

Unravelling the therapeutic potential of *Dioscorea deltoidea* against breast cancer: a combinational approach via network pharmacology and molecular docking

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Dioscorea deltoidea, a tuberous plant which is extensively grown in tropical and subtropical climates, has a wide array of therapeutic uses. The therapeutic potential of *D. deltoidea* was further explored by the interaction of different phytochemicals and multiple signalling pathways associated with breast cancer using a network pharmacology approach involving preliminary screening of active phytochemicals, target prediction, Kyoto Encyclopedia of Genes and Genomes/Gene Ontology pathway enrichment and molecular docking and results were further validated by the molecular dynamics simulation study. The present article provides a detailed insight into the action mechanism of *D. deltoidea* against breast cancer via network pharmacology and molecular docking thus, deciphering the therapeutic potential of *D. deltoidea* against breast cancer.

Keywords: Dioscin, *Dioscorea deltoidea*, molecular docking, molecular dynamics simulation, network pharmacology.

is the primary source of diosgenin, a secondary metabolite extracted from plants. Its anti-cancer, anti-diabetic, anticoagulant, anti-thrombosis, anti-inflammatory, antiviral, anti-ageing and other qualities make it a significant molecule in the pharmaceutical industry⁶. At higher concentrations, diosgenin, a steroidal saponin which is derived naturally from wild yams has the potential to eliminate highly chemorefractory and pro-metastatic breast cancer stem like cells⁷. Through cell cycle arrest, dioscin inhibits the proliferation of breast cancer stem-like cells by modulating the phosphoinositide 3 kinase (PI3K)/AKT mammalian (or mechanistic) target of rapamycin (mTOR) and p38 mitogen-activated protein kinase signalling pathways⁸. Some findings have shown the ability of deltonin to reduce cell growth is associated with its ability to induce apoptosis through activation of the extracellular signal-regulated kinase (ERK)/phosphoinositide 3-kinase/protein kinase B (AKT) signalling pathways and mitochondrial dysfunction due to reactive oxygen species. As a result, deltonin may be useful as a chemotherapeutic medication for the treatment of breast cancer⁹.

The *D. deltoidea*, a tuberous plant, which is a member of the Dioscoreaceae family, is a potentially effective medicinal plant for breast cancer. Studies have