

Treatment of Liver Disease using Secondary Metabolites of *Azadirachta indica* by Molecular Docking and Molecular Dynamics Simulations

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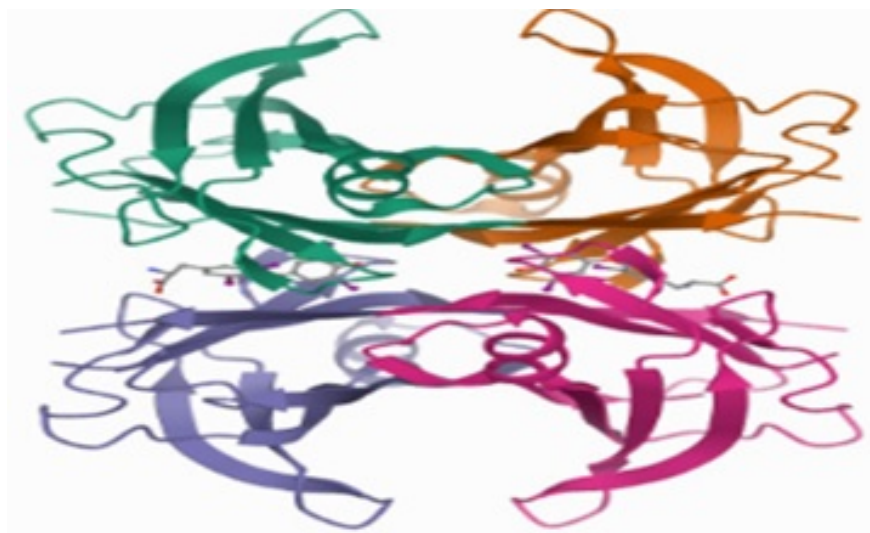
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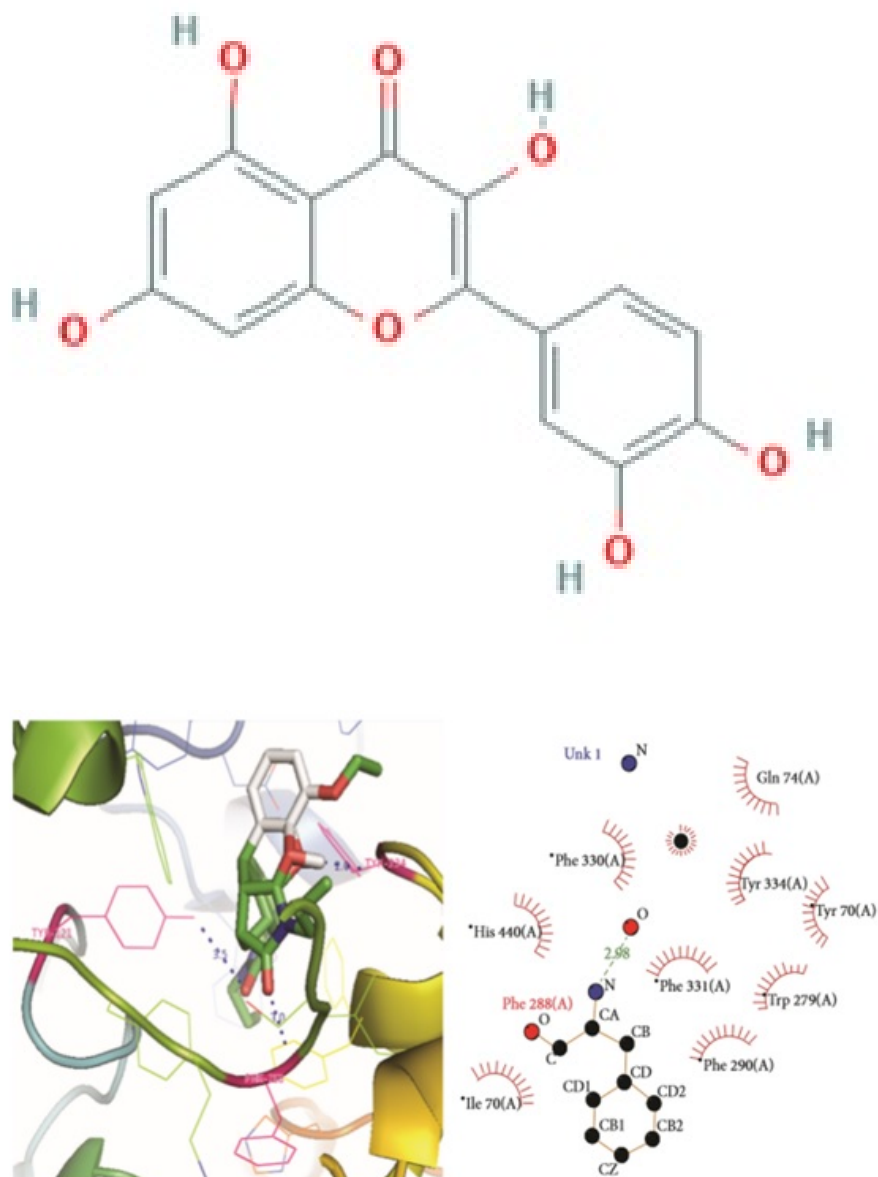
Abstract

