Article

Exploring the Therapeutic Potential of *Premna obtusifolia* and *Oxalis corniculata*: A Combined *in Vitro* Bioassay and Molecular Docking Study

Arifa Sultana [1], Rajib Das [2,3], Amit Roy [1], Mst. Nowsad Zahan Sathi [4], Najmus Sakib Minhaj [4], Md. Reaz Uddin [5,6], and Sitesh Chandra Bachar [1,*]

[1] Department of Pharmacy, Faculty of Pharmacy, University of Dhaka, Dhaka 1000, Bangladesh
[2] Department of Clinical Pharmacy and Pharmacology, Faculty of Pharmacy, University of Dhaka, Dhaka 1000, Bangladesh
[3] Department of Pharmacy, School of Life Sciences, United International University, Dhaka 1212, Bangladesh
[4] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Dhaka, Dhaka 1000, Bangladesh
[5] Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Dhaka, Dhaka 1000, Bangladesh
[6] Department of Molecular and Cellular Biology, Kennesaw State University, Kennesaw, GA 30144, USA
* Correspondence: bacharsc@du.ac.bd

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Abstract: Background: *Premna obtusifolia* (Lamiaceae) and *Oxalis corniculata* L. (Oxalidaceae) are two ethnomedicinal plants widely used in Bangladesh for the management of infections and inflammatory disorders. Although they belong to distinct botanical families and differ chemically, *P. obtusifolia* being rich in diterpenoids and *O. corniculata* abundant in flavonoids, both are traditionally associated with antioxidant and antimicrobial effects. The present study comparatively evaluated their methanolic extracts and solvent fractions using DPPH radical scavenging assay, total phenolic content (TPC) determination, and disc diffusion antimicrobial screening. Materials and Methods: After powdering the leaves and extracting them with methanol, the fractions were separated into n-hexane and chloroform. Using the DPPH radical scavenging experiment, antioxidant activity was evaluated, and IC_{50} values were computed. This was done using the disc diffusion method to measure antimicrobial activity. To determine the total phenolic content (TPC), the Folin–Ciocalteu technique was employed. To provide mechanistic insight, previously reported 14 phytochemicals from these species were subjected to molecular docking against human carbonyl reductase 1 (CBR-1; PDB ID: 4Z3D) and *Staphylococcus aureus* dihydrofolate reductase (DHFR; PDB ID: 2W9S). Results: The crude methanolic extract of *P. obtusifolia* showed an IC_{50} of 31 µg/mL, while *O. corniculata* exhibited stronger antioxidant activity (IC_{50} = 15.61 µg/mL). Both extracts demonstrated significant antimicrobial effects, whereas n-hexane and chloroform fractions showed moderate antimicrobial activity. The antioxidant potential of *P. obtusifolia* and *O. corniculata* was correlated with TPC values of 185.82 mg GAE/g and 154.90 mg GAE/g, respectively. Diosmetin-7-O-β-D-glucopyranoside, Quercetin, Arucadiol, and Swertisin demonstrated binding affinities comparable to reference ligands under the same docking conditions, according to molecular docking, indicating their potential as antioxidants and antimicrobials. Conclusion: The substantial antibacterial and antioxidant properties of the crude methanolic extracts support the traditional usage of *Oxalis corniculata* and *Premna obtusifolia* and suggest that these plants may be used as natural sources of bioactive chemicals for medicinal purposes.

Keywords: *Premna obtusifolia*; *Oxalis corniculate*; antioxidant; antimicrobial; total phenolic content

1. Introduction

Plants have long served as one of the most vital sources of medicine for humans. Since prehistoric times, human civilizations have relied on plants not only for food but also for treating various ailments. Traditional medical systems have emerged as a result of this dependence, especially in poor nations where as many as eighty percent of the people still uses herbal medicines for basic medical requirements [1,2]. Bioactive substances called phytochemicals, which have a variety of therapeutic qualities such as anti-inflammatory, anti-bacterial, anti-cancer and antioxidant effects, are primarily responsible for the pharmacological effectiveness of medicinal plants [3]. With advancements in phytochemical screening and drug discovery technologies, including high-throughput analysis, researchers can now analyze thousands of compounds weekly, facilitating the identification of new

therapeutic leads [4]. The structural diversity of naturally derived phytochemicals offers an invaluable resource for the development of novel, low-molecular-weight drug candidates, distinguishing them from conventional synthetic compounds [5]. Consequently, increasing attention has been directed toward plant-based drug discovery as a key area within complementary and alternative medicine (CAM) [6]. In Bangladesh, despite the country being rich in medicinal flora with over 500 documented medicinal plants still the scientific exploration and pharmacological validation of these species remain limited [7].

Premna obtusifolia (family: Lamiaceae) and *Oxalis corniculata* L. (family: Oxalidaceae) are notable among Bangladesh's numerous medicinal plants due to their ethnomedical significance and documented biological activity. *Premna obtusifolia* is a moderately sized plant that is native to the shoreline parts within the Andaman Islands and is also widely dispersed in Bangladesh, especially in the Sundarbans, Chittagong, and Sylhet districts. Indigenous communities refer to it as the "headache tree" or "Kritma" [8]. Being a member of the Lamiaceae family, which has more over 7000 varieties worldwide [9], *P. obtusifolia* is highly regarded for its antibacterial, analgesic as well as anti-inflammatory qualities. Traditionally, the leaves have been used to treat convulsions, rheumatism, fever and gastrointestinal disturbances, while the roots are used for stomachic and hepatic disorders [10,11]. Phytochemical investigations have identified bioactive constituents such as tannins, alkaloids, diterpenoids, and β-sitosterol from various parts of the plant, supporting its traditional use in folk medicine [12,13]. Similarly, *Oxalis corniculata* L., known locally as "Amrul" or "Amboli," is a small, herbaceous plant widely distributed across Bangladesh, including urban and rural regions such as Dhaka, Sylhet, and Chittagong. A member of the Oxalidaceae family, which comprises around 570 species, *O. corniculata* is recognized for its medicinal and nutritional value [14]. It has historically been used to cure fevers, skin disorders, scurvy, diarrhea, as well as dysentery. In addition to having cooling and antibacterial qualities, leaves are high in vitamin C. However, excessive intake may interfere with calcium absorption due to the high oxalate content [15]. Ethnobotanical reports from the Chittagong Hill Tracts also document its use by the Marma and Chakma communities to manage intestinal infections [11]. Pharmacologically, the plant exhibits antibacterial activity, particularly in alcoholic extracts that inhibit *Staphylococcus typhi* and *S. albus* at concentrations as low as 6.5 mg/mL [5]. Additionally, a crystalline compound isolated from the plant has demonstrated hypoglycemic effects in animal models [11].

Because of their importance in the treatment of infectious and chronic illnesses, plant-based pharmacological research has recently turned its attention to investigating antioxidant and antibacterial qualities. Age, diabetes, neurological illnesses, and cancer are all influenced by oxidative stress, which is caused by an excess of reactive oxygen species (ROS) such hydroxyl, superoxide, and hypochlorous acid [16–18]. Antioxidants neutralize these harmful radicals, thereby preventing cellular damage. The Brand-Williams approach, sometimes called the DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging test, is frequently used to assess the antioxidant capacity of plant compounds [19]. Concurrently, there has been a resurgence of interest in plant-derived chemicals having antibacterial and antifungal effects due to the growing issue of antimicrobial resistance. Alkaloids, tannins, glycosides, and flavonoids are examples of secondary metabolites that are known to stop microbial development in a number of ways [20]. Among the various *in vitro* methods for assessing antimicrobial activity, the agar disc diffusion technique is one of the most commonly employed. In this method, zones of inhibition around the sample-impregnated discs indicate antibacterial efficacy, which is measured in millimeters [21,22].

Although antioxidant and antimicrobial activities of *Oxalis corniculata* and several Premna species have been previously reported, comparative pharmacological evaluation of *P. obtusifolia* and *O. corniculata* collected from Bangladesh under a unified experimental framework remains limited. Furthermore, integration of *in vitro* bioassays with systematic molecular docking against mechanistically relevant antioxidant and antibacterial targets (CBR1 and *S. aureus* DHFR), followed by ADMET prioritization of reported phytoconstituents, has not been comprehensively performed for these species. Therefore, the present study adopts an integrated validation strategy to identify potential lead molecules while providing region-specific pharmacological evidence.

Although *Premna obtusifolia* and *Oxalis corniculata* belong to different botanical families and possess distinct phytochemical profiles, both are traditionally used in Bangladesh for similar therapeutic indications, particularly infections and inflammatory conditions. Investigating these two chemically diverse species under a unified experimental framework allows comparative evaluation of their antioxidant and antimicrobial potential while identifying phytochemical classes that may contribute to their biological activities. This approach provides ethnopharmacological validation rather than chemotaxonomic comparison and supports rational prioritization of bioactive scaffolds from locally available medicinal plants.

The current study intends to assess the antioxidant and antibacterial properties of the methanolic extracts and corresponding solvent fractions of *Premna obtusifolia* and *Oxalis corniculata* L. in light of their traditional and ethnopharmacological usage. Total phenolic content was also measured to assess its correlation with antioxidant

potential. This investigation seeks to provide scientific validation of the therapeutic claims associated with these plants and contribute to the search for novel natural compounds with pharmacological significance.

2. Materials and Methods

2.1. Plant Material Preparation and Collection

Fresh *Premna obtusifolia* leaves were gathered from the Khulna area, and *Oxalis corniculata* L. leaves were gathered from Sylhet, Bangladesh. The Bangladesh National Herbarium in Dhaka verified the authenticity of the plant specimens, and voucher samples were placed with accession numbers DACB-45941 for *P. obtusifolia* and DACB-45940 for *O. corniculata* L. After carefully washing the gathered leaves with clean water to get rid of dust and debris, they were then allowed to dry in the shade over a few days to stop the bioactive components from degrading. Once dried, the leaves were ground into a coarse powder utilizing a machine that grinds. Until they were used again in the experimental methods, the dried components were kept in clean, dry, sealed containers with the proper labels in a cool, dark place.

