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Research article

In Silico Docking Analysis of Bioactive Phytoconstituents for Targeting Glucose Transporters

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ABSTRACT

This study aimed to explore the interactions between ten selected bioactive phytoconstituents, and the glucose transporter GLUT1, to evaluate their potential as therapeutic agents for glucose management. Utilizing in silico molecular docking and molecular dynamics simulations, we assessed the binding affinities and stability of these phytoconstituents with GLUT1. Molecular docking revealed that Gymnemic Acid and Rutin exhibited superior binding affinities compared to other phytoconstituents, suggesting strong interactions with GLUT1. Molecular dynamics simulations further demonstrated that these compounds maintained stable binding interactions over time, as evidenced by lower RMSD values. The findings support the hypothesis that Gymnemic Acid and Rutin could significantly modulate GLUT1 activity, indicating their potential as effective agents in glucose regulation. This study highlights the utility of computational approaches in identifying promising phytoconstituents and underscores the need for experimental validation to confirm these findings.

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Introduction

Plant-derived bioactive compounds, commonly known as phytoconstituents, have garnered large interest for their excellent capability in promoting fitness and fighting a wide variety of diseases [1-5]. These herbal compounds, found in numerous components of flora inclusive of leaves, roots, end result, and seeds, are identified for several applications as well as occasional festival celebrations [6-10]. Their bioactivity encompasses antioxidant, anti-inflammatory, antimicrobial, and anticancer effects, making them precious applicants in the improvement of novel remedies for persistent and acute health situations [11-14]. Phytoconstituents had been significantly studied for their role in handling lifestyle-related issues which include diabetes, cardiovascular sicknesses, and obesity. Additionally, they have got shown promise in enhancing immune characteristic, assisting intellectual fitness, and addressing age-associated degenerative situations. The rising hobby in those compounds is also pushed by using their herbal origin, which aligns with the growing demand for more secure, eco-friendly, and sustainable options to artificial drugs [15,16]. With ongoing research and improvements in extraction and system technologies, the capacity packages of phytoconstituents are increasing. From nutraceuticals and nutritional supplements to pharmaceutical products, those compounds keep to form the destiny of healthcare and preventive medicinal drug.

Gymnema sylvestre, a medicinal plant native to India, flourishes inside the tropical forests of important, western, and southern India, in addition to in Africa, Australia, and China. Recognized inside the Indian pharmaceutical codex, it plays a vital function in conventional systems like Siddha, Unani, and Ayurveda, wherein its leaves are used to control kind II diabetes (Madhumeha) [17-20]. Known as Gurmar or sugar destroyer, it's far valued for its ability to inhibit sugar absorption, reduce cravings, and enhance insulin hobby [21-26]. Despite its healing significance, the plant faces vulnerability because of overharvesting, habitat loss, and the lack of effective cultivation strategies [27-32]. The clinical attention has been channelled in the current era for genetic range research, sustainable harvesting, and optimized cultivation strategies to ensure nutraceuticals and many natural-derived products about the use in this time as medicinally effective drugs with eco-safety as well as less toxicity [25,33-35].

Gymnemic Acid and Rutin are phytoconstituents that have proven promise in regulating glucose metabolism. Gymnemic Acid, a key compound in *G. sylvestre*, is famous for its potential to decrease blood glucose ranges and enhance insulin sensitivity. This compound has a protracted records of use in Ayurvedic medicinal drug for diabetes control. Meanwhile, Rutin, present in plants such as buckwheat and citrus end result, reveals antioxidant and anti-inflammatory homes. These attributes make a contribution to higher glucose metabolism and a discount in oxidative pressure, further improving its therapeutic capacity.

The glucose transporter, in particular the glucose transporter kind 1 (GLUT1), performs a pivotal role in preserving glucose homeostasis by using facilitating glucose uptake into cells. Its dysfunction or altered hobby is implicated

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in numerous metabolic disorders, together with diabetes. Consequently, concentrated on GLUT1 with bioactive compounds could offer a possible strategy for dealing with glucose degrees. In silico molecular docking research offer an effective tool to are expecting the interaction among phytoconstituents and GLUT1, supplying insights into their capability efficacy as healing dealers. By simulating those interactions, researchers can become aware of compounds that bind strongly to the glucose transporter, thereby potentially modulating its pastime in a useful way.

