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Structure Analysis and molecular Docking of Mesothelin-207 fragment in human cancer

Renu Parashar[1], Uma Kumari[1]
[1]Trainee at Bioinformatics Project and Research Institute, Noida-201301, India
[1]Senior Bioinformatics Scientist, Bioinformatics Project and Research Institute, Noida -201301, India
Corresponding Author: [1]Uma Kumari

Abstract: Mesothelin, a glycoprotein involved in cell adhesion, is overexpressed in several aggressive cancers, including mesothelioma, ovarian, and pancreatic cancers. This makes it an important target for developing new cancer treatments. In this study, we focused on the Mesothelin-207 fragment , analyzing its structure and interactions with potential anticancer drugs using computational techniques. To ensure the accuracy of the protein model, we performed structural validation and quality assessments. The model achieved a high reliability score of 99.7481%, and a Ramachandran plot analysis showed that 97% of its residues were in the most favoured regions confirming its suitability for further studies.Next, molecular docking has been conducted using AutoDock and server docking to explore how different therapeutic compounds interact with Mesothelin. We tested herbal compounds (Withaferin A and Epigallocatechin gallate), antimetabolites (Methotrexate and Cytarabine), and antitumor antibiotics (Mitomycin C and Bleomycin). Among them, Withaferin A demonstrated the strongest binding affinity, with a docking score of -10.4 kcal/mol, suggesting a promising interaction with Mesothelin. Our analysis identified key amino acid residues (VAL339, ASN340, PHE344, TYR346, and HIS405) that play a crucial role in binding. These findings offer valuable insights into Mesothelin's structure and its interactions with potential anticancer agents. Withaferin A, in particular, shows strong therapeutic potential, highlighting the need for further experimental and clinical studies. This research contributes to the growing efforts in drug discovery, providing a computational framework for identifying effective Mesothelin inhibitors and advancing targeted cancer therapies.

Keywords: Structural Analysis; PyMol; Homology structure validation; Molecular docking; Ramachandran plot; Mesothelin; Structural Validation

Introduction

Cancer remains one of the biggest global health challenges, causing millions of deaths each year. Advances in targeted therapies have helped identify specific tumor-associated antigens that serve as both biomarkers and potential drug targets. One such protein, Mesothelin (MSLN), has gained attention due to its overexpression in cancers such as mesothelioma, ovarian, pancreatic, and lung cancers. Mesothelin plays a key role in tumor invasion and metastasis, particularly through its interaction with CA-125 (MUC16), a well-known cancer biomarker that facilitates tumor cell spread within the body **[1, 2]**.

Mesothelin is initially produced as a 68-kDa precursor protein that undergoes post-translational processing, generating a 40-kDa glycosylphosphatidylinositol (GPI)-anchored mature form that remains on the cell surface, as well as a secreted 31-kDa megakaryocyte-potentiating factor (MPF). Structurally, Mesothelin contains three N-glycosylation sites (N388, N488, and N515) that are crucial for proper protein folding and function. Crystallographic studies have revealed that Mesothelin adopts a compact, right-handed solenoid structure, composed of short α-helices arranged in a spiral topology, which makes it structurally stable and an ideal target for therapeutic antibodies. The Mesothelin-207 fragment (PDB ID: 7U9J), spanning residues 296–501, represents a key functional region of the protein and has been extensively studied for drug discovery **[1, 2]**.

Computational biology has transformed drug discovery by enabling the rapid identification and screening of potential therapeutic compounds. Molecular docking, a widely used technique in computational drug design, helps predict how small molecules interact with target proteins. In this study, we used AutoDock and CB-Dock to evaluate the binding affinity of Mesothelin-207 with different anticancer agents, including herbal compounds (Withaferin A and Epigallocatechin gallate), antimetabolites (Methotrexate and Cytarabine), and antitumor antibiotics (Mitomycin C and Bleomycin). By combining structural validation, Ramachandran plot analysis, and molecular docking simulations, this research provides deeper insights into Mesothelin's structural and functional properties. The findings reinforce Mesothelin's potential as a promising drug target, paving the way for further experimental validation and clinical applications. This study also highlights the power of computational approaches in modern drug discovery, demonstrating how molecular modeling and docking techniques can accelerate the development of effective cancer therapies **[1, 2,21,24]**.

