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In silico Analysis of Interaction of Thymoquinone and its Analogues from Black Cumin Seeds with Proteins Involved in Parkinson's Disease †

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Abstract: Thymoquinone is the principal compound present in Nigella sativa seeds. It is an exemplary compound to treat diverse diseases. It is active against MPP+ and rotenone activity, which generally induces Parkinson's condition. Parkinson's disease (PD) is a progressive neurodegenerative disorder that causes the person to lose control of the body's functions. There is no specific test to identify and cure the disease. Less likely, it has various side effects. Long-term use of this drug can cause neuron degeneration. To overcome the side effects, thymoquinone can be incorporated with Levodopa. Thymoquinone may be a practicable option to avert quinone formation because of Levodopa (L-Dopa) auto-oxidation and can reflect the effects of the thymoquinone-levodopa drug on ameliorating the downside aspects of the native drug. It can also demonstrate the neuroprotective and antioxidant effect of the compound. Thus, this current research might provide some scope on the advantageous effects of thymoquinone against neurotoxicity. Molecular docking is an exemplary tool for the drug discovery process. Computational studies play a crucial role in the drug discovery pipeline by overcoming various challenges. The present docking study was carried out for five compounds against three PD proteins to ensure the use of a combination drug in PD to rescue neurons from neurotoxicity. From the above conducted *Insilco* analysis, we could conclude that the thymoquinone, thymol, thymohydroquinone can be combined with Levodopa to minimize secondary drug effects and also ameliorate PD conditions. This may instigate the use of black cumin seeds combined with Levodopa as combination drugs to compose the two compounds' drug profiles and eliminate unnecessary side effects. Further, *In vitro* analysis must be performed to scrutinize various effects on dopamine-producing cells. The forthcoming researches will determine the use of TQ subsumed Levodopa as a potential drug in PD. Although new efforts will be explored to control Parkinson's disease, further research must be performed to design a noble, highly potent drug that will rescue the dopaminergic neurons from their loss and ease the side effects of current treatment.

Keywords: Parkinson's disease; thymoquinone; Levodopa; L-Dopa; neurotoxicity.

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Conflicts of Interest

The authors declare no conflict of interest.