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Design of novel protein kinase inhibitors for the treatment of painful diabetic neuropathy using energy based pharmacophore modeling and docking studies

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Painful Diabetic Neuropathy (PDN) is an immensely debilitating condition affecting about 20% and 5% of type 2 and type 1 diabetes patients respectively. It involves progressive nerve damage and some of the symptoms like numbness, tingling, hyperalgesia and allodynia greatly affect all areas of patient's life including mood, sleep, self-worth, independence, ability to work and interpersonal relationships. Currently, the drugs available for PDN offer only symptomatic relief but they do not reverse the nerve damage. Pathogeneses include protein kinase C (PKC) activation, polyol pathway, advanced glycated end products and microangiopathy. In this study, the focus was on PKC, which belongs to the family of protein kinase enzymes which phosphorylate serine/threonine residues. Elevated blood glucose levels via a signaling cascade cause the activation of PKC leading to hyperalgesia and allodynia (through rho kinase activation). PKCβ2 was identified as the PKC isoform involved in PDN. In this study,3 point and 4 point energy based pharmacophores were generated using E-pharmacophore module of Schrodinger suit of softwares. The pharmacophore models were then used for virtual screening and the top ranked hits were docked to the receptor. Top ranked hits were then visually inspected and were shortlisted based on parameters like docking score, fitness score and number of hydrogen bonds. These molecules will be further studied in vitro.

Biography

M.Saketh is a final year B.Pharm(Hons.) student presently doing his thesis under Dr. P. Yogeeswari,(Head–Department of Pharmacy) at Birla Institute of Technology & Science-Pilani (BITS-Pilani), Hyderabad Campus since January, 2012.

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