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Computational Investigation of *Phyllanthus niruri* Phytoconstituents Against Iron Homeostasis and Thalassemia-Associated Molecular Targets Using Molecular Docking and Network Pharmacology

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Abstract: ***Thalassemia is a hereditary condition that affects haemoglobin formation, leading to ineffective erythropoiesis, anaemia, and iron overload, resulting in serious complications and reduced quality of life. While modern medical care, such as blood transfusions and iron chelation, has considerably extended patients' lifespan, prolonged therapy has been accompanied by various side effects, financial burden, and low compliance. In addition, due to the complex pathogenesis of thalassemia, which includes oxidative stress, inflammation, disrupted iron homeostasis, and cellular damage, there is a need to develop new methods that can address all these processes simultaneously. This fact has led researchers to show great interest in plant-based remedies containing naturally active biological substances. In this study, we explored the therapeutic efficacy of the plant Phyllanthus niruri by investigating its association with target proteins and biological pathways related to iron homeostasis in thalassemic patients, employing a comprehensive bioinformatics approach. Active compounds found in Phyllanthus niruri were recognized and filtered. Then, target identification, along with disease-gene associations, was performed for common diseases and compounds. For biological insights, targets associated with thalassemia and phytoconstituents were analysed employing network pharmacology, protein-protein interaction networks, Gene Ontology enrichment, and KEGG pathway analyses. In vitro molecular docking experiments to predict interactions between phytoconstituents and their targets were performed, and ADMET analysis was conducted to assess pharmacokinetics and drug-likeness. Among the identified hub genes were those associated with iron metabolism, oxidative stress, inflammation, and erythrocyte formation. The pathways enriched in the functional enrichment analysis included those associated with iron metabolism, cytokine signalling, apoptosis, and cellular responses to stress. The molecular docking study revealed favourable interactions between the phytoconstituents, particularly corilagin, geraniin, and quercetin, and the target proteins. ADMET predictions indicated favourable pharmacokinetics for some compounds. All in all, the results demonstrate the multitarget potential of Phyllanthus niruri as an important source of bioactive substances that can address complications of thalassemia, especially in cases of iron overload. The study lays an important foundation for the subsequent experimental verification of the results.***

Index Terms: ***Phyllanthus niruri, Thalassemia, Iron Homeostasis, Network Pharmacology, Gene Ontology, Molecular Docking, Pharmacokinetics, ADMET, Disease Gene Association***

Nomenclature:
GO: Gene Ontology
KEGG: Kyoto Encyclopedia of Genes and Genomes
ADMET: Absorption, Distribution, Metabolism, Excretion, and Toxicity
SMILES: Simplified Molecular Input Line Entry System
STRING: Search Tool for the Retrieval of Interacting Genes/Proteins
PDB: Protein Data Bank
PPI: Protein-Protein Interactions

I. INTRODUCTION

Thalassemia is a common genetic disorder of haemoglobin and has been a major public health problem, especially in the developing world, where there is a high incidence of thalassemia carriers [1]. This condition arises from mutations that impair globin chain production, leading to failure of haemoglobin formation and ineffective erythropoiesis, resulting in chronic anaemia and excessive iron deposition in critical organ systems. Iron overload, driven by frequent blood transfusions and enhanced iron absorption, plays a crucial role in the pathogenesis and mortality of the disease [1].

The regulation of iron levels in the body depends on a tightly regulated network comprising hepcidin, ferroportin, transferrin, ferritin, and other transporters that govern iron uptake, storage, and utilisation. Thalassemia is associated with disturbances in these processes, leading to iron accumulation and oxidative stress in mice, which, in turn, worsen the development of the condition [2]. Formation of reactive oxygen species in the presence of excess iron leads to lipid peroxidation, protein oxidation, DNA damage, and inflammation.

Existing therapies include frequent blood transfusions and iron chelation therapy [1]. Although these treatments have been very effective in improving patients' lifespans,

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their long-term use may lead to complications and noncompliance. Therefore, there is a great need to explore other therapeutic drugs that can target multiple mechanisms simultaneously.

Medicinal plants still play an important role in modern drug discovery and are rich sources of biologically active compounds. *Phyllanthus niruri* is a plant species that has gained prominence in recent years due to its traditional use and multifaceted pharmacological activity [3]. This plant has traditionally been used for treating diseases such as liver ailments, kidney stones, inflammatory conditions, infectious agents, and metabolic diseases [4].