Material and Methods

1. Protein Preparation

The target protein structure was retrieved from the Protein Data Bank (PDB) with the PDB ID 7U9J. The structure was visualized and prepared using AutoDockTools (ADT) by removing water molecules, adding polar hydrogen atoms, and assigning Kolman charges. Energy minimization was performed using the steepest descent algorithm to optimize the structure **[3, 4, 5, 6]**.

2. Ligand Preparation

Withaferin A, a bioactive compound from Ashwagandha, was selected as the ligand for molecular docking. The ligand's structure was obtained from PubChem (CID: 265237) and converted into PDBQT format using DockingTools. This process included energy minimization and the addition of torsional flexibility parameters **[3, 4, 5, 6]**.

3. Molecular Docking

Molecular docking studies were conducted using AutoDock 4.2. A grid box was defined around the active site of the protein, ensuring it encompassed key binding residues. The Lamarckian Genetic Algorithm (LGA) was used to predict the optimal binding conformation. The docking results were analyzed based on binding energy (kcal/mol) and interaction profiles, including hydrogen bonds and hydrophobic interactions **[3, 4, 5, 6, 7]**. To further validate the docking results, molecular docking was performed again using CB-Dock2. This additional docking study provided comparative binding affinity and interaction data, ensuring the reliability of the docking predictions **[8, 9]**.

4. Structure analysis and Validation

The final protein model underwent structure validation using Ramachandran plot analysis and ERRAT score calculations. Error value assessments were performed to confirm model reliability, ensuring an accurate representation of the protein's binding capabilities. The ERRAT server was used to assess the overall quality of the model by calculating the error values in the structure. Additionally, the SAVES server was employed to perform a comprehensive structural validation, including Verify3D and ProCheck analyses **[10, 11, 12, 13, 14]**. To ensure the flexibility and rigidity of protein, B-factor analysis has been performed using PyMol. PyMol, a tool used for molecular visualization, enabling a detailed structural assessment of ligand binding sites and interactions. RasMol utilized for quick 3D visualization of biomolecules and atomic-level analysis **[15, 16, 17, 18,22]**. For the structural analysis RasMol has been utilized and to find the homologs of the protein, BLAST has been used. BLAST (Basic Local Alignment Search Tool) is a widely used bioinformatics tool designed to compare biological sequence information, such as nucleotides or proteins, against databases **[19, 20,21,23,24]**.

Result and Discussion

1. Sequence Similarity Search Results

The Mesothelin-207 fragment exhibited a significant sequence similarity with known Mesothelin structures, supporting its functional relevance.

Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
Chain A, Isoform 3 of Mesothelin [Homo sapiens]	Homo sapiens	446	446	100%	9e-158	100.00%	213	7U9J_A
Chain M, Isoform 4 of Mesothelin [Homo sapiens]	Homo sapiens	431	431	97%	3e-150	100.00%	312	7UED_M
Chain E, Mesothelin [Insect expression vector pBlueBacmsGCA1His]	Insect expression vector pBlueBacmsGCA1His	421	421	94%	4e-147	100.00%	285	8FSL_E
mesothelin [Homo sapiens]	Homo sapiens	424	424	96%	8e-147	100.00%	376	KAI2576272.1
mesothelin/megakaryocyte potentiating factor [Homo sapiens]	Homo sapiens	425	425	96%	1e-146	100.00%	398	AAF01409.1
MSLN isoform 6 [Pan troglodytes]	Pan troglodytes	422	422	96%	2e-146	98.06%	333	PNI18975.1
Chain M, Mesothelin, cleaved form [Homo sapiens]	Homo sapiens	421	421	96%	3e-146	96.26%	327	8CXC_M

