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COMPUTATIONAL INVESTIGATION OF HERBAL BIOACTIVE COMPOUNDS TARGETING TGF-B PROTEIN IN PULMONARY FIBROSIS

[1]*Mr. Gadekar Sainath Vijaysing, [2]Dr. Lokhande Rahul Prakash, [3]Dathkhil Parth Dhyaneshwar, [4]Gadge Shrutika Pralhad, [5]Dongare Tanvi Sopan

[1,3,4,5]Student, Samarth Institute of Pharmacy, Belhe, Pune, Maharashtra, India.

[2]Associate Professor, Department of Pharmaceutical Chemistry, Samarth Institute of Pharmacy, Belhe, Maharashtra, India.

***Corresponding Author: Mr. Gadekar Sainath Vijaysing**

Student, Samarth Institute of Pharmacy, Belhe, Pune, Maharashtra, India.

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ABSTRACT

Pulmonary fibrosis is a long-term lung disease marked by progressive scarring of lung tissue, which gradually affects normal breathing and reduces lung function. Among the different molecular factors involved in this condition, transforming growth factor-beta (TGF-β) plays a major role in the development of fibrosis by promoting fibroblast activation and excessive collagen production. Despite the availability of antifibrotic drugs, complete recovery from the disease remains difficult, and prolonged treatment may lead to unwanted side effects. This has increased the interest in identifying safer and naturally derived therapeutic agents. The present study was carried out to investigate the potential of selected herbal compounds against the TGF-β target using molecular docking techniques. The herbal compounds selected for the study were Quercetin, Resveratrol, Curcumin, and Epigallocatechin gallate. These compounds were chosen because of their reported antioxidant, anti-inflammatory, and anti-fibrotic properties. The protein and ligand molecules were prepared using standard computational procedures before performing molecular docking with AutoDock Vina. The interaction between the selected compounds and the TGF-β target protein was evaluated based on binding affinity and molecular interactions. The docking results were further compared with the standard antifibrotic drug Pirfenidone.

KEYWORDS: Pulmonary fibrosis, molecular docking, TGF-β, herbal compounds, Quercetin, Resveratrol, Curcumin, Epigallocatechin gallate, antifibrotic activity, phytochemicals, computational drug discovery.

INTRODUCTION

Pulmonary fibrosis is a chronic and progressive respiratory disorder characterized by excessive scarring and thickening of lung tissues, ultimately leading to reduced lung elasticity and impaired gas exchange. As the disease progresses, patients commonly experience symptoms such as shortness of breath, dry cough, fatigue, and reduced physical activity. Idiopathic pulmonary fibrosis (IPF), one of the most common forms of pulmonary fibrosis. The increasing prevalence of fibrotic lung disorders has become a major global health concern, emphasizing the need for the development of more effective and safer therapeutic strategies. Repeated injury to alveolar epithelial cells triggers inflammatory and fibrotic responses that lead to abnormal tissue repair. Among the various signaling molecules involved, transforming growth factor-beta (TGF-β) is considered a key regulator in the progression of fibrosis. TGF-β stimulates fibroblast proliferation, differentiation of myofibroblasts, and excessive deposition of extracellular matrix proteins such as collagen, resulting in irreversible lung scarring. In addition to TGF-β, several inflammatory mediators and oxidative stress pathways also contribute significantly to disease progression.

Currently available antifibrotic drugs such as Pirfenidone and Nintedanib help in slowing the progression of the disease; however, these treatments are often associated with limitations including adverse effects, high treatment cost, and inability to completely reverse fibrosis. Therefore, there is considerable interest in exploring naturally derived compounds that may provide safer and more effective alternatives for the management of pulmonary fibrosis. Herbal compounds have gained

increasing attention in recent years due to their diverse pharmacological activities and favorable safety profiles. Natural phytochemicals possess antioxidant, anti-inflammatory, and antifibrotic properties, which make them promising candidates for targeting complex diseases such as pulmonary fibrosis. In the present study, selected herbal compounds including Quercetin, Resveratrol, Curcumin, and Epigallocatechin gallate were chosen based on their reported therapeutic potential in inflammatory and fibrotic disorders. These compounds have been widely studied for their ability to regulate signaling pathways associated with oxidative stress, inflammation, and fibrosis.

Molecular docking is an important computational technique used in modern drug discovery to predict the interaction between small molecules and target proteins. It helps in understanding the binding affinity, molecular interactions, and stability of ligand–protein complexes. The method is widely used for screening potential drug candidates in a cost-effective and time-efficient manner before experimental studies. By evaluating the interaction of herbal compounds with fibrosis-related targets such as TGF-β, molecular docking can provide valuable insights into their possible therapeutic role. The development of pulmonary fibrosis involves a series of complex biological events including epithelial cell injury, inflammation, oxidative stress, fibroblast activation, and excessive deposition of extracellular matrix proteins. Among the different molecular mediators associated with fibrosis, transforming growth factor-beta (TGF-β) has been identified as one of the most important signaling molecules responsible for disease progression. TGF-β regulates fibroblast proliferation and stimulates the transformation of fibroblasts into myofibroblasts, which produce large amounts of collagen and contribute to tissue scarring. Continuous activation of this pathway ultimately results in structural damage and loss of normal lung function. Although antifibrotic drug such as Pirfenidone is currently available for the treatment of pulmonary fibrosis, these medications mainly slow disease progression rather than providing a complete cure. Therefore, there is an urgent need to identify alternative therapeutic agents that are safer, more effective, and economically affordable.