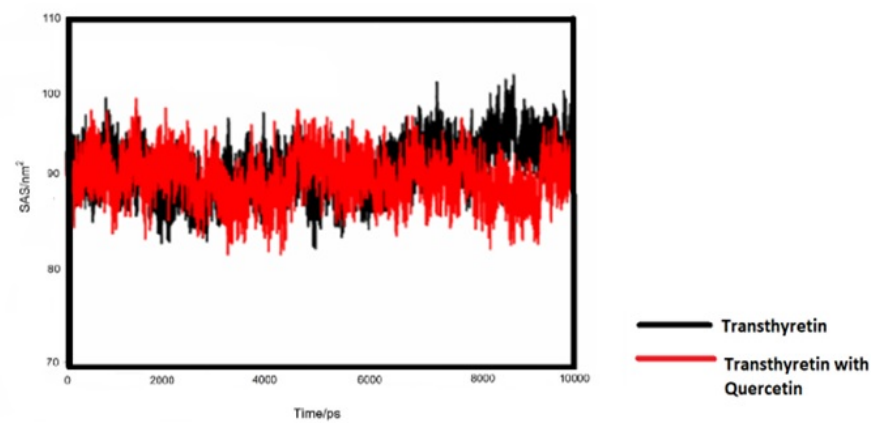
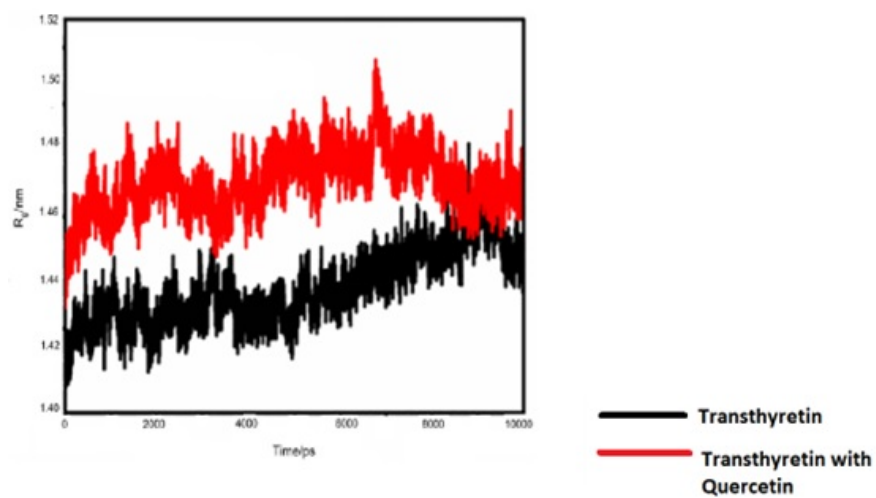
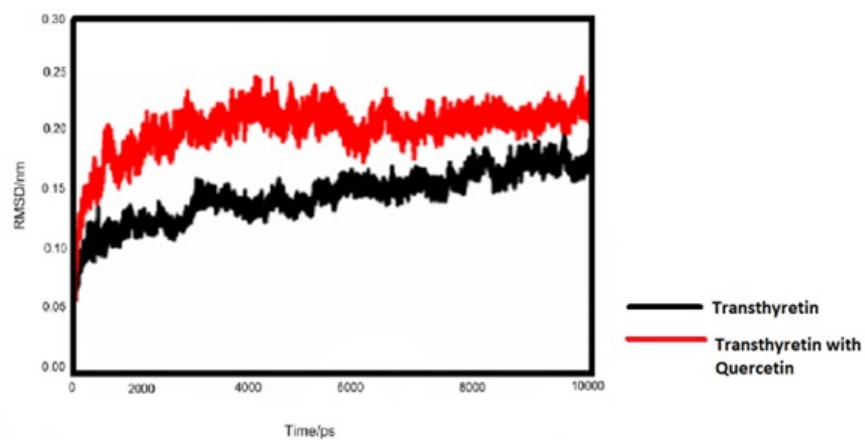
Transthyretin acts as a best protein target for which the medication could be intended as an inhibitor to treat the disease. Various flavonoids and alkaloids were retrieved from *Azadirachta indica* plant as an agent to bind the pockets of the protein. In order to investigate the binding patterns of flavanoids and alkaloids against Transthyretin (PDB ID: 1ICT) and to use simulations of molecular docking and molecular dynamics, the current in- silico research was performed. The molecular docking result indicates that Quercetin (CID: 5280343) binds to the region of active Transthyretin. pkCSM and molinspiration were used to analyse all of the candidate's properties. For the molecular dynamic simulation studies the best compound Quercetin has been chosen. The Molecular Dynamics Simulations analysis showed that 3000 ps of Transthyretin and Transthyretin-Quercetin complex were stable. Finally, the in silico research predicts that Quercetin may serve as a good inhibitor for the treatment of the disease and that its therapeutic potential may be demonstrated by further in vitro and in vivo studies.

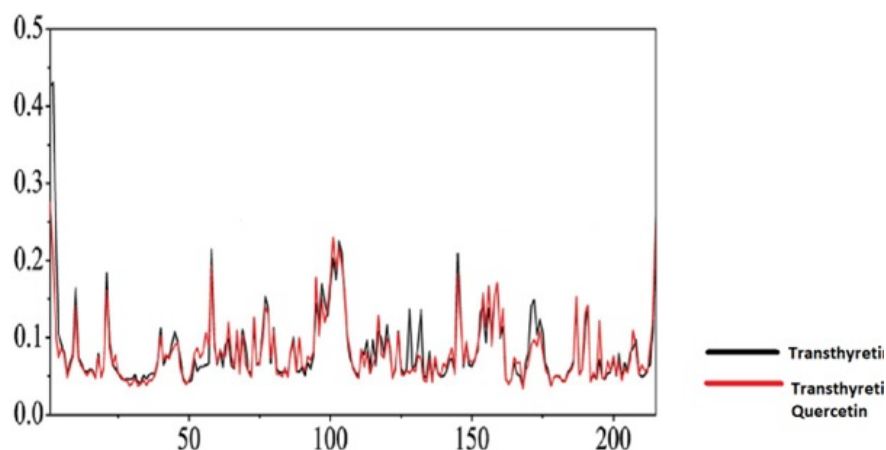
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