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In silico screening of potent natural inhibitor compounds against Human DOPA Decarboxylase for management of Parkinson's Disease

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Abstract

Loss of dopaminergic neurons of the *substantia nigra* of the mid brain is a well studied pathophysiology of Parkinson's disease (PD), is the second most common neurodegenerative disorder. To compensate dopamine levels at the Central Nervous System (CNS) exogenous L-Dopa is generally administered. But the major part of the L-Dopa is metabolized by Dopa decarboxylase (DDC, E.C. 4.1.1.28), a pyridoxal 5'-phosphate (PLP) enzyme, which is abundant in CNS and hence, only 1-5% of L-Dopa reaches to dopaminergic neurons. In this context, co-administration of peripheral DDC inhibitors (carbidopa or benserazide) has been successfully used for the symptomatic treatment of PD patients. But, due to use of synthetic drugs many adverse effects have been reported during treatment. Therefore, the current study is planned to discover some plant based potent natural inhibitors against human DDC as an alternative way for the management of PD. This study was conducted through virtual screening and molecular docking of DDC enzyme with phytochemicals like *withania somnifera* (ashwagandha), *glycine max* (soybean), *vicia faba* (broad bean), and *marsilea quadrifolia* (sunsunia) etc to evaluate their inhibition properties. *In silico* study results shown a good binding affinity and predicted some of the phytochemicals as potent natural inhibitors against human DDC. This work could be validated further through experimental procedures.

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