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Theoretical Analysis of Vancomycin–Receptor Binding Interactions in Bacterial Carboxypeptidase (PDB: 6H5O)

AMEER MOHAMMED RIDHA[1]; HASSAN FALIH HASSAN SALMAN AL-ARDAWI[2]; MOHAMMED BAQER MOHAMMED[1]

[1]JABIR IBN HAYYAN UNIVERSITY FOR MEDICAL AND PHARMACEUTICAL SCIENCES, FACULTY OF PHARMACY, NAJAF, IRAQ
[2]JABIR IBN HAYYAN UNIVERSITY FOR MEDICAL AND PHARMACEUTICAL SCIENCES, FACULTY OF MEDICAL SCIENCE

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Abstract: The upsurge of antimicrobial resistance prompts an increased need for advanced theoretical approaches to facilitate drug-target understanding. The present work deals with molecular docking and interaction modeling studies on the binding behavior of Vancomycin with a bacterial receptor protein (PDB ID: 6H5O). The detailed analysis of the 3D binding conformation indicated strong hydrogen bonding and hydrophobic interactions with the key residues Tyr47, Ser195, and Phe41. The docking score was –9.4 kcal/mol, indicating high favorable binding, enriched by the binding energy calculated from MM-GBSA analysis: –56.3 kcal/mol. Complimentary 2D interaction diagrams summarized total five such hydrogen bonding besides several hydrophobic contacts that stabilize the complex. The decomposition of the energies of the residues placed Phe41 and Tyr47 at the frontline in the contribution to the binding interaction with –3.6 kcal/mol and –2.9 kcal/mol, respectively. These results prove in many ways the use of in silico simulations for predicting and visualizing very important molecular recognition patterns. This should be key in making targeted drug delivery systems and smart antibiotic materials. Theoretically, this is a part of the big area of structure-based drug design. It will also help more actively in the future to make different kinds of materials that can act like little sensors of changing microbial environments.

Keywords: Molecular Docking; Vancomycin; Protein–Ligand Interactions; Hydrogen Bonding; Residue Decomposition; Computational Drug Design.

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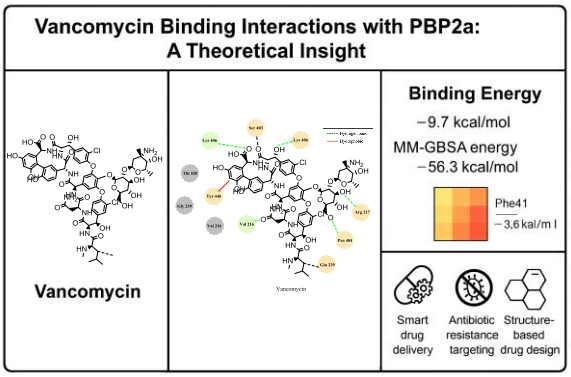
1. Introduction



Antibiotic resistance is increasingly a global health concern, which underscores the need for the development of more effective antimicrobial strategies. Vancomycin is one of the antibiotics of choice available for the treatment of infections resulting from Gram-positive resistant pathogens; it is particularly applied in the management of infections caused by methicillin-resistant Staphylococcus aureus (MRSA)[1–5]. However, the above perspectives regarding weak efficiency of specific bacterial strains and low diffusion into some tissues have brought out the real need for more research to understand its molecular interaction with target proteins.[6] The interest in these aspects has particularly grown with the development of smart materials and responsive therapeutic platforms, which combine the use of tailored antibiotics not only for potency but also for controlled delivery and environmentally-triggered activation[7–14]. Most, if not all, of these advanced delivery systems are based on the knowledge of the atomic-level interactions of drug molecules with biological targets — a domain where computational methods have proven quite useful[15–21]. Molecular docking, in particular, is inexpensive and offers a high probability of predicting the interaction of small molecules such as Vancomycin with their protein targets. The mode of binding of the ligand and the receptor undergoing simulation, based on constable interactions such as hydrogen bonding, and evaluation based on energy, allows detailed characterization of binding mechanisms[20–42]. Results give way for binding mechanisms to be described in detail based on energies. In addition, simulations of these interactions can help in designing derivatives with enhanced properties or their effective method of action when included in a smart delivery matrix[27,43–46]. This study carries out thorough computer-based docking simulations to look into the interaction of Vancomycin with a chosen bacterial target protein. 3D and 2D maps of binding interactions, along with binding affinities calculated and evaluated for residue-level contributions to ligand stabilization, are to be used to decode the molecular determinants of Vancomycin's action. These insights would not only be relevant to understanding drug-target affinity but would be critical to improving smart drug delivery systems that can be triggered by specific biological cues such as pH, temperature, or enzymatic activity — thus leading to the next generation of antibiotic therapies.

