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In Silico Evaluation of Antidiabetic Phytocompounds from Acacia albida and Vitex negundo Using Molecular Docking

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Abstract: *Diabetes Mellitus (DM) is one of the most prevalent chronic metabolic disorders worldwide and represents a major global health challenge due to its increasing incidence, associated complications, and economic burden. Type 2 Diabetes Mellitus (T2DM) is characterized by persistent hyperglycemia resulting from insulin resistance, impaired insulin secretion, or both. According to the International Diabetes Federation, the number of diabetic patients has increased dramatically over the years and is expected to continue rising in the future. Factors such as obesity, sedentary lifestyle, unhealthy dietary habits, stress, and genetic predisposition significantly contribute to the development of diabetes. Common symptoms include polyuria, polydipsia, and polyphagia, while long-term complications may involve cardiovascular diseases, nephropathy, neuropathy, and retinopathy.*
Current antidiabetic therapies are effective in controlling blood glucose levels but are often associated with adverse effects, high costs, and limitations in long-term management. Consequently, there is growing interest in medicinal plants and natural products as alternative therapeutic agents because of their comparatively lower toxicity and better safety profile. Numerous plant-derived bioactive compounds have demonstrated promising hypoglycemic activity and potential benefits in diabetes management.

Keywords: *Diabetes Mellitus*

I. INTRODUCTION

Background

The global burden of Diabetes Mellitus (DM) has been rising steadily across all populations. According to the International Diabetes Federation (2011), around 366 million individuals were living with diabetes at that time, with projections suggesting this number could increase to 552 million by 2030. Earlier estimates indicated that approximately 171 million adults worldwide had Type 2 Diabetes Mellitus in 2000. This figure grew significantly over time, reaching about 415 million cases by 2015.(1)

Managing diabetes without causing adverse effects remains a significant challenge in modern healthcare. As a result, there is growing interest in natural products that may help control blood glucose levels while producing fewer side effects.(2)

Diabetes Mellitus is a group of metabolic disorders characterized by persistent high blood glucose levels. It occurs when the pancreas does not produce sufficient insulin or when body cells do not respond effectively to insulin, a condition known as insulin resistance. In earlier terminology, this condition was referred to as non-insulin dependent diabetes mellitus (NIDDM).The main symptoms of Diabetes Mellitus include frequent urination (polyuria), excessive thirst (polydipsia), and increased appetite (polyphagia). Type 2 diabetes is commonly associated with factors such as unhealthy lifestyle habits, obesity (typically defined as a body mass index above 30), lack of regular physical activity, excess body weight, poor dietary patterns, and stress.(3)

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molecular docking has emerged as an important computational approach in diabetes research for drug discovery and development. It enables scientists to understand how small molecules, including natural compounds and synthetic drugs, interact with specific protein targets involved in glucose metabolism. Key targets often studied include enzymes like α-amylase and α-glucosidase, which regulate carbohydrate digestion, as well as proteins such as dipeptidyl peptidase-4 (DPP-4) that influence insulin activity. By simulating the binding of ligands to these targets, docking studies help predict the strength and nature of molecular interactions, providing insights into their potential inhibitory or activating effects. Tools such as AutoDock and Discovery Studio are commonly used to perform these analyses.[4]

Introduction

Diabetes Mellitus (DM) is one of the earliest documented diseases and remains among the most common chronic endocrine disorders worldwide Estimates from 2014 suggested that about 387 million people were living with diabetes, with nearly 90% of these cases being Type 2 Diabetes Mellitus (T2DM). During the period from 2012 to 2014, diabetes was responsible for approximately 1.5 to 4.9 million deaths annually. Projections indicate that the global number of diabetes cases may reach 439 million by 2030, including around 87 million individuals in India (Bachchawat et al., 2011). Additionally, the worldwide economic burden of diabetes was estimated at about 610 billion USD in 2014, and the condition has been officially recognized as a global epidemic by the World Health Organization.[5]

These challenges highlight the need for therapies that are safer, more effective, easy to administer, and affordable As a result, increasing attention is being given to traditional treatment approaches that utilize plant-derived antidiabetic compounds. Natural products are generally considered to have fewer adverse effects compared to synthetic drugs .[6]

Molecular docking is a computational technique widely used to investigate potential drug candidates for the treatment of diabetes mellitus, particularly in targeting proteins involved in glucose metabolism and insulin regulation. In diabetes research, docking studies focus on key enzymes such as α-amylase, α-glucosidase, dipeptidyl peptidase-4 (DPP-4), and insulin receptors, which play critical roles in controlling blood sugar levels.[7]

During docking, specialized software such as AutoDock or Schrödinger predicts the binding orientation and interaction of ligands within the active site of the target protein. The software calculates binding affinity, expressed as docking scores or binding energy values, which indicate how strongly a compound can interact with the protein. Lower binding energy suggests a more stable and potentially effective inhibitor.[8]

In diabetes-related studies, molecular docking helps identify compounds that may inhibit carbohydrate-digesting enzymes or enhance insulin sensitivity, thereby reducing blood glucose levels. Additionally, docking is often combined with ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis to evaluate the pharmacokinetic and safety profiles of promising molecules. Overall, molecular docking provides a cost-effective and time-saving strategy to discover and optimize novel antidiabetic agents before proceeding to laboratory and clinical studies.[9]

Literature Survey

Diabetes Mellitus is one of the most common chronic metabolic disorders worldwide and represents a major public health concern. According to reports from the International Diabetes Federation, approximately 366 million individuals were living with diabetes in 2011, and the number is projected to rise to 552 million by 2030. Earlier epidemiological studies estimated that nearly 171 million adults were affected by type 2 diabetes mellitus (T2DM) in 2000, which increased significantly to around 415 million cases by 2015. India is considered one of the countries most severely affected by diabetes, with projections suggesting that the number of diabetic patients may continue to rise substantially in the coming decades.