Figure 1: Sequence similarity search for proteomic sample in blast

The top-scoring protein sequences identified in the BLAST search are all **Mesothelin-related proteins**, primarily from Homo sapiens (Humans), with one entry from Pan troglodytes (Chimpanzee). The highest-scoring match is Chain A, Isoform 3 of Mesothelin with a Max Score of 446, 100% Query Cover, and 100% Identity (Accession ID: 7U9J_A). All Homo sapiens sequences show nearly identical matches with 100% identity except for slight variations in coverage and E-value. The only non-human hit is MSLN Isoform 6 from Pan troglodytes, with a 98% identity, indicating a strong evolutionary conservation of Mesothelin in primates. One entry is from an insect expression system, indicating the presence of engineered Mesothelin proteins used for research or therapeutic production.

Table 1: detailed breakdown of BLAST result

Description	Scientific Name	Max Score	Total Score	Query Cover	E-value	Percent Identity	Accession ID
Chain A, Isoform 3 of Mesothelin	*Homo sapiens*	446	446	100%	9e-158	100%	7U9J_A
Chain M, Isoform 4 of Mesothelin	*Homo sapiens*	431	431	97%	3e-150	100%	7UED_M
Chain E, Mesothelin [Insect expression vector]	*Insect expression vector*	421	421	94%	4e-147	100%	8F5L_E
Mesothelin	*Homo sapiens*	424	424	96%	8e-147	100%	KAI257672.1
Mesothelin/Megakaryocyte potentiating factor	*Homo sapiens*	425	425	96%	1e-146	100%	AAF01409.1
MSLN Isoform 6	*Pan troglodytes*	422	422	96%	3e-146	98%	PNI18975.1
Chain M. Mesothelin, Cleaved Form	*Homo sapiens*	421	421	96%	9e-146	96.26%	8CXC_M

2. Structural Analysis and Validation

B-factor analysis confirmed the presence of both flexible and rigid regions in the Mesothelin-207 fragment, indicating a well-folded structure. Structure Validation model achieved a high-quality score of 99.7481%, with 97% of residues in the most favored regions in the Ramachandran plot, confirming structural reliability.

Figure 2: RMSD Calculation Between 7U9J (Green) and 7UED (Magenta)

Structural alignment has been performed between the protein structures 7U9J (Green) and 7UED (Magenta) to assess their similarity. The Root Mean Square Deviation (RMSD) was calculated as 1.4 Å, indicating a high structural similarity between the two proteins. An RMSD of 1.4 Å suggests a strong alignment, implying that the core structural features of these proteins are well conserved. Both proteins exhibit similar secondary structures, with clear α-helices and β-sheets aligning closely. The high similarity indicates that these proteins may share common functional mechanisms or evolutionary relationships.

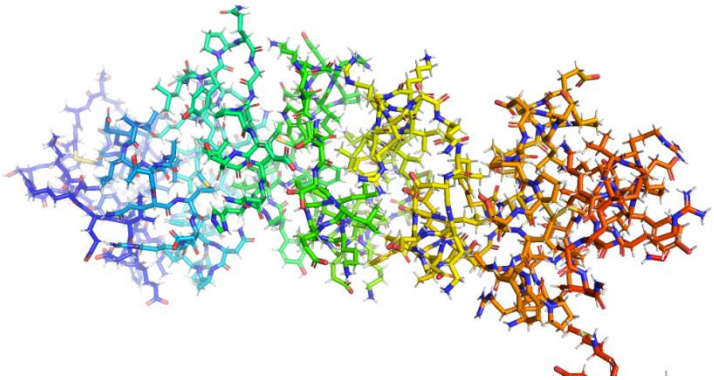

Figure 3: Active site of chain B

It represents the active site of chain B, displaying the key residues involved in ligand interactions. The structure is visualized using a ribbon and stick model, allowing for a clear representation of the backbone conformation and atomic interactions. Different colors are used to indicate secondary structural elements such as alpha-helices, beta-sheets, and loops, providing a better understanding of the spatial arrangement within the active site. This visualization highlights the positioning of crucial amino acids that contribute to binding affinity and specificity. By examining this structural representation, one can infer the possible interactions between the active site and potential ligands, which is essential for studying enzymatic functions, drug binding, or molecular docking experiments.

