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Screening of phytochemicals for the inhibition of JAK2 by molecular docking

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Janus kinases-2 (JAK2) is a member of the Janus Kinase family and has been implicated in signaling by members of the type II cytokine receptor family. JAK2 is involved in the regulation of various pathways of cell growth, development, differentiation or histone modifications. Inhibition of JAK down-regulates phosphorylation of transcription factors known as STAT and blocks the JAK-STAT signaling pathway which is vital for tumorigenesis. In the present study molecular docking was carried out to elucidate the interaction of phytochemicals with Protein Kinase 2 domain for the inhibition of JAK2 to block cytokine signaling. PDB ID code 4C61 from the Protein Data Bank was used to retrieve JAK2 crystal structure at 2.45- Å resolution and utilized for molecular docking under Schrodinger platform. Phytochemical, demethoxycurcumin from *Curcuma longa* as JAK2 inhibitor to modulate the JAK/STAT pathway. It is found that the phytochemical is potent to block the access at the site of Protein Kinase 2 domain. The efficacy was evaluated based on scoring function employed in Glide XP. Further ADME/Tox studies validate the efficacy of the phytochemical to possess druggable like characteristics pertaining to standard drugs. Pharmacophore modeling of demethoxycurcumin showed binding energy with substitution of different R-groups.

Biography

Shalini Koshle is a Senior Research Fellow in Department of Biotechnology, Sri Jayachamarajendra College of Engineering. She is currently pursuing PhD from Visvesvaraya Technological University, India. She has been awarded with Rajiv Gandhi National Fellowship, University Grant Commission, Government of India. She has published two papers in reputed journal and given oral presentation National Conference on "Technological Advancements in Chemical and Environmental engineering".

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