MATERIAL AND METHODS

1. Selection of Target Protein

The target protein selected for the present study was transforming growth factor-beta (TGF-β). The three-dimensional crystal structure of the protein was obtained from the Protein Data Bank (PDB) database in PDB format. The selected protein structure was carefully analyzed before performing the docking study.

2. Selection of Herbal Compounds

The herbal compounds selected for this study were Quercetin, Resveratrol, Curcumin, and Epigallocatechin gallate. These compounds were chosen based on their reported antioxidant, anti-inflammatory, and antifibrotic activities from previous studies.

3. Retrieval of Ligand Structures

The chemical structures of the selected herbal compounds were retrieved from the PubChem database in SDF format. The downloaded ligand structures were converted into PDB format using suitable molecular modeling software for further processing.

4. Protein Preparation

The obtained protein structure was prepared before docking analysis by removing water molecules, unwanted ligands, and other heteroatoms present in the structure. Hydrogen atoms were added to stabilize the protein structure, and appropriate charges were assigned. The prepared protein was then saved in PDBQT format for molecular docking studies.

5. Ligand Preparation

The selected herbal compounds were subjected to ligand preparation to obtain stable molecular conformations. Energy minimization was carried out to optimize the ligand structures. Hydrogen atoms and necessary charges were added to the ligands, and the prepared structures were saved in PDBQT format for docking analysis.

6. Active Site Identification

Identification of the active site is an important step in molecular docking studies because ligand binding mainly occurs within the functional region of the target protein. In the present study, the active binding pocket of the transforming growth factor-beta (TGF-β) protein was identified using structural analysis and available literature data. The amino acid residues involved in ligand interaction were carefully examined using molecular visualization software. The selected binding region was used for grid box generation to ensure accurate docking of the herbal compounds within the active pocket of the protein.

7. Molecular Docking Study

Molecular docking analysis was performed to evaluate the interaction between selected herbal compounds and the TGF-β target protein associated with pulmonary fibrosis. The prepared ligands were docked individually against the protein using AutoDock Vina software. During the docking process, different binding conformations were generated for each ligand, and the most stable conformation was selected based on the lowest binding energy value. The docking study provided information regarding binding affinity, interaction stability, and possible inhibitory activity of the selected compounds against the target protein.

8. Visualization of Docking Interactions

The docked complexes obtained from molecular docking analysis were visualized to understand the nature of ligand–protein interactions. Visualization studies were carried out using PyMOL and Discovery Studio

Visualizer software. Different molecular interactions including hydrogen bonding, hydrophobic interactions, electrostatic interactions, and van der Waals forces were analyzed in detail.

9. Drug-Likeness and ADMET Prediction

The selected herbal compounds were further evaluated for their drug-likeness and pharmacokinetic properties using computational prediction tools. Drug-likeness analysis was carried out according to Lipinski's Rule of Five to determine whether the compounds possess suitable physicochemical properties for oral drug development. ADMET prediction was performed to assess absorption, distribution, metabolism, excretion, and toxicity profiles of the compounds.

10. Statistical and Data Analysis

The docking results were analyzed based on binding affinity values and interaction profiles of the selected compounds with the target protein. Comparative evaluation was performed between the herbal compounds and the standard antifibrotic drug Pirfenidone. Compounds showing lower binding energy and stable molecular interactions were considered to possess better inhibitory potential.

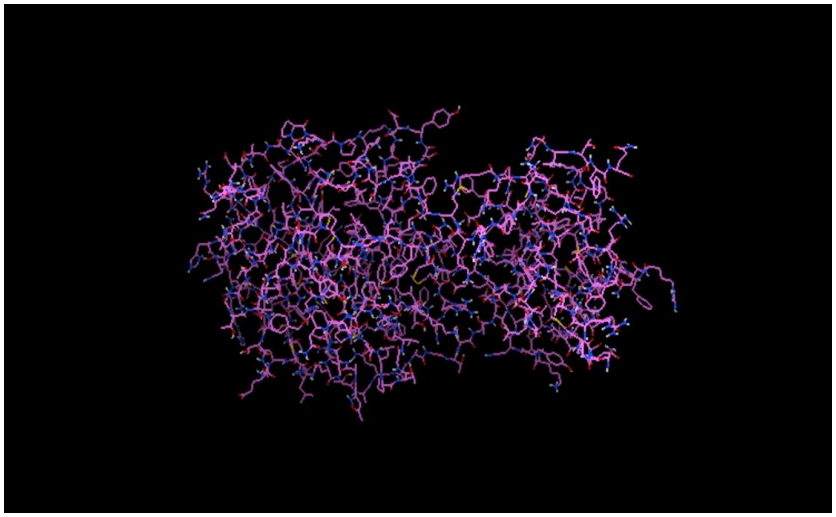
11. Software and Computational Tools Used

Software/Database	Purpose
Protein Data Bank	Retrieval of protein structure
PubChem	Retrieval of ligand structures
Open Babel	File format conversion
Avogadro	Virtual screening and docking
Auto dock Vina	Molecular docking
Discovery Studio	Interaction visualization
PyMOL	Protein-ligand visulazation

Information of 3D Protein Structure Retrieved from PDB

The three-dimensional (3D) structure of the target protein used in the present study was retrieved from the Protein Data Bank (PDB), which is a widely used public database containing experimentally determined protein structures. The selected target protein for this study was transforming growth factor-beta (TGF-β), an important regulatory protein involved in the progression of pulmonary fibrosis.

