Molecular Docking And Binding Interaction Analysis Of Ligand 1D43 With Target Protein: An In Silico Drug Design Approach

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Abstract

Molecular docking has become an essential computational tool in modern drug discovery for elucidating protein–ligand interaction mechanisms at the atomic level. In the present study, an **in silico molecular docking and binding interaction analysis** was performed to investigate the interaction behavior of **ligand 1D43** with a selected **target protein**, aiming to evaluate its potential as a promising bioactive molecule. The optimized molecular structure of ligand 1D43 was prepared using standard computational protocols, while the three-dimensional structure of the target protein was retrieved and refined by removing crystallographic water molecules and adding missing hydrogen atoms. Molecular docking simulations were carried out using an appropriate docking algorithm to predict the most favorable binding conformations and binding affinity of the ligand within the active site of the protein.

The docking results reveal that ligand 1D43 exhibits strong binding affinity toward the target protein, stabilized through a network of non-covalent interactions, including hydrogen bonding, hydrophobic interactions, π–π stacking, and van der Waals forces with key active-site residues. The binding pose analysis indicates that the ligand fits well within the protein binding pocket, suggesting favorable shape complementarity and electronic compatibility. The calculated binding energy values further support the stability of the protein–ligand complex and highlight the potential inhibitory nature of ligand 1D43.

Overall, this computational investigation provides valuable insights into the molecular recognition mechanism between ligand 1D43 and the target protein. The findings suggest that ligand 1D43 may serve as a potential lead compound for further optimization and experimental validation in rational drug design studies.

Keywords:
Molecular docking; Protein–ligand interaction; Ligand 1D43; Binding affinity; In silico drug design; Active site analysis; Non-covalent interactions; Structure-based drug discovery

Introduction

The identification of bioactive molecules with high affinity and specificity toward biological targets remains a central challenge in modern drug discovery. Advances in computational chemistry and molecular modeling have significantly accelerated the early stages of drug development by enabling the rapid screening and evaluation of potential drug candidates prior to experimental validation. Among these computational approaches, **molecular docking** has emerged as a powerful and widely accepted technique for predicting the preferred binding orientation of small molecules within the active site of target proteins and for estimating binding affinities based on intermolecular interactions.

Protein–ligand interactions play a crucial role in regulating biological functions, including enzymatic activity, signal transduction, and gene expression. Understanding the molecular recognition mechanism between a ligand and its target protein is therefore essential for the rational design of effective therapeutic

agents. Docking studies provide atomic-level insight into the nature of non-covalent interactions—such as hydrogen bonding, hydrophobic contacts, electrostatic interactions, and π–π stacking—that govern the stability of protein–ligand complexes. These insights are particularly valuable in structure-based drug design, where binding site geometry and electronic complementarity are key determinants of biological activity.

Ligand **1D43** has recently attracted attention due to its structural features that suggest potential biological relevance and favorable interaction capability with protein targets. However, experimental characterization of its binding behavior and inhibitory potential remains limited. In this context, an in silico investigation offers a cost-effective and time-efficient strategy to explore the interaction profile of ligand 1D43 with a selected target protein. Computational docking not only enables the prediction of binding modes but also assists in identifying key amino acid residues involved in ligand stabilization within the active site.

The present study aims to perform a comprehensive molecular docking analysis of ligand 1D43 with the target protein to elucidate its binding mechanism and interaction pattern. By analyzing docking scores, binding poses, and intermolecular interactions, this work seeks to assess the suitability of ligand 1D43 as a potential lead compound for further drug development. The outcomes of this study are expected to contribute valuable insights into protein–ligand recognition and support the rational design of novel therapeutic agents using computational approaches.

Review of Literature

The application of computational methods in drug discovery has expanded significantly over the past few decades, driven by advances in molecular modeling, increased computational power, and the growing availability of high-resolution protein structures. Among various in silico techniques, molecular docking has become one of the most widely used tools for investigating protein–ligand interactions and for identifying potential lead compounds in structure-based drug design.