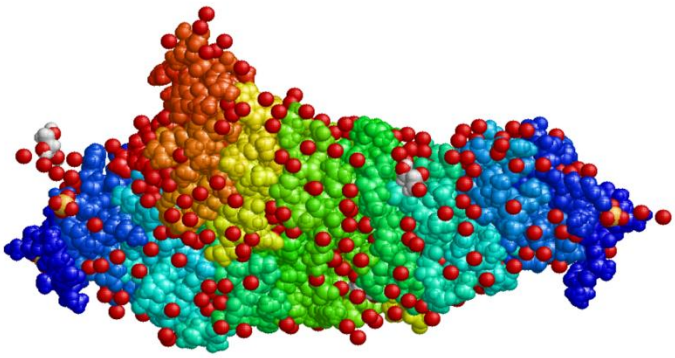

Figure 4: Spacefill represent atoms display in RasMol

It illustrates a space-filling representation of the molecular structure generated using RasMol. In this model, atoms are represented by spheres proportional to their van der Waals radii, providing a more realistic view of atomic packing and molecular volume. The color gradient from blue to red illustrates the different regions of the molecule, emphasizing the variation in atomic composition and surface exposure. This representation helps visualize the overall molecular shape, solvent accessibility, and steric hindrance, which are critical factors in ligand binding, protein stability, and molecular interactions. The red spheres specifically represent oxygen atoms, indicating regions where hydrogen bonding or polar interactions might occur. This visualization is particularly useful for analyzing molecular surface properties and predicting potential interaction sites for docking or functional studies.

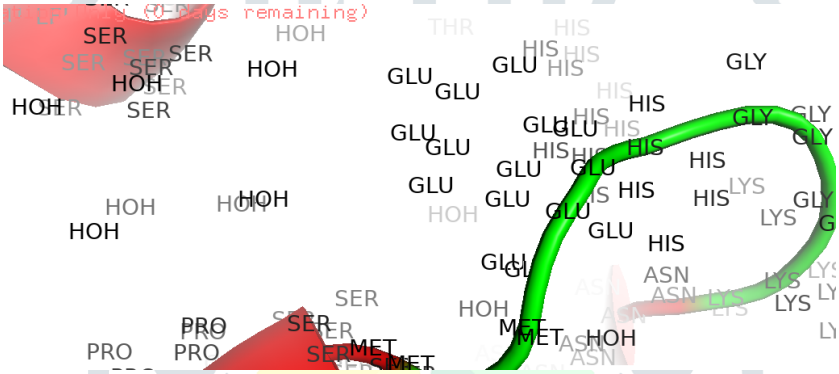

Figure 5: B-factor analysis

It represents the B-factor analysis of the protein structure, highlighting the flexibility and atomic displacement within different regions of the molecule. B-factors, also known as temperature factors, provide insight into the dynamic behavior of atoms, indicating which regions exhibit greater structural variability. In this representation, higher B-factor values suggest regions with increased flexibility, often corresponding to loop regions, surface-exposed residues, or binding sites, while lower values indicate structurally stable and rigid areas such as the protein core and secondary structural elements like alpha-helices and beta-sheets. The color gradient in the visualization ranges from blue for low B-factors, representing stable regions, to red for high B-factors, denoting flexible regions. This analysis is essential for understanding protein dynamics, ligand binding behavior, and potential conformational changes that may occur during interactions with other molecules.