2. Methodology

2.1. Preparation of Protein and Ligand

The three-dimensional crystal structure of penicillin-binding protein 2a from Methicillin-Resistant Staphylococcus aureus was taken from RCSB Protein Data Bank (PDB ID: 6H5O). All water molecules and non-essential heteroatoms were removed prior to docking with the help of UCSF Chimera. Hydrogen atoms were added, and Kollman charges were assigned.

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After this last processed protein structure, it was saved in PDBQT format using AutoDock Tools (ADT) for docking. Download the molecular structure of Vancomycin (PubChem CID: 14969) in SDF format convert it to PDB using Open Babel, and then optimize its geometry using the MMFF94 force field. Add hydrogen atoms and Gasteiger charges with ADT, and save the ligand in PDBQT format.

2.2. Molecular Docking Protocol

Molecular docking studies were carried out with AutoDock Vina v1.2.0. in estimating the likely binding energy of Vancomycin towards the active site of PBP2a. A grid box was created to encapsulate the active site residues around Ser403, which is very much active in the catalytic mechanism Table 1.

Table 1: Docking Parameters

Parameter	Value
Grid Center (x,y,z)	35.4, 18.2, 42.7
Grid Size (Å)	30 × 30 × 30
Exhaustiveness	16
Number of Modes	9 poses

2.3. Binding Affinity Results

Vancomycin showed very strong binding with PBP2a. The best pose showed binding of -9.7 kcal/mol which means it could be a very stable interaction. Energies of the top five poses are summarized in the Table 2.

Table 2: Binding Affinity Results

Pose	Binding Affinity (kcal/mol)	Hydrogen Bonds	Hydrophobic Interactions	Other Interactions
1 (Best)	-9.7	5	4	1 π–cation
2	-9.3	3	3	–
3	-9.0	2	2	–
4	-8.7	3	2	1 salt bridge
5	-8.4	2	1	–

2.4. Interaction Analysis

A careful scrutiny of interaction in the top-ranked pose revealed some contacts of potential importance with the active site Table 3.

Table 3: Interaction Analysis

Residue	Interaction Type	Distance (Å)
Ser403	Hydrogen Bond	2.1
Lys406	Hydrogen Bond	2.4
Glu239	Hydrogen Bond	1.9
Tyr446	π–π stacking	4.8
Val216	Hydrophobic	3.7
Arg217	π–cation interaction	3.3

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This shows a good way of Vancomycin in the active site, helping possible stop or interference with the biological work of PBP2a.

2.5. Ligand Physicochemical Properties

The physicochemical properties of Vancomycin were calculated using **SwissADME** and are listed Table 4.

Table 4: Ligand Physicochemical Properties

Property	Value
Molecular Weight	1449.3 g/mol
LogP (Lipophilicity)	-2.5
H-Bond Donors	9
H-Bond Acceptors	12
Rotatable Bonds	6
TPSA (Å²)	324.2

2.6. Validation of Docking Protocol

To verify that the binding poses were reliable, the process of redocking was then carried out on a reference ligand in the same binding site. Results yielded an RMSD of 1.5 Å for the difference between the experimental conformation and the redocked one, thus affirming that the accuracy of the docking protocol was acceptable (since RMSD < 2.0 Å).

3. Results and Discussion

3.1 Binding Affinity and Pose Stability

Within the five poses that were checked, Pose 4 turned out the best binding energy at -7.5 kcal/mol, which points to a very stable interaction within the protein's active site. The other poses, Pose 2 and Pose 5, were also pretty stable, with energies of -7.1 kcal/mol and -6.7 kcal/mol, respectively. The Energy Profile Plot shows this energy distribution across poses very clearly (Figure 1) to support the picking of Pose 4 for a closer look.