The phytochemical analysis of this medicinal plant has revealed the presence of several biologically active compounds, namely corilagin, geraniin, quercetin, rutin, kaempferol, gallic acid, ellagic acid, catechin, phyllanthin, and hypophyllanthin. All these compounds possess antioxidant, anti-inflammatory, hepatoprotective, immunomodulatory, and chelation abilities that can be effective against certain diseases [5].

The emergence of computational biology approaches has enabled studies of the relationships among phytochemicals, proteins, genes, and signalling pathways using a systems biology approach. Network pharmacology is a technique that can be used effectively to understand the multiple components and targets that characterise herbal drugs. With the integration of molecular docking, protein-protein interaction, and pharmacokinetics predictions, network pharmacology becomes an effective way of exploring natural product therapies [6].

Several recent studies using network pharmacology and molecular docking have yielded valuable insights into the biological activities of Phyllanthus and other herbal plants [7]. These studies have demonstrated interactions between phytochemicals and proteins involved in the inflammatory response, oxidative stress, metabolic activity, and cellular protection, particularly those located in the liver [8]. Nevertheless, very few studies have examined the potential effects of compounds from Phyllanthus niruri on thalassemia and iron-metabolism proteins.

Consequently, the current research is focused on examining the therapeutic effect of *Phyllanthus niruri* plant metabolites against the biological targets associated with thalassemia via a comprehensive computational approach, including target prediction, network pharmacology, protein-protein interactions analysis, Gene Ontology enrichment, Kyoto Encyclopedia of Genes and Genomes pathway analysis, Docking and Absorption, Distribution, Metabolism, Excretion, and Toxicity evaluation. In addition, the study will attempt to identify bioactive compounds, targets, and signalling pathways that might be useful for the treatment of thalassemia and iron overload.

II. MATERIALS AND METHODS

A. Identification and Selection of Phytoconstituents

An extensive literature survey was conducted to gather information on the bioactive phytoconstituents of *Phyllanthus niruri*. Literature surveys were conducted using various published articles and reviews to gather information on the plant's phytochemicals and pharmacological properties. The selected major phytoconstituents, including corilagin, geraniin, quercetin, rutin, kaempferol, gallic acid, ellagic acid, catechin, phyllanthin, and hypophyllanthin, were identified for their biological importance and therapeutic potential. The structures of these phytoconstituents were obtained from the PubChem database, which is a comprehensive resource for chemical information [9]. Canonical SMILES structures and three-dimensional structures were selected for target prediction and docking studies.

B. Prediction of Compound-Associated Targets

The possible protein targets associated with the chosen phytoconstituents were identified using computerised target prediction techniques. The canonical SMILES format of each molecule was entered into Swiss Target Prediction, a well-known database that predicts molecular biological targets based on similarity and ligand-protein interaction information. Only predicted targets for Homo sapiens were retrieved, assembled into a consolidated list, and duplicate targets were removed. Protein identifiers were standardized according to the UniProt naming system [10].

C. Collection of Disease-Associated Targets

Genes involved in thalassemia, iron overload, iron metabolism, oxidative stress, and erythropoiesis have been identified by mining databases and literature. Disease-related genes were selected using tools such as GeneCards [11], DrugBank [12], and the literature on iron homeostasis and haematological diseases. Keywords like “thalassemia,” “iron overload,” “iron homeostasis,” “anaemia,” “oxidative stress,” and “erythropoiesis” were used while searching for targets. Redundant targets and non-human targets were filtered out from the retrieved list of genes.

D. Identification of Common Therapeutic Targets

To identify potential therapeutic targets, compound-associated protein targets were compared with disease genes using comparative analysis techniques. The resulting overlap was deemed to represent potential therapeutic proteins through which Phyllanthus *niruri* phytochemicals exert their effects on the biology of thalassemia. The set of overlapping target proteins became the starting point for further network pharmacology analysis, protein-protein interaction studies, pathway enrichment analysis, and molecular docking experiments.

E. Construction of Compound–Target Interaction Network

Compound-target interaction networks were created to illustrate the relationship between bioactive phytoconstituents and drug targets [13]. This network analysis was performed using Cytoscape, a popular tool for analysing biomolecular interactions and visualising networks [14]. In the generated network, nodes represented phytoconstituents and therapeutic targets, and edges represented interactions between them. Various network topology properties, such as degree, betweenness, and closeness centralities, were evaluated to identify high-degree compounds and hub targets.

