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Molecular Docking of Arjuna Tree Phytocompounds for Ischemic Heart Disease

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Abstract

Heart disease is a serious condition that can be caused by several lifestyle changes and sometimes genetic problems. The primary protein component of apolipoprotein is the LDL receptor, which indicates that a reduction in LDL levels can reduce the risk of ischemic heart disease. Apolipoprotein levels are associated with increased levels of ischemic heart disease. Using ADMET analysis, drug likelihood prediction, and molecular docking, this work attempted to find natural chemicals from Terminalia arjuna (T. arjuna) that have several medicinal uses in Indian Ayurveda to prevent disease. The PDB database provided the 3D structure of the apolipoprotein, while the PubChem database provided 2D SDF format for the phytocompounds from T. arjuna. The Pyrx tool was used to analyse and remove the ligands with low binding affinity and was used for docking. BIOVIA Visualizer was used for visualization. The statistical distribution of the combinations of the protein's backbone dihedral angles ϕ and ψ is displayed via Ramachandran plot analysis. Five chemicals from T. arjuna have been identified by molecular docking experiments as having the capacity to attach to the apolipoprotein. Five compounds were found to have drug-like qualities based on the ADMET profile and drug likeness prediction. According to the current study, two chemicals have distinct binding affinities and may be employed as ischemic heart disease therapeutic strategies.

Keywords: Apolipoprotein, CHD, *Terminalia arjuna*, ADMET, molecular docking, Pyrx tool

INTRODUCTION

Heart issues brought on by constricted heart (coronary) arteries that feed blood to the heart muscle is referred to as ischemic heart disease, coronary heart disease (CHD), or coronary artery disease. Atherosclerosis, or plaque accumulation, is the most common cause of the narrowing, though blood clots and blood vessel constriction can also be the reason. A heart attack, also known as a myocardial infarction (MI), occurs when the heart muscle's cells die due to a complete blockage of blood flow to the heart muscle. Angina pectoris is the pain that occurs when the heart muscle does not receive enough oxygen [1].

Apolipoprotein E (ApoE) is involved in both dementia and ischemic heart disease and is essential for lipoprotein metabolism in the brain and peripheral tissues. It has only recently been determined whether ApoE plasma levels are linked to an elevated risk of dementia and ischemic heart disease in the general population, and whether these correlations are unrelated to the APOE polymorphism, lipids, and lipoproteins [2].

The main protein component of LDL is apolipoprotein, which the LDL receptor uses as a ligand to remove LDL from the bloodstream [3, 4]. Triglyceride-rich residual particles are cleared by the LRP/heparin sulfate proteoglycan with the

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help of ApoE [5, 6]. By interacting with surface proteoglycans in hepatic cells, ApoE in lipoproteins that include ApoB (ApoB) and HDL particles can help regulate absorption in the liver [7]. Additionally, the sequence that has the highest affinity for arterial proteoglycans – a crucial phenomenon for lipoprotein deposition in the artery wall – is shared by ApoE and ApoB. Increased ApoE content in lipoproteins that contain ApoB may lead to more deposition in the artery wall and a rise in atherosclerosis [2].

A decrease in plasma low-density lipoprotein (LDL) cholesterol levels lowers the incidence of ischemic heart disease and the corresponding death rate, as elevated LDL cholesterol levels are causally linked to ischemic heart disease [3]. Triglyceride-rich lipoproteins may be the mediator of the link between elevated plasma levels of ApoE and an increased risk of ischemic heart disease [4].

Terminalia arjuna (*T. arjuna*) also known as "Arjuna," is one of the medicinal plants that are native to India. It has been used as a cardiotonic in the treatment of various human ailments, including heart failure, ischemic stroke, cardiomyopathy, atherosclerosis, and myocardium necrosis. According to reports, *T. arjuna* has potent hydrolipidemic qualities. It is believed that *T. arjuna's* saponin glycosides may be the cause of its inotropic effects, while flavonoids and phenolics may provide vascular amplification and antioxidant activity, thereby validating the plant's numerous cardio-protective properties [5].