Traditional herbal formulations have also attracted considerable scientific interest in diabetes research. Donguibogam describes a traditional Korean herbal formulation known as Saeng-Ji-Hwang-Ko (SJHK), which has historically been used for the treatment of So-gal, a condition corresponding to modern type 2 diabetes mellitus. Bioactive compounds including agnuside, betulinic acid, caffeic acid, casticin, ellagic acid, gallic acid, kaempferol, luteolin, quercetin, rutin,

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ursolic acid, and vitexin have shown promising pharmacological activities related to glucose metabolism and antioxidant defense.

In recent years, molecular docking has emerged as an important computational tool in antidiabetic drug discovery. Molecular docking is a technique used to predict the interaction between small molecules and target proteins at the molecular level. It helps identify the binding orientation, affinity, and stability of ligands within the active site of proteins associated with diabetes. Important protein targets commonly investigated in diabetes research include α-amylase, α-glucosidase, dipeptidyl peptidase-4 (DPP-4), and insulin receptors, all of which play essential roles in glucose regulation and carbohydrate metabolism.

The molecular docking process generally begins with protein preparation. Protein structures are retrieved from the Protein Data Bank (PDB) based on specific selection criteria such as X-ray crystallography resolution and biological relevance. After downloading the protein structure, unnecessary molecules such as water are removed, hydrogen atoms are added, and the active binding site is identified. Ligands are then prepared by downloading their structures from databases such as PubChem or DrugBank and converting them into suitable formats for docking analysis. Software tools including AutoDock Vina and BIOVIA Discovery Studio are commonly used for protein–ligand interaction studies and visualization.

Objectives

1. Epidemiological Objective

To assess the prevalence, incidence, and demographic distribution of diabetes in a defined population, and to identify associated risk factors such as age, obesity, sedentary lifestyle, and genetic predisposition.

2. Pathophysiological Objective

To study the molecular and physiological mechanisms involved in diabetes, including insulin resistance, pancreatic β-cell dysfunction, and impaired glucose metabolism.

3. Pharmacological Objective

To evaluate the efficacy and safety of antidiabetic drugs such as Insulin, and other oral hypoglycemic agents in controlling blood glucose levels and preventing complications.

4. Clinical Objective

To analyze diagnostic methods (fasting blood glucose, HbA1c levels) and treatment outcomes in diabetic patients, and to determine the effectiveness of lifestyle modifications such as diet, physical activity, and weight management.

5. Computational / Docking Objective To perform molecular docking studies of selected bioactive compounds against target proteins involved in diabetes, such as:

Alpha-glucosidase

DPP-4

in order to identify potential inhibitors with high binding affinity and therapeutic potential.

6. Preventive Objective

To explore preventive strategies and public health interventions that can reduce the burden of diabetes and associated complications such as cardiovascular diseases, neuropathy, and nephropathy.[10]

Disease Importance

Diabetes mellitus is one of the most significant chronic metabolic disorders affecting global public health. It is characterized by persistent hyperglycemia resulting from impaired insulin secretion, insulin resistance, or both. The disease has become a major medical and socioeconomic burden due to its rapidly increasing prevalence, long-term complications, and impact on quality of life. According to the World Health Organization and the International Diabetes Federation, the number of diabetic patients is continuously rising worldwide because of urbanization, sedentary lifestyles, obesity, unhealthy dietary habits, and genetic predisposition. Diabetes is now considered one of the leading causes of morbidity and mortality across both developed and developing countries.

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The importance of diabetes in research is primarily associated with its severe complications and complex pathophysiology. Chronic uncontrolled diabetes can lead to cardiovascular diseases, nephropathy, neuropathy, retinopathy, stroke, peripheral vascular disease, and impaired wound healing. These complications significantly reduce life expectancy and increase healthcare expenditures. In addition, diabetes is strongly associated with oxidative stress, chronic inflammation, endothelial dysfunction, and metabolic imbalance, making it a multifactorial disease that requires continuous scientific investigation.

Research on diabetes is essential for the discovery of safer and more effective therapeutic agents. Although several antidiabetic drugs such as are available, many of these medications are associated with limitations including gastrointestinal disturbances, hypoglycemia, weight gain, reduced efficacy over long-term use, and adverse effects on organs.

Molecular docking and computational drug discovery approaches have gained considerable importance in diabetes research because they help predict ligand–protein interactions, binding affinity, and inhibitory mechanisms before experimental testing. These methods reduce research cost, save time, and assist in the rapid screening of phytochemicals against important diabetic targets such as α-glucosidase, α-amylase, DPP-4, PPAR-γ, and SGLT2.

Diabetes research is also important for understanding disease mechanisms at the molecular level. Advances in genomics, proteomics, metabolomics, and bioinformatics have improved knowledge regarding insulin resistance, pancreatic β-cell dysfunction, inflammatory pathways, and genetic susceptibility. Such studies contribute to the development of personalized medicine and targeted therapy for diabetic patients.[11]

Known Plant Activity

The flowers of Acacia albida and Vitex negundo have attracted scientific interest because of their potential antidiabetic properties and rich phytochemical composition. Both plants contain important bioactive constituents such as flavonoids, phenolic compounds, tannins, saponins, iridoid glycosides, and essential oils, which are known to play significant roles in glucose regulation and metabolic balance. These compounds may help lower blood glucose levels by improving glucose metabolism, enhancing insulin sensitivity, and promoting glucose uptake in body tissues. The antioxidant properties of the flower extracts are especially important in diabetes management, as they help reduce oxidative stress and protect pancreatic β-cells from free radical damage, thereby supporting normal insulin secretion and glucose homeostasis. In addition, the flowers may inhibit carbohydrate-digesting enzymes, which can help control postprandial hyperglycemia. Traditional medicinal systems have also utilized these flowers for managing diabetes and associated metabolic disorders. Furthermore, their anti-inflammatory and lipid-regulating activities may help reduce diabetic complications such as tissue damage, neuropathy, and inflammation, indicating their potential value in the development of natural antidiabetic therapies.[12]