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Higher-degree compounds were considered highly responsible for the pharmacology of *Phyllanthus niruri*. High-degree proteins, on the other hand, could be classified as biological targets.

F. Protein–Protein Interaction Network Analysis

To analyse protein interactions, a protein–protein interaction analysis was conducted using the STRING database [15]. This database contains not only experimentally confirmed protein-protein interactions but also predicted ones, along with the interaction information extracted from the literature. The overlapping target proteins were mapped on the STRING database, and a protein-protein interaction network was constructed. The constructed interaction network was analysed to identify hub proteins that participate in essential biological processes. In particular, those proteins that had the highest degree of interaction and were located centrally in the network were selected for further interpretation of their biological roles.

G. Gene Ontology Enrichment Analysis

GO enrichment analysis was conducted to assess the biological relevance of the discovered therapeutic targets [16]. GO groups genes into three broad categories: Biological Process, Molecular Function, and Cellular Component. GO enrichment analysis was conducted to identify the biological processes enriched among the therapeutic targets. Biological Process was used to study the physiological processes involved, while Molecular Function and Cellular Component were used to determine the biochemical activities and subcellular locations, respectively. GO-enriched terms were ranked based on their statistical significance scores.

H. KEGG Pathway Enrichment Analysis

To reveal the pathways contributing to the identified therapeutic targets, KEGG pathway enrichment analysis was performed. The KEGG offers an overview of the functional roles of various biological systems at both the molecular and cellular levels [17]. The identified target proteins were then assigned to pathways in the KEGG database based on their contributions to signal transduction processes related to thalassemia, oxidative stress, inflammation, iron metabolism, apoptosis, and erythropoiesis. Enriched pathways were further analyzed biologically.

I. Ligand Preparation

For molecular docking analysis, the selected phytochemicals were prepared using established computational methods. Three-dimensional structures available from PubChem were prepared for docking by converting them into suitable formats and optimising their energy to obtain stable structures [9]. Where required, hydrogen atoms were added to the structures, and molecular geometry was optimised to facilitate accurate docking. The prepared ligands were subsequently used in protein-ligand interaction studies.

J. Protein Preparation

Specific therapeutic targets identified through network pharmacology and PPI analyses were selected for molecular docking studies. High-resolution protein structures were obtained from the Protein Data Bank, a worldwide database of experimentally determined biomolecular structures [18]. Preparation of protein structures involved deleting water molecules, crystallisation ligands, and any unnecessary heteroatoms. Hydrogen atoms were added, and active site domains were delineated using structural data and knowledge of the binding sites of ligands. These proteins served as receptors during docking.

K. Molecular Docking Analysis

Docking experiments were conducted to analyse the affinity and interaction patterns between selected phytochemicals and the target proteins used in drug development. AutoDock Vina was used for docking experiments owing to its speed and reliability in predicting protein-ligand interactions [19]. Affinity score values were generated for all the protein-ligand pairs. Affinities of protein-ligand pairs having lower affinity scores were analyzed. Docked protein-ligand pairs were analysed for hydrogen bonds, hydrophobic interactions, pi-pi interactions, and electrostatic interactions that helped stabilise them [19]. Ligands with lower affinity scores and stable interaction patterns were chosen as potential drug molecules.

L. ADMET and Drug-Likeness Evaluation

The pharmacokinetics and toxicity of the selected plant-derived chemical entities were predicted using various computational tools, including SwissADME [20]. Drug-likeness properties, including molecular weight, lipophilicity, hydrogen-bond donor and acceptor counts, and topological polar surface area, were evaluated in accordance with medicinal chemistry guidelines. ADMET parameters were determined to determine the suitability of the pharmacokinetics of the respective compound. Parameters concerning gastrointestinal absorption, oral bioavailability, blood-brain barrier penetration, and toxicity were also assessed. The suitable and safe compounds were selected as good prospects for further experimentation.

III. RESULTS AND DISCUSSION

A. Identification of Bioactive Phytoconstituents

Several important phytoconstituents isolated from *Phyllanthus niruri* that exhibited various pharmacological activities were selected for computational studies. This list includes corilagin, geraniin, quercetin, rutin, kaempferol, gallic acid, ellagic acid, catechin, phyllanthin, and hypophyllanthin. The selected phytoconstituents represent different classes of natural products, including tannins, flavonoids, lignans, and polyphenols, which exhibit antioxidant, anti-inflammatory, metal-chelating, and hepatoprotective activities [21]. They can interact with various biological receptors involved in thalassemia and iron balance. The information on the chemical structures of these molecules was obtained from the PubChem database.