The primary medicinal component of *T. arjuna* for therapeutic purposes is its bark. Minerals, like calcium and magnesium, are present in it. The main phytocompounds in Arjuna bark include lactones, phenolic acids like ellagic and gallic acid, phenolic acids like terminic acid and arjunolic acid, glycosides like arjunetic and arjunosides I–IV, flavons, tannins, oligomeric Proanthocyanidins, β-sitosterol, and casuarinin. The bark of Arjuna terminalia is used in a variety of methods, including decoction, powder, juice, and more. Most people find all Arjuna formulations to be extremely safe and well-tolerated when taken as directed [8]. Long-term use of Arjuna bark powder shows no negative side effects and is most likely safe for the liver and kidneys. Laboratory and clinical indicators show no indications of a significant change [9].

Several phytocompounds found in *T. arjuna*, also referred to as the arjuna tree, may help prevent ischemic heart disease. These phytocompounds can attach to apolipoprotein and can be utilized in the production of medications that treat ischemic heart disease. Adsorption, distribution, metabolism, excretion, and toxicity (ADMET) filters are used in pharmacological screening to make sure the chemical is appropriate before choosing these antagonists. To choose possible medication candidates, molecular docking is also used to model the compound's interaction with apolipoprotein.

METHODS

Protein Preparation

The Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) (https://www.rcsb.org/) gave the 3D structure of the protein apolipoprotein (PDB ID:1GS9) in protein data bank format. The protein is made up of A chain with 165 amino acids in its sequence. It features a 1.70Å crystal resolution. Prior to docking, the protein was purified using BIOVIA Discovery Studio Visualizer's standard procedure. Water molecules were removed before to docking since they have the potential to impact docking scores. To make binding easier with the ligands selected for the study, the prebound ligands are removed from the crystal structures. While other chains had been removed off to make the protein structures simpler, Chain A was kept whole for study. Purified structures are improved in quality by the addition of polar hydrogen atoms, as shown in Figure 1(a) and (b).

Preparation of Ligand

The phytocompounds found in *T. arjuna* were gathered from Indian medicinal plants, phytochemistry, and therapies (IMPPAT) (https://cb.imsc.res.in/imppat/) using data gathered from previous research [11, 12]. The 2D SDF (Two-Dimensional Structure Data File) format was utilized to

extract the canonical SMILES from 39 compounds that were obtained from the PubChem chemical database(https://pubchem.ncbi.nlm.nih.gov). The process of ligand preparation involved ligand optimization, energy minimization, and conversion to PDB format using the PyRx program [10, 13].

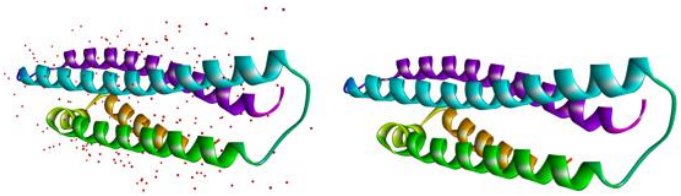

Figure 1. Three-dimensional structure of apolipoprotein acquired using BIOVIA. a) 3D structure of apolipoprotein and, b) 3D structure of purified apolipoprotein.

Ramachandran Plot

The Ramachandran plot is a representation of the torsional angles of a peptide's amino acids, phi and psi [10]. Using PDB sum (http://www.ebi.ac.uk/pdbsum/), the plot was obtained [14]. After uploading the Protein (1GS9) PDB file, a Ramachandran plot analysis was performed using outliers identified by residue type, residue number, and chain, exhibiting all the labels [10].

Drug Likeliness of Ligands

In pharmacokinetics and pharmacology, the phrase ADME, or "absorption, distribution, metabolism, and excretion," describes how a drug is eliminated from the body. Since each of the four criteria affects drug levels and the kinetics of drug exposure to tissues, they all influence the compound's pharmacological activity and overall effectiveness as a medicine. Occasionally, toxicity is also considered; this is known as an ADMET [15]. An ADMET quality assessment is used to evaluate a possible chemical for medicinal development.

The SWISS-ADME tool was also used to do the analysis [16]. For ADME analysis, the Lipinski rule of five was considered. When a molecule meets two or more requirements, Lipinski's rule of five predicts whether a drug similarity will be successful or not.