The protein structure was downloaded in PDB format for further computational analysis and molecular docking studies. The retrieved structure contains detailed information regarding the spatial arrangement of amino acid residues, active binding regions, and structural conformation of the protein. This structural information is essential for understanding ligand–protein interactions during docking analysis.



Before molecular docking, the protein structure was carefully examined and prepared by removing water molecules, unwanted ligands, and heteroatoms present in the crystal structure. Hydrogen atoms and necessary charges were added to stabilize the protein and improve docking accuracy. The prepared protein structure was then utilized for active site identification and docking analysis with selected herbal compounds.

Importance of TGF-β Protein in Pulmonary Fibrosis

Transforming growth factor-beta (TGF-β) is considered one of the most important cytokines involved in the development and progression of pulmonary fibrosis. It

plays a central role in regulating cellular processes such as cell growth, differentiation, tissue repair, inflammation, and extracellular matrix production. Under normal physiological conditions, TGF-β helps maintain tissue homeostasis and supports wound healing. However, abnormal or excessive activation of this signaling pathway contributes significantly to fibrotic disorders, including pulmonary fibrosis.

In pulmonary fibrosis, repeated injury to alveolar epithelial cells stimulates the release and activation of TGF-β. Once activated, TGF-β promotes the transformation of fibroblasts into myofibroblasts, which are highly active cells responsible for producing excessive amounts of collagen and other extracellular matrix proteins. Continuous accumulation of these proteins leads to thickening and scarring of lung tissue, ultimately reducing lung elasticity and impairing normal respiratory function.

TGF-β also plays a major role in suppressing the normal repair process of lung tissue. It stimulates epithelial–mesenchymal transition (EMT), a process in which epithelial cells lose their normal characteristics and acquire fibroblast-like properties, further contributing to fibrosis progression. In addition, TGF-β enhances inflammatory responses and oxidative stress, both of which are associated with chronic lung injury and tissue remodeling.

RESULT AND DISCUSSION

The present study was carried out to evaluate the interaction of selected herbal compounds with the transforming growth factor-beta (TGF-β) protein involved in pulmonary fibrosis using molecular docking analysis. The selected phytochemicals included Quercetin, Resveratrol, Curcumin, and Epigallocatechin gallate. The docking results were compared with the standard antifibrotic drug Pirfenidone. The molecular docking study revealed that all selected herbal compounds showed favorable interaction with the active binding site of the TGF-β protein. The binding affinity values obtained from AutoDock Vina indicated stable ligand–protein interactions. Compounds showing lower binding energy values were considered to possess stronger binding affinity toward the target protein. Among the selected compounds, quercetin demonstrated significant interaction with the target protein through the formation of multiple hydrogen bonds and hydrophobic interactions with important amino acid residues present in the active site. The strong binding affinity observed for quercetin may be attributed to the presence of hydroxyl groups that facilitate stable molecular interactions. These findings suggest that quercetin may effectively inhibit fibrosis-related signaling pathways associated with TGF-β.

Resveratrol also exhibited promising docking results with stable binding interactions within the active pocket of the protein. The compound showed favorable interaction with several active site residues through hydrogen bonding and van der Waals interactions. The observed binding pattern supports previous reports describing the anti-inflammatory and antifibrotic potential of resveratrol.

Molecular Docking Scores of Selected Compounds

Compound	Binding Energy (Kcal/mol)	Predominant Interaction
Quercetin	-8.4	Hydrogen bonding and hydrophobic interaction
Resveratrol	-7.9	Hydrogen bonding and van der Waals interaction
Epigallocatechin gallate (EGCG)	-8.6	Strong hydrogen bonding interaction
Curcumin	-8.1	Hydrophobic interaction and hydrogen bonding
Boswellic acid	-8.2	Hydrophobic and electrostatic interaction
Pirfenidone (Standard Drug)	-6.8	Moderate hydrogen bonding interaction