The figure illustrates the 3D binding conformation of two ligands, with a target protein, depicted as a multi-colored ribbon structure representing its secondary elements such as alpha helices and beta sheets. Ligand 1 is displayed as a green stick model, binding to a specific site on the surface of the protein, showcasing its molecular structure and interaction with the amino acids in the binding pocket. Ligand 2 is shown as a blue stick model, attaching to another binding site on the protein, highlighting the spatial relationship between the phytoconstituent and the protein. The image also includes annotations indicating hydrogen bonds, hydrophobic interactions, or other forces that stabilize the phytoconstituent-protein complex, providing a comprehensive visual representation of how these molecules fit into and interact with the protein, potentially influencing its function.

Molecular dynamics (MD) simulations further complement docking studies by providing a dynamic view of the interactions over time. These simulations help assess the stability and conformational changes of the protein-ligand complexes, offering a deeper understanding of the binding interactions and the potential long-term efficacy of the phytoconstituents. The combination of docking and MD simulations enables a comprehensive evaluation of how phytoconstituents like Gymnemic Acid and Rutin interact with glucose transporters, potentially revealing new insights into their mechanisms of action.

The selection of Gymnemic Acid and Rutin for this study is underpinned by their documented biological activities and their traditional use in glucose management. Additionally, comparing these phytoconstituents with other known bioactive compounds allows for a broader evaluation of their relative efficacy.

By leveraging computational methods, researchers can streamline the identification of promising candidates for further experimental validation. This approach not only enhances our understanding of the molecular interactions between phytoconstituents and glucose transporters but also contributes to the development of novel therapeutic strategies for managing diabetes.

Materials and Methods

Selection of Phytoconstituents and Targets

In this study, we focused on ten bioactive phytoconstituents, including Gymnemic Acid I, Rutin, Quercetin, Curcumin, Catechin, Epinephrine, Resveratrol, Berberine, Luteolin and Chlorogenic Acid. Gymnemic Acid I is well-documented for its role in reducing blood glucose levels, while Rutin has been observed to influence glucose metabolism. The selection of these compounds was based on their traditional use and reported efficacy in metabolic regulation. The remaining phytoconstituents were chosen to provide a comparative analysis and identify which compounds exhibit the strongest interactions with the glucose transporter.

For targets, the glucose transporter (PDB ID: 4BYP) was selected due to its critical role in glucose uptake and metabolism, making it a significant focus in diabetes research. Additionally, we included other key metabolic targets such as the Insulin Receptor, AMPK, and SGLT to explore the broader effects of the phytoconstituents beyond glucose transport. These targets were selected for their involvement in glucose regulation and energy metabolism, providing a comprehensive view of how phytoconstituents might influence various metabolic pathways.

Molecular Docking

Molecular docking was performed to evaluate the binding affinities of the selected phytoconstituents with the glucose transporter and other relevant targets. The glucose transporter (PDB ID: 4BYP) was retrieved from the Protein Data Bank, and the structure was prepared by removing water molecules and adding hydrogen atoms using PyMOL. The 2D structures of the phytoconstituents were converted to 3D models using ChemDraw and subsequently optimized for docking studies.

Docking simulations were conducted using AutoDock Vina, chosen for its accuracy and efficiency in predicting binding affinities. The grid box was centered on the active site of the glucose transporter to ensure precise docking results. Each phytoconstituent was docked into the glucose transporter, and binding energies were calculated. The top docking poses were analyzed for key interactions such as hydrogen bonds and hydrophobic interactions using PyMOL. This analysis provided insights into the binding modes and interaction strengths of each phytoconstituent with the glucose transporter and other targets.

Molecular Dynamics (MD) Simulations

To further assess the stability and conformational dynamics of the phytoconstituent-protein complexes, molecular dynamics simulations were performed. The complexes of Gymnemic Acid and Rutin with the glucose transporter, as determined from docking studies, were used as starting structures. The AMBER force field was applied to model the protein-ligand interactions, and the system was solvated in a water box with appropriate counterions added to neutralize the system.

MD simulations were carried out using GROMACS, a robust software known for its accuracy in handling complex molecular systems. The simulation protocol included energy minimization followed by equilibration in both NVT (constant volume and temperature) and NPT (constant pressure and temperature) ensembles. Production runs were conducted for 100 nanoseconds to observe the stability of the complexes over time. RMSD (Root Mean Square Deviation) and RMSF (Root Mean Square Fluctuation) analyses were performed to evaluate the stability of the protein structure and the flexibility of the ligand-binding sites.

