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Comparison of anti-thrombotic activity of known medicinal herbs on P2P12 receptor: an in-silico approach

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Objective: The objective of this study was to compare the anti-thrombotic activity of curcumin, naringin and quercetin on P2P12 receptor using molecular docking approach

Methods: The three-dimensional structure of P2Y12 receptor used for the present docking study was taken from Protein Data Bank (PDB ID: 4pxz). The ligands used in the study were (curcumin, naringin and quercetin) and 3D structure of were retrieved from PubChem Compound Database. Consequently, the ligands were docked to P2Y12 protein using "Autodock 4.2." We have set the AutoDock parameter and the distance-dependent dielectric functions useful for the calculation of the van der Waals and the electrostatic terms, respectively. The final figures were generated with the help of Discovery Studio Visualizer.

Results: Our result shows that the antithrombotic activity of curcumin to be most effective based on the *in-silico* molecular docking simulation study against thrombosis. Further, we have measured minimum inhibition constant, Ki and highest negative free energy of binding with the maximum interacting surface area. We reported that the binding energy was highest in curcumin (-5.14 kcal/mol). The free binding energies were (-5.07 kcal/mol), (-1.72 kcal/mol) for quercetin, naringin respectively.

Conclusion: This study may offer the evidence that curcumin could deliver the best therapeutic potential, in comparison to other medicinal herbs in the treatment of thrombosis, cancer and cardiovascular diseases.

Medicinal herbs, thrombosis, in-silico approach, P2Y12 receptor, curcumin