2.2. Extraction and Solvent-Solvent Partitioning

A total of 500 g of powdered leaf material from *Premna obtusifolia* and *Oxalis corniculata* L. were subjected to cold maceration in 2 L of methanol. The mixtures were kept in tightly sealed containers and stirred intermittently over a period of 15 days at room temperature to ensure efficient extraction of phytoconstituents. Following extraction, Whatman No. 1 filter paper was used to filter the extracts. The raw extracts were then obtained by concentrating the filtrates at low temperature and decreased pressure in a rotary evaporator. The rough methanolic portion yields were 20.08 g for *P. obtusifolia* and 15 g for *O. corniculata* L. Following extraction, each crude extract was resuspended in 50 mL of a solvent system consisting of 90% distilled water and 10% methanol to remove impurities. Following the transfer of the resultant solution into a separatory funnel, n-hexane along with chloroform was used in a sequential manner to perform liquid-liquid partitioning. Initially, 50 mL of n-hexane was included in the aqueous suspension and then five minutes of vigorous shaking were applied to the mixture. The upper organic layer (n-hexane fraction) was collected, and the process was repeated to ensure maximum extraction. The remaining aqueous layer was then subjected to a similar partitioning process using 50 mL of chloroform. After two rounds of extraction, the chloroform layers were also collected. For further biological and phytochemical investigations, the separated organic fractions such as n-hexane and chloroform as well as the leftover aqueous fractions were concentrated using an evaporator that rotates and kept in airtight containers. The obtained fractions were designated as follows: HMEPO (n-hexane fraction of *P. obtusifolia* methanolic extract), MMEPO (methanol fraction of *P. obtusifolia*), CMEPO (chloroform fraction of *P. obtusifolia*), HMEOC (n-hexane fraction of *O. corniculata*), MMEOC (methanol fraction of *O. corniculata*), and CMEOC (chloroform fraction of *O. corniculata*). These coded designations were consistently used throughout biological evaluations.

2.3. Anti-Oxidant Activity Test

2.3.1. Activity of Free Radical Scavenging by DPPH Assay

The antioxidant potential of *Premna obtusifolia* and *Oxalis corniculata* L. was evaluated using the 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging assay [1,2]. This method is based on the reduction of the purple-colored DPPH radical to a yellow-colored diphenylpicrylhydrazine upon reaction with antioxidant compounds. A DPPH stock solution (20 µg/mL) was prepared in methanol. The plant extracts were initially dissolved in ethanol to obtain a stock solution of 1000 µg/mL, from which serial dilutions were prepared. The final concentrations used for IC_{50} determination were 31.25, 62.5, 125, 250, and 500 µg/mL. For each concentration, 2 mL of DPPH solution was mixed with the extract solution to make a final volume of 4 mL. The reaction mixtures were incubated in the dark at room temperature for 30 min. After incubation, absorbance was measured at 517 nm using a UV–Vis spectrophotometer. A decrease in absorbance indicated increased free radical scavenging activity. Ascorbic acid and tert-butyl-1-hydroxytoluene (BHT) were used as positive controls for comparison.

The percentage of DPPH radical inhibition was calculated using the following equation:

$$\text{Inhibition (\%)} = [1 - (\text{Absorbance of control}/\text{Absorbance of sample})] \times 100$$

All antioxidant experiments were performed in triplicate (n = 3), and results were expressed as mean ± standard deviation. IC_{50} values were determined by nonlinear regression analysis of percentage inhibition versus concentration using Microsoft Excel. The IC_{50} value was defined as the concentration of extract required to scavenge 50% of DPPH radicals and was used as an indicator of antioxidant capacity.

2.3.2. Total Phenolic Content Measured with the Folin-Ciocalteu Reagent

Gallic acid was used as the standard phenolic compound in the Folin–Ciocalteu colorimetric technique to assess the total phenolic content (TPC) of the crude methanolic extracts of *Premna obtusifolia* and *Oxalis corniculata* L. [23]. This approach is predicated on the oxidation of phenolic compounds by the Folin–Ciocalteu reagent, resulting in a quantifiable blue complex spectrophotometrically. For the assay, 1 mg of each crude extract was dissolved in methanol. An aliquot of 0.2 mL of the diluted extract was mixed with 0.1 mL of Folin–Ciocalteu reagent. Once the mixture has had time to react for 5 min at room temperature, 2.0 mL of sodium bicarbonate solution (70 g/L) was added. The reaction mixture was then incubated for 30 min in the dark at room temperature. The absorbance was determined at 765 nm using a UV-visible spectrophotometer. A calibration curve was prepared using gallic acid solutions of known concentrations (0–250 μg/mL), and the amounts of gallic acid on the x-axis were plotted against the absorbance values on the y-axis. The standard curve was used to determine the plant extracts' total phenolic content, which was then reported as milligrams of gallic acid equivalents (mg GAE) per gram of dry extract.

2.4. Antibacterial Activity Test

2.4.1. Bacterial Strains Used as Test Organisms

Pure cultures of bacterial strains were acquired from the Biomedical Research Lab, Curzon Hall, University of Dhaka. The test organisms comprised both Gram-positive (*Bacillus cereus*, *Bacillus subtilis*) and Gram-negative (*Salmonella paratyphi*, *Escherichia coli*) bacteria. These strains were selected based on their clinical relevance and prevalence in infectious diseases.

2.4.2. Antibacterial Activity Using Disc Diffusion Technique

The conventional disc diffusion method was used to assess the antibacterial properties of the raw methanolic isolates of *Premna obtusifolia* and *Oxalis corniculata* L. [3]. Bacterial cultures were grown within nutrient-rich broth and maintained at 37 °C for 24 h. Methanol was used to dissolve the plant extracts, resulting in concentrations of 200 and 400 μg/disc. Mueller-Hinton agar plates that had previously been inoculated with suspensions of bacteria were covered with sterile filter paper discs (6 mm in diameter) that had been soaked with the extract solution. A disc impregnated with methanol served as the negative control, while a standard antibiotic disc containing Ciprofloxacin (5 μg/disc) was used as the positive control. For a whole day, the plates were incubated at 37 °C. Following incubation, the antimicrobial activity was assessed by measuring the diameter of the zone of inhibition around each disc in millimeters. Every experiment was carried out in triplicate, and the mean ± standard deviation was used to report the results. The disc diffusion assay provides a preliminary assessment of antimicrobial activity and does not determine minimum inhibitory concentration (MIC) or minimum bactericidal concentration (MBC). Therefore, further quantitative assays are required to confirm potency.

2.5. Antifungal Activity Test

2.5.1. Fungal Strains Used as Test Organisms

Saccharomyces cerevisiae, *Aspergillus niger*, and *Candida albicans* were among the fungus strains acquired from the University of Dhaka's Biomedical Research Laboratory in Curzon Hall. These fungi were selected based on their importance in clinical and foodborne infections.

2.5.2. Antifungal Activity by Disc Diffusion Approach

The antifungal properties of the plant extracts was assessed by means of the disc diffusion method [3]. Fungal cultures were uniformly inoculated on Potato Dextrose Agar (PDA) plates. Sterile filter paper discs were impregnated with plant extract solutions (200 and 400 μg/disc in methanol) and placed on the agar surface. Griseofulvin discs served as the positive control, while methanol-loaded discs served as the negative control. For a whole day, the plates were placed in incubators at 28 °C. The diameter of the zones of inhibition surrounding each disc, measured in millimeters, was used to assess the antifungal efficacy following incubation. The data were displayed as mean ± standard deviation, and each test was run in triplicate. The disc diffusion assay provides a preliminary assessment of antimicrobial activity and does not determine minimum inhibitory concentration (MIC) or minimum bactericidal concentration (MBC). Therefore, further quantitative assays are required to confirm potency.

2.6. In-Silico Molecular Docking Study of Major Bioactive Compounds Reported from Both Crude Extracts

To explore potential molecular interactions, computational docking analyses were carried out using major phytochemicals previously reported from *Oxalis corniculata* and *Premna obtusifolia* [24,25]. These compounds were selected based on documented phytochemical investigations and were not isolated in the present study. Structural details, including molecular formula, molecular weight, PubChem CID, and canonical SMILES, were retrieved from the PubChem database to construct a curated ligand library. Two-dimensional structures were prepared in ChemDraw and converted into optimized three-dimensional conformations prior to docking.

Drug-likeness and pharmacokinetic characteristics were assessed using SwissADME and ProTox-3.0 platforms to predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties. The crystallographic structures of the target proteins were downloaded from the RCSB Protein Data Bank. Ligand preparation involved hydrogen addition and energy minimization using BIOVIA Discovery Studio, followed by conversion to PDB format. Protein structures were refined by removing crystallographic water molecules, co-crystallized ligands, and non-essential heteroatoms while retaining the appropriate chain, after which energy minimization was performed using Swiss-PDB Viewer.

Docking simulations were conducted using AutoDock Vina integrated within the PyRx environment. A blind docking strategy was applied by defining a grid box large enough to cover the entire protein surface, allowing unbiased identification of potential binding regions. Grid dimensions were defined in angstrom units (Å). The exhaustiveness parameter was set to 8, and nine binding conformations were generated for each ligand. Binding poses were clustered using a root-mean-square deviation (RMSD) threshold of 2.0 Å, and the lowest-energy conformation from the most populated cluster was selected for further analysis. Interaction visualization and examination of hydrogen bonding, hydrophobic contacts, and bond distances were performed using PyMOL and BIOVIA Discovery Studio Visualizer.

Although this workflow enables initial screening of ligand–protein interactions, it should be emphasized that redocking validation with native co-crystallized ligands was not undertaken. Furthermore, advanced post-docking refinement methods such as MM-GBSA rescoring or molecular dynamics simulations were beyond the scope of this study. Consequently, the reported binding affinities should be regarded as preliminary computational indicators intended for prioritizing candidate compounds rather than definitive evidence of binding stability or biological efficacy.

2.7. Statistical Analysis

All experiments were conducted in triplicate (n = 3), and data are expressed as mean ± standard deviation (SD). Statistical analysis was performed using IBM SPSS version 26.0. Differences among multiple groups were analyzed using one-way analysis of variance (ANOVA), followed by Tukey's post hoc test where appropriate. A p-value < 0.05 was considered statistically significant.

3. Results

3.1. Antioxidant Activity Test

3.1.1. DPPH Based Free Radical Scavenging Activity

The methanolic extracts' antioxidant capacity of *Premna obtusifolia* and *Oxalis corniculata* L. leaves was assessed using the DPPH radical scavenging assay, with the standard baseline being ascorbic acid. The indicator of antioxidant potential was the IC_{50} value, which is the concentration needed to scavenge 50% of DPPH free radicals. The methanolic portion of *Oxalis corniculata* L. exhibited the highest antioxidant action, with an IC_{50} value of 15.61 µg/mL. The extract of *Premna obtusifolia* also demonstrated significant radical scavenging activity, yielding an IC_{50} value of 31 µg/mL. In comparison, the standard antioxidant ascorbic acid showed the strongest activity, with an IC_{50} value of 9.48 µg/mL. These findings suggest that both plant extracts possess notable antioxidant properties, with *Oxalis corniculata* L. being more potent than *Premna obtusifolia*. The IC_{50} values of the test samples and standard are graphically represented in Figure 1.

