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In silico study of cannabinoids in neurodegenerative disorders

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Oxygen is requisite in biological systems to converge their energy demands and supply of nutrients in our body. The generation of free radicals is the most common consequence of oxygen consumption which may lead to the damaging of cells. Importantly, antioxidant system of the body has a pertinent role in prevention of any loss that arises due to the generation of free radicals. However, dysfunction of antioxidant system or due to overproduction of free radicals may lead to some serious consequences which affect normal brain functionality. The brain tissue is greatly prone to the effects of reactive oxygen species due to its high demand for oxygen. Apart from several other environmental factors, oxidative stress (OS) plays a critical role in free-radical attack on neural cells leads to the loss of function that eventually contributes to neurodegeneration. However, antioxidants have defensive role against such kind of oxidative stress to prevent neuronal damage. Antioxidants may also be used as a therapeutic agent against intense neuronal loss, as they have the ability to neutralize free-radicals. Diet is a chief source of antioxidants, as well as medicinal herbs are also found to be a commercial source of antioxidants at present. Currently, we have focused on the natural compounds with good antioxidant and anti-inflammatory property that elicit neuroprotection. Herein, using different *in silico* techniques, we have validated the potential protective role of Cannabinoids in neurodegeneration. Furthermore, *in silico* techniques encompass string database for protein-protein interaction and docking for finding proper interaction between drugs and protein molecules have been identified.

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Molecular evolution of antimicrobial peptides Cecropin, Defensin and Gambicin in Mosquitoes

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Mosquitoes are vectors of many deadliest diseases-malaria, dengue, chicken guinea, Japanese encephalitis, yellow fever, etc. The endogenous peptides, which are constitutively expressed or induced, provide a fast and effective means of defense against the parasites to the mosquito. The use of bioinformatics tools for phylogenetic relationships of three antimicrobial peptides of mosquito, cecropin, defensin and gambicin based on amino acid sequence information was elucidated. The presence of non-polar residues in the primary structure of peptides confirm their hydrophobic nature. Conserved signature sequence motif, W-x(0,2)-[KDN]-{Q}-{L}-K-[KRE]-[LI]-E-[RKN] in N-terminal of cecropin and C-x(3)-C-x(6,9)-[GAS]-K-C-[IMQT]-x(3)-C-x-C in defensin is identified which is responsible for their antimicrobial nature. Mosquito defensin shows presence of cystein residues that may form disulphide bond and provide stability to antimicrobial peptide. The presence of catalytic and non-catalytic domains is in accordance with presence of conserved signature sequence. Gambicin is the novel antimicrobial as it does not show sequence similarity with any other antimicrobial gene. The study will leads to identification of novel antimicrobial compound which could be used as a drug in human against many pathogenic diseases.

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