

ABSTRACT

Thymol, a monocyclic phenolic monoterpene derived from essential oils of plants such as *Origanum* and *Thymus vulgaris*, exhibits notable biological activities including anti-inflammatory, antioxidant, antitumor, and antibacterial effects. This study aimed to elucidate the binding affinity of Thymol with caspase-9, a critical initiator enzyme in the intrinsic apoptotic pathway, using molecular docking methodologies. The research employed BIOVIA Discovery Studio, Swiss PDB Viewer, and AutoDock Vina to analyze the interaction between Thymol and caspase-9. Their 3D structures were sourced from the Pubchem database and Protein Data Bank, respectively. Our docking analysis revealed a binding free energy of -6.0 kcal/mol, indicative of significant hydrogen bonding and hydrophobic interactions stabilizing the complex. The findings suggest that Thymol effectively binds to caspase-9, supported by strong hydrophobic interactions, positioning caspase-9 as a viable target for thyme's anticancer potential. This study provides a foundation for further exploration into Thymol-based therapies for cancer treatment, leveraging its binding efficacy with caspase-9.