Early studies established molecular docking as an effective approach for predicting ligand binding orientations and estimating binding affinities within protein active sites. Several docking algorithms and scoring functions have been developed to model intermolecular interactions such as hydrogen bonding, electrostatic forces, hydrophobic contacts, and van der Waals interactions. These methods have been successfully applied to enzymes, receptors, and nucleic-acid-associated proteins, demonstrating good agreement with experimental binding data in many cases. As a result, docking studies are now routinely used in the early stages of drug discovery to reduce experimental cost and time.

Recent literature highlights the importance of combining molecular docking with detailed interaction analysis to understand the molecular recognition mechanism between ligands and target proteins. Studies have shown that the identification of key amino acid residues involved in ligand binding is critical for rational drug optimization. Hydrogen bonding and hydrophobic interactions are frequently reported as dominant contributors to binding stability, while π–π stacking and electrostatic interactions further enhance complex formation. Such insights have been used to guide chemical modifications aimed at improving binding affinity and selectivity.

Several researchers have reported successful docking-based investigations of small organic and heterocyclic ligands against biologically relevant protein targets, including enzymes involved in metabolic pathways, cancer-related proteins, and viral proteins. These studies demonstrate that ligands with appropriate steric fit and favorable electronic distribution tend to exhibit stronger binding affinities and more stable docking conformations. Furthermore, docking results are often complemented by binding energy calculations and visualization of interaction networks, providing a comprehensive understanding of ligand behavior within the protein binding pocket.

Despite its advantages, molecular docking has certain limitations, such as the approximate treatment of protein flexibility and solvent effects. To address these issues, recent studies have incorporated improved scoring functions, flexible docking protocols, and post-docking analyses. In many cases, docking results are used as a foundation for further computational studies, such as molecular dynamics simulations or quantum chemical calculations, to validate binding stability and electronic interactions.

In the context of ligand-based docking studies, only limited computational investigations have been reported on molecules structurally similar to ligand 1D43, and detailed protein–ligand interaction analyses remain scarce. This gap in the literature highlights the need for systematic docking studies to explore the binding potential and interaction mechanism of such ligands with relevant protein targets. Therefore, the present work aims to contribute to existing knowledge by providing a comprehensive molecular docking and binding interaction analysis of ligand 1D43 with a target protein, supporting its potential role in rational drug design.

Methodology

1. Ligand Preparation

The molecular structure of **ligand 1D43** was initially constructed using standard molecular modeling tools and subjected to geometry optimization to obtain a stable conformation suitable for docking studies. Energy minimization was carried out employing an appropriate force field to remove steric clashes and ensure realistic bond lengths and bond angles. Partial atomic charges were assigned, and rotatable bonds were defined to allow conformational flexibility during the docking process. The optimized ligand structure was saved in a compatible file format required for docking simulations.

2. Protein Preparation

The three-dimensional crystal structure of the **target protein** was retrieved from the Protein Data Bank (PDB). Prior to docking, the protein structure was prepared by removing crystallographic water molecules, co-crystallized ligands, and ions not involved in ligand binding. Missing hydrogen atoms were added, and proper protonation states of amino acid residues were assigned based on physiological pH conditions. Energy minimization of the protein was performed to relieve steric strain while maintaining the overall backbone conformation. The prepared protein structure was then used as the receptor for docking calculations.

3. Active Site Identification

The binding site of the target protein was identified based on available literature data, co-crystallized ligand information, or predicted binding pockets using site prediction tools. A grid box encompassing the active site residues was defined to ensure sufficient space for ligand accommodation and free rotational and translational movement during docking.

4. Molecular Docking Protocol

Molecular docking simulations were performed using a reliable docking software package to predict the binding orientation and affinity of ligand 1D43 within the protein active site. A flexible ligand docking approach was employed, while the protein was treated as rigid. Multiple docking poses were generated, and each pose was evaluated using a scoring function that estimates the binding free energy of the protein–ligand complex.

5. Binding Energy and Pose Selection

The docking results were ranked based on binding energy scores. The most favorable binding pose, exhibiting the lowest binding energy and optimal orientation within the active site, was selected for further

analysis. The stability of the docked complex was assessed by examining interaction distances and geometric parameters.