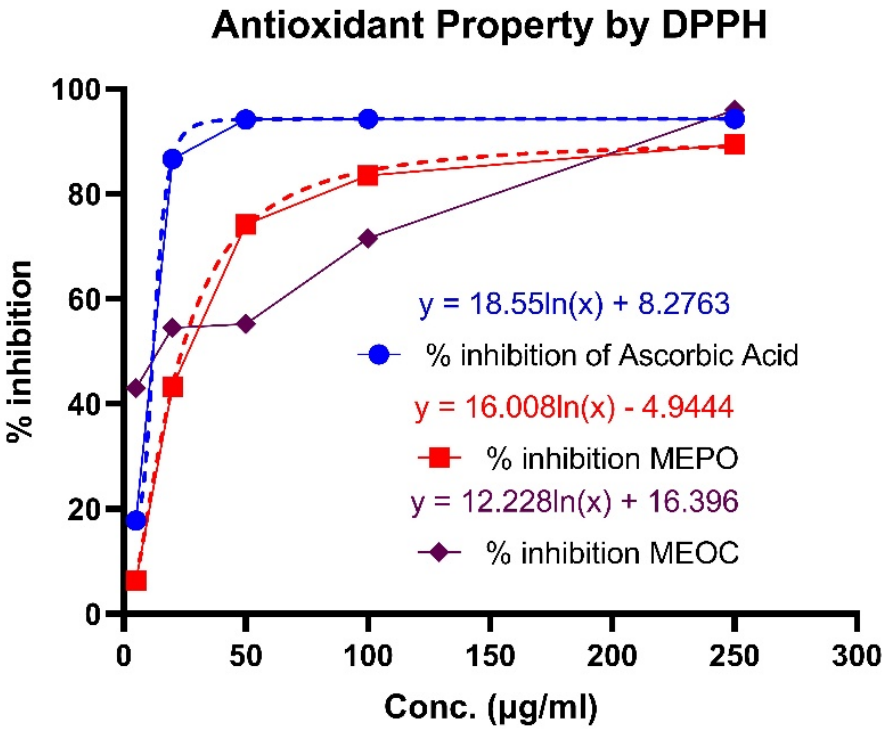


Figure 1. Antioxidant potential (IC_{50} values) of ascorbic acid (standard), methanol extract of *Premna obtusifolia* (MEPO), and methanol extract of *Oxalis corniculata* L. (MEOC) as determined by DPPH free radical scavenging assay. Lower IC_{50} values indicate higher antioxidant activity.

3.1.2. Total Phenolic Content Measured with the Folin-Ciocalteu Reagent

Phenolic content overall (TPC) of the methanolic extracts of *Premna obtusifolia* and *Oxalis corniculata* L. was determined utilizing the Folin–Ciocalteu colorimetric assay. The results were reported in milligrams of gallic acid equivalents per gram of dry extract (mg GAE/g), with gallic acid serving as the benchmark. A curve of calibration was constructed with gallic acid standard solutions, and the final equation was $Y = 0.011X + 0.156$ with an association coefficient of $R^2 = 0.947$, where X is the phenolics concentration in mg GAE/g and Y is the absorbance at 765 nm. (Figure 2). Based on the standard curve, the methanolic extract of *Premna obtusifolia* exhibited a higher phenolic concentration of 185.82 mg GAE/g**,** while *Oxalis corniculata* L. exhibited a slightly lower but still substantial content of 154.90 mg GAE/g. These values indicate a strong existence of phenolic substances in both extracts from plants, suggesting a possible correlation with their observed antioxidant activities. The detailed values of phenolic content overall are summarized in Table 1. To further explore the relationship between phenolic content and antioxidant activity, Pearson correlation analysis was performed between total phenolic content (TPC) and DPPH IC_{50} values. A negative correlation was observed ($r = -0.91$), indicating that higher phenolic content is associated with stronger radical scavenging activity. Although based on a limited number of samples, this quantitative analysis supports the proposed contribution of phenolic compounds to antioxidant potential.

Table 1. Total phenolic content of methanol extract of *Premna obtusifolia* (MEPO) and *Oxalis corniculata* L. (MEOC).

Plant Extract	Absorbance	Average	Total Phenolic Content (mg/g GAE)
MEPO	2.23 2.20 2.18	2.20	185.82 mg
MEOC	1.89 1.86 1.83	1.86	154.90 mg

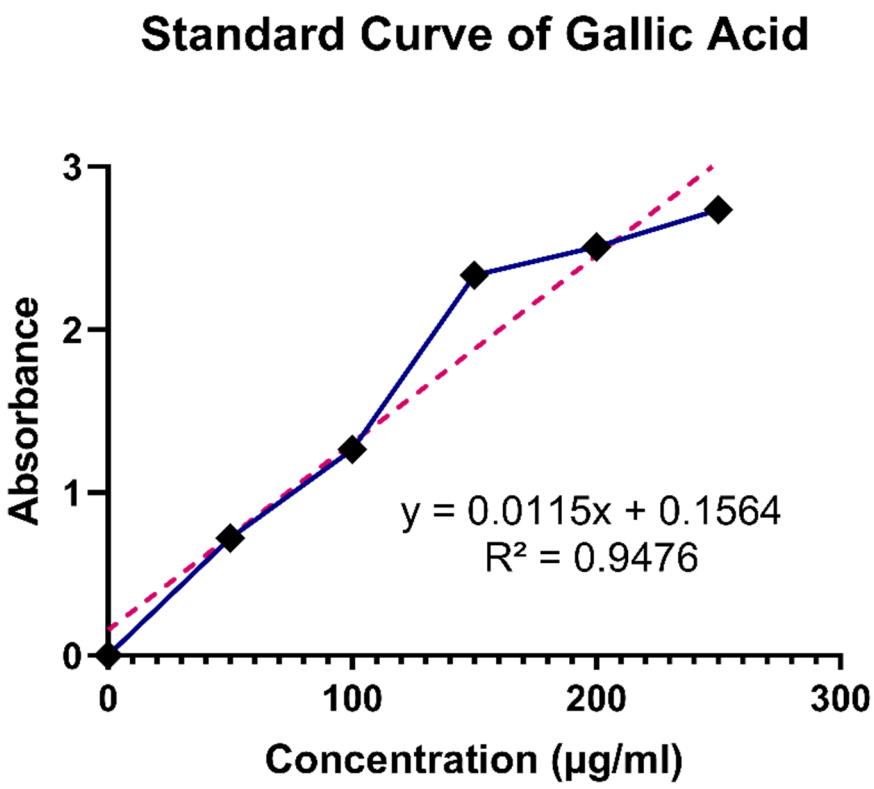


Figure 2. Standard curve for galic acid for total phenolic content determination.

3.2. Antimicrobial Activity

The antimicrobial potential of the methanolic extracts and their respective solvent fractions (n-hexane, methanol, and chloroform) of *Premna obtusifolia* and *Oxalis corniculata* L. was evaluated in comparison to a panel of thirteen bacterial strains and three fungal strains using the disc diffusion method. The antibacterial and antifungal assays employed griseofulvin and ciprofloxacin (20 µg/disc) as positive controls, accordingly, and methanol as the negative control.

3.2.1. Antibacterial Activity

All test extracts demonstrated varying degrees of antibacterial activity. The methanol fraction of *Oxalis corniculata* (MMEOC) exhibited the highest antibacterial activity, particularly at 400 µg/disc, showing significant zones of inhibition against *Bacillus megaterium* (14.67 ± 0.58 mm), *Escherichia coli* (14 ± 1 mm), *Salmonella typhi* (14 ± 1 mm), and *Shigella boydii* (13.33 ± 2.08 mm). Similarly, the methanol fraction of *Premna obtusifolia* (MMEPO) also showed appreciable zones of inhibition against *Salmonella paratyphi* (12.67 ± 2.08 mm) and *Bacillus cereus* (12.33 ± 1.53 mm). The chloroform and n-hexane fractions of both plants displayed mild to moderate antibacterial effects, generally ranging from 6 to 11 mm in zone diameter. Among all fractions, the methanol-soluble ones consistently showed higher antibacterial activity, indicating better solubility and bioavailability of active constituents in methanol. However, all plant extracts produced significantly lower inhibition zones compared to the standard antibiotic ciprofloxacin (25–27.33 mm), indicating moderate but promising antibacterial potential ($p < 0.05$). Table 2 displays the comprehensive antimicrobial information. Significant differences were observed among groups (one-way ANOVA, $p = 0.032$).

Table 2. Zone of inhibition diameter of the methanolic extract of *Oxalis corniculate* L. and *Premna obtusifolia*.

