Short Communication

iMedPub Journals
http://www.imedpub.com

Journal of Biomarkers in Drug Development

2021
Vol. 2 No. 2 :109

A Pharmacoinformatic Approach to Possible Phytocompounds in Parkinson's Disease Medication Development

Khorana Jung*

Department of Hematology and Medical Oncology, Cleveland Clinic, Cleveland, USA

Corresponding author:
Khorana Jung

Khorana.j.@ccf.org

Citation: Jung K (2021) A Pharmacoinformatic Approach to Possible Phytocompounds in Parkinson's Disease Medication Development. J Biomark Drug Dev. Vol.2 No.2:109

Abstract

Parkinson's disease (PD) is the second most prevalent neurodegenerative ailment and is caused by human physiological function. Dopamine agonists, which replicate dopamine's natural activity in the brain and directly stimulate dopamine receptors, are one of the most popular treatments for Parkinson's disease now available. Pharmaceutical medications currently available only provide brief respite from the condition. Because Phytocompounds can form secondary metabolites with novel chemical structures, they have been highlighted as a prospective research target in the search for new medicinal molecules. The drug development of Parkinson's disease has been studied utilising computational tools in the future.

Keywords: Phytocompounds, Parkinson's disease, Neurodegenerative

Received: October 29, 2021; **Accepted:** November 12, 2021; **Published:** November 19, 2021

Introduction

With each passing day, modern life has become more hectic. All stress-related ailments are caused by a lack of physical activity and mental calm. Tension and restlessness influence the body and mind, particularly the central nervous system, which serves as the regulating system's midway. Neurodegeneration is a disorder that occurs as a result of a neuropath logical condition and the ageing of the brain [1]. Cerebrovascular disorders include stroke, vascular dementia, and other types of cerebrum dysfunction. Neurodegenerative illness kills a lot of people all around the world. According to recent data, the total death rate in the twenty-first century is low. Cognitive dysfunction, neuropsychiatric and neurodegenerative illnesses, such as schizophrenia and depression, are the most common health issues. Parkinson disease is the second most common neurological ailment, and it has a significant impact on a person's quality of life, causing reliance and premature death. Pathological characteristic signs of Parkinson's disease include bradykinesia, rigidity, postural instability or facial dyskinesia, muscle stiffness, and tremor. Neurodegeneration is not reduced in half by current therapeutic techniques. With the use of computational chemistry, drug researchers are focusing on identifying new medicines based on phytochemical ingredients and food supplements for neuroprotective effects in Parkinson's disease [2]. In recent years, current medicines for neuropsychiatric and neurodegenerative illnesses have provided symptomatic alleviation rather than long-term relief. Treatment techniques to slow the progression of Parkinson's disease have yet to be devised, but this research is a step in the right direction. Computational chemistry has evolved into a cost-effective method for drug development and lead molecule identification. When combined with natural products, this allows a medicinal chemist to examine the choices more quickly and with less effort. Parkinson's disease is characterised by bradykinesia, rigidity, postural instability or facial dyskinesia, muscular stiffness, and tremor on a pathological level. Other linked consequences include sleep difficulties, cognitive impairment, depression, mood changes, psychosis, and dementia. Although the cause of neuronal cell death is unknown, mitochondrial malfunction, oxidative stress, and consequent apoptotic cell death have all been proposed as underlying processes. Despite the fact that current medications for this ailment provide symptomatic alleviation, effective options for decreasing disease progression have yet to be established [3].

A variety of plant-based natural medicines as well as manmade synthetic neuroprotective agents have been identified. Synthetically created neuroprotective compounds, on the other hand, have been shown to have specific detrimental effects in humans, such as dry mouth, exhaustion, sluggishness, drowsiness, stress or apprehension, difficulty with balance, and so on. In the current scenario, plant-based goods have sparked widespread interest through research and efforts at the national and global levels [4,5]. Some phytochemicals exhibit biological activities that are linked to cognitive function, although neither

the reported effects nor the mechanisms of action are well understood. Structure-based drug design is a combination of methods integrating molecular biology, computational chemistry, and bioinformatics that is a big aspect of drug discovery. With the help of the Schrodinger computational suite, computational figures were drawn and designed. The structure of a chemical compound or drug can be determined using X-ray crystallography or NMR spectroscopy, and structure-based drug design can anticipate how the intended drug molecule binds and interacts with the target protein using computational techniques.

Chemical compound design and structure-based medication design are complementary. Structure-based drug design entails the creation of new compounds that can fit into the active site of a target protein and complement it in terms of shape, charge, energy, and other binding properties. The hypothesised shape of a protein-ligand combination is frequently predicted via molecular docking. Docking is commonly utilised in virtual screening trials in conjunction with scoring algorithms to predict ligand binding affinities. A good docking function's ultimate goal is to distinguish between various types of true and false solutions. The docking procedure includes determining the enzymes' optimal kinetic performance and maximum ligand binding. Both empirical and theoretical bounds must be considered when calculating the free energy of ligand binding. The empirical data also reveals a substantial tendency of lower contributions per atom as the relative molecular mass of the ligand increases, according to this review. These findings are used to guide drug development efforts.

Conclusion

The standard medicines and treatments available today have proven ineffectual in treating Parkinson's disease's multifaceted pathogenic processes. Medicinal plant bioactive chemicals, on the other hand, have been proven to have the ability to modify or reduce the progression of Parkinson's disease. Identification of new bioactive chemicals is becoming increasingly important in the development of new and effective medications. To comprehend the drug-receptor interaction, a pharmacoinformatic method must be used in current drug design. With a better understanding of drug and receptor interactions, this concludes that modern computational tools can greatly assist and facilitate the discovery of innovative, effective, and more potent inhibitors for Parkinson's disease. The computational techniques make it possible to save time, avoid danger, and detect efficient compounds with the chosen target at a reasonable cost.

References

1. Jung P, Lushniak BD (2018) Do preventive medicine physicians practice medicine? Prev Med 111: 459-462.
2. Kumar GP, Farhath K (2012) Neuroprotective potential of phytochemicals. Pharmacogn Rev 6: 81-90.
3. Sermin G, Zeynep Z, Stefan H, Kursad HG (2012) The Adverse Effects of Air Pollution on the Nervous System. J Toxicol 2:1-23.
4. Jankovic J (2008) Parkinson's disease: clinical features and diagnosis. J Neurol Neurosurg Psychiatr 79:368-376.
5. Khanna R, Zou G, D'Haens G (2015) A retrospective analysis: the development of patient reported outcome measures for the assessment of Crohn's disease activity Aliment Pharmacol Ther 41:77-86.