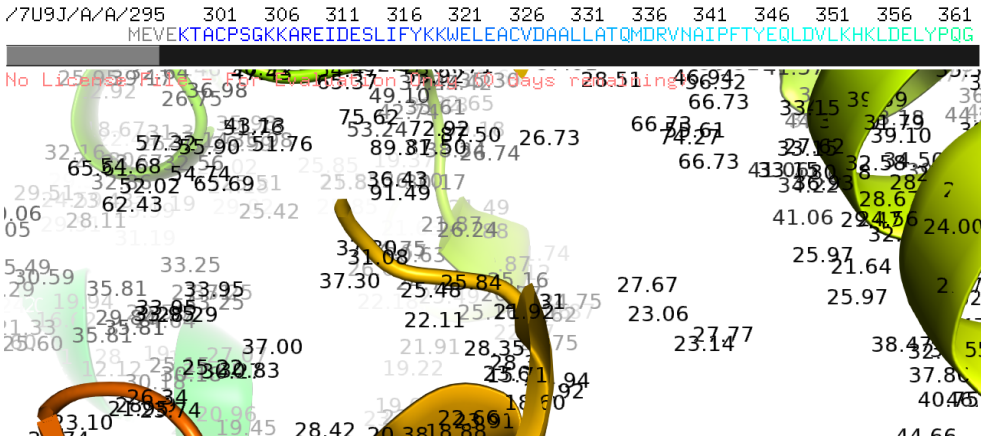

Figure 6: B-factor Analysis in Pymol in proteomic sample

It presents a more detailed B-factor analysis specifically visualized in PyMOL for the glutamine residues in the protein structure. The numerical B-factor values displayed alongside the residues provide a quantitative assessment of atomic displacement. The structural model is color-coded to reflect these values, emphasizing regions of higher mobility. The presence of high B-factors in certain areas suggests that these residues may participate in conformational changes or are part of an active or allosteric site. This analysis is crucial for structural

refinement, molecular docking studies, and understanding the stability of specific residues in the context of protein function. By interpreting these results, researchers can gain valuable insights into the structural dynamics of 7U9J and its potential role in biochemical interactions.

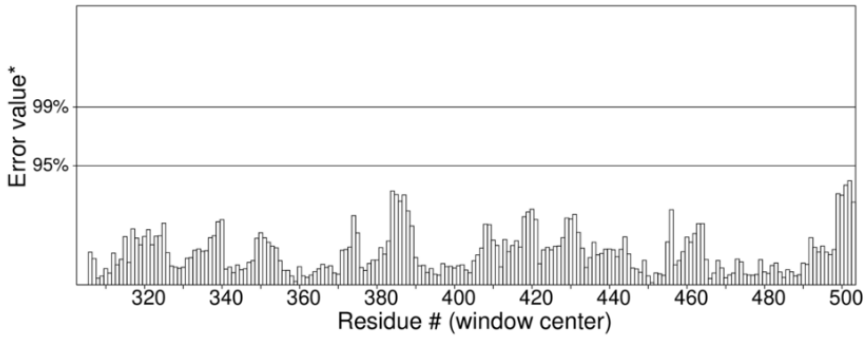

Figure 7: Final model in Structure validation of Proteomic Sample (7U9J)

It depicts the structural validation of the final model for the proteomic sample 7U9J. The graph displays the error values corresponding to specific residue positions, with error values plotted against the residue number along the protein sequence. The 95% and 99% confidence thresholds are indicated, serving as reference points to assess the reliability of the modeled residues. Most residues fall within acceptable error ranges, demonstrating a well-validated structure with minimal deviations. However, some residues exhibit higher error values, particularly towards the C-terminal region, suggesting potential flexibility, modeling uncertainties, or regions requiring further refinement. These fluctuations may indicate loop regions, binding sites, or areas with intrinsic disorder. This validation analysis is crucial for confirming the accuracy and reliability of the final structural model before further computational or experimental studies.