Test Microorganism	Diameter of Zone of Inhibition (mm)												
	Standard	HMEPO		MMEPO		CMEPO		HMEOC		MMEOC		CMEOC	
	20 µg/disc	200 µg/disc	400 µg/disc	200 µg/disc	400 µg/disc	200 µg/disc	400 µg/disc	200 µg/disc	400 µg/disc	200 µg/disc	400 µg/disc	200 µg/disc	400 µg/disc
Bacteria													
Bacillus cereus	25.67 ± 2.89	8.33 ± 1.53	10.67 ± 1.53	8.00 ± 1.73	12.33 ± 1.53	8.33 ± 0.58	11.00 ± 1.00	7.33 ± 1.53	11.33 ± 3.21	8.33 ± 1.15	13.00 ± 0.00	8.00 ± 2.00	9.67 ± 0.58
Bacillus megaterium	25.00 ± 1.73	8.67 ± 0.58	10.00 ± 1.00	7.00 ± 1.00	11.67 ± 1.53	8.00 ± 1.73	10.67 ± 2.89	7.33 ± 2.31	14.67 ± 0.58	7.00 ± 1.00	10.67 ± 2.08	8.33 ± 2.08	9.33 ± 1.15
Bacillus subtilis	25.67 ± 1.73	9.33 ± 0.58	10.33 ± 0.58	7.33 ± 1.53	11.67 ± 3.06	7.33 ± 1.15	10.67 ± 0.58	8.67 ± 1.15	10.67 ± 0.58	8.33 ± 1.53	13.33 ± 0.58	7.67 ± 0.58	11.00 ± 1.73
Salmonella paratyphi	26.00 ± 1.00	8.33 ± 2.08	9.33 ± 0.58	7.33 ± 1.53	12.67 ± 2.08	7.67 ± 1.15	13.00 ± 2.65	7.33 ± 2.31	13.00 ± 2.00	8.33 ± 2.08	13.00 ± 1.73	8.33 ± 0.58	10.00 ± 1.00
Salmonella typhi	27.33 ± 2.31	8.00 ± 1.73	10.67 ± 1.53	6.67 ± 1.15	9.67 ± 2.08	6.67 ± 0.58	10.67 ± 1.53	7.67 ± 1.53	14.00 ± 1.00	8.67 ± 1.15	10.33 ± 0.58	9.33 ± 0.58	10.33 ± 2.08
Vibrio parahemolyticus	27.33 ± 1.15	7.67 ± 1.53	9.33 ± 2.31	7.67 ± 1.53	13.00 ± 1.73	7.67 ± 1.53	11.33 ± 2.08	8.33 ± 2.08	10.00 ± 1.00	9.33 ± 0.58	13.67 ± 0.58	7.33 ± 1.15	9.67 ± 1.53
Vibrio mimicus	26.67 ± 2.52	8.67 ± 2.31	10.67 ± 0.58	6.67 ± 1.15	9.33 ± 1.15	7.33 ± 1.53	10.67 ± 1.53	6.67 ± 1.15	12.00 ± 3.00	7.67 ± 1.53	13.00 ± 2.00	8.00 ± 2.00	10.67 ± 1.53
Staphylococcus aureus	27.33 ± 1.53	8.00 ± 2.00	11.00 ± 1.73	6.67 ± 1.15	11.00 ± 2.65	6.67 ± 0.58	11.33 ± 3.21	6.33 ± 0.58	12.33 ± 2.08	7.67 ± 1.53	13.33 ± 2.08	7.33 ± 1.53	8.67 ± 0.58
E. coli	27.00 ± 1.00	7.67 ± 1.15	10.33 ± 1.15	6.00 ± 0.00	12.00 ± 1.73	7.67 ± 0.58	12.33 ± 1.53	7.33 ± 1.15	14.00 ± 1.00	7.67 ± 1.53	11 ± 1.73	8.00 ± 2.00	10.33 ± 1.53
Shigella dysenteriae	25.67 ± 1.53	7.33 ± 1.15	10.00 ± 1.00	8.00 ± 1.73	11.33 ± 0.58	7.00 ± 1.73	10.33 ± 2.31	8.67 ± 1.53	11.00 ± 2.00	7.33 ± 2.31	11 ± 1.73	8.67 ± 1.53	10.67 ± 1.53
Pseudomonas aeruginosa	27.00 ± 2.00	7.00 ± 1.00	9.00 ± 1.73	8.67 ± 0.58	9.67 ± 2.89	8.67 ± 0.58	11.00 ± 1.73	8.67 ± 0.58	9.67 ± 1.15	7.67 ± 2.08	13.00 ± 1.00	6.67 ± 1.15	10.33 ± 2.08
Sarcina lutea	25.67 ± 0.58	8.67 ± 1.53	8.67 ± 2.31	7.33 ± 1.53	9.33 ± 0.58	7.67 ± 1.53	11.33 ± 3.21	7.67 ± 2.08	10.00 ± 0.00	8.67 ± 1.53	11.33 ± 2.31	7.00 ± 1.73	10.33 ± 1.53
Shigella boydii	27.33 ± 2.52	8.67 ± 1.53	10.33 ± 0.58	7.33 ± 1.15	11.33 ± 3.06	7.33 ± 1.15	11.67 ± 1.53	8.00 ± 2.00	11.33 ± 1.53	7.33 ± 2.31	9.67 ± 0.58	10.67 ± 1.15	13.33 ± 2.08
Fungus													
Saccharomyces cerevisiae	26.67 ± 2.08	9.67 ± 0.58	10.33 ± 0.58	6.33 ± 0.58	12.00 ± 3.00	7.33 ± 1.53	14.33 ± 1.15	8.33 ± 2.08	10.67 ± 1.53	7.67 ± 1.53	11.33 ± 1.53	8.67 ± 1.15	8.67 ± 1.15
Candida albicans	27.67 ± 2.08	8.33 ± 1.15	10.00 ± 2.00	8.33 ± 0.58	9.33 ± 2.31	7.67 ± 1.53	13.33 ± 2.89	9.33 ± 0.58	11.33 ± 2.52	8.67 ± 2.31	13.00 ± 1.00	7.67 ± 2.08	9.33 ± 1.15
Aspergillus niger	26.33 ± 2.52	6.67 ± 1.15	8.67 ± 0.58	7.00 ± 1.00	11.00 ± 2.65	7.67 ± 1.53	12.67 ± 2.52	7.33 ± 1.15	12.67 ± 2.08	9.33 ± 0.58	12.33 ± 3.06	9.33 ± 1.15	10.33 ± 0.58

3.2.2. Antifungal Activity

The assessment of antifungals revealed that all extracts demonstrated weak to medium efficacy against *Aspergillus niger*, *Candida albicans*, and *Saccharomyces cerevisia* species. Among them, the portion of methanol of *Oxalis corniculata* (MMEOC) at 400 µg/disc showed the highest antifungal activity, with inhibition zones of 14.33 ± 1.15 mm against *S. cerevisiae* and 13.33 ± 2.89 mm against *C. albicans*. The methanol fraction of *Premna obtusifolia* (MMEPO) also showed moderate activity with inhibition zones up to 12 mm. The n-hexane and chloroform fractions demonstrated relatively lower antifungal effects, with inhibition zones generally below 10 mm. All plant extracts showed significantly ($p < 0.05$) smaller inhibition zones than the standard antifungal agent griseofulvin, which exhibited zones exceeding 26 mm against all tested fungi. Significant differences were observed among groups (one-way ANOVA, $p = 0.041$). These results suggest that methanol extracts, particularly from *Oxalis corniculata* L., possess promising antimicrobial properties, supporting their traditional use in treating infectious diseases.

All examined bacterial strains showed considerably ($p < 0.05$) lower zones of inhibition values for MEPO and MEOC than for conventional ciprofloxacin and Griseofulvin. The results are shown as the mean ± SD of three separate tests. Abbreviations: *Premna obtusifolia* methanolic extract's n-hexane portion (HMEPO), Methanol portion of *Premna obtusifolia'*s methanolic extract (MMEPO), Chloroform fraction of methanolic extract of *Premna obtusifolia* (CMEPO), n-Hexane fraction of methanolic extract of *Oxalis corniculata* L. (HMEOC), Methanol fraction of methanolic extract of *Oxalis corniculata* L. (MMEOC), Chloroform fraction of methanolic extract of *Oxalis corniculata* L. (CMEOC).

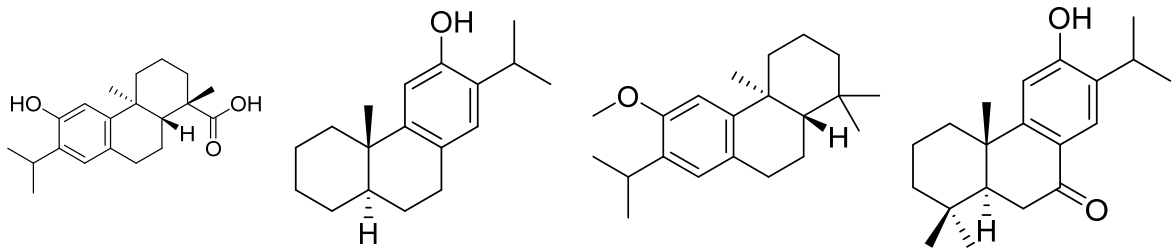
3.3. Molecular Docking and ADMET Study of Previously Reported Major Compounds

All 14 compounds reported from *Oxalis corniculata* and 10 reported from *Premna obtusifolia* satisfied Lipinski's rule of five criteria (molecular weight < 500 Da, hydrogen bond donors < 5, hydrogen bond acceptors < 10, logP < 5, adequate water solubility) and exhibited drug-like ADMET profiles, justifying their selection for molecular docking (Figures 3 and 4). Compound (**8**) demonstrated optimal pharmacokinetics with high absorption, moderate solubility, low clearance, and no hepatotoxicity, carcinogenicity, mutagenicity, or cytotoxicity. Compound (**5**), (**7**), (**13**), (**14**), (**19**), (**20**) and (**21**) also showed favorable toxicity profiles.

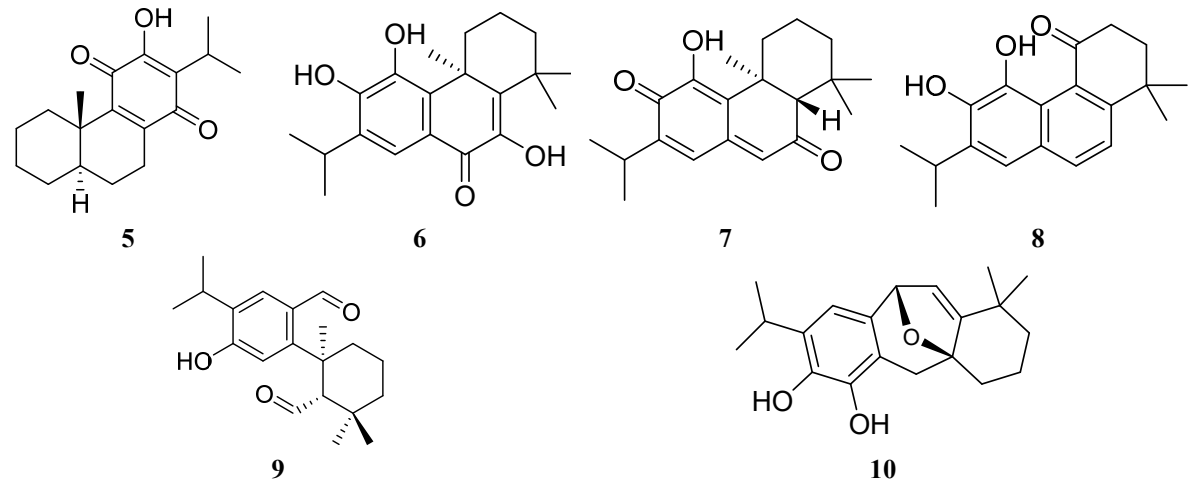
For antioxidant activity, compounds were docked against human carbonyl reductase 1 (CBR-1; PDB ID: 4Z3D) using β-carotene as standard (−8.5 kcal/mol) (Figure 5). The grid box was centered at X = −0.0146, Y = 0.0172, and Z = 33.2897 Å, with dimensions of 90.4202 × 91.1517 × 92.4536 Å. From *Oxalis corniculata*, compound (**18**) and (**13**) achieved the highest binding affinities of −9.4 kcal/mol, followed by compound (**14**) (−9.2 kcal/mol), compound (**21**) (−9.1 kcal/mol), compound (**20**) (−8.7 kcal/mol), and compound (**17**) (−8.6 kcal/mol) (Table 3, Figure 6). From *Premna obtusifolia*, Compound (**8**) exhibited −9.4 kcal/mol affinity, with compound (**6**) (−7.8 kcal/mol), compound (**7**) (−7.6 kcal/mol), compound (**5**) (−7.4 kcal/mol), and compound (**10**) (−7.4 kcal/mol) showing moderate binding (Table 4).

For antimicrobial activity, docking targeted Staphylococcus aureus dihydrofolate reductase (DHFR; PDB ID: 2W9S) using ceftriaxone as standard (−9.0 kcal/mol) (Figure 5). The grid box measured 48.9284 Å (X), 44.9892 Å (Y), and 58.2850 Å (Z), centered at X = −0.7507, Y = −0.2193, Z = 0.3092. Compound (**14**) from *Oxalis corniculata* showed the highest affinity of −10.0 kcal/mol, followed by compound (**17**) (−9.2 kcal/mol), compound (**20**) (−9.0 kcal/mol), and compound (**16**) (−9.0 kcal/mol) (Table 5, Figure 6). From *Premna obtusifolia*, compound (**8**) achieved −9.4 kcal/mol, with compound (**5**) demonstrating comparable efficacy (Table 6).