Lipinski rules:

1. Molecular mass < 500 Dalton,
2. logP < 4.15,
3. H-bond donor < 5,
4. H-bond acceptor < 10,
5. 40 < molar refractivity < 130
6. GI absorption – High

Molecular Docking

The molecular docking method simulates the interaction between a tiny molecule and a protein at the atomic level, allowing us to better understand fundamental biological processes and quantify how small molecules behave at the binding site of target proteins [10]. For molecular docking studies, PyRx-virtual screening tool software was utilized. PyRx is a virtual docking tool that aids in simulating ligand-protein interaction to better understand the characteristics of the binding [10]. Eight phytocompounds from *T. arjuna* were docked with the 1GS9 using the PyRx program.

Prepared receptors and ligand files were chosen to establish the target for the docking investigation. After loading and converting the protein into a macromolecule for docking, ligands were generated by loading them using the tool's open-babel tab [10, 17]. While the phytocompounds were submitted as

sdf files, the purified protein was loaded as the macromolecule and converted to AutoDock.pdbqt format. Applying the universal force field and converting the ligands to pdbqt format allowed for energy minimization. The ligands were evaluated for docking after the grid (Center X:17.7908 Y:42.1403 Z:50.2586; and Dimensions X:25.0000 Y:25.0000 Z:25.0000) was created. By default, the parameters PyRx takes nine distinct conformations to achieve the best match with the protein, assuming that the ligands are flexible and the macromolecules' three-dimensional structures are stiff. Compounds with the lowest binding affinities were chosen using the interaction data that was gathered [11]. Following docking, we obtained a table with each ligand's binding affinity. Based on the ligand's highest binding affinity, the top five ligands were chosen for more research. The PDB file format was used to store the top five compounds as seen in Figure 2. Using BIOVIA Discovery Studio Visualizer, a 2D/3D interactive visualization study was completed [18].

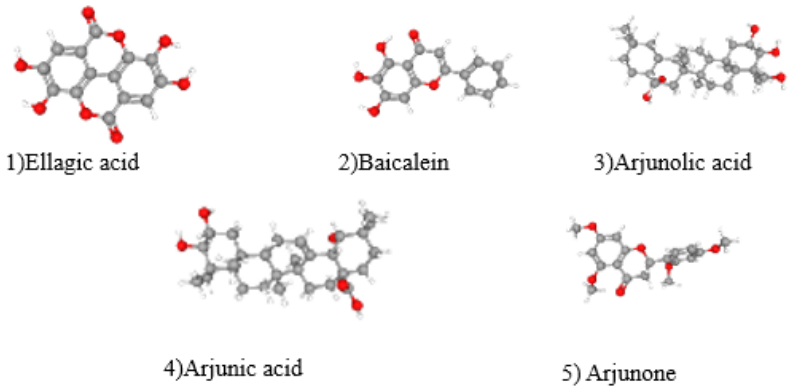

Figure 2. (1–5) are the 3D models of phytocompounds after docking.

RESULTS

Protein Structure Analysis

Secondary Structure

The secondary structure of apolipoprotein was examined using PDB sum. This tool displays the molecules that comprise the three-dimensional structure along with their schematic interactions. Five helices, ten helix-helix contacts, and three beta twists make up the secondary structure of apolipoprotein, according to the data shown in Figure 3. Variants, like Leu28Pro, Arg158Cys and Arg145Cys, are available. There are 144 residues in the structure overall.