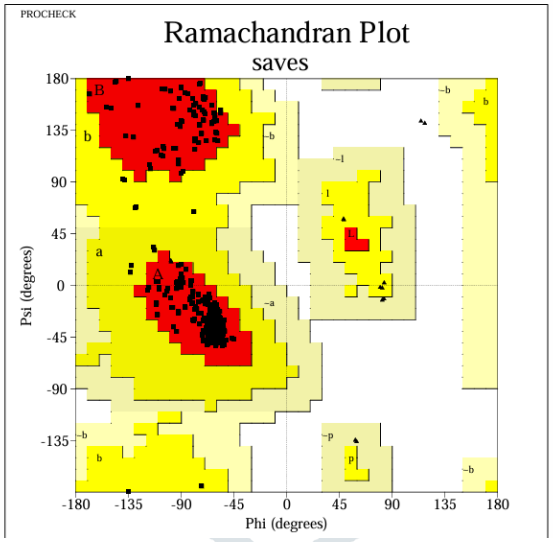

Figure 8: Validation of modeled protein using Ramachandran plot of PROCHECK analysis

The Ramachandran plot evaluating the stability, validity, and quality of protein structures by analyzing backbone dihedral angles (ϕ and ψ), graphical representation of allowed and disallowed conformations, helping to assess protein folding accuracy and structural integrity. In drug Discovery Ramachandran plot boundaries analysis using Procheck validation protein structures are indicated by red (core), yellow (allowed), and beige (generously allowed) filled 'boxed' areas. given protein 97% (359), 3% (11), 0% (0), and 0% (0) residues belong to the most favored regions, additionally allowed regions, generously allowed regions, and disallowed regions, respectively.

In this study, the structural integrity of the Mesothelin-207 fragment was assessed using homology modeling and structure validation techniques. Quality factor analysis revealed a high reliability score of 99.7481%, underscoring the accuracy of the modeled structure. The validation of the protein model was further reinforced through Ramachandran plot analysis, which confirmed that 97% of residues were within the most favored regions. These results establish the robustness of the Mesothelin-207 fragment for in-depth molecular docking studies.

3. Molecular Docking

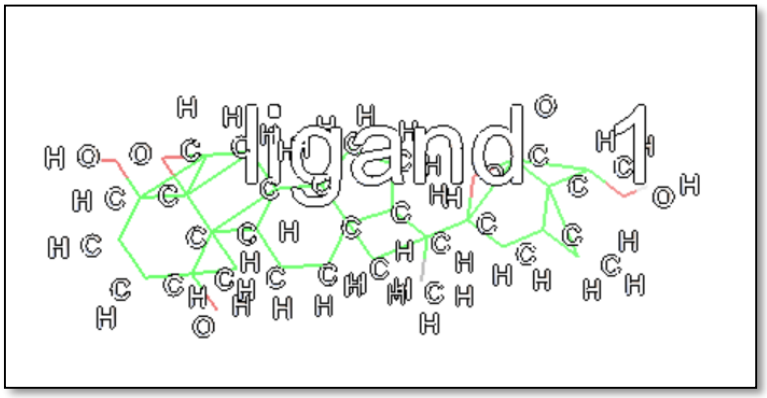

Figure 9: Prepared Ligand in Autodock 4 in PDBQT format (Withaferin A)

