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Addressing new targets and cytoprotective compounds against neurodegenerative diseases

Bruno Andrade
Universidade Estadual do Sudoeste da Bahia, Brazil

Parkinson's disease, Alzheimer's disease and Autism comprise the most common neurodegenerative disorders. Sometimes, they share common metabolic pathways with between them and with other neurodegenerative disorders of the central nervous system. In general these disorders are related to abnormal high level of peptides and catabolites, such as that derived from Amyloid Precursor Protein (APP), which plays a key role in Alzheimer's disease. In this study we proposed to evaluate the role of new targets involved with neurodegenerative diseases, using computational tools (systems biology and cheminformatics), as well as propose new natural compounds which can act in neuroprotection. All protein targets were transcribed from hub genes (picked by search ensemble approach algorithm (SEA) and its ligands were subjected to molecular docking studies. In addition we performed 20 nanoseconds molecular dynamics using MMPBSA protocol. Small molecules Docking studies were performed by Audodock 4.0, while peptide-protein and protein-protein interactions were calculated by Rosetta Online Server. PyMol 1.7 and Discovery Studio 4.0 were used to evaluate docking results and generating 2D maps. The suite GROMACS 5.0.5 was used to simulate MMPBSA Molecular Dinamics.

Biography

Bruno Andrade has completed his PhD in Biotechnology in 2011 from the State University of Feira de Santana, Brazil. He has experience in structural and functional analysis of molecules isolated from microorganisms, animals and plants with pharmacological potential, and working on the following topics: Homology Molecular Modeling, Docking and Virtual Screening. He is currently Adjunct Professor at the State University of Southwest Bahia, Brazil, School of Medicine. He has published over 30 works (including 10 papers) in reputed journals and international meetings.

bandrade@uesb.edu.br

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