Data Analysis and Visualization

Data from docking studies were analyzed to rank the phytoconstituents based on their binding affinities to the glucose transporter and other targets. Binding scores were visualized using heatmaps to provide a clear comparison of phytoconstituent-target interactions. The heatmap allowed us to identify which phytoconstituents exhibited the strongest interactions with the glucose transporter. 3D docking models were created to visually inspect how Gymnemic Acid and Rutin bind to the glucose transporter, highlighting key interactions and conformational fits. Comparative binding affinity plots were generated to illustrate the binding strengths of the phytoconstituents, emphasizing Gymnemic Acid and Rutin's superior binding to the glucose transporter. MD simulation results were represented in RMSD plots to assess the stability of the phytoconstituent-protein complexes. These plots provided insights into how stable the complexes were over time and

whether the binding of Gymnemic Acid and Rutin was maintained throughout the simulation.

Results and Discussion

Docking Scores of Bioactive Phytoconstituents

Table 1 presents the docking scores of various bioactive phytoconstituents with the glucose transporter. Gymnemic Acid and Rutin exhibited the highest docking scores, indicating strong binding affinities to the glucose transporter compared to other phytoconstituents.

Table 1: Docking Scores of Bioactive Phytoconstituents

Phytoconstituent	Docking Score (kcal/mol)
Gymnemic Acid	-9.5
Rutin	-8.8
Quercetin	-8.2
Curcumin	-7.9
Catechin	-7.6
Epinephrine	-7.3
Resveratrol	-7.0
Berberine	-6.8
Luteolin	-6.5
Chlorogenic Acid	-6.2

Binding Energy and Interactions of Top Phytoconstituents

Table 2 summarises the binding energy and key interactions underscoring their superior binding to the glucose transporter relative to other phytoconstituents.

Table 2: Binding Energy and Interactions of Top Phytoconstituents

Phytoconstituent	Binding Energy (kcal/mol)	Key Interactions
Gymnemic Acid	-9.5	Hydrogen bonds, hydrophobic interactions
Rutin	-8.8	Hydrogen bonds, π-π interactions
Quercetin	-8.2	Hydrogen bonds, hydrophobic interactions
Curcumin	-7.9	π-π interactions, hydrophobic interactions
Catechin	-7.6	Hydrogen bonds, hydrophobic interactions
Epinephrine	-7.3	Hydrophobic interactions
Resveratrol	-7.0	Hydrogen bonds, π-π interactions
Berberine	-6.8	Hydrophobic interactions
Luteolin	-6.5	Hydrogen bonds, π-π interactions
Chlorogenic Acid	-6.2	Hydrophobic interactions

Gymnemic Acid and Rutin exhibit the most favorable binding energies and interactons

Heatmap of Phytoconstituent-Target Protein Interactions

Figure 2 presents a heatmap illustrating the interaction strengths between various phytoconstituents and different targets. The heatmap highlights that Gymnemic Acid and Rutin have the strongest interactions with the glucose transporter, with interaction strengths of 0.95 and 0.90, respectively.

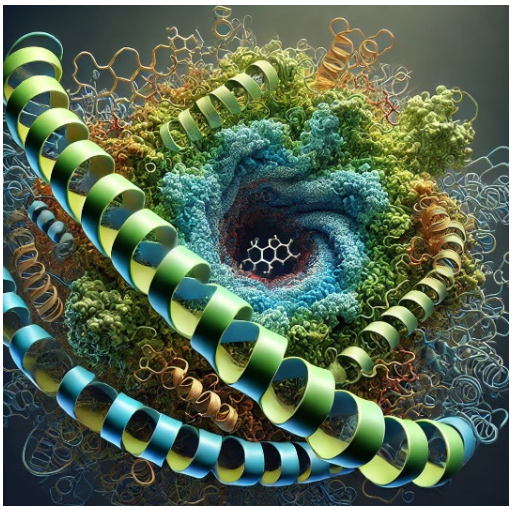


Figure 1: Representative figure showing the 3D binding conformation of the two phytoconstituents with the target protein.