Protein-ligand interactions revealed extensive hydrogen bonding, π-π stacking, and hydrophobic contacts in the active sites of both targets (Figure 6. All top-ranking compounds exhibited binding energies superior to or comparable with standards. ADMET profile of the major compounds from *Premna obtusifolia* and *Oxalis corniculate* are mentioned in Table 7 and 8.



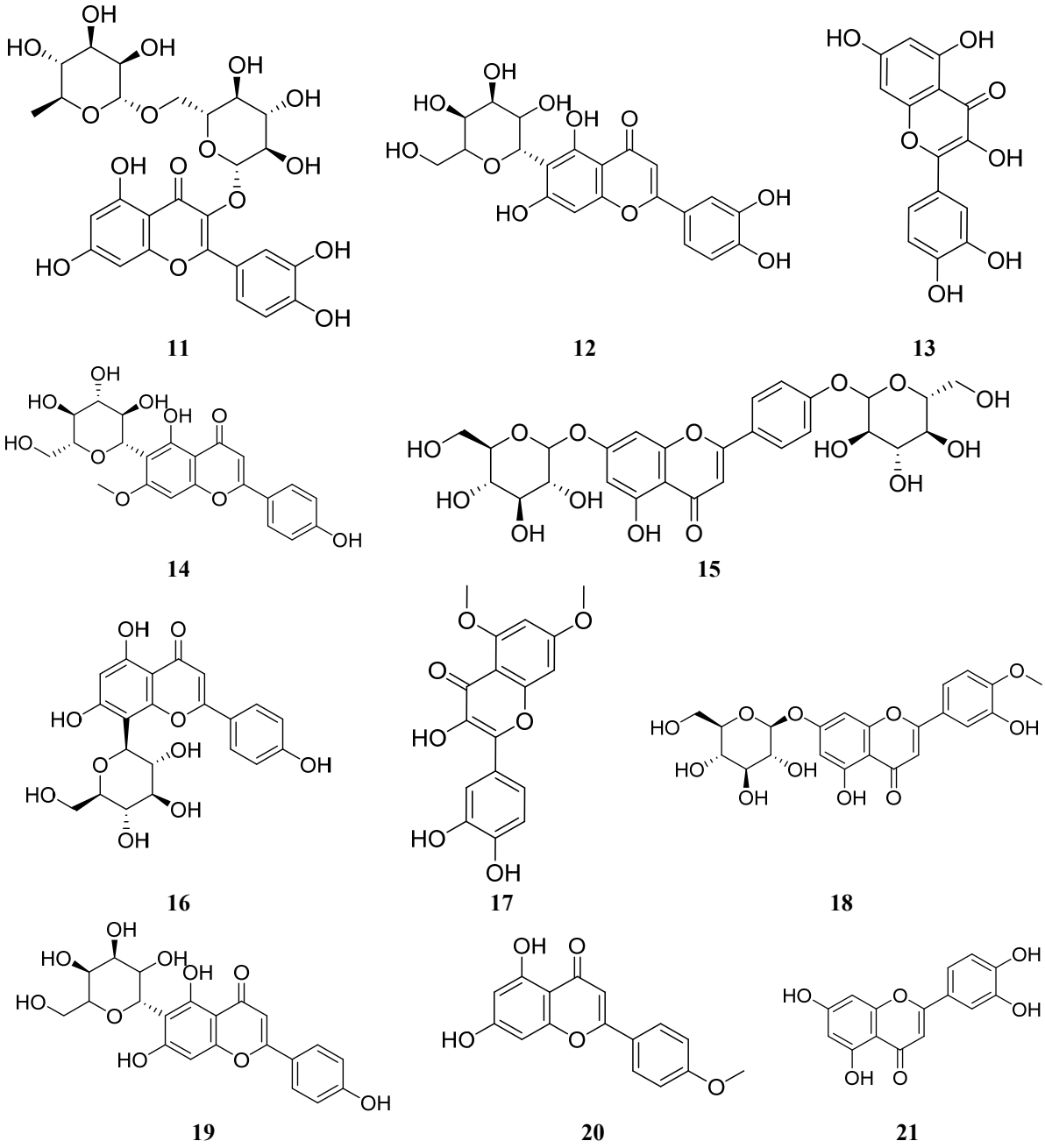
1 **2** **3** **4**



5 **6** **7** **8**

9 **10**

Figure 3. Structures of compounds from *Premna obtusifolia* [25]. Lambertic (**1**), Ferruginol (**2**), O-methyl ferruginol (**3**), Sugiol (**4**), Royleanone (**5**), 14-deoxycoleon (**6**), Taxodion (**7**), Arucadiol (**8**), 12-hydroxy-6,7-secoabieta-8,11,13-triene-6,7-dial (**9**), Salviasperanol (**10**).



11 **12** **13**

14 **15**

16 **17** **18**

19 **20** **21**

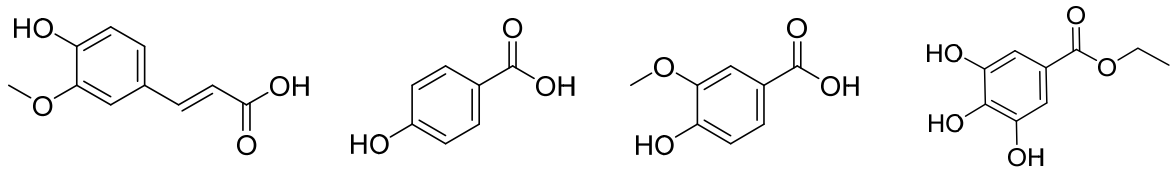


Figure 4. Compounds isolated from *Oxalis corniculate* [24]. Rutin (**11**), Isoorientin (**12**), Quercetin (**13**), Swertisin (**14**), Apigenin 7,4′-diglucoside (**15**), Vitexin (**16**), 5,7-dimethoxy-3,3′,4′-trihydroxy flavone (**17**), Diosmetin-7-O-beta-D-glucopyranoside (**18**), Isovitexin (**19**), Acacetin (**20**), Luteolin (**21**), Ferulic acid (**22**), p-Hydroxybenzoic acid (**23**), Vanillic Acid (**24**), Ethyl gallate (**25**).

The RCSB protein Data Bank provided the 3D crystal structure of human CBR-1 protein (PDB ID: 4Z3D) and dihydrofolate reductase protein (PDB ID: 2W9S) of *Staphylococcus aureus,* determined by X-ray diffraction. Figure 5 shows these protein's 3D structure.

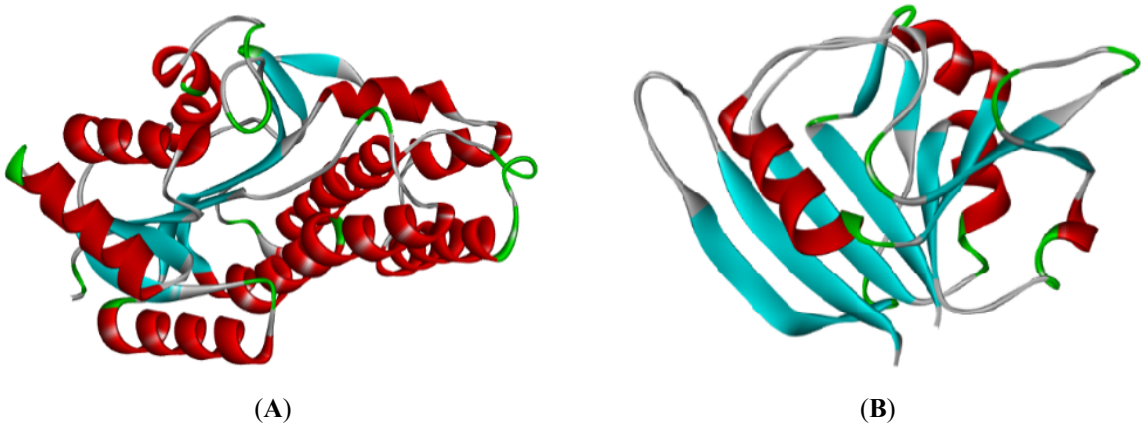


Figure 5. The 3D structure of selected target protein (**A**) CBR-1 protein (PDB ID: 4Z3D) and (**B**) dihydrofolate reductase protein (PDB ID: 2W9S).

Table 3. Binding affinity of ligands (*Oxalis corniculata*) with targeted protein CBR-1 (PDB ID: 4Z3D).

SL No.	Ligands	Binding Affinity (kcal/mol)	Interacting Amino Acids
1	Beta Carotene (Control)	−8.5	Ala235(A), Val230(A), Met234(A), Ile16(A), Val137(A), Pro227(A), Ile92(A), Phe94(A)
2	Diosmetin-7-O-beta-D-glucopyranoside	−9.4	Ala235(A), Met234(A), Phe94(A), Lys14(A), Trp229(A), Pro227(A), Ile16(A)
3	Quercetin	−9.4	Pro227(A), Lys197(A), Lys14(A), Asn89 (A), Gly228(A), Met234(A), Ile16(A)
4	Swertisin	−9.2	Phe94(A), Ala235(A), Trp229(A), Met234(A), Ile16(A), Pro227(A), Lys14(A)
5	Luteolin	−9.1	Met234(A), Ala235(A), Val230(A), Ile16(A), Pro227(A), Lys197(A), Tyr193(A), Asn89(A), Gly91(A)
5	Acacetin	−8.7	Lys197(A), Ser138(A), Gly228(A), Ile16(A), Pro227(A), Met234(A), Lys14(A)
6	5,7-dimethoxy-3,3′, 4′-trihydroxy flavone	−8.6	Pro227(A), Ile16(A), Met234(A), Gly238(A), Ser138(A), Lys14(A), Lys197(A)
7	5-hydroxy-6,7,8, 4′-tetra methoxy flavone	−8.4	Pro227(A), Ile16(A), Met234(A), Gly17(A), Gly91(A), Ile92(A), Asn89(A), Asn13(A), Lys14(A)
8	Vitexin	−8.2	Ile16(A), Met234(A), Ala93(A), Asn13(A), Lys14(A)
9	Isovitexin	−7.8	Leu27(A), Asp84(A), Leu255(A), Pro135(A), His5(A)
10	Ferulic acid	−6.3	Pro227(A), Ile16(A), Met234(A), Gly17(A), Gly228(A), Ile16(A), Asn89(A), Val230(A), Tyr193(A)

Table 4. Binding affinity of ligands (*Premna obtusifolia*) with targeted protein CBR-1 protein (PDB ID: 4Z3D).