Gap : Combination not studied

The gap combination study of Acacia albida and Vitex negundo in diabetes research highlights an important unexplored area in herbal medicine. Individually, both plants have demonstrated promising antidiabetic activities due to the presence of flavonoids, phenolic compounds, tannins, alkaloids, terpenoids, and antioxidants. Studies on Acacia albida reported significant antihyperglycemic, antihyperlipidemic, and antioxidant effects in streptozotocin-induced diabetic models. The plant extract was found to reduce blood glucose levels, improve lipid profile, and protect pancreatic tissues from oxidative damage.

Similarly, Vitex negundo has shown strong α-glucosidase inhibitory activity, antioxidant potential, and molecular docking affinity toward diabetic target enzymes. The plant contains bioactive compounds such as vitexin, casticin, luteolin derivatives, and agnuside, which may contribute to glucose regulation and improved insulin sensitivity. Several studies also suggest that Vitex negundo can reduce oxidative stress and inflammatory responses associated with diabetes mellitus.

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However, despite the individual pharmacological importance of these plants, there is very limited scientific evidence regarding their combined or synergistic antidiabetic activity. No detailed experimental research has comprehensively evaluated the combined extract of Acacia albida and Vitex negundo for diabetes management, especially concerning molecular mechanisms, enzyme inhibition, pancreatic β-cell protection, or long-term metabolic regulation. This creates a significant research gap in phytopharmacology and herbal drug development.[13]

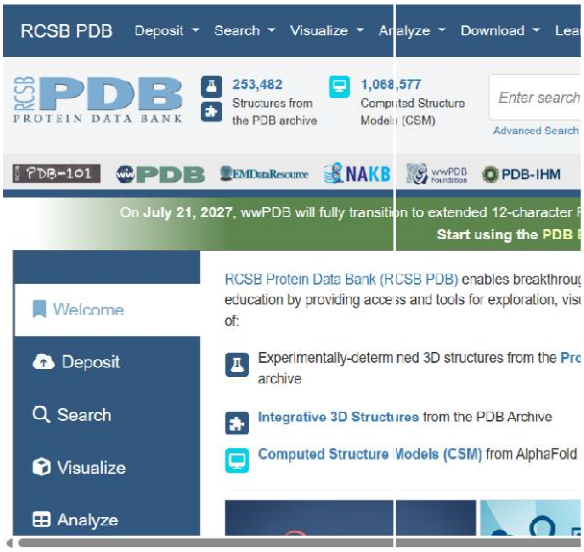
A combination study of these two medicinal plants may provide enhanced therapeutic benefits because both plants possess complementary phytochemicals with antioxidant and antihyperglycemic properties. Their combined formulation could potentially produce synergistic effects by improving glucose uptake, inhibiting carbohydrate-digesting enzymes, reducing oxidative stress, and protecting pancreatic cells more effectively than single-plant therapy. Such studies may also help in developing safer polyherbal formulations with fewer side effects compared to synthetic antidiabetic drugs.

Future research should focus on phytochemical standardization, in vitro enzyme inhibition assays, in vivo diabetic animal models, molecular docking analysis, toxicity studies, and clinical evaluation of the combined extracts.[14]

Molecular Docking Procedure

1.Protein Preparation

The initial stage of site-specific molecular docking involves preparing the protein structure for analysis. This begins by accessing the Protein Data Bank (PDB) to retrieve the required protein. A protein is then carefully selected according to the study's target, ensuring it meets quality standards, such as being resolved through X-ray diffraction with a resolution better than 2 Å. The source of the protein is also considered, with Homo sapiens commonly chosen for studies related to human biology. Once an appropriate structure is identified, it is downloaded from the protein data bank and saved in PDB file format using the available options. This prepared file can then be used for subsequent docking studies.[15]



Access Protein Data Bank (PDB)

↓

Select target protein based on research objective

↓

Apply selection criteria:

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↓

Download selected protein structure

↓

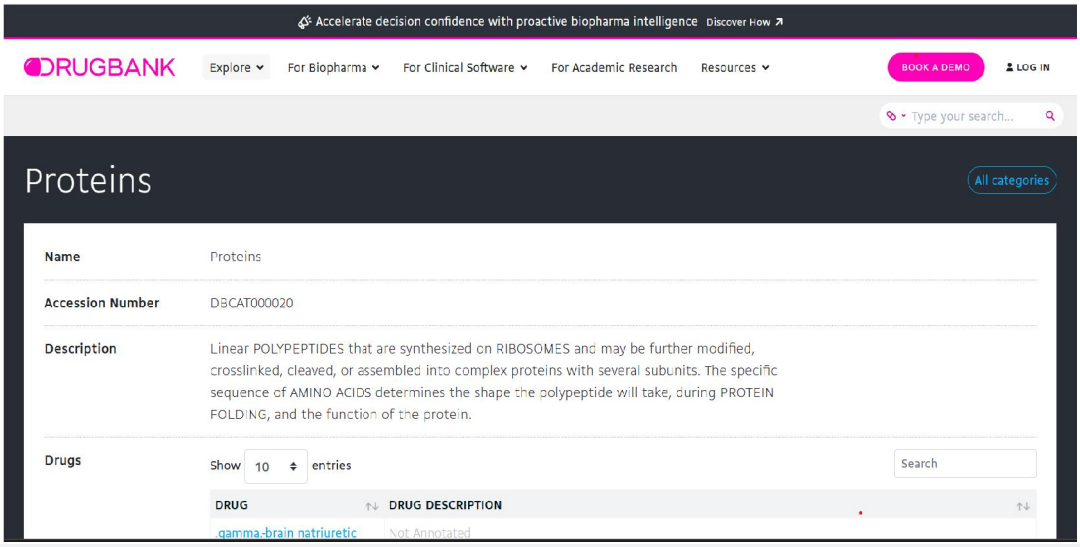
Right-click and choose PDB file format

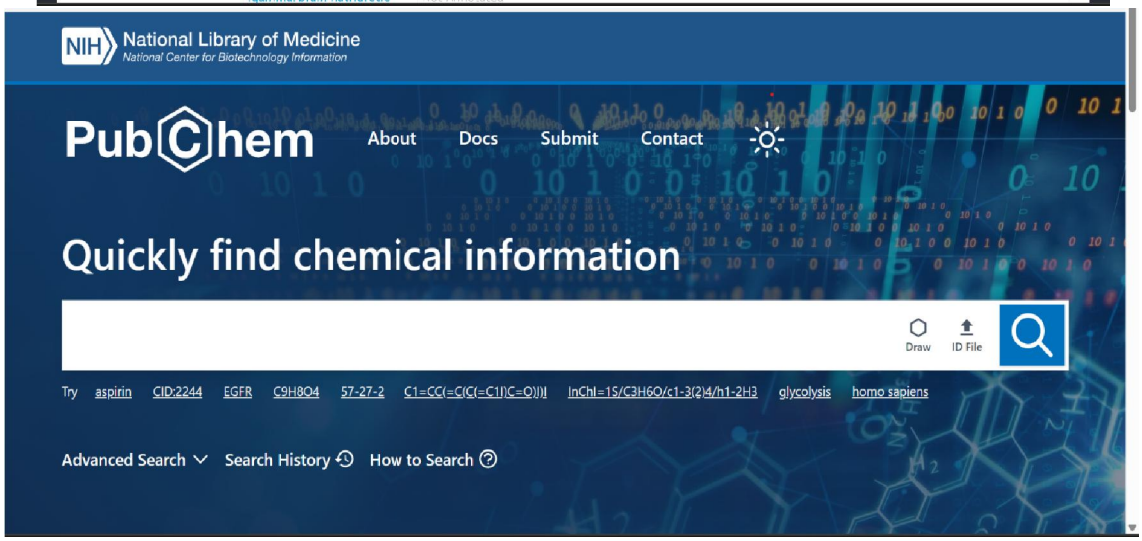
↓

Save the file to local system

2. Ligand Preparation

The second step in molecular docking involves ligand preparation, where the compound of interest (drug) is selected and its structural data is obtained. Initially, the name of the drug is identified, and relevant information is searched in chemical databases such as DrugBank or PubChem. From DrugBank, the ligand structure can be downloaded and typically saved in PDB format. Alternatively, PubChem provides the option to download the compound in 3D SDF format, which contains detailed three-dimensional structural information. These downloaded ligand files are then used for further processing and analysis in the docking study.[16]





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3. Drug Discovery Studio

The third step in the molecular docking workflow involves using Drug Discovery Studio for visualization and further processing of the protein structure. In this step, the software is opened and the required file is selected through the "File" option. The protein structure is then loaded into the workspace for analysis. Once the protein is displayed, the view can be adjusted by expanding the screen to obtain a clearer and more detailed visualization. This step helps in properly examining the protein structure before proceeding with docking and interaction studies.

In the subsequent step of molecular docking, the protein structure is refined and the binding site is defined using appropriate tools. Initially, all water molecules present in the structure are removed to avoid interference during docking. The ligand group within the protein is then expanded and selected for further analysis. Using the tools menu, receptor–ligand interactions are examined, and the binding site is defined and modified based on the selected region. A binding sphere is created from the current selection to represent the active site, and its size is adjusted by expanding or compressing it as required. After finalizing the sphere, its properties are accessed by right-clicking, allowing the user to note important parameters such as the radius and the X, Y, and Z coordinates. These details are essential for accurately setting up the docking process.

In this stage of molecular docking, the protein structure is further refined to prepare it for accurate analysis. Initially, any bound ligand present in the protein is removed to avoid interference with the docking process. The cleaned protein structure is then selected, and under the chemistry options, hydrogen atoms are added—particularly polar hydrogens—to improve the accuracy of interaction studies. After completing these modifications, the prepared protein is saved in Protein Data Bank (PDB) format for further use.

For ligand preparation, if the drug file is available in SDF format, it is opened using Drug Discovery Studio and then converted by saving it in PDB format. This ensures compatibility of both protein and ligand files for subsequent docking procedures.[17]

4. Docking Folder

In this step of the molecular docking procedure, a dedicated working directory is created to organize all necessary files. A new folder is made, typically in the Windows "C" drive, where all AutoDock Vina-related files and the configuration file are stored together for easy access. The configuration file is then prepared by specifying key parameters, including the receptor and ligand file names in PDBQT format, as well as the desired output file name. Additionally, the coordinates for the docking search space—center X, center Y, and center Z—are entered based on the previously determined binding site values. These parameters define the region where docking will occur. Finally, the output file is assigned an appropriate name, ensuring that all inputs are properly organized for running the docking simulation.[18]

5. Autodock Folder

In this step, the prepared protein is processed using the AutoDock tool to make it suitable for docking. The procedure begins by opening the file and loading the molecule into the software using the "read molecule" option. Once loaded, the protein structure is displayed on the screen, allowing for visualization and selection. The macromolecule option is then chosen to define the protein for docking purposes, and grid settings are applied to specify the region of interest. The desired protein is selected by clicking on its name, and the molecule is confirmed for further processing. Finally, the prepared protein is saved in PDBQT format, which is required for compatibility with AutoDock-based docking simulations.[19]