B. Identification of Potential Therapeutic Targets

Target prediction studies of the selected Phyllanthus niruri phytoconstituents yielded a complete list of targets likely

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responsible for the plant's physiological functions. Upon incorporating phytochemical targets with target genes involved in thalassemia development, excess iron accumulation, oxidative stress, and erythropoiesis, an overlapping set of targets was identified. The overlapping targets could be considered a set of potential drug targets through which the actions of *Phyllanthus niruri* phytoconstituents may occur as biological responses against thalassemia-induced disorders. The targets were involved in regulating intracellular iron levels, inflammation, oxidative stress, apoptosis, and hematopoiesis. The presence of overlapping targets supports the assumption that Phyllanthus niruri can engage in multi-target therapeutic activities affecting multiple biological pathways simultaneously.

C. Compound–Target Interaction Network Analysis

The interaction network between phytoconstituents and their therapeutic targets provided insights into the relationship from a systems-biology perspective. This was achieved using interconnected nodes comprising both the compounds and proteins based on the biological interactions predicted by the network [22]. A topological analysis of the network demonstrated that certain phytochemicals had comparatively high degrees of connectivity, indicating multiple interactions with therapeutic proteins. Among the phytoconstituents under investigation, corilagin, geraniin, quercetin, and kaempferol showed the highest degree of value.

These highly connected phytoconstituents may act as bioactive components and be responsible for the pharmacologic actions of *Phyllanthus niruri* through their interaction with multiple targets, thereby resulting in a synergistic mechanism of action, as is expected in herbal medicine. Similarly, there were target proteins with comparatively high centrality values, thus occupying strategic positions in the interaction network. Such proteins would play important roles in regulating disease progression and thus be potential therapeutic targets. This network organisation is consistent with the theory that phytoconstituents mediate their pharmacological effects by modulating multiple targets rather than acting through single protein interactions.

D. Protein–Protein Interaction Network Analysis

Protein–protein interaction analysis was performed to explore the functional interrelationships among the identified drug targets [23]. The PPI network revealed an intricate interconnectedness among proteins involved in iron metabolism, inflammation, oxidative stress response, and cell survival pathways. Certain proteins were characterised as hub proteins due to their high-degree interactions and network positions. It was observed that these proteins were strongly associated with several pathways related to iron metabolism, cytokine signalling, erythropoiesis, and cell stress responses.

The occurrence of such highly connected proteins suggests that targeting them can affect a variety of signal transduction pathways. This feature becomes extremely useful when treating complex diseases such as thalassemia, which involve multiple biological systems. Proteins identified through protein-protein interaction analysis were then considered as candidates for functional enrichment and molecular docking studies owing to their probable biological importance.

E. KEGG Pathway Enrichment Analysis

KEGG pathway analysis was performed to identify biological pathways significantly associated with the identified targets [17]. Some pathways showed significant enrichment, including oxidative stress response, inflammatory signalling, apoptosis-related, cytokine signalling, cellular proliferation, and iron metabolism. Some of these pathways included those involved in regulating reactive oxygen species and the inflammatory response. Excess iron accumulation due to thalassemia results in oxidative stress and inflammation. This results in tissue injury leading to the development of the disorder. Significant enrichment in apoptosis-related pathways indicates that the identified phytoconstituents affect apoptotic processes, thereby reducing iron-induced cellular injury. Furthermore, pathways associated with erythropoiesis and hematopoietic regulation were identified. It shows the importance of the thalassemia targets.

F. Molecular Docking Analysis

Docking was performed on selected phytoconstituents to examine potential interactions with therapeutic target proteins [24]. The docking results indicated satisfactory binding properties for some ligand-protein complexes, suggesting the potential to form stable molecular complexes. The negative binding energy values for most docked complexes indicated spontaneous, thermodynamically favourable binding. In addition to these, hydrogen bonding, hydrophobic interactions, electrostatic interactions, and aromatic interactions were detected.

Corilagin, among the studied phytoconstituents, exhibited excellent binding properties toward several target proteins. Geraniin, quercetin, kaempferol, and ellagic acid had also shown similar potential for interaction with the selected target proteins. The results suggest that the selected compounds have the appropriate structural arrangement for interacting with the proteins of interest.

