A182 · In-Silico Characterization of Plumbagin Binding to Multiple Protein Targets Using Molecular Docking

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Plumbagin is a naphthoquinone compound with diverse biological activities, including antimicrobial and anticancer effects. However, the protein interactions underlying these effects remain incompletely characterized. This study investigated the interactions of plumbagin with eight protein targets associated with processes relevant to its impact: the bacterial cell-division protein FtsZ and the human proteins Keap1, NF-κB, DDX3X, PI3K, AMPK, GPX4, and NOX4, with FtsZ being included as a reference target based on previous evidence of plumbagin binding. Structural similarity between FtsZ and the human protein targets was evaluated using MatchMaker in ChimeraX, potential ligand binding sites were predicted using COACH-D, and molecular docking evaluated predicted plumbagin-protein interactions.Docking scores were used to classify the targets as strong, moderate, or weak predicted binders according to predefined score thresholds. COACH-D C-scores ranged from 0.50 to 1.00, with FtsZ and Keap1 receiving the highest scores of 1.00 and 0.99, respectively. SwissDock docking scores ranged from −6.136 to −4.770 kcal/mol, resulting in two strong, four moderate, and two weak predicted binders. Keap1 and NOX4 were classified as strong predicted binders, FtsZ, NF-κB, DDX3X, and PI3K were moderate predicted binders; and weak predicted binders were AMPK and GPX4. Comparison of COACH-D and docking-associated residues revealed varying levels of residue-level similarity among the targets, with identical residues identified for FtsZ but not across the remaining proteins. Overall, the results demonstrate differences in the predicted interaction of plumbagin with selected protein targets and identify Keap1 and NOX4 as candidates for further experimental investigation.

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