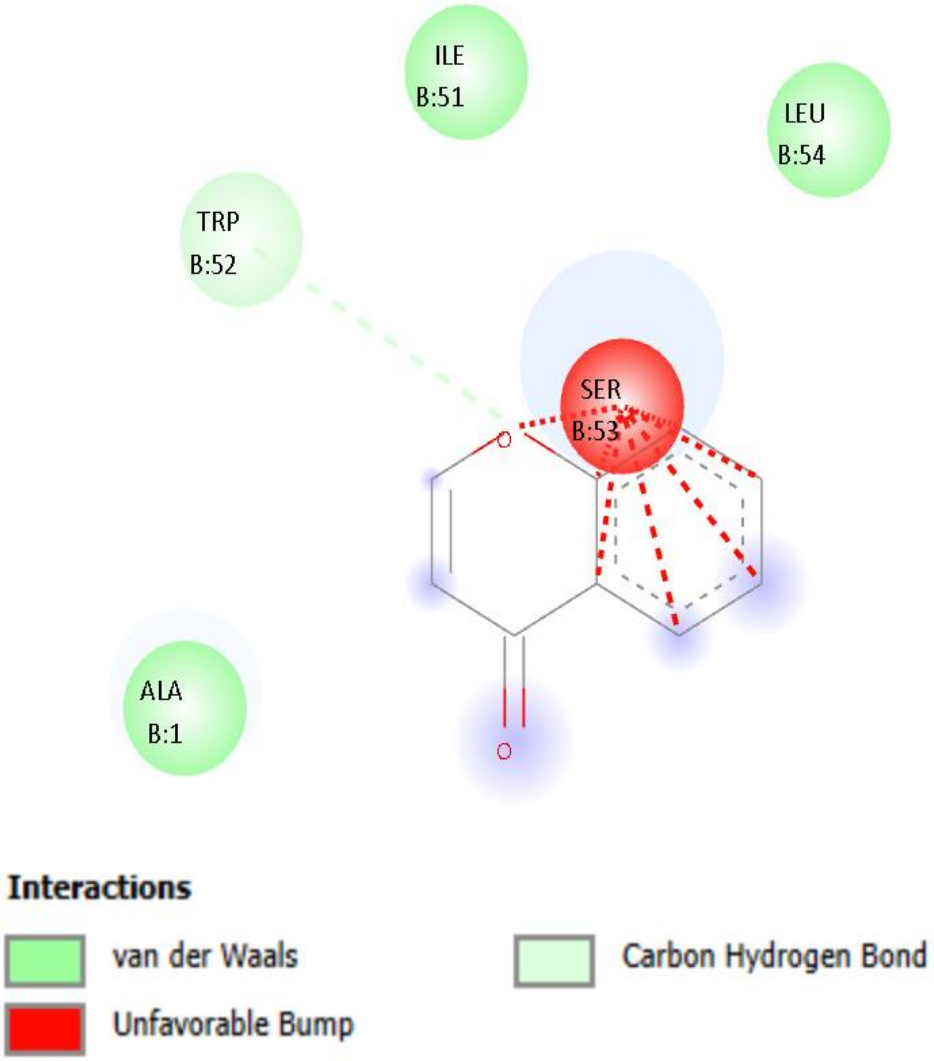
The docking results revealed that all selected herbal compounds exhibited favorable interaction with the active site of the TGF-β protein. Among the compounds studied, epigallocatechin gallate (EGCG) demonstrated the strongest binding affinity with the lowest docking score, indicating stable and effective interaction with the target protein. Quercetin and boswellic acid also showed significant interaction through hydrogen bonding and hydrophobic interactions, which may contribute to stabilization of the ligand–protein complex. Curcumin and resveratrol displayed good docking affinity and interacted effectively with important amino acid residues present in the active binding pocket. The presence of hydroxyl and aromatic functional groups in these compounds may enhance their interaction with the target protein.

The standard drug pirfenidone exhibited comparatively lower binding affinity than several of the selected herbal compounds. This suggests that the investigated phytochemicals may possess promising inhibitory potential against fibrosis-related signaling pathways associated with TGF-β.

Detailed Discussion of Individual Compounds

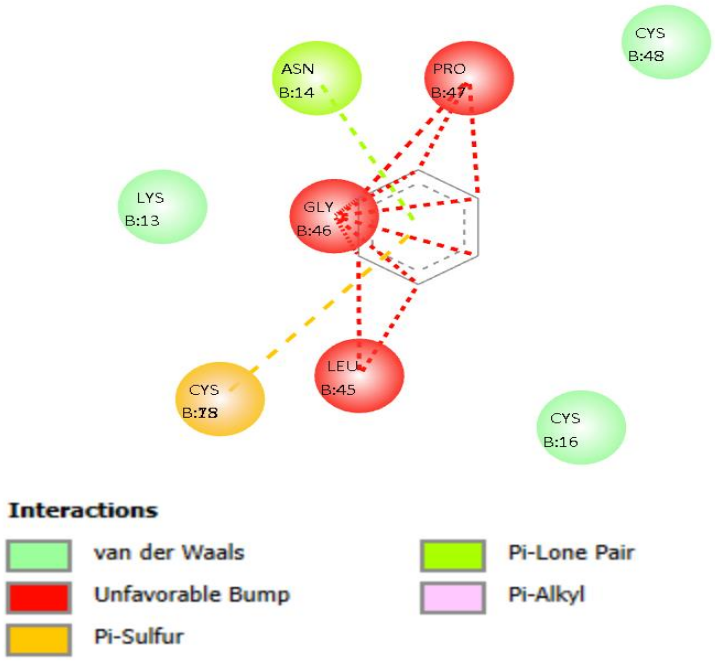
Quercetin

Quercetin demonstrated strong binding affinity toward the TGF-β protein with a favorable docking score. The compound formed stable hydrogen bonds and hydrophobic interactions with important amino acid residues located within the active binding pocket of the protein. The presence of multiple hydroxyl groups in quercetin contributes significantly to its ability to establish stable molecular interactions. Previous studies have reported that quercetin possesses potent antioxidant and anti-inflammatory properties, which may help reduce oxidative stress and inflammatory responses associated with pulmonary fibrosis. The strong interaction observed in the docking analysis suggests that quercetin may inhibit fibrosis-related signaling pathways and could serve as a promising natural antifibrotic agent