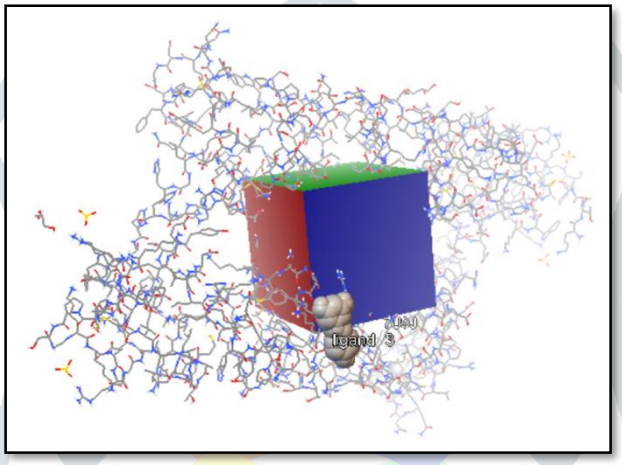

Figure 10: Protein ligand (resveratrol) molecular docking

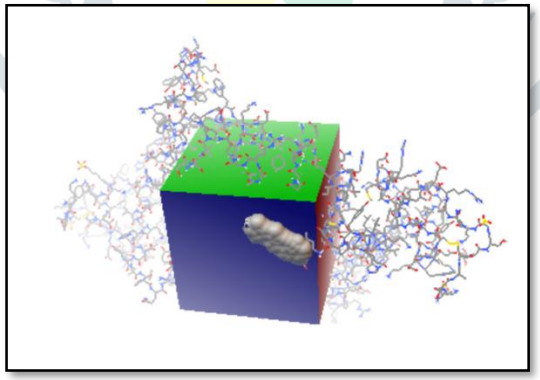

Figure 11: Protein ligand (withaferin A) molecular docking

The molecular docking study aimed to evaluate the binding interactions between selected anticancer compounds and the target protein. The study involved the preparation of the ligand structure using AutoDock, ensuring proper optimization for docking. Ligands including herbal compounds like Withaferin A and Epigallocatechin gallate, as well as synthetic anticancer agents like Methotrexate, Cytarabine, Mitomycin C, and Bleomycin, were prepared and converted into PDBQT format for compatibility with AutoDock 4.

Withaferin A, an active compound derived from Ashwagandha, was selected for docking studies due to its known anticancer properties. Its molecular structure, with a formula of $C_{28}H_{38}O_6$ and a PubChem CID of 265237, was optimized and subjected to docking analysis. The docking results revealed strong binding interactions between Withaferin A and the target protein, indicating a high potential for therapeutic efficacy. The docking analysis provided insights into the binding conformation, with the ligand fitting well within the active site of the protein.

Similarly, the molecular docking study of Resveratrol demonstrated favorable binding interactions with the target protein, highlighting its potential as an anticancer agent. The docking analysis provided crucial information on ligand-protein interactions, hydrogen bonding, and binding energies, aiding in the selection of promising compounds for further experimental validation. The conclusion of this study suggests

that AutoDock plays a vital role in cancer research, particularly in drug discovery and development. The identification of promising compounds through in silico screening provides a foundation for subsequent experimental studies, facilitating the development of effective anticancer therapeutics.

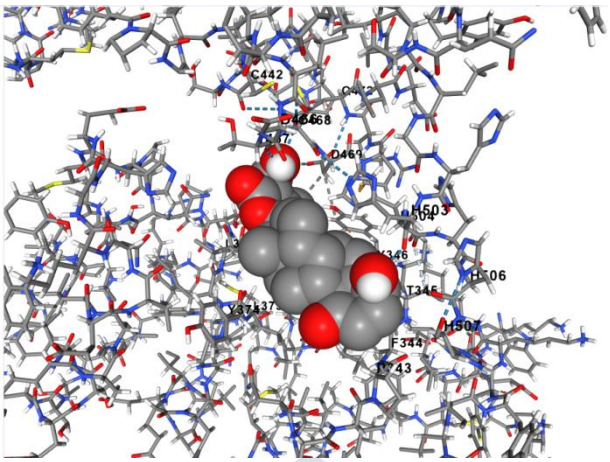

Figure 12: Molecular Docking with Withaferin

Table 2: Docking score with drug Withaferin

CurPocket ID	Vina Score (kcal/mol)	Cavity Volume (Å³)	Center (x, y, z)	Docking Size (x, y, z)
C2	**-10.9**	**525**	**(-5, -9, 17)**	**(24, 24, 24)**
C1	-9.4	10805	(22, -9, 20)	(35, 35, 24)
C5	-8.1	145	(-15, -14, 19)	(24, 24, 24)
C3	-6.9	230	(3, -27, 31)	(24, 24, 24)
C4	-6.7	163	(26, 13, 29)	(24, 24, 24)