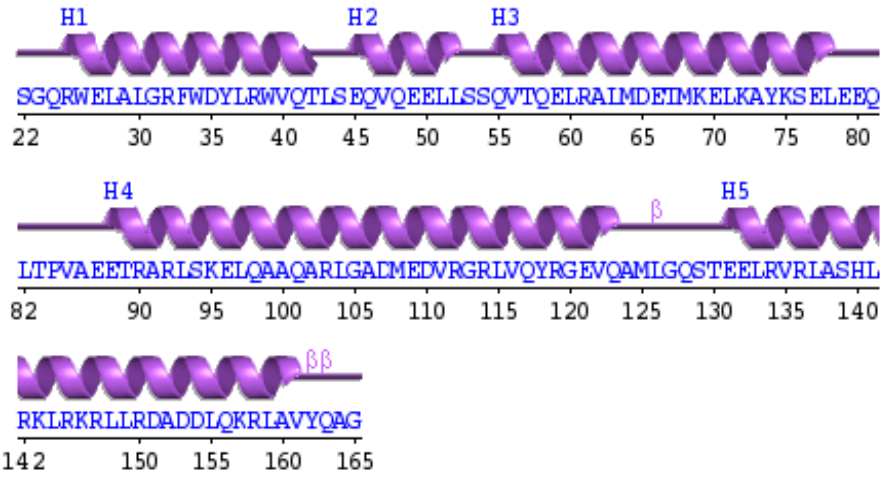

Figure 3. Secondary structure of apolipoprotein.

Ramachandran Plot

The Ramachandran plot visualizes energetically permitted regions for the torsions angle ψ vs φ of amino acids in a protein structure. PROCHECK statistics present in PDBsum was used to generate the Ramachandran plot of apolipoprotein, as shown in Figure 4. The red sections on the graph represent the sterically permissible regions in which peptide conformation is stable. While 5.2%, or one residue, of the amino acid residues lie in the disallowed zone, about 94.1%, or 127 residues, fall in the allowed region. The subregions contain the remaining 0.7%. Seven glycine residues, one proline residue, one end-residue, and 135 non-proline and non-glycine residues make up the 144 residues.

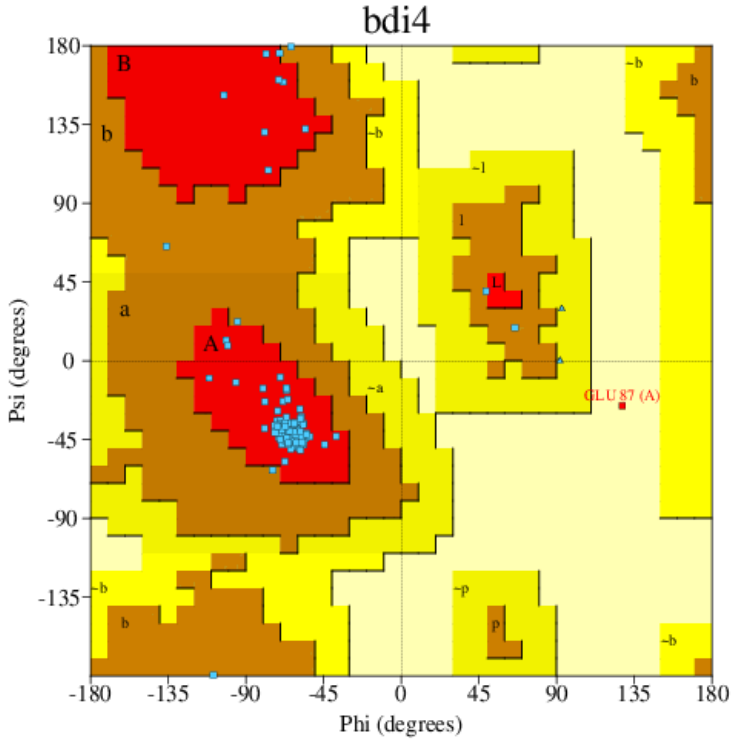

Figure 4. Ramachandran plot of apolipoprotein.

ADME Analysis

The phytocompounds from *T. arjuna* with highest binding affinity with the protein apolipoprotein was observed in Table 1.

Table 1. Top five phytocompounds from *T. arjuna* having highest binding affinity with apolipoprotein.

S.N.	PubChem Compound ID	Name of Phytocompound	Binding Energy (Kcal/mol)
1	5281855	Ellagic acid	–6.5
2	5281605	Baicalein	–5.9
3	73641	Arjunolic acid	–5.8
4	15385516	Arjunic acid	–5.6
5	14034821	Arjunone	–5.3

Key characteristics of ADME analysis include the blood-brain barrier's (BBB) ability to limit a compound's ability to enter the brain. A high level of gastrointestinal (GI) absorption is necessary to increase the drug's effectiveness. Additionally, the chemical need to dissolve readily. Less negative solubility values are therefore permitted. Toxicity prediction was also done using tool called Protox (https://tox.charite.de/). The process of screening compounds according to ADME characteristics is seen in Table 2.