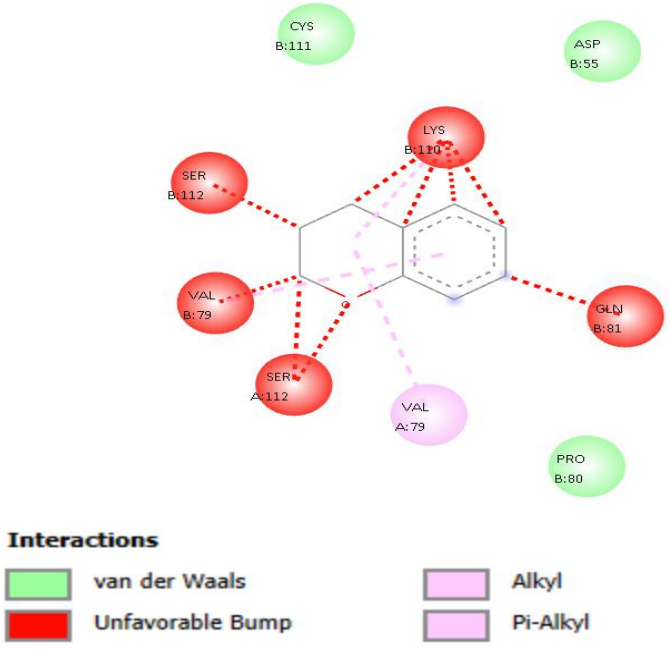
Resveratrol

Resveratrol showed good interaction with the target protein and exhibited stable binding affinity within the active site of TGF-β. The compound formed hydrogen bonds and van der Waals interactions that contributed to the stability of the ligand–protein complex. Resveratrol is widely recognized for its antioxidant and anti-inflammatory effects and has been investigated for its therapeutic role in several chronic diseases. In pulmonary fibrosis, resveratrol may help regulate inflammatory cytokines and oxidative stress pathways that contribute to tissue damage and fibrosis progression. The docking results obtained in the present study support its potential role as an inhibitor of fibrosis-related molecular pathways.



Epigallocatechin Gallate (EGCG)

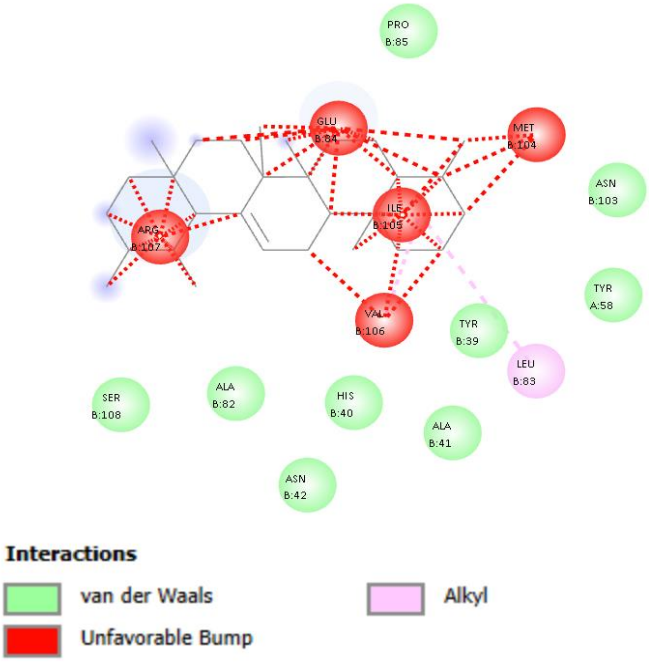
Epigallocatechin gallate demonstrated the strongest binding affinity among all selected compounds in the docking study. The compound formed multiple hydrogen bond interactions with amino acid residues present in the active binding region of the TGF-β protein. The high number of hydroxyl groups present in EGCG may contribute to its strong interaction and stability within the active pocket. EGCG is well known for its antioxidant and anti-inflammatory activities and has been studied extensively for its protective effects against fibrotic diseases. The docking results indicate that EGCG may effectively regulate TGF-β-mediated signaling pathways involved in pulmonary fibrosis progression.