6. For Ligand Preparation

in this stage, the ligand is prepared for docking using the appropriate software tools. The process begins by selecting the ligand input file and opening it within the program. Once opened, the desired drug molecule is chosen, and its structure is displayed on the screen for visualization. After confirming the correct ligand, it is processed and directed to the output option, where it is saved in PDBQT format, which is required for docking studies. It is important to note that

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both the prepared protein and ligand files, now in PDBQT format, should be stored together in the designated docking folder, ensuring proper organization and readiness for the docking simulation.[20]

7. Command Prompt

In this step, the molecular docking process is executed using the command prompt. First, the command prompt is opened, and the path of the docking folder is copied and navigated to by typing the "cd" command followed by the folder address. Once inside the correct directory, the functionality of AutoDock Vina can be checked by running the command "vina.exe --help," where the double hyphen indicates command options. After confirming proper setup, the docking process is initiated by executing the command "vina.exe --config conf.txt --log log.txt," which uses the configuration file and generates a log file of the docking results. This completes the docking execution and prepares the results for further analysis.

8. 2D, 3D Structure of Protein

In this final step, Drug Discovery Studio is used to analyze the docking results and visualize molecular interactions. The prepared protein structure in PDBQT format, along with all the split ligand poses generated after docking, is loaded into the software. The interaction analysis option is then selected to study how the ligand binds with the protein. A specific ligand pose is chosen, defined, and examined for its interactions within the active site. The interaction details, particularly non-bonded interactions, are visualized by selecting the appropriate display options. To explore different docking poses, the user can navigate through them using the up and down arrows. Additionally, a two-dimensional (2D) interaction diagram can be generated for clearer representation, which can then be saved as an image file for documentation and further analysis. In this step, a high-quality three-dimensional (3D) visualization of the protein–ligand complex is generated for presentation or publication purposes. The process begins by accessing the visualization or script options within the software and selecting settings that enhance the image to publication-quality standards. To clearly identify important residues, labels are added by right-clicking on the structure and choosing the labeling option. The object type is set to amino acids, and attributes such as the three-letter residue code along with the corresponding ID number are selected for display. The appearance of the labels is then customized by choosing a suitable font, such as Arial, and adjusting the font size (e.g., size 18) for better clarity. After applying these settings and confirming the changes, the final image is saved as an image file, making it suitable for reports or research publications.[21]

PHYTOCONSTITUENT	LIPINSKI	BIOAVAILABILITY	TOXICITY PREDICTIONS	GEL ABSORPTION	BBB PERMANT
AGNUSIDE	NO	O.17	NO	LOW	NO
BETEULINIC ACID	YES	O.85	NO	HIGH	NO
CAFFIC ACID	YES	0.56	NO	HIGH	NO
CASTICIN	YES	O.55	NO	HIGH	NO
DIMETHYL TRIPTAMINE	YES	O.55	NO	HIGH	YES
ELLAGIC ACID	YES	0.55	NO	HIGH	NO
GALLIC ACID	YES	0.56	NO	HIGH	NO
KAEMPFEROL	YES	0.55	NO	HIGH	NO
LUPEOL	YES	0.55	NO	LOW	NO
LUTEOLIN	YES	0.55	NO	HIGH	NO
LUTEOLIN 7-O GLYCOSIDES	NO	0.17	NO	LOW	NO
N-METHYL TRYPTAMINE	YES	0.56	NO	HIGH	NO

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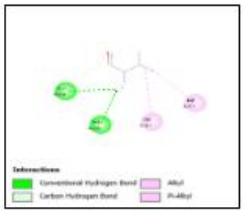
QUERCETIN	YES	0.55	NO	HIGH	NO
RUTIN	NO	0.17	NO	LOW	NO
SAPONINS	YES	0.56	NO	HIGH	YES
URSOLIC ACID	YES	0.85	NO	LOW	YES
VITEXIN	YES	0.55	NO	LOW	NO

ADMET Properties Of Phytoconstituent

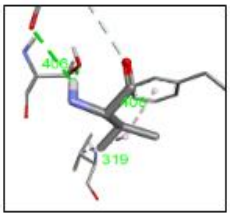
Interaction Diagram

1HOO

2D

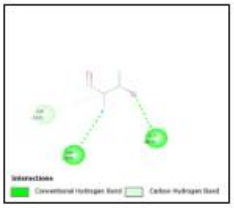


3D

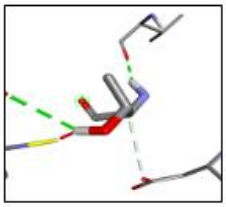


2CBZ

2D

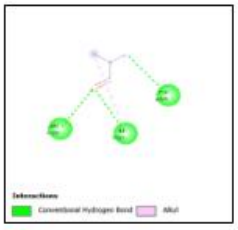


3D



3DHP

2D



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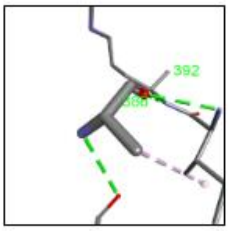
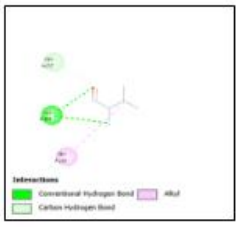


3FEE

2D



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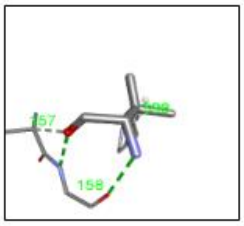
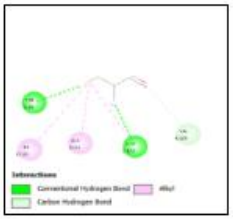


