

Investigating Anti-Tumourigenic and Anti-Angiogenic Effects of Resveratrol in Breast Carcinogenesis Using in-Silico Algorithms

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Abstract : Breast cancer is the most common cancer among females worldwide and is estimated that more than 450,000 deaths are reported each year. It accounts for about 14% of all female cancer deaths. Angiogenesis plays an essential role in Breast cancer development, invasion, and metastasis. Breast cancer predominantly begins in luminal epithelial cells lining the normal breast ducts. Breast carcinoma likely requires coordinated efforts of both increased proliferation and increased motility to progress to metastatic stages. Resveratrol: a natural stilbenoid, has anti-inflammatory and anticancer effects that inhibits proliferation of variety of human cancer cell lines, including breast, prostate, stomach, colon, pancreatic, and thyroid cancers. The objective of this study is: To investigate anti-neoangiogenesis effects of Resveratrol in breast cancer and to analyze inhibitory effects of resveratrol on aromatase, ER α , HER2/neu, and VEGFR. Docking is the computational determination of binding affinity between molecule (protein structure and ligand). We performed molecular docking using Swiss-Dock and to determine docking effects of (1) Resveratrol with Aromatase, (2) Resveratrol with ER α (3) Resveratrol with HER2/neu and (4) Resveratrol with VEGFR2. Docking results of resveratrol determined inhibitory effects on aromatase with binding energy of -7.28 kcal/mol which shows anticancerous effects on estrogen dependent breast tumors. Resveratrol also show inhibitory effects on ER α and HER2/new with binding energy -8.02, and -6.74 respectively; which revealed anti-cytoproliferative effects upon breast cancer. On the other hand resveratrol v/s VEGFR showed potential inhibitory effects on neo-angiogenesis with binding energy -7.68 kcal/mol, angiogenesis is the important phenomenon that promote tumor development and metastasis. Resveratrol is an anti-breast cancer agent conformed by in silico studies, it has been identified that resveratrol can inhibit breast cancer cells proliferation by acting as competitive inhibitor of aromatase, ER α and HER2 neo, while neo-angiogenesis is restricted by binding to VEGFR which authenticates the anti-carcinogenic effects of resveratrol against breast cancer.

Keywords : angiogenesis, anti-cytoproliferative, molecular docking, resveratrol

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