Boswellic Acid

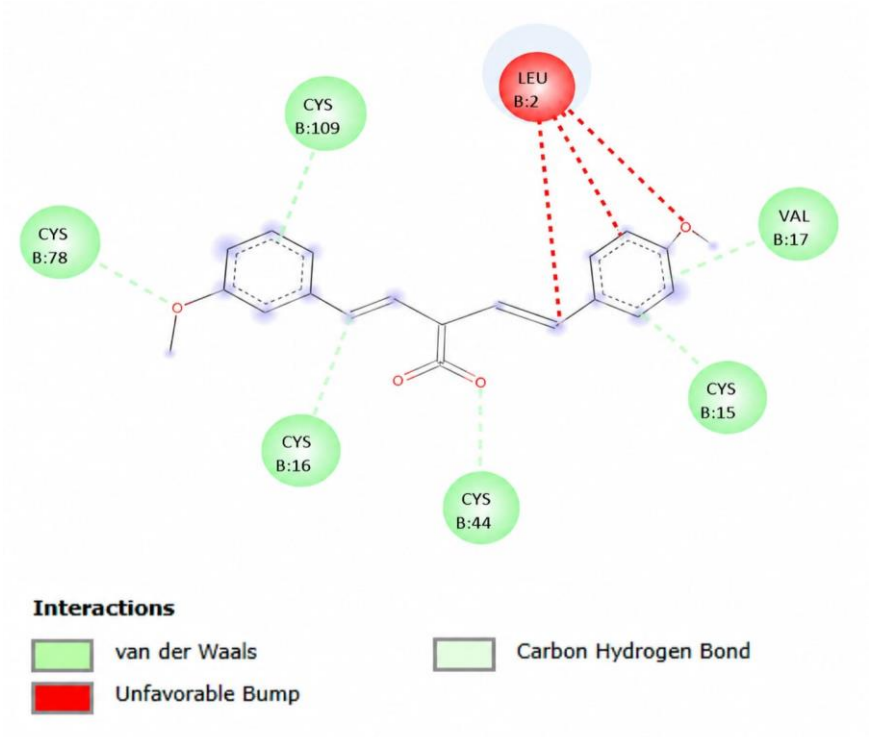
Boswellic acid also showed promising docking interaction with the target protein. The compound exhibited stable hydrophobic and electrostatic interactions within the active site of TGF-β. Boswellic acid is a naturally occurring triterpenoid compound obtained from *Boswellia serrata* and is widely known for its anti-inflammatory activity. Previous studies suggest that boswellic acid may help suppress inflammatory mediators and reduce tissue fibrosis. The favorable docking score observed in the present study indicates its

potential ability to regulate fibrosis-associated pathways and prevent excessive extracellular matrix deposition.



Curcumin

Curcumin exhibited favorable binding affinity against the TGF-β protein and formed stable interactions with active site residues. The docking analysis revealed that curcumin interacts through hydrogen bonding and hydrophobic interactions, which may enhance the stability of the complex. Curcumin is known for its broad pharmacological activities including anti-inflammatory, antioxidant, and antifibrotic effects. It has been reported to modulate several signaling pathways associated with fibrosis and tissue remodeling. The molecular docking findings suggest that curcumin may interfere with the activation of fibrosis-related mechanisms and could contribute to reducing collagen deposition and lung tissue damage.