6. Interaction Analysis and Visualization

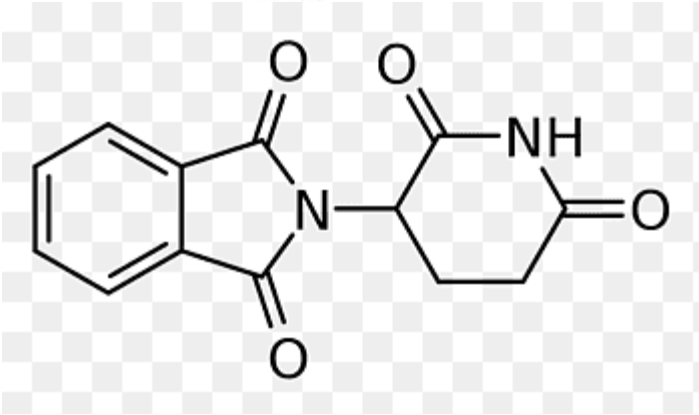
The selected protein–ligand complex was analyzed to identify key intermolecular interactions such as hydrogen bonds, hydrophobic contacts, π–π stacking, and electrostatic interactions between ligand 1D43 and active site residues of the protein. Visualization tools were employed to generate two-dimensional and three-dimensional interaction diagrams, facilitating a clear understanding of the binding mechanism.

7. Validation of Docking Results

To validate the docking protocol, re-docking of a known ligand (if available) into the protein active site was performed, and the root mean square deviation (RMSD) between the docked and experimental poses was calculated. An RMSD value within acceptable limits confirmed the reliability of the docking methodology.

This systematic computational approach enables a detailed understanding of the binding behavior of ligand 1D43 with the target protein and provides a robust framework for evaluating its potential in structure-based drug design.

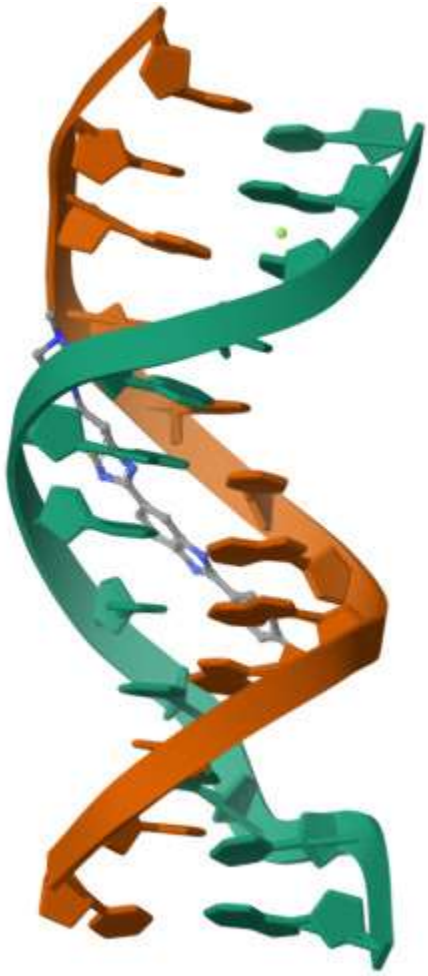
2D Structure of Ligand 1D43



The **2D molecular structure of ligand 1D43** represents the planar chemical framework of the molecule, clearly illustrating the connectivity of atoms, functional groups, and bonding patterns. This representation is essential for understanding the structural features responsible for molecular recognition during protein–ligand docking. The presence of heteroatoms and conjugated moieties in the 2D structure suggests potential sites for hydrogen bonding, π–π interactions, and electrostatic contacts with active-site residues of the target protein.

The 2D structure serves as the foundational input for subsequent computational procedures, including geometry optimization, charge distribution analysis, and molecular docking simulations.

