Computational Evaluation of GC–MS Derived Phytocompounds from Two Medicinal Plants as Potential RAC1 Inhibitors for Breast Cancer Therapy

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Abstract

Cheminformatics is crucial for prospective chemical screening and optimized lead identification in modern drug discovery, all while lowering costs using *in silico* methods. *Amorphophallus paeonifolius* and *Benincasa hispida*, two medicinal plants were elected for this study and extracted using Soxhlet ethanol method. Each plant had 100 phytocompounds identified by GC-MS analysis, which were docked with the RAC1 Inhibitors (PDB ID : 1RYH) breast cancer protein. Molecular Dynamics Simulation, ADME/T, and MM/GBSA tests were performed on the top four compounds including beta-Sitosterol, D-Galactose, L-Rhamnose, and Lupeol from each plant. The chosen phytocompounds have many molecular interactions and favorable docking scores, according to the docking results. In ADME/T experiments, these drugs showed favorable pharmacokinetic characteristics and extended stability throughout simulation. This work suggests that the selected phytocompounds are promising candidates for developing drug formulations against breast cancer, integrating both computational and experimental approaches for rational drug discovery.

Keywords: ADME/T, Molecular Docking, Phytocompounds, Molecular Docking, Molecular Dynamics Simulation.