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In silico exploration of anti-Alzheimer's compounds present in hexane extract of Erythroxylum monogynum leaves using GC-MS/MS.

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Erythroxylum monogynum Roxb. (Syn. Red cedar or Bastard sandal), has been used to cure many ailments of human beings. Literature survey reveals that it has many pharmacological activities i.e. antidiabetic, antihyperlipidemic activity, dyspepsia, stomachic, fever, oedema etc. The aim of the present study is to identify the novel plant-derived anti-Alzheimer's activity phytoconstituents from E. monogynum to understand the molecular basis of anti-Alzheimer's activity. E. monogynum hexane leaves extract is subjected to GC-MS/MS analysis further identification of novel phytoconstituents. Virtual screenings of these phytoconsistituents was tested against therapeutic targets for the identification of Amyloid β (Aβ) inhibition activity and acetylcholinesterase (ACHE) inhibition activity. iGEMDOCK, admetSAR, LigPlot analysis were carried out for docking studies, drug likeness prediction and intermolecular interactions of the identified phytoconstituents. From the docking score 10 compounds are showing Aβ inhibition activity more than the standard curcumin, where as 41 compounds are showing ACHE inhibition activity more than the standard galantamine. Top 5 compounds of both targets are tested for drug-likeness prediction. Further, two lead compounds are subjected to LigPlot analysis to understand intermolecular interactions and their strengths. The docking score, drug-likeness and LigPlot analysis reveals that docosane, 11-decyl-, 2-methyloctacosane, hexadecanoic acid, 1-(2-aminoethoxy)hydroxyphos phenyl, docosane, 11-decyl- beta D-glucopyranoside, 4-nitrophenyl, gamma-tocopherol and andrographolide compounds are having potential anti-Alzheimer's effect. Our study shows that phytoconsistuents of E. monogynum are very potential anti-Alzheimer's candidates. Using the modern techniques these molecules can be used to develop an effective drug for the treatment of Alzheimer's disease from natural products.

Biography

I Subash.P doing PhD at the age of 29 years from Department of Pharmacy Indira Gandhi National Tribal University, Amarkantak, Madhya Pradesh under the guidance and supervision of Dr. K.Srinivasa rao, My research topic is Phytochemical investigation and evaluation of selected Indian medicinal plants for anti-Alzheimer's activity.

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