SL No.	Ligands	Binding Affinity (kcal/mol)	Interacting Amino Acids
1	Beta Carotene (Control)	−8.5	Ala235(A), Val230(A), Met234(A), Ile16(A), Val137(A), Pro227(A), Ile92(A), Phe94(A)
2	Arucadiol	−7.9	Asp84(A), Arg133(A), Pro258(A), His5(A)
3	14-deoxycoleon	−7.8	Pro258(A), Pro130(A), Leu20(A), His5(A), Phe28(A)
4	Taxodion	−7.6	Pro258(A), Gln131(A), Leu255(A), His5(A), Phe28(A)

Table 4. *Cont.*

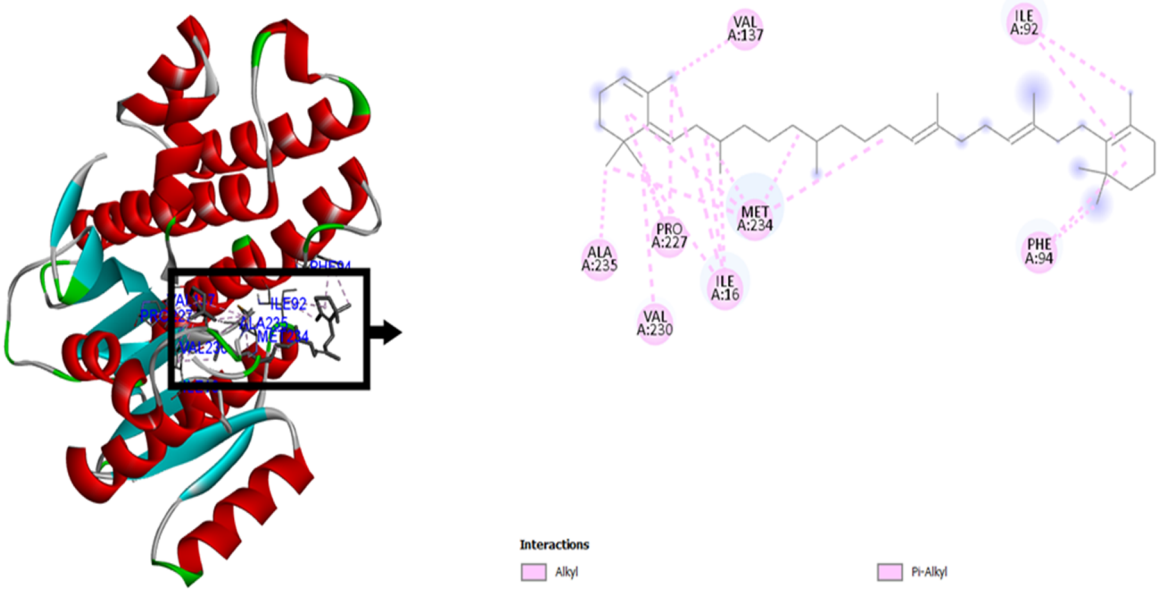
SL No.	Ligands	Binding Affinity (kcal/mol)	Interacting Amino Acids
5	Salviasperanol	−7.4	Pro258(A), Leu255(A), Leu256(A), His5(A), Phe28(A), Leu27(A), Ser29(A)
6	Royleanone	−7.4	Leu255(A), His5(A), Phe28(A), Pro258(A)
7	Ferruginol	−7.3	His183(A), Lys95(A), Phe102(A), Gln105(A)
8	Sugiol	−7.2	Lys197(A), Ile16(A), Tyr193(A), Met234(A), Pro227(A)
9	O-methyl ferruginol	−6.9	Asp84(A), Leu255(A), His5(A), Phe28(A), Pro227(A)

Table 5. Binding affinity of ligands (*Premna obtusifolia*) with targeted protein dihydrofolate reductase (PDB ID: 2W9S).

SL No.	Ligands	Binding Affinity (kcal/mol)	Interacting Amino Acids
1	Ceftriaxone (Control)	−9.0	Ala7(A), Met234(A), Leu20(A), Ile92(A), Phe94(A), Gly93(A), Gln19(A), Ser49(A), Ala7(A)
2	Arucadiol	−9.4	Leu20(A), Ile14(A), Ile50(A), Leu28(A), Asn18(A)
3	Royleanone	−9.3	Thr46(A), Leu20(A), Ile14(A), Ile31(A), Ala7(A), Ser49(A), Phe92(A)
4	Taxodion	−8.9	Phe92(A), Ile50(A), Leu20(A), Ile14(A)
5	Salviasperanol	−8.8	Leu20(A), Ala7(A), Phe92(A)
6	Ferruginol	−8.8	Leu20(A), Leu28(A), Ile50(A), Ile31(A)
7	14-Deoxycoleon	−8.7	Leu20(A), Leu28(A), Ile50(A), Ile31(A), Ser49(A), Phe92(A)

Table 6. Binding affinity of ligands (*Oxalis corniculata*) with targeted protein dihydrofolate reductase (PDB ID: 2W9S).

SL No.	Ligands	Binding Affinity (kcal/mol)	Interacting Amino Acids
1	Ceftriaxone (Control)	−9.0	Ala7(A), Met234(A), Leu20(A), Ile92(A), Phe94(A), Gly93(A). Gln19(A), Ser49(A), Ala7(A)
2	Swertisin	−10.0	Thr121(A), Tyr98(A), Ile14(A), Ile31(A), Ile50(A), Leu20(A), Leu54(A), Leu28(A), Gly15(A), Gln19(A), Asn18(A), Ser49(A), Thr46(A)
3	5,7-dimethoxy-3,3′, 4′-trihydroxy flavone	−9.2	Thr121(A), Lys45(A), Thr46(A), Asn18 (A), Gln19(A), Leu20(A), Gly94(A)
4	Acacetin	−9.0	Phe92(A), Ala7(A), Asn18 (A), Leu20(A), Ile31(A), Ile5(A), Ser49(A), Thr46 (A)
5	Vitexin	−9.0	Leu20(A), Ala7(A), Val6(A), Ile31(A), Ile5(A), Tyr193(A), Gly94(A), Asp27(A)
6	5-hydroxy-6,7,8,4′-tetra methoxy flavone	8.4	Leu20(A), Asn18 (A), Ser49(A), Thr121(A), Thr46(A), Ile14(A), Tyr98(A), Phe92(A), Ile5(A), Val6(A), Ala7(A), Ile31(A), His30(A), Asp27(A)
7	Isovitexin	−8.3	Leu20(A), Lys29(A), Ile50(A)



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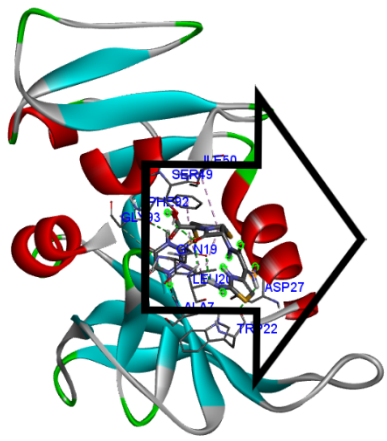
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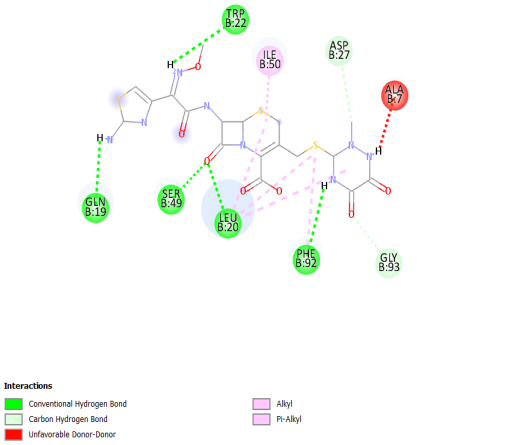
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Interactions
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Carbon Hydrogen Bond
Unfavorable Donor-Donor
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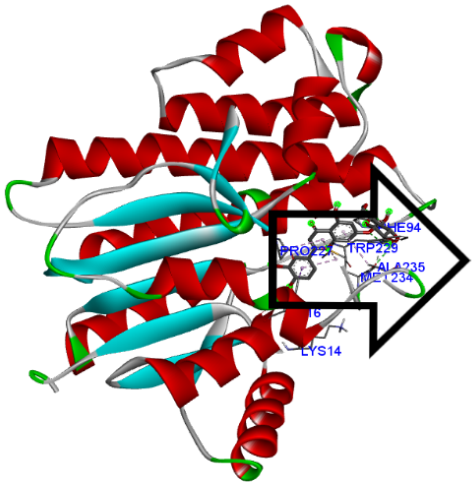
Pi-Alkyl

(B)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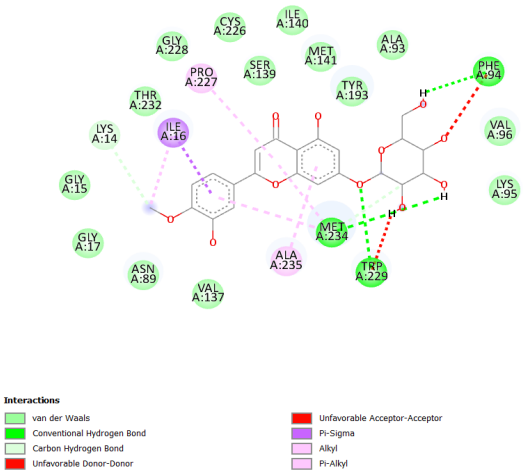
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ILE A:16
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ALA A:235
ASN A:89
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Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
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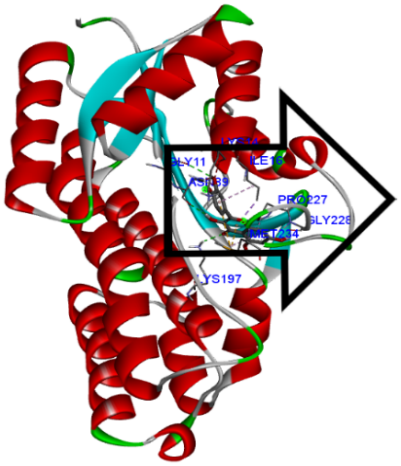
Pi-Sigma
Alkyl
Pi-Alkyl

