs, mutations and migrations (Jones et al., 1997). GOLD imports the partial flexibility to proteins and full flexibility to inhibitors. The compounds are docked into the active site of angiotensin, calcium channel and cholesterol absorption inhibitor and the interaction of these ligands with the active site residues are thoroughly studied using calculations of molecular mechanics.

3 Results and discussion

The concept of docking is important to determine the properties associated with protein-ligand interactions such as binding energy, electron distribution, hydrogen bond donor acceptor properties and hydrophobicity. In the present study, CASTp server was used to found the possible binding site of Calcium Channel (Fig. I). The anti stress compounds were docked into calcium channel using GOLD 3.0.1 and all docking solutions for calcium Channels were ranked according to the GOLD fitness function (Fig. II). The docking results showed that all the Anti stress compounds are active Calcium Channel inhibitors.

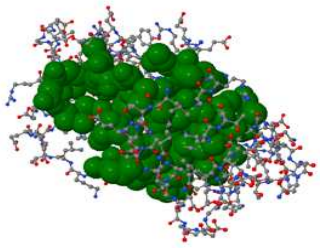

Fig.I: active site of Calcium Channel

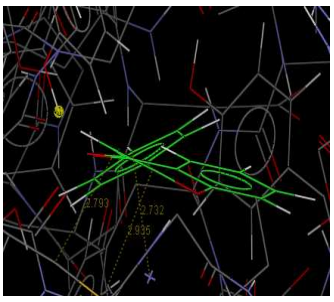

Fig.II: Docking studies of Calcium Channel

These compounds were subjected to ADME studies to identify the activity. Toxicity and mutagenic studies were also performed. These can be synthesized further and used as antistress drugs in future.

4 Refferences

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