5CIQ

2D



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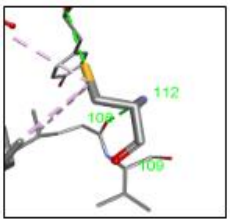
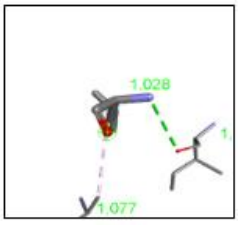


6MBO

2D

3D



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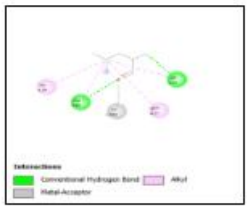
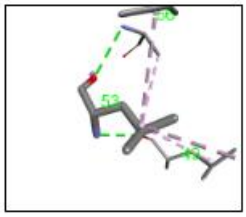
6ZRC

2D

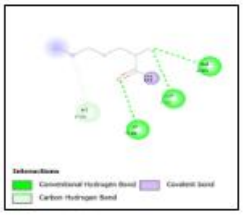


3D



7NH5

2D



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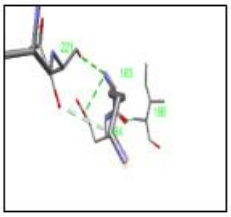
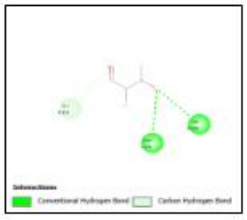


8AK8

2D



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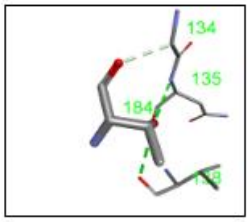
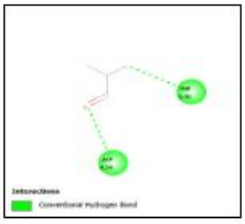


8WGT

2D



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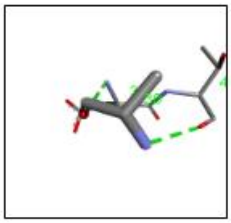

Results

Binding Energy Table

PHYTOCONSTITUENT	1HOO	2CBZ	3DHP	3FEE	5CIQ	6MBO	6ZR6	7NH5	8AK8	8WGT
AGUNISIDE	-10.9	-6.2	-6.3	-6.5	-6.1	-4.5	-5.6	-5.5	-5.7	-4.7
BETULINIC ACID	-10.0	-6.4	-6.3	-5.7	-6.2	-4.6	-6.3	-5.7	-6.2	-4.5
CAFFEIC ACID	-5.0	-5.0	-5.3	-5.4	-4.8	-4.2	-4.7	-4.2	-5.1	-4.2
CASTICIN	-5.6	-6.0	-6.1	-5.9	-4.8	-4.0	-5.2	-5.0	-5.7	-4.3
DIMETHYLTRIPTAMINE	-0.9	-3.9	-4.1	-4.9	-4.1	-3.4	-4.1	-3.9	-4.2	-3.2
ELLAGIC ACID	-6.7	-6.8	-5.8	-5.7	-5.0	-4.1	-5.6	-5.3	-5.7	-4.3
GALLIC ACID	-5.8	-6.3	-6.2	-5.9	-5.9	-5.0	-5.7	-5.3	-6.3	-4.9
KAEMPFEROL	-5.6	-6.2	-5.8	-5.7	-5.5	-4.6	-5.6	-5.0	-6.2	-5.0
LUPEOL	-6.1	-8.4	-7.8	-8.4	-7.3	-5.6	-7.5	-7.1	-7.5	-5.6
LUTEOLIN	-5.5	-6.1	-5.6	-6.1	-5.4	-4.2	-5.7	-5.2	-5.5	-4.5
LOTEOLIN 7 O GLUCOSIDES	-6.6	-7.3	-6.5	-6.9	-6.5	-5.0	-6.0	-6.2	-7.0	-5.3
N-METHYLTRYPTAMINE	-1.1	-1.2	-1.5	-1.2	-1.2	-1.5	-1.7	-1.3	-1.2	-1.4
QUERCETIN	-6.0	-6.6	-6.0	-5.9	-5.2	-4.1	-5.4	-4.9	-5.3	-4.3
RUTIN	-7.6	-8.7	-6.8	-6.8	-6.6	-5.7	-6.5	-6.7	-7.6	-4.8

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SAPONINS	-2.7	-3.8	-2.7	-2.9	-2.7	-2.7	-2.7	-2.4	-2.7	-2.4
URSOLIC ACID	-7.1	-8.9	-8.7	-9.1	-7.5	-6.1	-7.9	-8.0	-8.1	-5.7
VITEXIN	-6.2	-7.6	-6.1	-5.9	-5.3	-4.7	-6.1	-5.7	-6.0	-4.8
SITAGLIPTIN (S.D)	-6.8	-4.7	-4.9	-5.3	-4.7	-3.4	-4.3	-3.8	-4.4	-3.8

The molecular docking study revealed significant variations in the binding affinities of the selected phytoconstituents against the target proteins (1HOO, 2CBZ, 3DHP, 3FEE, 5CIQ, 6MBO, 6ZR6, 7NH5, 8AK8, and 8WGT). Binding energy values ranged from weak interactions in compounds such as N-methyltryptamine and dimethyltryptamine to very strong interactions in compounds like Aguniside, Ursolic acid, Lupeol, and Rutin. In molecular docking studies, more negative binding energy values indicate stronger ligand–protein interactions and better binding stability.

Among all the phytoconstituents, Aguniside exhibited the strongest binding affinity, particularly against protein 1HOO with a docking score of −10.9 which was significantly better than the standard drug Sitagliptin (−6.8). Aguniside also demonstrated favorable interactions with several other target proteins, indicating its broad-spectrum binding potential and possible antidiabetic activity. Similarly, Ursolic acid showed consistently high binding affinities across multiple proteins, including −9.1 against 3FEE, −8.9 against 2CBZ, and −8.7 against 3DHP, all of which were markedly superior to Sitagliptin. These findings suggest that Ursolic acid possesses strong inhibitory potential and stable interaction with diabetic target proteins.