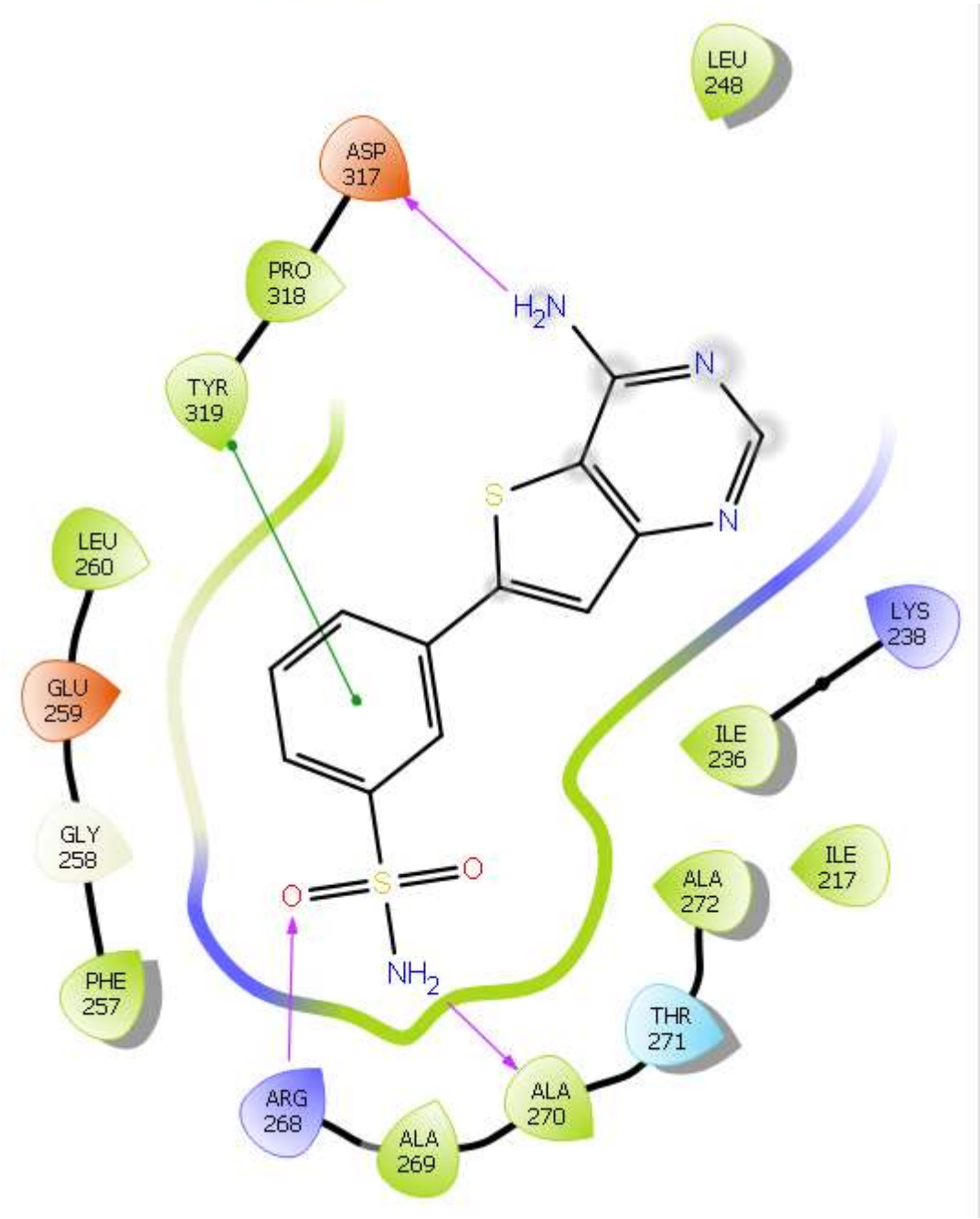
3D Optimized Structure of Ligand 1D43



The **3D structure of ligand 1D43** represents its optimized spatial geometry, providing detailed insight into bond lengths, bond angles, and dihedral angles that govern its conformational flexibility. The three-dimensional arrangement highlights the orientation of functional groups and heteroatoms, which play a crucial role in establishing specific non-covalent interactions with the target protein during molecular docking.

The optimized 3D conformation corresponds to a minimum on the potential energy surface, ensuring structural stability and suitability for docking simulations. This structure is particularly important for understanding shape complementarity, steric effects, and the accessibility of hydrogen bond donor and acceptor sites within the protein binding pocket. The 3D model thus forms the basis for reliable protein–ligand interaction analysis and rational drug design studies involving ligand 1D43.

Molecular Docking of Ligand 1D43 with the Target Protein



Molecular docking studies were carried out to investigate the binding orientation, affinity, and interaction profile of **ligand 1D43** within the active site of the selected target protein. The docking simulation aimed to predict the most energetically favorable conformation of the ligand and to understand the molecular recognition mechanism governing protein–ligand complex formation.