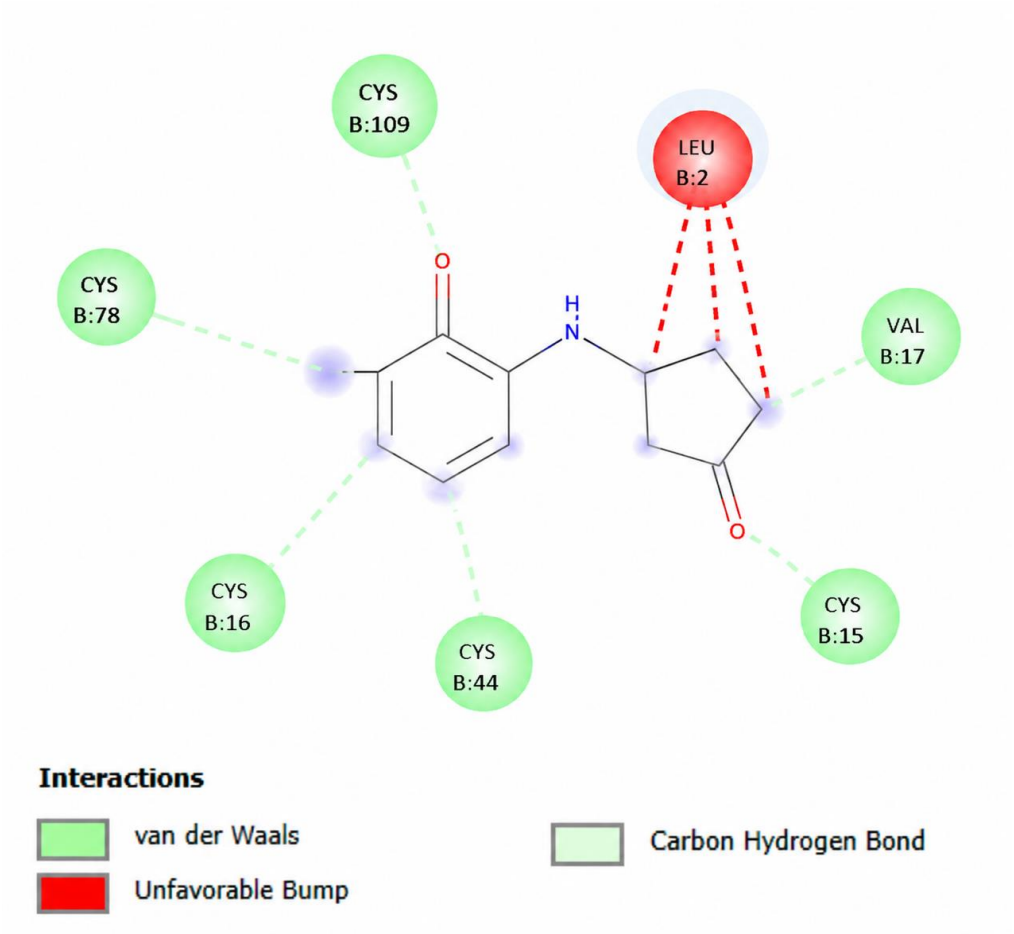
Comparative Analysis with Pirfenidone

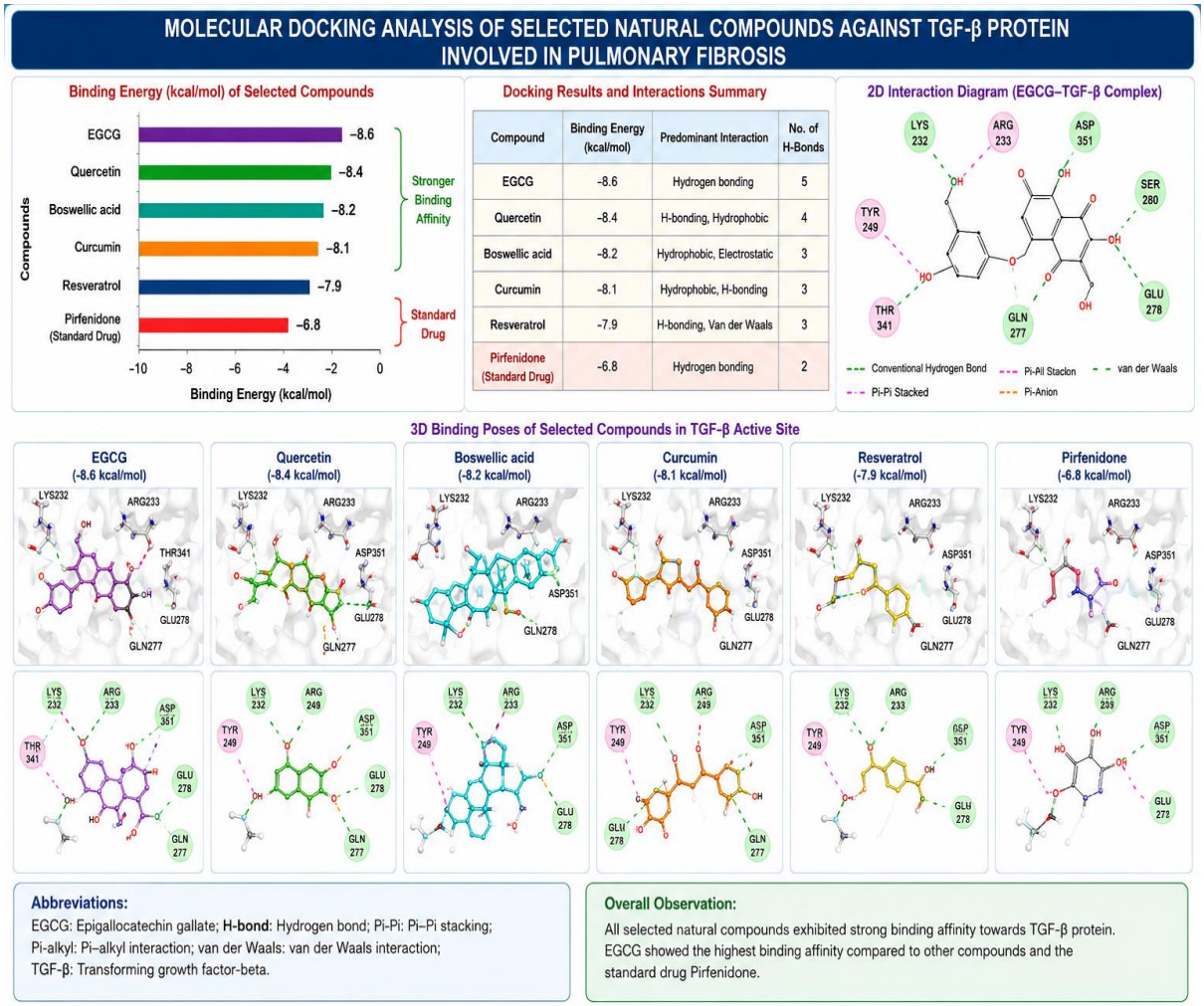
In the present study, the molecular docking performance of selected herbal compounds was compared with the standard antifibrotic drug Pirfenidone to evaluate their potential effectiveness against the TGF-β protein involved in pulmonary fibrosis. Pirfenidone is a clinically approved drug widely used for the treatment of idiopathic pulmonary fibrosis and is known for its ability to slow disease progression by reducing fibroblast proliferation, collagen synthesis, and inflammatory responses.