Table 2. ADME data obtained using Swiss ADME.

S.N.	Ligands	GI absorption	Solubility	Toxicity level
1	Ellagic acid	High	Soluble	4
2	Baicalein	High	Moderately soluble	5
3	Arjunolic acid	High	Poorly soluble	4
4	Arjunic acid	High	Poorly soluble	4
5	Arjunone	High	Soluble	4

Pharmacological Parameters

Pharmacological properties, including molecular weight, hydrogen bond donor, hydrogen bond acceptor, and molar refractivity, are displayed in Table 3 according to the Lipinski rules that are discussed in the Methods section.

Table 3. ADME analysis of best docked compounds based on Lipinski's rule.

S.N.	Ligand Name	Molecular Weight (g/mol)	H-Bond Donor	H-Bond Acceptor	LogP	Molar Refractivity
1	Ellagic acid	302.19	8	4	0.79	75.31
2	Baicalein	270.24	5	3	2.43	73.99
3	Arjunolic acid	488.7	5	4	3.11	138.98
4	Arjunic acid	488.7	5	4	3.31	138.98
5	Arjunone	344.36	6	0	3.35	91.47

Molecular Docking Analysis

Table 3 was chosen for further analysis based on Lipinski's rule.

The drugs' inhibitory action, binding affinity, and docking score were all assessed using PyRx. A scoring algorithm known as the "docking score" is used to predict how well a protein and ligand will bind when they are docked. Compounds present in Table 1 were appropriate compounds with the highest negative binding affinity, were selected for additional examination once the docking findings were received. Dassault Systems' BIOVIA Discovery Studio Visualizer was used for visualization, and the resulting two-dimensional (2D) and three-dimensional (3D) models are shown in Figures 5 and 6.

With a binding affinity of –6.5, the ligand ellagic acid formed strong contact with the amino acid A chain. ASP35, TRP34, and ASP153 were all interacting with the ligand.

While TRP A:34 displayed Pi-Pi stacking, ASP A:35, and ASP A:153 exhibited a conventional hydrogen bond with the ligand.

With a binding affinity of -5.9, the ligand Baicalein formed strong contact with the amino acid A chain. LEU149, LEU28, GLN156, GLU27, and TRP34 were all interacting with the ligand.

While TRP A:34 displayed Pi-Pi stacking, GLN A:156, and GLU A:27 exhibited a conventional hydrogen bond with the ligand, LEU A:149 exhibited Pi-Alkyl, LEU A:28 exhibited van der Waals force.

DISCUSSION

Around the world, ischemic heart disease is still quite common. Among the leading preventable causes of death is heart disease. The disease is primarily attributed to bad lifestyle choices, while some genetic factors may play a role. These include unhealthy eating habits, seldom exercise, tobacco use, drug or alcohol misuse, and elevated stress levels. Many doctors in the 18th and 19th centuries were perplexed by angina, a tightness in the chest that is frequently a sign of ischemic heart disease [19].

One of the most important apolipoproteins in the central nervous system, apolipoprotein E (Apo E) can repair neurons. Significant correlations were found between Apo E genetic variations and the risk of degenerative disorders of the nervous system, such as Alzheimer's disease, vascular dementia, and cerebrovascular disease. One of the coronary risk factors is the measurement of blood lipid and lipoprotein levels. Studying the vulnerability to CHD requires an understanding of the apolipoprotein genes involved in lipoprotein production and metabolism [20].