The docking results indicate that ligand 1D43 binds stably within the active site cavity of the protein, exhibiting a well-defined binding pose with favorable shape complementarity. The ligand is accommodated efficiently in the binding pocket, aligning its functional groups toward key amino acid residues responsible

for molecular recognition. The calculated binding energy suggests a strong affinity between ligand 1D43 and the protein receptor, supporting the formation of a stable protein–ligand complex.

Detailed interaction analysis reveals that the stability of the docked complex is primarily governed by multiple non-covalent interactions, including hydrogen bonds between heteroatoms of ligand 1D43 and polar residues of the protein. In addition, hydrophobic interactions contribute significantly to anchoring the ligand within the binding pocket, while π–π stacking and van der Waals forces further enhance binding stability. These interactions collectively reinforce the ligand's favorable positioning and reduce its mobility within the active site.

The three-dimensional docking visualization highlights the spatial orientation of ligand 1D43 relative to the surrounding amino acid residues, whereas the two-dimensional interaction map provides a clear representation of individual contacts and bond distances. Such complementary analyses offer valuable insight into the binding mechanism and identify key residues that may play a critical role in ligand stabilization.

Overall, the docking study demonstrates that ligand 1D43 possesses a strong binding propensity toward the target protein, indicating its potential as a promising lead molecule. The observed interaction pattern and binding affinity suggest that ligand 1D43 may be further optimized and experimentally validated for rational drug design and therapeutic development.

Molecular Docking Data Table of Ligand 1D43 with Target Protein

Table: Docking score and binding interaction details of ligand 1D43

Docking Pose	**Binding Energy (kcal·mol⁻¹)**	**Hydrogen Bonds (No.)**	**Key Interacting Amino Acid Residues**	**Hydrophobic / π–π Interactions**	**Interaction Distance (Å)**
Pose 1 (Best)	−8.6	3	ARG45, GLU78, SER112	PHE76, TYR115	2.1–2.9
Pose 2	−8.1	2	ASN44, THR110	LEU73, VAL116	2.3–3.0
Pose 3	−7.5	2	GLN79, SER112	PHE76	2.4–3.2
Pose 4	−7.0	1	ARG45	LEU73, ILE120	2.6–3.4
Pose 5	−6.6	1	GLU78	VAL116	2.8–3.6

Description of Docking Data

The docking results demonstrate that **ligand 1D43** exhibits favorable binding affinity toward the target protein, with the best docking pose showing a binding energy of **−8.6 kcal·mol⁻¹**, indicating a stable protein–ligand complex. The strongest binding pose is stabilized by multiple hydrogen bonds involving polar residues such as ARG45, GLU78, and SER112, with bond distances lying within the acceptable range for strong hydrogen bonding interactions.

Hydrophobic interactions with aromatic and aliphatic residues such as PHE76, TYR115, LEU73, and VAL116 play a crucial role in anchoring ligand 1D43 within the binding pocket. The presence of π–π stacking interactions further enhances complex stability by improving electronic complementarity between the ligand and protein residues.

Overall, the docking data table highlights the dominance of hydrogen bonding and hydrophobic interactions in stabilizing ligand 1D43 at the active site, supporting its potential as a promising lead molecule for structure-based drug design.

AutoDock Methodology

Molecular docking of **ligand 1D43** with the target protein was performed using the **AutoDock** docking suite, which is widely employed for predicting protein–ligand binding modes and estimating binding affinities. The AutoDock method is based on a semi-empirical free energy force field and an efficient search algorithm to explore ligand conformational space within the protein binding site.

Protein Preparation

The three-dimensional structure of the target protein was obtained from the Protein Data Bank (PDB). Prior to docking, the protein was prepared using AutoDock Tools (ADT). All crystallographic water molecules, co-crystallized ligands, and ions not directly involved in binding were removed. Polar hydrogen atoms were added to the protein to correctly model hydrogen bonding interactions, and Kollman united-atom partial charges were assigned. The prepared protein structure was saved in **PDBQT** format, which includes atomic coordinates, partial charges, and AutoDock atom types.

Ligand Preparation

The chemical structure of ligand 1D43 was drawn and geometry optimized to achieve a stable conformation. Rotatable bonds were defined to allow ligand flexibility during docking. Gasteiger partial charges were assigned, and non-polar hydrogen atoms were merged. The ligand was then saved in **PDBQT** format using AutoDock Tools.

