

SHORT COMMUNICATION

Anti-Metastatic Potential of Pakistani Spice Box

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Inhibition of vascular endothelial growth factor 2 (VEGFR2), cyclooxygenase-2 (COX-2), NFκB inhibiting kinase (NIK) and hypoxia inducible factor-2 α (HIF-2 α) nexus can block cancer spread.¹ This study aimed at finding phytochemicals in spices for inhibition of above mentioned target proteins in order to prevent/ treat cancer. The crystal structures for VEGFR2, COX-2, NIK and HIF-2α were downloaded from RCSB protein data bank with PDB IDs of 3VHE, 5IKQ, 4IDT & 4XT2 respectively. (The chemical constituents of the spices: nutmeg, cinnamon, black pepper, red chili, clove, black caraway seed, fennel, star anise, turmeric and coriander were collected from Dr. Duke's phytochemical and ethnobotanical databases. Next the 3D structures of the chemicals were downloaded from PubChem.

These chemicals were then docked against crystal structures of the target proteins using Glide docking software from Schrodinger. The chemicals that docked successfully against 3VHE (vascular endothelial growth factor receptor 2) included: Apiin, kaempferol, quercetin, cymaroside and capsorubin from red chili with dock scores of (-11.301, -11.076, -10.990, -10.196, -9.82) kcal/mol respectively, quercetin and trichostachine from black pepper with dock scores -11.546 kcal/mol and -9.017 kcal/mol, curcumin from turmeric with -9.019 kcal/mol score, quercetin, isokaemferide, rhamnetin and apigetrin from coriander with dock scores of -11.574 kcal/mol, -10.894 kcal/mol, -10.484, -10.364 cal/mol; foeniculoside ii from fennel with dock score -9.065 kcal/mol, procyanidin B-2 from cinnamon with dock score of -9.218 kcal/mol and kaempferide, rhamnocitrin, myricetin, rhamnetin from clove with dock scores of -10.927 kcal/mol, -10.593 kcal/mol, -10.467 kcal/mol, -9.931 kcal/mol -10.59 kcal/mol respectively. For cyclooxygenase-2 (5IKQ), Rhamnetin 3, 3', 4'-triglucoside from black pepper and procyanidin from cinnamon showed successful docking. For NFκB-inducing kinase (4IDT), cubebin from black pepper and riboflavin from coriander showed successful docking. Successfully docked compounds against 4XT2 (hypoxia inducible factor-2) included AC1NQWCK [tert-butyl N-[(2S)-1-[(2S,4R)-2-[[1-(cyclopropylsulfonyl)carbamoyl]cyclobutyl]carbamoyl]-4-(7-methoxy-2-phenylquinolin-4-yl)oxypyrrolidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]carbamate] from red chili and catechin from cinnamon. Because of successful in-silico docking with the target proteins, these spices can be predicted as cancer curbing agents. In future these compounds can be tested in vitro and in vivo for their potential inhibitory activity.

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