G. Discussion

Thalassemia is an intricate haematological condition characterised by defective erythropoiesis, persistent anaemia, oxidative stress, inflammation, and gradual iron accumulation. Because multiple biological processes contribute to disease development, drugs that target multiple molecules could significantly improve treatment outcomes. The current research employed network pharmacology and molecular docking to evaluate the effectiveness of plant molecules from Phyllanthus niruri in treating thalassemia-associated targets [7]. The analysis of the compound-target network suggested that corilagin, geraniin, quercetin, and kaempferol exhibited strong interactions with proteins involved in iron metabolism, oxidative stress, inflammatory response, apoptosis, and erythropoiesis.

The results from the protein-protein interaction analysis identified hub proteins associated with iron

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metabolism and cell stress response pathways, suggesting potential molecular mechanisms through which the herb could treat iron overload-associated diseases. Moreover, the GO and KEGG enrichment analyses identified biological processes associated with oxidative stress, inflammation, apoptosis, and iron homeostasis, which are highly implicated in the pathogenesis of thalassemia. The results of molecular docking analysis also provided supporting evidence for the use of phytochemicals from Phyllanthus niruri in the treatment of thalassemia. The phytochemical corilagin exhibited high affinity for binding to various target molecules due to its ability to form stable hydrogen-bond interactions. The other molecules, such as geraniin, quercetin, kaempferol, and ellagic acid, were also observed to exhibit binding affinities for their respective targets.

These results align with past literature indicating the antioxidant and anti-inflammatory nature of the phytochemicals in *Phyllanthus niruri.* Such characteristics can be especially helpful in patients with thalassemia, who have elevated iron levels, which can increase reactive oxygen species production and cellular damage. In addition, ADMET analysis highlighted some components with good pharmacokinetic behaviour and safety profiles; however, some larger tannins had low predicted intestinal absorption rates, thereby necessitating formulation optimisation. One of the advantages of this research is that multiple tools, such as target prediction, network pharmacology, protein interaction, functional analysis, molecular docking, and pharmacokinetics, are integrated, enabling a comprehensive analysis of the medicinal potential of *Phyllanthus niruri.* Nonetheless, this is based solely on computations and requires additional confirmation through in vivo/in vitro experiments, as well as possibly clinical trials [25]. In conclusion, *Phyllanthus niruri* is a promising source of multitarget phytochemicals for the treatment of thalassemia and its consequences.

IV. CONCLUSION

In the current study, a comprehensive computational approach was used to examine the efficacy of *phytochemicals from Phyllanthus niruri against* thalassemia-related molecular targets and iron homeostasis pathways. Through network pharmacology, protein–protein interactions, GO, KEGG pathway enrichment, molecular docking, and ADMET studies, various active compounds and potential targets were determined. The findings indicate that major phytochemicals, such as corilagin, geraniin, quercetin, kaempferol, and ellagic acid, interact with proteins involved in processes including iron metabolism, oxidative stress, inflammation, apoptosis, and erythropoiesis. Network pharmacology and PPI analyses indicated the multitarget nature of Phyllanthus niruri and identified hub proteins implicated in thalassemia.

Molecular docking revealed favourable binding properties between the selected phytochemicals and potential therapeutic targets. Corilagin emerged as having the most favourable binding profile, whereas geraniin, quercetin, and kaempferol were found to have promising therapeutic potentials. ADMET studies revealed acceptable pharmacological features in several compounds. The present results indicate that the *plant Phyllanthus niruri contains potential multi-target bioactive compounds that can modulate pathways implicated* in thalassemia and iron-overload disorders. The study opens up an avenue for future experimentation on *Phyllanthus niruri*-based drugs for the treatment of blood diseases.

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FUTURE SCOPE

Further research efforts must be directed towards validating the computational results through experiments using in vitro and in vivo methods. Biochemical methods can be used to assess the inhibitory effects of selected phytoconstituents on target proteins involved in iron metabolism and oxidative stress. Further animal trials and clinical investigations will be essential in determining the pharmacokinetics and safety of the selected compounds.

The use of omics techniques, along with an AI-based approach, in drug discovery and formulation design can help advance the *Phyllanthus niruri* phytoconstituents as therapeutic candidates for treating thalassemia and other disorders of iron overload.

DECLARATION STATEMENT

Some of the references cited are outdated, noted explicitly as [14] and [16]. However, these works remain significant for the current study, as they are pioneering in their fields.

After aggregating input from all authors, I must verify the accuracy of the following information as the article's author.

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