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Patterns of interaction of major active components of the blue green algae S*pirulina fusiformis* against chosen orphan nuclear receptors: an *in silico* study

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Abstract : Objective: Hepatotoxicity is a metabolic disorder, caused due to oxidative stress which leads to liver damage. Non -steroidal anti-inflammatory drugs like diclofenac are the agent for hepatotoxicity. The aim of our study is to predict the inhibitory effect of ligands like 3'-hydroxy-4'-methoxydiclofenac, 3'-hydroxydiclofenac, (3Z)-phycocyanobilin, beta carotene, vitamin B12 and diclofenac sodium with the receptors like apo human pregnane X receptor, nuclear bile acid receptor FXR, constitutive androstane receptor and LXR. Molecular docking techniques are used in this experiment to predict the interacting residue and hydrogen bond of ligand-protein complex.Patch dock server is used to dock ligand with a receptor. The 3D structure of the docked complex is analyzed using PyMol molecular viewer. Vitamin B12 showed significant interaction with all the receptor compared to other ligand. We predicted that vitamin B12 will have good effectiveness against hepatotoxicity; its potential effects can be further studied *in vivo* models.
Keywords: Hepatotoxicity, docking, diclofenac, vitamin B12.

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