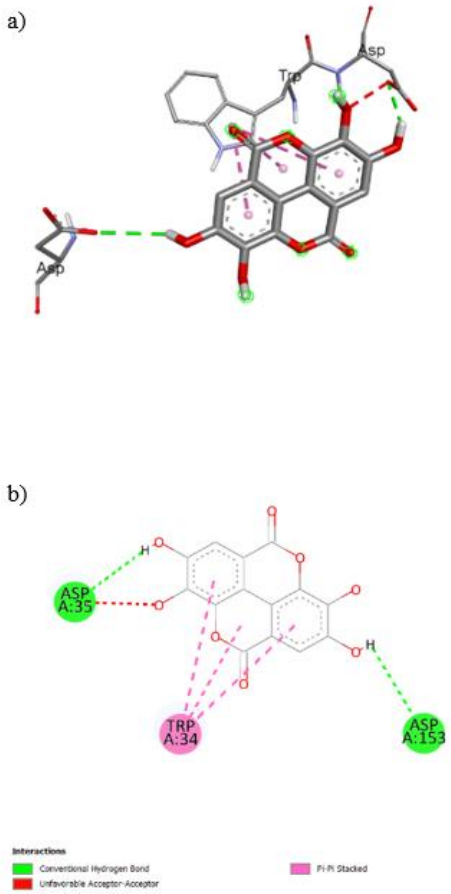

Figure 5. Visualization of molecular interaction between ellagic acid and apolipoprotein. a) 3D interaction diagram and. b) 2D interaction diagram.

The study demonstrated the function of *T. arjuna* phytocompounds, which have several therapeutic benefits according to Ayurveda [10]. Since natural phytocompounds from medicinal plants like *T. arjuna* are less harmful than manufactured ones, they can be utilized. It has been demonstrated that in silico techniques including molecular docking, ADME analysis, and molecular dynamic simulation are useful for future studies that examine the ligands' stability, interactions, and binding affinity with the target [10].

To confirm the protein's purity, apolipoprotein (PDB ID:1GS9) was subjected to a Ramachandran plot analysis. Additionally, for the in-silico investigation, eight compounds were selected based on their binding affinities to be tested against apolipoprotein using the molecular docking technique. Five of these phytocompounds – ellagic acid, baicalein, arjunic acid, arjunolic acid, and arjunone – from *T. arjuna* shown have a high affinity for binding to the protein. Following a molecular docking research, ADME analysis was performed on all five compounds to confirm their toxicity and drug likeliness. It was discovered that the two substances having the highest binding affinities to apolipoprotein were ellagic acid and baicalein.

