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(57) Abstract :

This present invention investigates the anticancer potential of secondary metabolites from Asparagus racemosus through molecular docking studies targeting Estrogen Receptor a and Aromatase, two key proteins implicated in cancer progression. Phytoconstituents were selected from PubChem, and the protein structures were optimized for docking. Each compound was visualized in ChemDraw and docked using the Glide module in Schrödinger Suite 2020, allowing precise measurements of binding affinities. The study highlights specific interactions between plant compounds and cancer-related proteins, offering valuable insights into natural compounds with strong binding affinity and potential therapeutic applications. This work presents a promising in-silico approach for screening plant-based anticancer agents, paving the way for safer, plant-derived alternatives in cancer treatment.

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