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Insilico Molecular interaction study of Non-terpenoid and non-steroid constituents of neem (A. indica) against Breast cancer inducing protein (AXL receptor tyrosine kinase).

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Abstract

Breast cancer is a global concern among women. The patients benefit from the availability of diagnostics, prognoses, and treatments, but researchers continue to work on improving the quality of life for breast cancer patients. At present, breast cancer does not have a single known treatment that can render it cured. The goal of identifying molecular targets for treating cancer has been a research priority for decades. Growth arrest-specific protein 6 (GAS6) is a high-affinity ligand of the AXL protein, which is in the TAM family. In addition to tumor cell growth, metastasis, invasion, Epithelial-Mesenchymal Transition (EMT), angiogenesis, and drug resistance, the Gas6/AXL signaling pathway is involved in immune regulation, stem cell maintenance, and drug resistance. The cancer-associated protein Axl is also a potential therapeutic target for the discovery and development of novel therapeutics. The objective of the present study was to screen the Non-Terpenoid and non-steroid phyto constituents against Breast cancer inducing protein (AXL receptor tyrosine kinase).

Methods: In this study we have screened 15 Non-Terpenoid and non-steroid phyto constituents from neem (A. indica) which is reported previously. These compounds further screened Pharmacophore analysis by ChemMine Tools (OpenBabel Descriptors). The Lipinski rule passed compounds carried out their Molecular interaction and ADMET study by Cavity-detection guided Blind Docking and pkCSM online tools against AXL receptor tyrosine kinase. These compounds were further evaluated for Pharmacokinetic (ADMET) properties Analysis along with FDA approved anti breast cancer drug molecule Anastrozole.

Results and conclusion: In the present study we screened 15 bioactive among all 6 compounds were fulfilled the Lipinski's rule of 5. These compounds were used for against Breast cancer inducing protein (AXL receptor tyrosine kinase) inhibitors through molecular docking studies. The results were shown with high energy Compound Name and with CB-Dock Vina score Isorhamnetin (-8) > Nimbiol (-7.3) > Quercetin (-7.7) and Sugiol (-7.7), Kaemferol (-7.6) > 5-Hydroxy-methyl furfural (-4.6). And further these compounds need to be evaluated invitro and invivo as well performed on animal models to confirm the anti-Breast cancer activity.

Key Words: Receptor Tyrosine Kinase, Breast cancer, Molecular Docking, Pharmacokinetic properties, Non-terpenoid, non-steroid constituents, Epithelial-Mesenchymal Transition.

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