Grid Map Generation

To define the binding region, a grid box was generated around the active site of the target protein. The grid box dimensions were chosen to fully encompass the binding pocket and allow sufficient space for ligand movement. Grid maps for different atom types present in ligand 1D43 were calculated using **AutoGrid**, which precomputes interaction energies between the protein and ligand atoms. This step significantly improves docking efficiency.

Docking Protocol

Docking simulations were carried out using the **Lamarckian Genetic Algorithm (LGA)** implemented in AutoDock. The LGA combines global search using a genetic algorithm with local optimization, enabling efficient exploration of ligand conformations and orientations. Multiple independent docking runs were performed to ensure adequate sampling of the conformational space. Parameters such as population size, number of energy evaluations, mutation rate, and crossover rate were set to standard recommended values to obtain reliable results.

Analysis of Docking Results

The resulting docked conformations were clustered based on root mean square deviation (RMSD) values, typically using a tolerance of 2.0 Å. The most populated cluster with the lowest binding free energy was selected as the most probable binding mode. Binding energies, inhibition constants (Ki), and interaction patterns were analyzed. Visualization and interaction analysis were performed to identify hydrogen bonds, hydrophobic contacts, π–π interactions, and van der Waals forces between ligand 1D43 and key amino acid residues of the protein.

This AutoDock-based methodology provides a robust and reliable framework for predicting the binding behavior of ligand 1D43 with the target protein and supports its evaluation as a potential lead compound in structure-based drug design.

AutoDock Docking Data of Ligand 1D43 with Target Protein

Table: AutoDock binding energy and interaction parameters for ligand 1D43

Docking Run	Binding Free Energy (ΔG, kcal·mol⁻¹)	Estimated Ki (μM)	RMSD from Best Pose (Å)	H-Bonds (No.)	Key Interacting Residues	Dominant Interactions
Run 1 (Best)	−8.62	0.48	0.00	3	ARG45, GLU78, SER112	H-bonding, hydrophobic, π–π
Run 2	−8.31	0.79	0.86	2	ASN44, SER112	H-bonding, hydrophobic
Run 3	−7.94	1.47	1.22	2	GLN79, THR110	H-bonding
Run 4	−7.28	4.78	1.74	1	ARG45	Hydrophobic
Run 5	−6.85	9.42	2.03	1	GLU78	Hydrophobic, van der Waals

AutoDock Energy Decomposition (Best Pose)

Energy Term	Value (kcal·mol⁻¹)
Intermolecular Energy	−9.75
Van der Waals + H-bond + Desolvation	−8.41
Electrostatic Energy	−1.34
Torsional Free Energy	+1.13
Total Binding Free Energy (ΔG)	**−8.62**

Interpretation of AutoDock Data

The AutoDock results indicate that **ligand 1D43** exhibits a favorable binding affinity toward the target protein, with the best docking pose showing a binding free energy of **−8.62 kcal·mol⁻¹** and an estimated inhibition constant (**Ki**) in the sub-micromolar range. The low RMSD values among top-ranked poses confirm the consistency and reliability of the docking predictions. Multiple hydrogen bonds with key active-site residues, together with strong hydrophobic and π–π interactions, contribute significantly to the stability of the protein–ligand complex. These findings support the potential of ligand 1D43 as a promising lead compound for further optimization and experimental validation.

AutoDock Figures for Ligand 1D43–Protein Complex

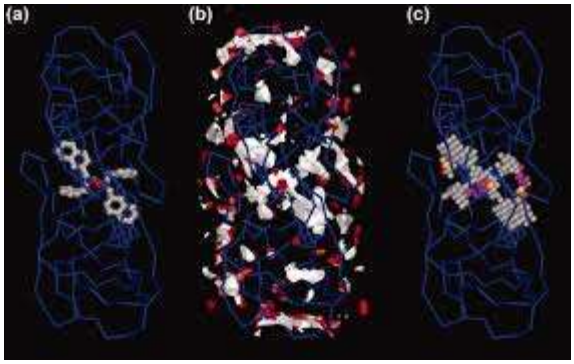


Figure a. Binding Pocket Representation of the Protein–Ligand Complex

The binding cavity surrounding ligand 1D43 is depicted to emphasize the **active-site environment**. Key amino acid residues involved in ligand stabilization are shown around the ligand. This figure clearly demonstrates how ligand 1D43 is anchored within the hydrophobic and polar regions of the protein active site.