Discussion

Diabetes Mellitus (DM) is a rapidly growing metabolic disorder that has become a major global health concern because of its increasing prevalence, chronic complications, and socioeconomic impact. The rising number of diabetes cases reported worldwide highlights the urgent need for effective prevention and treatment strategies. According to global estimates, the burden of Type 2 Diabetes Mellitus (T2DM) has increased dramatically over the past few decades due to urbanization, sedentary lifestyles, obesity, unhealthy dietary habits, and genetic susceptibility. The condition is characterized by persistent hyperglycemia caused by impaired insulin secretion, insulin resistance, or both, leading to serious complications such as cardiovascular diseases, nephropathy, neuropathy, and retinopathy. These complications significantly reduce the quality of life and increase healthcare expenditures worldwide.

Conventional antidiabetic therapies, including insulin and oral hypoglycemic agents such as metformin, are widely used for glycemic control. Although these treatments are effective, they are often associated with adverse effects, long-term dependency, and financial burden. Therefore, there is increasing scientific interest in identifying safer and more affordable alternatives from natural sources. Traditional medicinal systems have long utilized herbal formulations for the management of diabetes, and many medicinal plants have demonstrated significant hypoglycemic potential because of their rich phytochemical composition.

Saeng-Ji-Hwang-Ko (SJHK), a traditional Korean herbal formulation described in the historic medical text Donguibogam, has attracted attention for its possible therapeutic role in Type 2 Diabetes Mellitus. The formulation has historically been used to treat So-gal syndrome, which resembles modern diabetic conditions. The present study emphasizes the importance of exploring the active phytoconstituents of SJHK and understanding their interactions with molecular targets associated with diabetes through computational approaches such as molecular docking and network pharmacology.

Molecular docking has become an essential tool in modern drug discovery and diabetes research because it provides detailed insight into ligand–protein interactions at the molecular level. In this study, docking analysis was carried out against important diabetic target proteins such as α-glucosidase and DPP-4, which are directly involved in glucose metabolism and insulin regulation. The docking approach helps predict the binding affinity and stability of phytochemicals within the active site of target proteins. Lower binding energy values indicate stronger and more stable interactions, suggesting better inhibitory potential against diabetic targets.

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The docking workflow included systematic protein and ligand preparation using databases such as the Protein Data Bank (PDB), PubChem, and DrugBank. The use of software tools including Discovery Studio and AutoDock Vina enabled proper protein refinement, ligand optimization, binding site identification, docking simulation, and visualization of protein–ligand interactions in both two-dimensional and three-dimensional forms. These computational methods provide a reliable and cost-effective strategy for the early screening of potential antidiabetic compounds before experimental validation.

ADMET analysis further supported the evaluation of phytoconstituents by predicting their pharmacokinetic and toxicity profiles. Most compounds demonstrated favorable bioavailability and low toxicity, indicating their suitability for drug development. Compounds such as betulinic acid, ursolic acid, quercetin, kaempferol, luteolin, vitexin, and caffeic acid exhibited acceptable drug-likeness properties according to Lipinski's rule and showed good gastrointestinal absorption. On the other hand, certain compounds such as agnuside, rutin, and luteolin-7-O-glycosides displayed lower bioavailability, suggesting possible limitations in absorption and oral effectiveness. The absence of predicted toxicity for most compounds further supports their therapeutic potential as safer alternatives to synthetic drugs.

The findings of this study suggest that plant-derived bioactive compounds may serve as promising inhibitors of diabetic target proteins and could contribute to the development of novel antidiabetic therapies. Molecular docking combined with ADMET analysis offers an efficient platform for identifying bioactive molecules with favorable pharmacological profiles. However, computational results alone are not sufficient to confirm therapeutic efficacy. Therefore, further in vitro, in vivo, and clinical studies are required to validate the antidiabetic activity, mechanism of action, safety, and efficacy of these phytoconstituents.

Overall, the present study highlights the significance of integrating traditional medicinal knowledge with modern computational techniques in the search for effective antidiabetic agents. The use of natural compounds with favorable docking interactions and pharmacokinetic properties may provide safer, cost-effective, and more accessible therapeutic options for the management of Diabetes Mellitus in the future.

II. CONCLUSION

Diabetes Mellitus is a major chronic metabolic disorder that continues to pose a serious global health challenge because of its rapidly increasing prevalence, associated complications, and economic burden. The growing incidence of Type 2 Diabetes Mellitus is strongly linked with unhealthy lifestyles, obesity, physical inactivity, stress, and genetic predisposition. Despite the availability of conventional antidiabetic therapies such as insulin and oral hypoglycemic agents, long-term treatment is often associated with adverse effects, high costs, and limited effectiveness in preventing complications. Therefore, the search for safer, more effective, and affordable therapeutic alternatives remains an important area of research.

Traditional medicinal plants and herbal formulations have gained significant attention as potential sources of antidiabetic agents due to their rich phytochemical composition and comparatively lower toxicity. Saeng-Ji-Hwang-Ko (SJHK), a traditional Korean herbal formulation, represents a promising natural therapeutic candidate for the management of diabetes. The present study highlights the importance of investigating plant-derived bioactive compounds and their mechanisms of action through modern computational techniques such as molecular docking and ADMET analysis.

Molecular docking proved to be an effective and reliable approach for predicting the interaction between phytoconstituents and important diabetic target proteins such as α-glucosidase and DPP-4. The docking procedure enabled the identification of compounds with favorable binding affinity and stable protein–ligand interactions, suggesting their possible role as inhibitors involved in glucose metabolism regulation. The use of software tools such as AutoDock Vina and Discovery Studio facilitated protein preparation, ligand optimization, docking execution, and visualization of molecular interactions in both 2D and 3D forms.