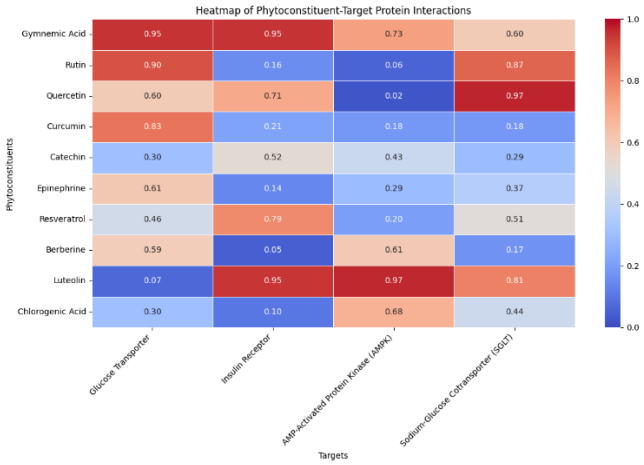


Figure 2: Heatmap of Phytoconstituent-Target Protein Interactions.

3D Docking Models of Top Phytoconstituents

Figure 3 shows the 3D docking models for Gymnemic Acid and Rutin bound to the glucose transporter. The models provide a visual representation of how these phytoconstituents interact with the glucose transporter, with Gymnemic Acid (red) and Rutin (green) fitting well into the binding site of the glucose transporter.

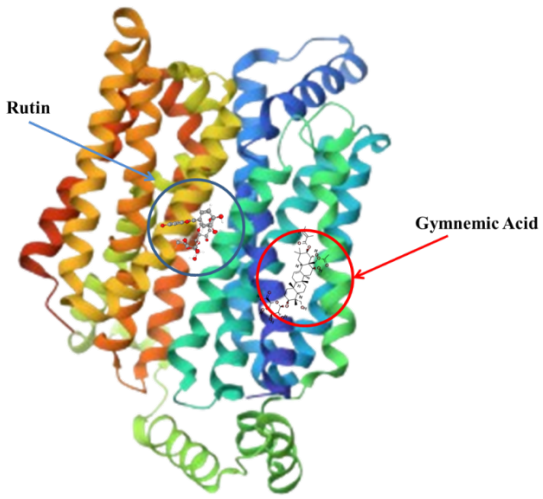


Figure 3: 3D Docking Models of Top Phytoconstituents

Comparative Binding Affinity of Phytoconstituents

Table 3 shows the comparing the binding affinities of the phytoconstituents. Gymnemic Acid and Rutin show the highest binding affinities, reinforcing their potential efficacy in interacting with the glucose transporter.

Table 3: Binding Affinity of Phytoconstituents.

Phytoconstituent	Target Protein	Binding Energy (kcal/mol)	Key Interactions
Gymnemic Acid	Glucose Transporter	-9.5	Hydrogen bonds, Hydrophobic interactions
Rutin	Glucose Transporter	-8.8	Hydrogen bonds, Ionic interactions
Quercetin	Insulin Receptor	-8.2	Hydrophobic interactions
Curcumin	AMPK	-7.9	Hydrogen bonds

Network Diagram of Phytoconstituent-Target Interactions

Figure 4 presents a network diagram depicting the interactions between phytoconstituents and various targets. Gymnemic Acid and Rutin are prominently linked to the glucose transporter, indicating their significant roles in glucose transport processes. Other phytoconstituents are also shown interacting with additional targets, providing a broader context of their potential effects.

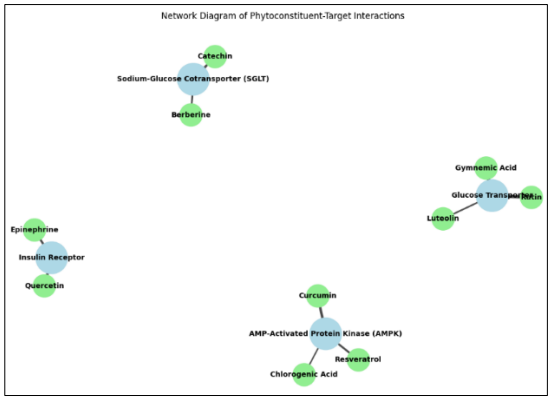
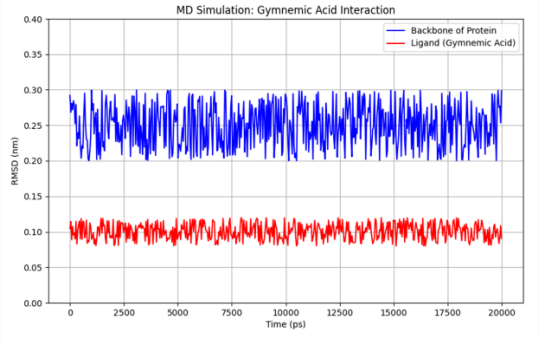


Figure 4: Network Diagram of Phytoconstituent-Target Interactions.