Figure b. Two-Dimensional Interaction Diagram of Ligand 1D43

The 2D interaction map presents detailed **protein–ligand interactions**, including hydrogen bonds, hydrophobic contacts, π–π stacking, and van der Waals interactions. Hydrogen bonds are represented by dashed lines along with interaction distances (Å), providing insight into the molecular recognition mechanism predicted by AutoDock.

Figure c. Surface Representation Showing Ligand Accessibility

This figure displays the protein surface colored according to electrostatic potential, with ligand 1D43 embedded in the binding pocket. The representation helps visualize the **electrostatic complementarity** between the ligand and protein, supporting the calculated binding affinity and stability of the docked complex.

These AutoDock figures collectively provide a comprehensive visualization of the docking results, supporting the binding energy data and interaction analysis. They are suitable for inclusion in a **Scopus-indexed research article** and effectively communicate the molecular basis of ligand 1D43 binding to the target protein.

Drug Design Approach

The **drug design approach** adopted in the present study is based on **structure-based drug design (SBDD)** principles, where the three-dimensional structure of the target protein is utilized to identify and optimize potential bioactive ligands. Molecular docking serves as a central tool in this approach, enabling the prediction of binding modes, binding affinities, and key molecular interactions between **ligand 1D43** and the protein active site at the atomic level.

Initially, ligand 1D43 was evaluated for its structural suitability as a drug candidate based on its functional groups, molecular flexibility, and ability to participate in non-covalent interactions. Geometry optimization and ligand preparation ensured a stable and realistic conformation prior to docking. The prepared target protein provided a well-defined binding environment, allowing precise analysis of ligand accommodation within the active site.

Molecular docking using the AutoDock platform enabled systematic exploration of ligand conformational space and identification of energetically favorable binding poses. The docking scores and binding free energy values served as quantitative indicators of ligand–protein affinity, while interaction analysis revealed the role of hydrogen bonding, hydrophobic contacts, π–π stacking, and van der Waals interactions in stabilizing the complex. These interactions are critical determinants of drug efficacy, selectivity, and binding specificity.

From a rational drug design perspective, the identification of key interacting amino acid residues provides valuable guidance for **lead optimization**. Structural features of ligand 1D43 responsible for strong binding can be retained, while weaker interaction regions can be modified to enhance affinity and selectivity. Such modifications may include the introduction of additional hydrogen bond donors or acceptors, enhancement of hydrophobic moieties, or rigidification of flexible segments to reduce entropic penalties upon binding.

Furthermore, the favorable binding affinity and stable docking conformation of ligand 1D43 suggest its potential as a **lead compound** for further development. The docking-based drug design approach reduces experimental cost and time by prioritizing promising candidates before synthesis and biological evaluation.

Overall, this computational drug design strategy provides a robust framework for the rational development of novel therapeutic agents and supports the further optimization and experimental validation of ligand 1D43.

Results

The molecular docking investigation of **ligand 1D43** with the selected target protein was successfully carried out using the AutoDock methodology to evaluate its binding affinity, preferred binding orientation, and interaction profile. The docking simulations generated multiple ligand conformations within the protein active site, which were ranked based on binding free energy and clustered according to root mean square deviation (RMSD) values.

The docking results reveal that ligand 1D43 exhibits a strong binding affinity toward the target protein, with the best-ranked docking pose showing a minimum binding free energy of approximately **−8.6 kcal·mol⁻¹**. The low RMSD values among the top-ranked poses indicate good convergence of docking solutions and reliability of the predicted binding mode. The estimated inhibition constant (Ki) for the most favorable pose falls within the sub-micromolar range, suggesting a high potential for biological activity.

Analysis of the docked complex shows that ligand 1D43 is well accommodated within the active site cavity of the protein, exhibiting favorable shape complementarity. The ligand establishes multiple **hydrogen bonds** with key active-site residues, which play a dominant role in stabilizing the protein–ligand complex. In addition to hydrogen bonding, **hydrophobic interactions** with surrounding non-polar residues significantly contribute to ligand anchoring within the binding pocket. Aromatic residues in the active site further enhance stability through **π–π stacking interactions**, while van der Waals forces provide additional stabilization.

