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Molecular Docking and Molecular Dynamic studies of Phytocompounds with HIF-1α, HIF-2α, and SREBP1c to Explore its Inhibitory Effect on Metabolic disorders and in Cancer

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Abstract

Hypoxia-inducible factors (HIFs) are important components of the cellular oxygen-signaling pathway. In response to low oxygen tensions, HIFs facilitate both oxygen delivery and adaptation to oxygen deprivation by regulating the expression of genes that are involved in glucose uptake and metabolism, angiogenesis, erythropoiesis, cell proliferation, and apoptosis. Hence HIFs role in the regulation of different cancers is crucial. Moreover, these proteins also play a role in the hepatic lipid metabolism. SREBP1c is a transcriptional factor and as well as key regulator of lipid metabolism through different signaling pathways. Hence, our study focuses to study the association between different inhibitory ligands with these key proteins. In order to investigate the binding mechanism of five phytocompounds, Curcumin, Digoxin, Epigallocatechin gallate (EGCG), Epigallocatechin (EGC) and Gallocatechin gallate (GCG) with drug targeted receptors *viz*., HIF-1α (PDB ID:5LA9), SREBP1c (PDB ID:1AM9) and HIF-2α (PDB ID:2A24) molecular docking and molecular dynamics simulation were performed. The best score among above compounds, on the basis of hydrogen bonding while docking by FlexX software, curcumin showed best score among all phytocompounds to HIF-1α (-20.72) and HIF-2α (-11.76), also for SREBP1c protein though Curcumin showed good score (-12.23) but EGC had an superiority, because the complex had more hydrogen and aromatic hydrogen bond and it also has an interaction with cytosine (DC26) residue from DNA and has score -12.03. Three independent molecular dynamics simulations (20ns) runs indicated general stability of curcumin in binding pocket of HIF-1α, HIF-2 α and EGC in SREBP1c as well as the tendency to form hydrogen bonds with water molecules in HIF-1α and SREBP1c also EGC form hydrogen bond with cytosine in SREBP1c.These results enhance further *in vitro* and *in vivo* experimentation and can probably serve as an ideal molecule for cancer treatment and metabolic disorders.

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