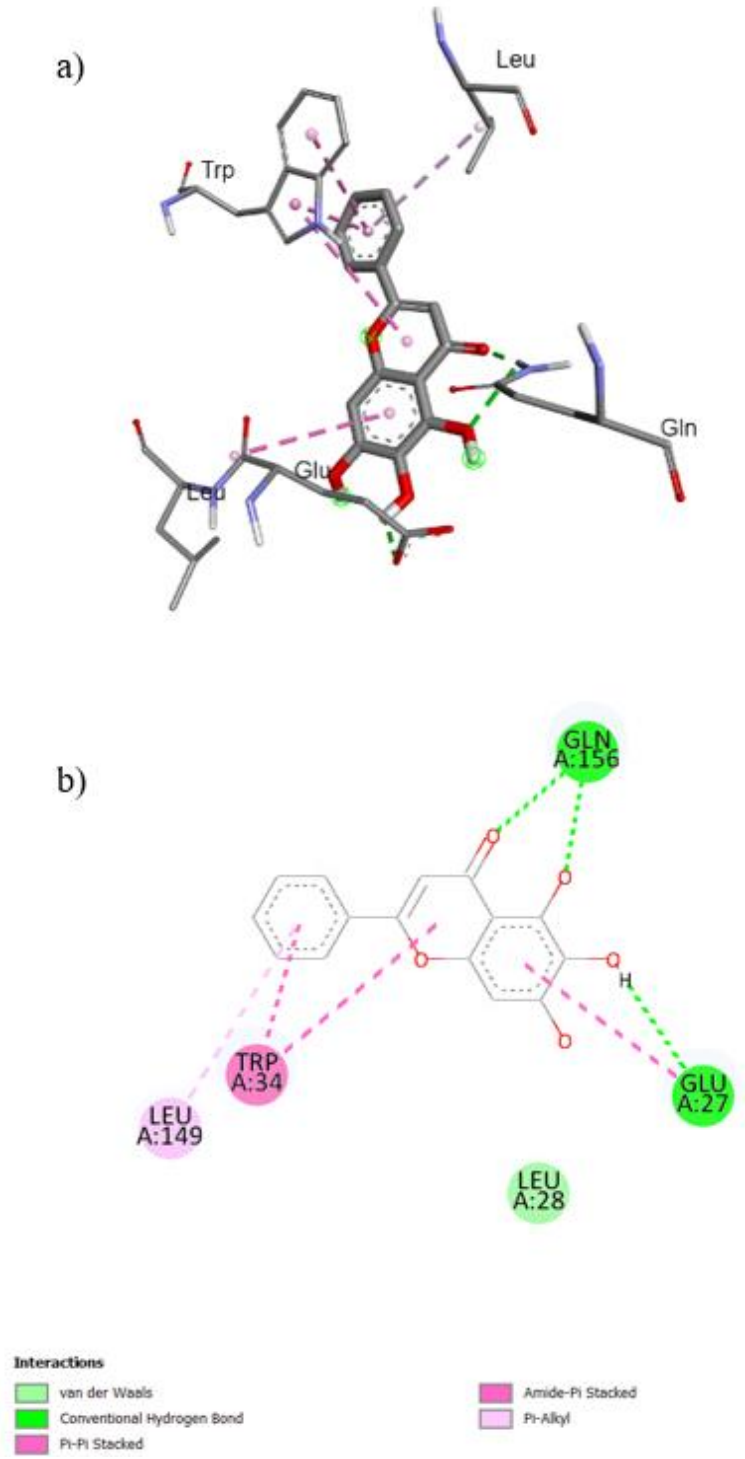

Figure 6. Visualization of molecular interaction between baicalein and apolipoprotein. a) 3D interaction diagram and b) 2D interaction diagram.

According to their molecular docking technique (binding affinity), drug likelihood as determined by Swiss ADME, and toxicity prediction using tools, such as Protox, these phytocompounds are found to be effective against the protein.

Despite the promising findings of in silico research, many compounds may have additional disadvantages that outweigh their promise as a therapeutic option. Constipation, vomiting, and

stomach pain are all known side effects of Baicalein. Mild nausea, Constipation, Headache are the side effects of Arjunic acid. Blood clotting may be slowed by *T. arjuna* . Bruising and bleeding may become more likely if *T. arjuna* is taken with drugs that also inhibit blood coagulation [21].

For the above reason, it is crucial to remember that in vitro and in silico research can yield different outcomes [11].

CONCLUSIONS

The goal of the study was to identify *T. arjuna'*s natural phytocompounds as a possible treatment for ischemic heart disease. It is a disease brought on by a poor lifestyle, including bad eating habits, insufficient exercise, and occasionally genetic issues. One ischemic heart disease protein that is known to contribute to the symptoms of ischemic heart disease is apolipoprotein, which is found in high concentrations leading to the disease.

Based on this study, we can try to target this protein with a medicinal plant like *T. arjuna* that can cause less harm in the hopes of lowering the risk of ischemic heart disease. This study demonstrated that certain *T. arjuna* phytocompounds, such as ellagic acid and baicalein have some of the highest binding affinities for apolipoprotein. As Ayurvedic treatments for ischemic heart disease, the best-docked phytocompounds with drug-like qualities, a safe ADMET profile, and efficacy could be beneficial in the development of specific inhibitors.

Abbreviation

ApoB	Apolipoprotein B
ApoE	Apolipoprotein E
ADMET	Adsorption, distribution, metabolism, excretion, and toxicity
Å	Angstrom
ß	Beta
BBB	Blood-brain barrier
CHD	Coronary heart disease
2D	2 Dimensional
3D	3 Dimensional
Figure	Figure
GI	Gastrointestinal
HDL	High density lipoprotein
IMPPAT	Indian medicinal plants, phytochemistry, and therapies
LDL	Low density lipoprotein
Ψ	Psi
Φ	Phi
%	Percentage
RCSB PDB	Research Collaboratory for Structural Bioinformatics Protein Data Bank
SDF	Structure Data File
T.arjuna	*Terminalia arjuna*

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