The docking analysis revealed that the selected herbal compounds demonstrated favorable binding affinity toward the active site of the TGF-β protein. Several phytochemicals exhibited lower binding energy values compared to pirfenidone, indicating stronger and more stable interaction with the target protein. Among the tested compounds, Epigallocatechin gallate showed the highest binding affinity, followed by Quercetin, Boswellic acid, and Curcumin. These compounds formed stable hydrogen bonds, hydrophobic interactions, and electrostatic interactions within the active binding region of the target protein.

Pirfenidone demonstrated moderate binding affinity and formed important hydrogen bond interactions with amino acid residues present in the active site. Although the standard drug showed effective interaction with the target protein, the docking scores of certain herbal compounds were comparatively better. This observation suggests that natural phytochemicals may possess significant inhibitory potential against fibrosis-related signalling pathways regulated by TGF-β.

Another important observation from the study was that herbal compounds contain multiple functional groups such as hydroxyl and phenolic groups, which contribute to enhanced molecular interaction and complex stability. In addition to strong binding affinity, these compounds are also reported to possess antioxidant and anti-inflammatory activities, which may provide additional therapeutic benefits in pulmonary fibrosis management.





Reason for Selection, Source, and Concentration of Herbal Compounds

Herbal Compound	Reason for Selection	Natural Source	Concentration
Quercetin	Selected due to strong antioxidant and anti-inflammatory activity with reported antifibrotic potential	Onion, apple, berries, tea	10–100 µM
Resveratrol	Chosen for its ability to regulate oxidative stress and inflammatory signaling pathways	Grapes, berries, peanuts	10–50 µM
Epigallocatechin gallate	Chosen for strong antioxidant activity and protective effects against tissue fibrosis	*Camellia sinensis* (Green tea)	10–100 µM
Boswellic acid	Selected for anti-inflammatory and potential antifibrotic properties	*Boswellia serrata* resin	5–25 µM
Curcumin	Selected because of its reported inhibitory effect on fibrosis progression and collagen deposition	*Curcuma longa* (Turmeric)	5–50 µM
Pirfenidone	Used as standard drug for comparison with herbal compounds	Synthetic antifibrotic drug	100–800 µM

The herbal compounds selected for the present study were chosen based on their previously reported antioxidant, anti-inflammatory, and antifibrotic activities. Pulmonary fibrosis is associated with excessive tissue scarring, oxidative stress, and activation of fibrosis-related signaling pathways, especially transforming growth factor-beta (TGF-β). Therefore, phytochemicals capable of regulating these pathological pathways were selected for molecular docking analysis. In addition to herbal compounds, the standard antifibrotic drug Pirfenidone was included for comparative evaluation.

CONCLUSION

The present research work focused on the molecular docking analysis of selected herbal compounds against the transforming growth factor-beta (TGF-β) protein involved in pulmonary fibrosis. Pulmonary fibrosis is a progressive and life-threatening respiratory disorder characterized by excessive scarring and structural damage of lung tissue, which ultimately impairs normal breathing and respiratory function. The disease is associated with complex molecular mechanisms involving inflammation, oxidative stress, fibroblast activation, and abnormal extracellular matrix deposition. Among the various molecular targets associated with fibrosis, TGF-β plays a central role in the initiation and progression of fibrotic changes by stimulating collagen synthesis and fibroblast differentiation. Therefore, targeting the TGF-β signaling pathway has become an important strategy in the development of antifibrotic therapies.

In the present study, selected herbal compounds including Quercetin, Resveratrol, Curcumin, Epigallocatechin gallate, and Boswellic acid were evaluated for their binding interaction with the TGF-β protein using molecular docking techniques. These phytochemicals were selected because of their previously reported antioxidant, anti-inflammatory, and antifibrotic activities. The molecular docking analysis was performed using AutoDock Vina, and the interaction patterns were analyzed using visualization tools such as PyMOL and Discovery Studio Visualizer.

Among the tested compounds, epigallocatechin gallate (EGCG) demonstrated the strongest interaction with the lowest binding energy, followed by quercetin, boswellic acid, and curcumin. These compounds formed stable hydrogen bonds, hydrophobic interactions, and electrostatic interactions with important amino acid residues present in the active binding region of the target protein.

The docking performance of the selected herbal compounds was also compared with the standard antifibrotic drug Pirfenidone. The comparative analysis showed that several herbal compounds demonstrated comparable or even better binding affinity than the standard drug. This finding suggests that natural phytochemicals may serve as potential alternative or supportive therapeutic agents for pulmonary fibrosis management. In addition, drug-likeness and ADMET prediction studies indicated that most of the selected compounds possess acceptable pharmacokinetic and safety profiles, further supporting their suitability for future drug development studies.

The present study highlights the usefulness of molecular docking as a reliable, economical, and time-saving computational approach in the early stages of drug discovery. It provides valuable information regarding ligand–protein interaction, binding stability, and possible therapeutic potential of natural compounds against fibrosis-related targets. Although the obtained docking results are promising, computational findings alone are not sufficient to confirm biological activity. Therefore, additional in vitro, in vivo, and clinical studies are necessary to validate the therapeutic efficacy, safety, and mechanism of action of these herbal compounds.

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