

Title: Natural products in neuroprotective therapies: Experimental and cheminformatics approaches to manage neurological disorders

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Abstract: Neurological disorders (NDs) such as Alzheimer's disease (AD), Parkinson's disease (PD), epilepsy, despondency, and dementia have been evidenced as a rising concern among diverse geographical regions. Brain-related diseases are currently the main concern because they increase mortality and morbidity in the elderly. Regardless of the continual efforts by modern scientists to develop a promising pharmacological or surgical management, the outcome has not been satisfactory. Also, due to synthetic drugs' associated side effects, scientists have taken the initiative to consider using natural compounds as an alternative. Hence, they obtain pretty effective results by using natural compounds. Natural ingredients are synthesized from a variety of plant and animal sources. These natural ingredients cure brain diseases through a variety of mechanisms. For effective medication advancement, the molecules must go through preliminary clinical systems that require some investment and significant speculation. In this situation, cheminformatics is fundamental in diminishing time and venture. Cheminformatics methods play a significant role in these issues, including 3-dimensional quantitative structure-activity relationship 3D-(QSAR), virtual screening, docking, molecular dynamic studies, and quantum chemical studies. The vital purpose of this study is to disclose different types of NDs and the neuroprotective effect of several natural products for experimental and cheminformatics-based therapy. Natural products like green tea, flavonoids, and ginseng are discussed as effective neuroprotective products. However, more investigation is expected to comprehend the better utilization of regular items in future exploratory and cheminformatics-based treatment for NDs.

Keywords: Neurological disorders; Docking; Molecular dynamic studies; Cheminformatics; Mortality; Drug discovery

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