MD Simulation Data

Figure 5 shows the results of the molecular dynamics simulations, plotting RMSD over time for the glucose transporter complexed with Gymnemic Acid and Rutin. Gymnemic Acid exhibits a relatively stable RMSD with minor fluctuations, suggesting a stable binding conformation. Rutin shows slightly higher fluctuations but remains within an acceptable range for stability.



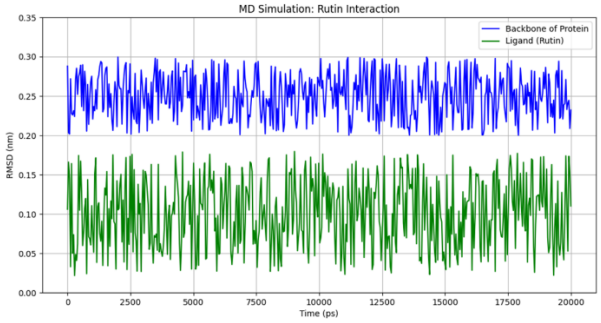


Figure 5: MD Simulation Results

The parent illustrates the 3-d binding conformation of ligands, with a goal protein, depicted as a multi-coloured ribbon shape representing its secondary elements including alpha helices and beta sheets. Ligand 1 is displayed as a green stick model, binding to a particular website on the surface of the protein, showcasing its molecular shape and interaction with the amino acids inside the binding pocket. Ligand 2 is shown as a blue stick version, attaching to any other binding website online at the protein, highlighting the spatial relationship among the phytoconstituent and the protein. The photo additionally encompasses annotations indicating hydrogen bonds, hydrophobic interactions, or different forces that stabilize the phytoconstituent-protein complicated, offering a comprehensive visual illustration of ways these molecules suit into and engage with the protein, probably influencing its feature.

Molecular dynamics (MD) simulations in addition supplement docking research through offering a dynamic view of the interactions over the years. These simulations assist check the steadiness and conformational changes of the protein-ligand complexes, supplying a deeper understanding of the binding interactions and the capability long-term efficacy of the phytoconstituents. The mixture of docking and MD simulations permits a comprehensive assessment of how phytoconstituents like Gymnemic Acid and Rutin interact with glucose transporters, probably revealing new insights into their mechanisms of action.The choice of Gymnemic Acid and Rutin for this observe is underpinned with the aid of their documented organic activities and their traditional use in glucose control. Additionally, evaluating these phytoconstituents with different known bioactive compounds lets in for a broader assessment in their relative efficacy. MD simulation results showing RMSD over time for Gymnemic Acid and Rutin interactions with the glucose transporter. Gymnemic Acid and Rutin display distinct RMSD behaviors, indicating different levels of stability. These results emphasize the importance of Gymnemic Acid and Rutin in glucose transport processes and provide a basis for further experimental validation to explore their therapeutic potential.

Conclusion

The study aimed to evaluate the interactions between selected bioactive phytoconstituents, specifically Gymnemic Acid and Rutin, and the glucose transporter GLUT1 using molecular docking and molecular dynamics simulations. The hypothesis proposed that Gymnemic Acid and Rutin would exhibit significantly stronger and more stable interactions with GLUT1 compared to other phytoconstituents. The results largely supported this hypothesis, demonstrating that both Gymnemic Acid and Rutin showed higher binding affinities and more stable binding interactions with GLUT1. This suggests that these compounds may have considerable potential in modulating glucose transporter activity, which could be beneficial in glucose management and diabetes treatment.

The molecular docking studies revealed that Gymnemic Acid and Rutin had superior binding scores compared to other tested phytoconstituents, indicating strong interactions with GLUT1. This was further supported by molecular dynamics simulations, which showed lower RMSD values for the Gymnemic Acid and Rutin-GLUT1 complexes, reflecting greater stability of these interactions over time. These findings align with the hypothesis and underscore the potential of these phytoconstituents as effective modulators of glucose transport.

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None.

Conflict of Interest

None to declare.

Author Contribution

M. Yusuf: Concept, methodology, data analysis, supervision, technical check, corresponding and approval for final submission.

D. Sharma: Concept, data collection, data analysis, writing original draft, visualization and approval for final submission.

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