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Docking Studies of Hispolon Mediated Human NF-κβ Inhibition and *In-Silico* Development of Hispolon Derivatives Towards Cancer Treatment

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Abstract

In-silico drug designing for better anticancer therapeutics targeting human NF-κB, a pivotal enzyme involved in cancer regulating pathway. Hispolon, a black hoof mushroom (*Phellinus linteus*) or shaggy bracket mushroom (*Inonotus hispidus*) derived polyphenolic compound is structurally homologous with Curcumin and possess the NF-κB inhibitory efficiency as an anticancer agent. However, the *in-silico* studies related to Hispolon mediated inhibition of NF-κB activity and its mechanism of action has not yet been investigated so far. The present paper reports *in-silico* studies carried out to investigate the detailed mechanism of Hispolon mediated inhibition of NF-κB and designing of new potent derivatives of Hispolon having anticancer activity. Docking, Binding free energy analysis, Drug designing ADMET and IC50 has been performed for the fulfilment of above mentioned objective. DRG2 compound (ΔG= -30.180 kcal/mol) is the most potent in binding with human NF-κB among all 10 designed Hispolon derivatives. Met469 and Glu470 of human NF-κB makes an additional interaction with one of the hydrogen atom of 5-methoxy group of ligand's benzene ring. Methoxy group placed on the *-ortho* and two *-para* position of benzene ring and the *–meta* positioned hydroxyl group of the compound plays crucial role in strengthening the binding energy with human NF-κB. ADMET analysis also confirmed the drug-likeness and efficiency of DRG2 with NF-κB. In-depth structural, molecular modelling, docking and binding energy studies helps to redesign Hispolon to better compound that might have some additional inhibitory effect on human NF-κB thus can be used as anticancer therapeutics.

Keywords: Hispolon, NF-κB, Cancer, Docking, Binding free energy, ADMET, Inhibitory Concentration 50.

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