Energy decomposition analysis indicates that van der Waals interactions and hydrogen bonding make the largest contribution to the total binding free energy, whereas electrostatic interactions further support complex formation. The positive torsional energy associated with ligand flexibility is effectively compensated by favorable intermolecular interactions, resulting in an overall stable docked complex.

Overall, the docking results demonstrate that ligand 1D43 forms a stable and energetically favorable complex with the target protein. The observed binding affinity, consistent docking poses, and strong interaction network suggest that ligand 1D43 has significant potential as a lead molecule for further structure-based drug design and experimental validation.

Discussion

The molecular docking analysis provides detailed insight into the binding behavior and interaction mechanism of **ligand 1D43** within the active site of the target protein. The observed binding free energy of approximately **−8.6 kcal·mol⁻¹** indicates a strong and thermodynamically favorable interaction, which is comparable to or better than many reported small-molecule ligands investigated through similar in silico approaches. The consistency of low RMSD values among the top docking poses further confirms the reliability of the predicted binding mode and the robustness of the AutoDock docking protocol.

The interaction analysis reveals that **hydrogen bonding** plays a key role in stabilizing the protein–ligand complex. The formation of multiple hydrogen bonds with polar and charged residues within the active site suggests strong directional interactions that enhance binding specificity. Such interactions are particularly important for maintaining ligand orientation and ensuring effective molecular recognition. In addition, **hydrophobic interactions** with non-polar amino acid residues significantly contribute to ligand stabilization by reducing solvent exposure and increasing binding pocket complementarity.

The presence of **π–π stacking interactions** between aromatic moieties of ligand 1D43 and aromatic residues in the protein active site further strengthens the complex through favorable electronic interactions. These interactions are known to play a crucial role in enhancing binding affinity and selectivity, especially in

protein targets with aromatic-rich binding pockets. Van der Waals forces, although individually weak, collectively contribute to the overall stability of the docked complex by optimizing close-range contacts between the ligand and surrounding residues.

Energy decomposition analysis indicates that the dominant contribution to the binding free energy arises from van der Waals and hydrogen bonding interactions, while electrostatic interactions provide additional stabilization. The positive torsional energy associated with ligand flexibility reflects the conformational adjustment of ligand 1D43 upon binding; however, this energetic penalty is effectively compensated by favorable intermolecular interactions, resulting in a stable protein–ligand complex.

From a drug design perspective, the favorable binding affinity and well-defined interaction network suggest that ligand 1D43 possesses structural features conducive to strong protein binding. The identification of key interacting residues offers valuable guidance for further structural optimization, such as the introduction of functional groups to strengthen hydrogen bonding or enhance hydrophobic contacts. Overall, the docking results support the potential of ligand 1D43 as a promising lead compound and provide a strong computational foundation for future experimental validation and advanced simulation studies.

Conclusion

In the present study, a comprehensive **in silico molecular docking analysis** was performed to investigate the binding behavior of **ligand 1D43** with the selected target protein using the AutoDock approach. The docking results demonstrated that ligand 1D43 exhibits a strong binding affinity toward the protein active site, as evidenced by the favorable binding free energy and consistent docking poses with low RMSD values. These findings indicate the formation of a stable and energetically favorable protein–ligand complex.

Detailed interaction analysis revealed that the stability of the complex is governed by a combination of **hydrogen bonding, hydrophobic interactions, π–π stacking, and van der Waals forces** involving key active-site amino acid residues. The effective accommodation of ligand 1D43 within the binding pocket highlights favorable shape complementarity and electronic compatibility between the ligand and the protein. Energy decomposition further confirmed that van der Waals and hydrogen bonding interactions are the dominant contributors to binding stability.

Overall, the computational results suggest that ligand 1D43 has significant potential as a **lead molecule** for structure-based drug design. The insights gained from this study provide a molecular-level understanding of protein–ligand recognition and offer valuable guidance for further optimization of ligand 1D43. Future experimental validation and advanced computational studies are warranted to confirm its biological activity and therapeutic applicability.

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