(C)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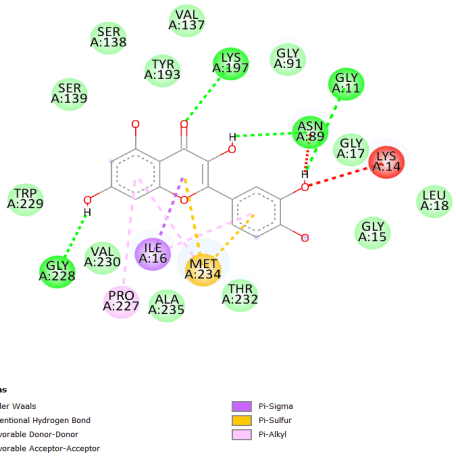
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Interactions
van der Waals
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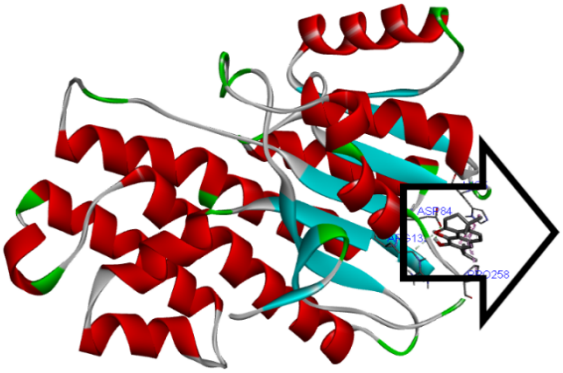
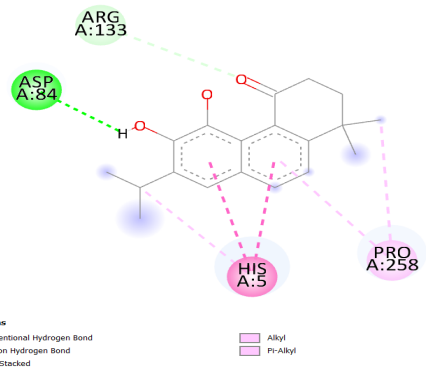
Pi-Sigma
Pi-Sulfur
Pi-Alkyl

(D)


ASP84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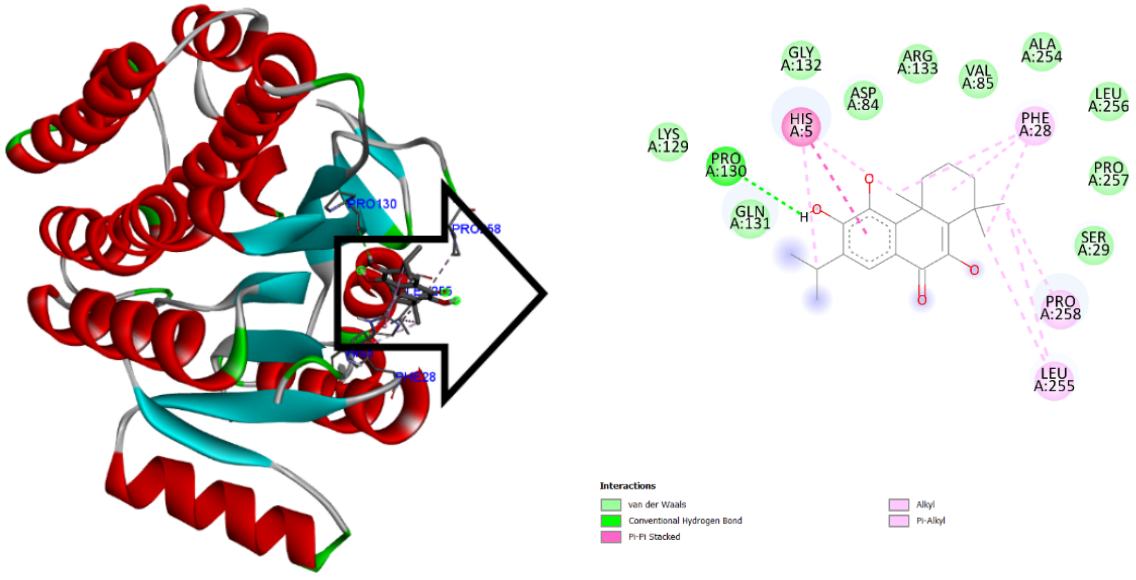
Pi-Alkyl

(E)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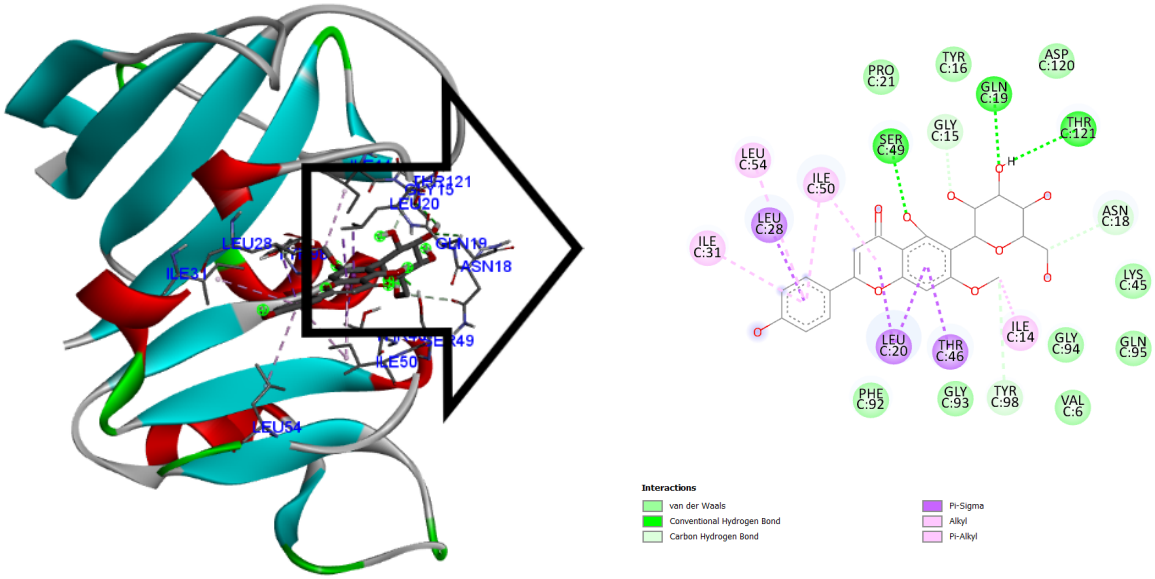
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi Stacked
Alkyl
Pi-Alkyl

(**F**)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ILE31
LYS45
LEU20
THR46
ILE14
GLY94
GLN95
PHE92
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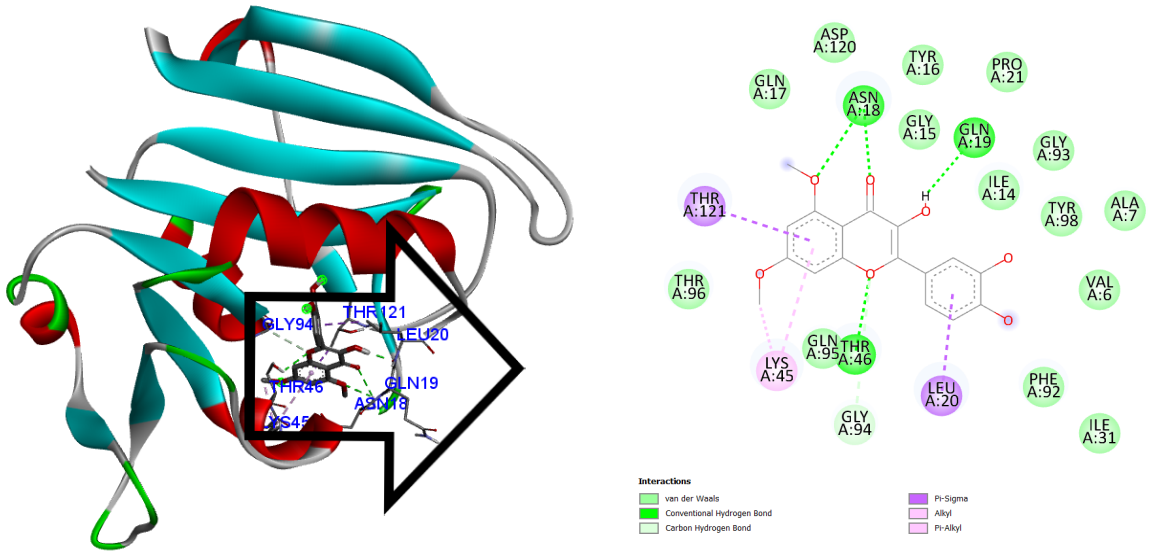
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl

(**G**)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TYR98
ALA7
THR96
VAL6
GLN95
THR46
LYS45
LEU20
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Pi-Alkyl

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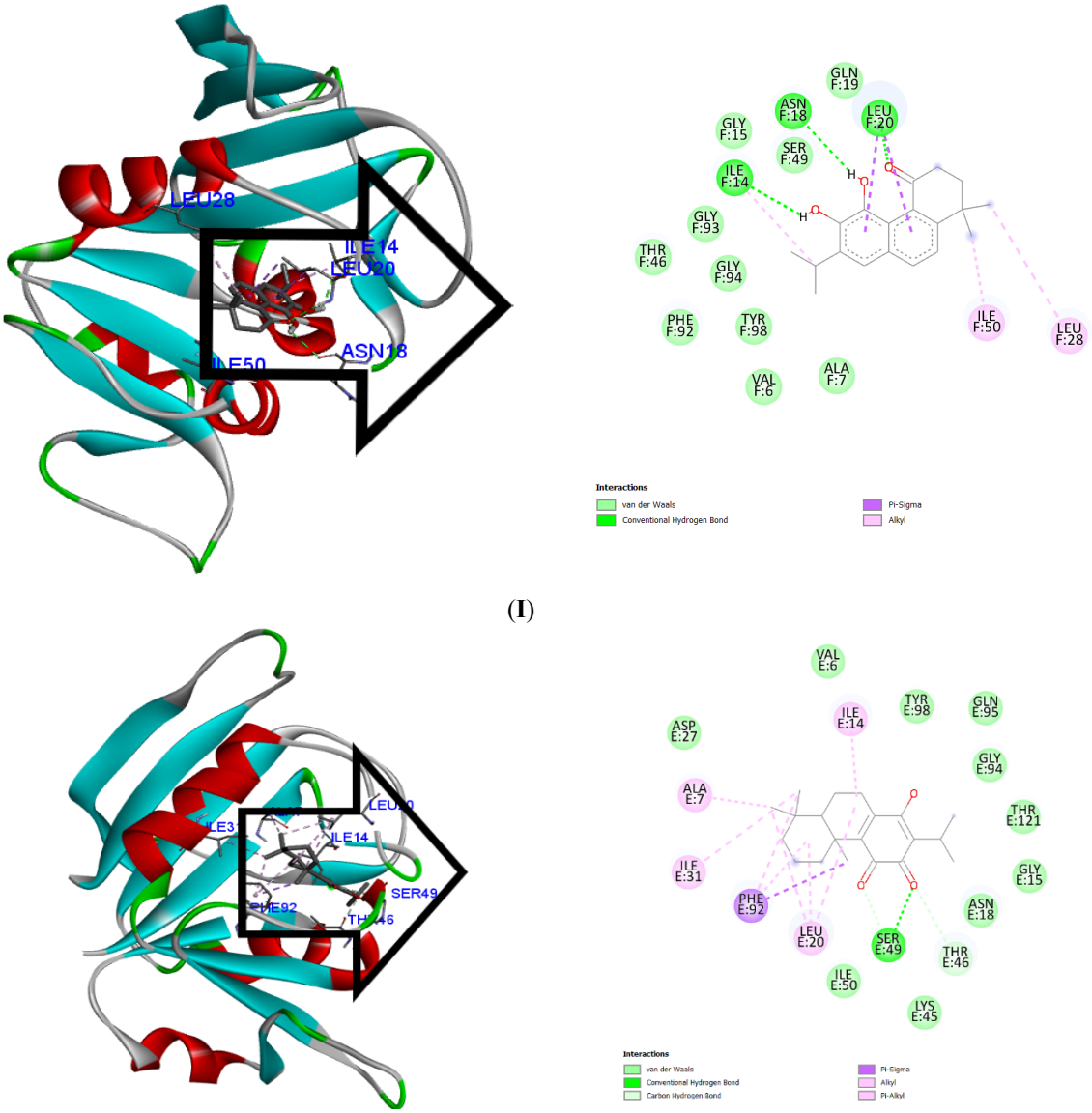

