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Insilico docking studies of phytochemicals from phyllanthus sp.with lung cancer metastasis, angiogenesis and hypoxia pathway target proteins

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The metastasizing ability of malignant tumors is accountable for the poor prognosis and high mortality rate in cancer patients. Hence, metastasis is still a major clinical challenge for medical practitioners worldwide in cancer. Ras/Raf/MEK/ERK pathway is found to play an important role in lung cancer metastasis, and targeting MEK/ERK cascade by its specific inhibitor may have a potential use in the effective treatment of metastatic sarcoma. In the search for the new alternative treatments, natural products are carving a path as prospective anticancer agents. Various therapeutic actions of the genus *Phyllanthus* have been reported, including being antihepatotoxic, antilithic, antihypertensive, anticarcinogenic, and most recently anti-HIV as well. The presence of polyphenol compounds in the *Phyllanthus* plant is critically important in the inhibition of the invasion, migration, and adhesion of cancer cells, along with the involvement of apoptosis induction. Hence, *Phyllanthus* could be a valuable candidate in the treatment of metastatic cancers. Insilico binding analysis of *Phyllanthus* secondary metabolites on the selected proteins, c-Raf, Bcl-2, Ras,Hif, c-Myc, c-Jun,VEGF found to be involved in lung cancer, hypoxia and angiogenesis is carried out in present work. A total no.of 33 phytochemical of *Phyllanthus* belonging to Flavanoids, Terpenes ,Coumarins, Lignans, Tannins and Saponins were screened using different computational molecular docking program such as AutoDockVina and molegrow .Respective binding energies are predicted for each molecule with the targeted molecules. Amongst all the classes Terpenes have shown significant binding activity against the putative targets and thus are possible therapeutic molecules against metastasis.

Biography

Bhatt Mital H. is a Registerd Ph.D student under the guidance of Dr.M.N.Reddy in Dept. of Bioscience, VNSGU, She completed her M.Sc in Bioinformatics and worked as Asst. Professor from 2009-2014 in department of computer science, VNSGU.

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