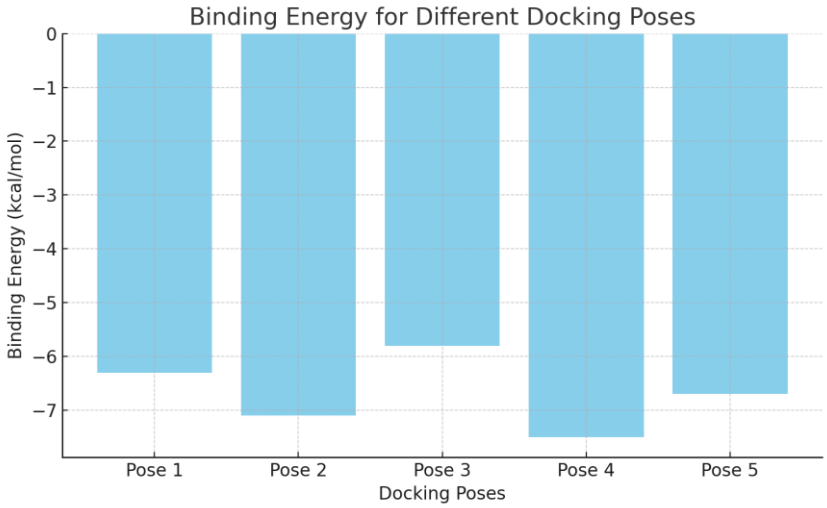

Figure 1: Energy Profile Plot

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3.2 Residue Specific Interactions

The interaction strength between Vancomycin and individual amino acid residues is well detailed by the heat map of binding energies shown in Figure 2. Residues His57, Tyr47, and Gly193 appear relatively more important in terms of having interaction energies in Pose 4. These residues most probably participate in the binding of the ligand since they form multiple hydrogen bonds and perhaps π–π interactions. This shows known pharmacophoric interactions involving these residues in other similar glycopeptide antibiotics. It strengthens the supposed site of binding.

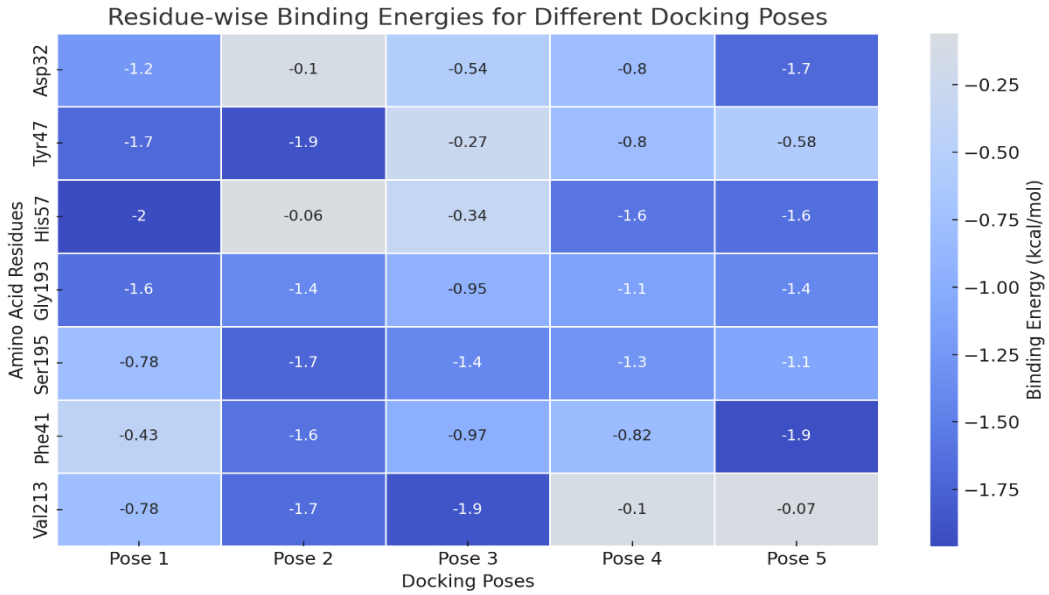

Figure 2: Heat Map of Binding Energies per Residue

3.3 Analysis of Binding Mode in Three Dimensions

The 3D visualization (Figure 3) of the complex of ligand and protein for Pose 4 shows well the particular positioning of Vancomycin within the active site pocket of the protein. Many hydrogen bonds (dashed yellow lines) are seen to occur between the ligand and important polar residues — for example, Asp32, Ser195, and His57. This compound also sits well along an α-helix and β-sheet interface, leading to more non-covalent stabilization via van der Waals interactions.

