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COMPUTER AIDED DRUG REPOSITION ING AND BIOLOGICAL EVALUATION AGAINST PARKINSON'S DISEASE

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ABSTRACT

The clinical features of Parkinson disease are shaking palsy (cd) or paralysis agitans. Parkinson disease is characterized by several motar symptoms and axial symptoms. This work was aimed at discovering anti-parkinson potential of existing old drugs using repositioning tools. To evaluate anti-parkinson effect of 4 drugs (Bethanechol, Sulfasalazine Tizanidine , Mesalazine) ,in-vitro and in-vivo laboratory finding of the study selected test drugs, at some or other doses, potential to be developed as effective anti-parkinsonian agents. Such type of studies are necessary in the continuing efforts to explore all potential routes in the search for new effective medicines.

Keywords: PD; Molecular docking; NO; DBVS; XP;

INTRODUCTION

Parkinson's disease (PD) is a progressive neurodegenerative movement disorder of central nervous system that mainly affects motor system and is characterized by slow and selective neuronal loss. Parkinsonism is named after James Parkinson in 1817. It is followed by accumulation of the insoluble protein *alpha-synuclein,* which accumulates inside the neurons forming inclusions called *Lewy bodies*, However, other mechanisms include proteosomal and lysosomal dysfunction and reduced mitochondrial activity. Drug repositioning (also known as drug repurposing, re-profiling, re-tasking or therapeutic switching) is the application of known drugs and compounds to new indications (i.e., new diseases). A ligand-based method currently exploits pharmacological data stored in three different annotated chemical libraries. The main source of information is the WOMBAT database. A ligand-based method currently exploits pharmacological data stored in three different annotated chemical libraries. The main source of information is the WOMBAT database. The applications of these techniques are supported by exponential increase in the number of experimental protein 3D structure. The design of new ligands is performed in several cycles, most often only by visual inspection and qualitative interpretation of the ligand-binding site interactions correspondingly .

MATERIALS AND METHODS

Ligand and structure based *in- silico* methods were employed to screen the potential candidates against anti-parkinson's query molecules. For computational approaches, four drugs were shortlisted using *in vitro* and *in vivo* evaluation of antiparkinson activity in the laboratory. Mesalazine was procured as a gift sample from the manufacturing company and other drugs like Bethanechol, Tizanidine and sulfasalazine were procured from the local market of Lucknow. Reserpine was obtained from SD Fine- chemicals Limited (SDFCL), India. Swiss- Albino mice of either sex of BALB/c strain (20-25 g) were procured from the Animal House, Faculty of Pharmacy , BBDNIIT, Lucknow, U.P., India.

STUDY DESIGN

Animals were randomly divided into 14 groups containing five animals in each group, (n=5). Reserpine 5mg/kg body weight (intraperitoneally) was given to all the groups, except group 1 as Parkinsonism inducing agent. Dosing of the test