ADMET evaluation further supported the therapeutic potential of several phytoconstituents by demonstrating acceptable pharmacokinetic properties, good gastrointestinal absorption, and low predicted toxicity. Compounds such

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as betulinic acid, ursolic acid, quercetin, kaempferol, luteolin, and vitexin showed promising drug-likeness characteristics and may serve as potential lead molecules for future antidiabetic drug development.

Overall, the integration of traditional medicinal knowledge with molecular docking and ADMET studies provides a cost-effective and time-saving strategy for the discovery of novel antidiabetic agents.

REFERENCES

1.Singh P, Singh VK, Singh AK. Molecular docking analysis of candidate compounds derived from medicinal plants with type 2 diabetes mellitus targets. Bioinformation. 2019 Mar 15;15(3):179–188. doi:10.6026/97320630015179. PMID: 31354193; PMCID: PMC6637395.

2.Natarajan A, Sugumar S, Bitragunta S, Balasubramanyan N. Molecular docking studies of (4Z, 12Z)-cyclopentadeca-4, 12-dienone from Grewia hirsuta with some targets related to type 2 diabetes. BMC Complement Altern Med. 2015;15:73. doi:10.1186/s12906-015-0588-5.

3.Zheng Y, Ley SH, Hu FB. Global aetiology and epidemiology of type 2 diabetes mellitus and its complications. Nat Rev Endocrinol. 2018;14(2):88–98. doi:10.1038/nrendo.2017.151.

4.Meng XY, Zhang HX, Mezei M, Cui M. Molecular docking: A powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011;7(2):146–157. doi:10.2174/157340911795677602.

5.Ahmed D, Khan MI, Kaithwas G, Roy S, Gautam S, Singh M, et al. Molecular docking analysis and antidiabetic activity of Rifabutin against STZ-NA induced diabetes in albino wistar rats. Egypt J Basic Appl Sci. 2017;4(3):232–245. doi: 10.1016/j.bjbas.2017.04.010

6.Meng FD, Yuan L, Xu DJ, Che MY, Hou SZ, Lu DD, et al. Exploring the targets and molecular mechanism of glycyrrhetinic acid against diabetic nephropathy based on network pharmacology and molecular docking. World J Diabetes. 2023 Nov 15;14(11):1672-1692. doi:10.4239/wjd.v14.i11.1672. PMID: 38077799; PMCID: PMC10704203.

7.Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, et al. AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. J Comput Chem. 2009;30(16):2785–2791. doi:10.1002/jcc.21256

8.Trott O, Olson AJ. AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. J Comput Chem. 2010;31(2):455–461. doi:10.1002/jcc.21334

9.Meng XY, Zhang HX, Mezei M, Cui M. Molecular docking: A powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011;7(2):146-157. doi:10.2174/157340911795677602.

10.Saeedi P, Petersohn I, Salpea P, Malanda B, Karuranga S, Unwin N, et al. Global and regional diabetes prevalence estimates for 2019 and projections for 2030 and 2045: Results from the International Diabetes Federation Diabetes Atlas, 9th edition. Diabetes Res Clin Pract. 2019;157:107843. doi:10.1016/j.diabres.2019.107843.

11.Ke C, Narayan KMV, Chan JCN, Jha P, Shah BR. Pathophysiology, phenotypes and management of type 2 diabetes mellitus in Indian and Chinese populations. Nat Rev Endocrinol. 2022;18(7):413-432. doi:10.1038/s41574-022-00669

12.Zheng Y, Ley SH, Hu FB. Global aetiology and epidemiology of type 2 diabetes mellitus and its complications. Nat Rev Endocrinol. 2018;14(2):88-98. doi:10.1038/nrendo.2017.151.

13.Forbes JM, Cooper ME. Mechanisms of diabetic complications. Physiol Rev. 2013;93(1):137-188. doi:10.1152/physrev.00045.2011.

14.Patel DK, Prasad SK, Kumar R, Hemalatha S. An overview on antidiabetic medicinal plants having insulin mimetic property. Asian Pac J Trop Biomed. 2012;2(4):320-330. doi:10.1016/S2221-1691(12)60032-X.

15.DeFronzo RA. From the triumvirate to the ominous octet: a new paradigm for the treatment of type 2 diabetes mellitus. Diabetes. 2009;58(4):773-795. doi:10.2337/db09-9028.

16.Meng XY, Zhang HX, Mezei M, Cui M. Molecular docking: a powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011;7(2):146-157. doi:10.2174/157340911795677602.

17.Kalaivani T, Mathew L. Free radical scavenging activity from leaves of Acacia nilotica (L.) Wild. ex Delile, an Indian medicinal tree. Food Chem Toxicol. 2010;48(1):298-305. doi:10.1016/j.fct.2009.10.003.

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18.Marles RJ, Farnsworth NR. Antidiabetic plants and their active constituents. Phytomedicine. 1995;2(2):137-189. doi:10.1016/S0944-7113(11)80059-0.
19.Patel SS, Goyal RK. Cardioprotective effects of gallic acid in diabetes-induced myocardial dysfunction in rats. Pharmacogn Res. 2011;3(4):239-245. doi:10.4103/0974-8490.89743.
20.Modak M, Dixit P, Londhe J, Ghaskadbi S, Devasagayam TP. Indian herbs and herbal drugs used for the treatment of diabetes. J Clin Biochem Nutr. 2007;40(3):163-173. doi:10.3164/jcbn.40.163.
21.Ekor M. The growing use of herbal medicines: issues relating to adverse reactions and challenges in monitoring safety. Front Pharmacol. 2014;4:177. doi:10.3389/fphar.2013.00177.