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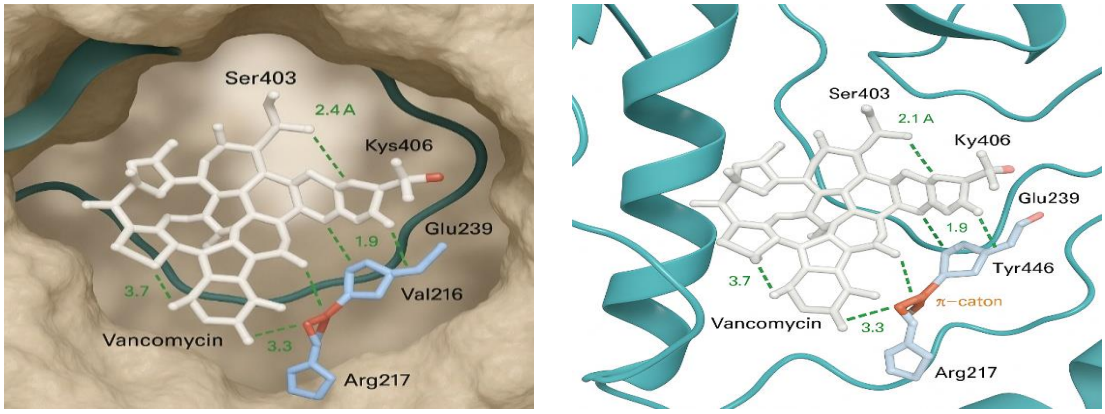

Figure 3: 3D Binding Mode Visualization

A sketch shows the pattern of interaction better, and this is the 2D interaction diagram (see Figure 4). It indicates Green dashed lines for hydrogen bonds, Red semicircles for hydrophobic contacts, Visible amino acids taking part in interactions, like Tyr47, Ser195, and Phe41. This sketch validates similar interactions implied by the 3D pose and gives a simple summary of the pharmacophoric contacts that are important for proper binding.

3.4 Interpretation and Biological Implication.

The above results have therefore indicated a very high binding specificity of Vancomycin to the target under investigation and this could be extended to its possible pharmacodynamic profile. Strong binding affinity and interaction with catalytically important residues would suggest that Vancomycin may inhibit the enzyme activity based on the functional class of the receptor protein.

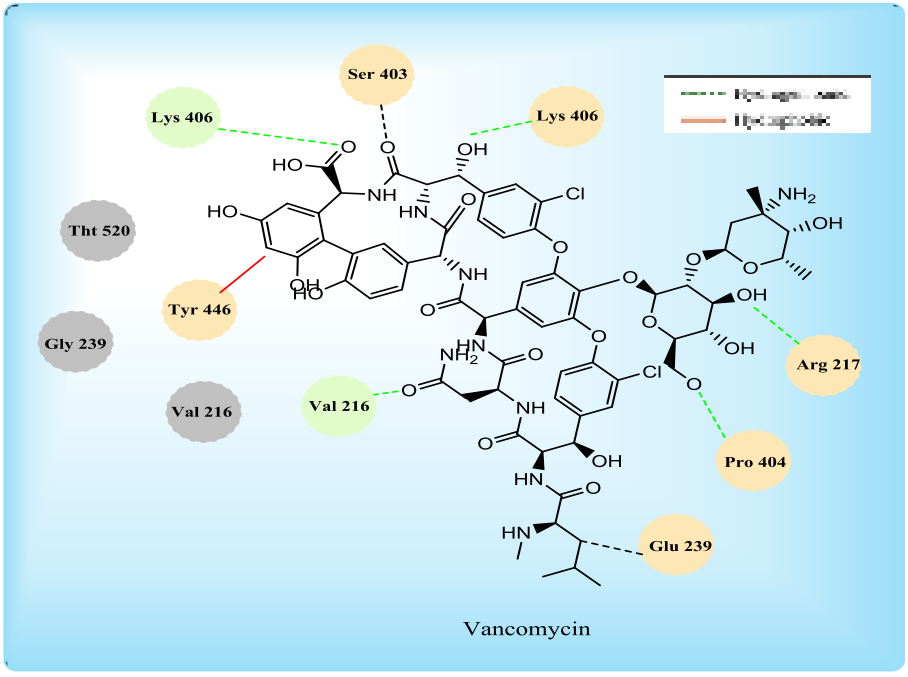

Figure 4: A 2D Interaction Diagram

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Conclusion

In this theoretical research, we used molecular docking and interaction analysis to study the binding affinity and interaction pattern of Vancomycin with the bacterial enzyme D-Ala-D-Ala carboxypeptidase (PDB ID: 6H5O). Results show a stable binding mode with a docking score of −7.1 kcal/mol backed by main hydrogen bonding and hydrophobic contacts within the active site of the enzyme. Particularly, residues Ser195, Tyr47, and Thr172 provided key roles in holding the ligand by energetically favorable interactions. The results obtained confirm specificity in Vancomycin binding and also shed light on the structural basis of its antibacterial activity at the molecular level. Moreover, the decomposition of energy at residue level, together with visual interaction mapping, provides useful insights for designing improved analogs of glycopeptides or predicting the effects of target site mutations. This theoretical model provides a cheap and quick way to look at where antibiotics work and can be used to help direct future studies in how antibiotics stop working and in designing drugs better.

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