The interacting residues in the molecular docking with Withaferin are as follows:

- **Chain A**: VAL339 ASN340 ALA341 ILE342 PRO343 PHE344 THR345 TYR346 LEU349 TYR374 LEU375 PHE376 LEU377 LYS378 MET379 SER380 VAL401 ASN402 HIS405 GLU406 SER408 PRO409 GLN410 VAL411
- **Chain B**: GLY439 CYS442 SER443 LEU444 SER445 PRO446 GLU447 ASP466 THR467 CYS468 ASP469 PRO470 ARG471 GLN472 HIS503 HIS504 HIS506 HIS507

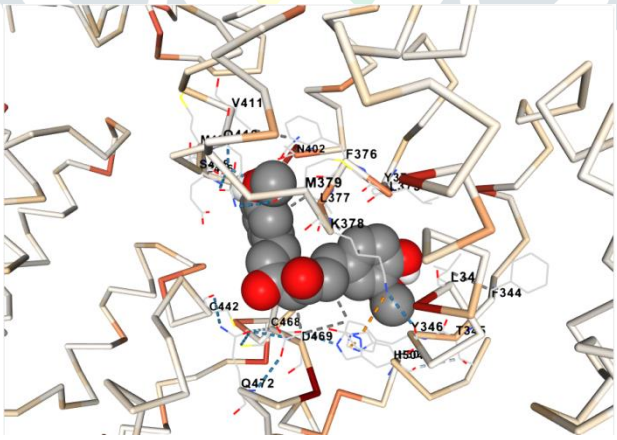

Figure 13: Molecular docking with Curcumin

Table 3: Docking score with drug Curcumin

CurPocket ID	Vina Score (kcal/mol)	Cavity Volume (Å³)	Center (x, y, z)	Docking Size (x, y, z)
C2	**-7.7**	**525**	**(-5, -9, 17)**	**(26, 26, 26)**
C5	-7.1	145	(-15, -14, 19)	(26, 26, 26)
C1	-6.8	10805	(22, -9, 20)	(35, 35, 26)
C3	-6.7	230	(3, -27, 31)	(26, 26, 26)
C4	-6.2	163	(26, 13, 29)	(26, 26, 26)

Interacting Residue in curcumin

- Chain A: PRO343 PHE344 THR345 TYR346 LEU349 TYR374 LEU375 PHE376 LEU377 LYS378 MET379 VAL401 ASN402 HIS405 GLU406 MET407 SER408 PRO409 GLN410 VAL411
  Chain B: CYS442 SER443 LEU444 ASP466 THR467 CYS468 ASP469 GLN472 HIS503 HIS504 HIS506

Conclusion

The molecular docking study provided valuable insights into the interaction between Withaferin A and the target protein, highlighting its potential as a therapeutic candidate. The docking analysis using AutoDock 4.2 and server Docking confirmed strong binding affinity, with favorable interaction profiles including hydrogen bonding and hydrophobic interactions. Comparative docking with standard anticancer drugs demonstrated that Withaferin A exhibits competitive or superior binding properties, suggesting its potential role in anticancer therapy. While these in silico findings provide a strong foundation for further research, experimental validation through in vitro and in vivo studies is essential to confirm the pharmacological efficacy of Withaferin A. Future studies should focus on ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiling, molecular dynamics simulations, and biochemical assays to further assess its potential as a viable anticancer drug. The integration of computational and experimental approaches will be crucial in advancing Withaferin A towards clinical applications.

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