Figure 6. Three-dimensional binding interactions of selected ligands with target proteins. (**A**) Beta carotene and 4Z3D; (**B**) Ceftriaxone and 2W9S; (**C**) Diosmetin-7-O-beta-D-glucopyranoside and 4Z3D; (**D**) Swertisin and 4Z3D; (**E**) Arucadiol and 4Z3D; (**F**) 14-deoxycoleon and 4Z3D; (**G**) Swertisin and 2W9S; (**H**) 5,7-dimethoxy-3,3′,4′-trihydroxy flavone and 2W9S; (**I**) Arucadiol and 2W9S; (**J**) Royleanone and 2W9S. Hydrogen bonds are shown as dashed lines.

Data from the ADMET study suggested that Arucadiol (**8**) emerges as the promising candidate owing to its high absorption, moderate solubility, acceptable clearance, and lack of hepatotoxicity, carcinogenicity, mutagenicity and cytotoxicity (Tables 7 and 8). Swertisin (**14**), Isovitexin (**19**), Acacetin (**20**), Luteolin (**21**), Quercetin (**13**), Royleanone (**5**) and Taxodion (**7**) also show a favourable profile, with minimal toxicity concerns, making these a feasible alternative for future investigation. Notably, Swertisin (**14**), Isovitexin (**19**), and Acacetin (**20**) exhibited low predicted gastrointestinal (GI) absorption in the SwissADME analysis, which may be attributed to their relatively high polarity and glycosidic nature. This suggests that although these compounds demonstrated promising biological interactions *in silico*, their oral bioavailability may be limited and could require structural modification or alternative delivery strategies for optimal therapeutic application. In contrast, compound such as Diosmetin-7-O-beta-D-glucopyranoside (**18**) and Isoorientin (**12**) exhibits certain limitations, including low GI absorption and high water solubility, which might influence their therapeutic value. These results suggest that Arucadiol from *Premna obtusifolia* and Swertisin from *Oxalis corniculata* may serve as promising candidates for future *in vitro* and *in vivo* investigations to further assess their biological potential and safety characteristics.

The present docking results should be interpreted as preliminary computational insights, as a blind docking approach was adopted to explore potential binding regions, which may require further validation through site-specific docking or molecular dynamics simulations.

Table 7. ADMET profile of the major compounds from *Premna obtusifolia.*

Name	CID ID	ADME Analysis					Pharmacokinetics		Druglikeness	Toxicity Prediction			
		M.W.	HBA	HBD	Lipophilicity (iLOGP)	Water. S.	GI Absorption	BBB Permeant	Lipinski Violation	Hepatotoxicity	Carcinogenicity	Mutagenicity	Cytotoxicity
lambertic acid	13370049	316.4	3	2	2.83	moderately Soluble	Low	Yes	0	Inactive	Inactive	Inactive	Inactive
ferruginol	442027	286.5	1	1	3.63	moderately Soluble	High	Yes	1	Inactive	Inactive	Inactive	Inactive
O-methyl ferruginol	484400	300.5	1	0	4.08	Poorly soluble	Low	No	1	Inactive	Inactive, 0.63	Inactive	Inactive
sugiol	94162	300.4	2	1	3.29	moderately Soluble	High	Yes	0	Inactive	Inactive	Inactive	Inactive
royleanone	442084	316.43	3	1	2.92	moderately Soluble	High	Yes	0	Inactive	active, 0.51	Inactive	Inactive
14-deoxycoleon	10735190	330.42	4	3	3.04	moderately Soluble	High	No	0	Inactive, 0.68	active, 0.51	Inactive	Inactive
taxodion	73588	314.4	3	1	3.13	moderately Soluble	High	Yes	0	Inactive	active, 0.5	Inactive	Inactive
arucadiol	11011966	298.4	3	2	3.14	moderately Soluble	High	Yes	0	Inactive, 0.58	Inactive, 0.58	Inactive, 0.63	Inactive
12-hydroxy-6,7-secoabieta-8,11,13-triene-6,7-dial	15404650	316.4	3	1	2.78	moderately Soluble	High	Yes	0	Inactive, 0.67	Inactive, 0.55	Inactive, 0.63	Inactive
salviasperanol	11709435	314.4	3	2	3.32	moderately Soluble	High	Yes	0	Inactive	Inactive, 0.54	Inactive	Inactive, 0.69

Table 8. ADMET profile of the major compounds from *Oxalis corniculata.*

Name	CID ID	ADME Analysis					Pharmacokinetics		Druglikeness	Toxicity Prediction			
		M.W.	HBA	HBD	Lipophilicity (iLOGP)	Water. S.	GI Absorption	BBB Permeant	Lipinski Violation	Hepatotoxicity	Carcinogenicity	Mutagenicity	Cytotoxicity
5-hydroxy-6,7,8,4′-tetra methoxy flavone	14137334	360.4	7	1	3.38	moderately Soluble	High	No	0	Inactive, 0.69	Inactive, 0.57	Inactive	Inactive
p-hydroxybenzoic acid	135	138.12	3	2	0.85	soluble	High	Yes	0	Inactive, 0.52	Inactive, 0.51	Inactive	Inactive
Ferulic acid	445858	194.18	4	2	1.62	soluble	High	Yes	0	Inactive, 0.51	Inactive, 0.61	Inactive	Inactive
Isoorientin	114776	448.4	11	8	1.6	soluble	Low	No	2	Inactive	Inactive	Active, 0.52	Inactive, 0.64
Swertisin	124034	446.4	10	6	2.5	soluble	Low	No	1	Inactive	Inactive	Inactive, 0.59	Inactive, 0.69
Vitexin	5280441	432.4	10	7	1.63	soluble	Low	No	1	Inactive	Inactive	Active, 0.52	Inactive
Vanillic Acid	8468	168.15	4	2	1.4	soluble	High	No	0	Inactive, 0.55	Inactive, 0.64	Inactive	Inactive
Ethyl gallate	13250	198.17	5	3	1.21	soluble	High	No	0	Inactive	Inactive	Inactive	Inactive
5,7-dimethoxy-3,3′,4′-trihydroxy flavone	26034	330.29	7	3	2.13	moderately Soluble	High	No	0	Inactive	Active. 0.52	Inactive	Inactive
Diosmetin-7-O-beta-D-glucopyranoside	11016019	462.4	11	6	2.45	soluble	Low	No	2	Inactive	Inactive	Inactive	Inactive
Isovitexin	162350	432.4	10	7	1.6	soluble	Low	No	1	Inactive	Inactive	Active, 0.52	Inactive
Acacetin	5280442	284.26	5	2	2.56	moderately Soluble	High	No	0	Inactive	Inactive	Active, 0.50	Inactive
Luteolin	5280445	286.24	6	4	1.86	soluble	High	No	0	Inactive	Active, 0.68	Active, 0.51	Inactive
Quercetin	5280343	302.2	7	5	1.63	soluble	High	No	0	Inactive	Active, 0.68	Active, 0.51	Inactive

4. Discussion

Premna obtusifolia and *Oxalis corniculata* L. are two ethnomedicinal plants that are widely used in Bangladeshi traditional medicine. The current study assessed the antioxidant and antibacterial qualities using methanolic extracts and solvent-partitioned portions (n-hexane, methanol, and chloroform). The results provide strong evidence supporting their folkloric applications in managing infections and oxidative stress-related conditions.

The antioxidant potential, assessed via the DPPH radical scavenging assay, demonstrated that both plant extracts possess significant radical neutralizing activity. Notably, *Oxalis corniculata* L. exhibited stronger antioxidant activity (IC_{50} = 15.61 μg/mL) than *P. obtusifolia* (IC_{50} = 31 μg/mL), despite this, neither was as effective as ascorbic acid, the reference benchmark (IC_{50} = 9.48 μg/mL). The results obtained suggest that the extracts can stabilize DPPH radicals by contributing electrons or hydrogen atoms. The observed antioxidant activity is likely attributed to the rich polyphenolic composition of the extracts, as shown by the significant total phenolic content (TPC) determined by the Folin–Ciocalteu test. Specifically, *P. obtusifolia* exhibited a slightly higher TPC (185.82 mg GAE/g) compared to *O. corniculata* L. (154.90 mg GAE/g). The positive correlation between TPC and radical scavenging activity aligns with previous reports highlighting the central role of phenolic compounds in neutralizing free radicals and protecting substances including proteins, lipids and DNA from oxidative degradation. Previous studies corroborate these findings. For example, *O. corniculata* has been found to have a total phenolic content of 6.424 mg equivalents to gallic acid each gram of dry mass [26], while other studies demonstrated higher TPC values across various solvent fractions, ranging from 21.0 to 162.0 μg GAE/mg in aqueous fractions, methanolic, hexane, chloroform, ethyl acetate, as well as n-butanol [27,28]. In the case of *P. obtusifolia*, prior investigations reported notable antioxidant activities, including DPPH scavenging (IC_{50} = 11.18 ± 0.03 μg/mL), reducing power (IC_{50} = 21.69 ± 0.02 μg/mL) and metal chelation (IC_{50} = 18.82 ± 0.46 μg/mL) [29–31].

In terms of antimicrobial activity, both plant extracts showed differential inhibitory effects against a group of harmful fungus and bacteria. The methanolic fraction of *Oxalis corniculata* (MMEOC) showed the strongest antibacterial action among the fractions that were evaluated, particularly against *Bacillus megaterium*, *E. coli*, *S. typhi*, and *Shigella boydii*. *Premna obtusifolia* also exhibited moderate activity, with MMEPO being the most effective among its fractions. These findings imply that the bioactive substances that are accountable for antibacterial action are more effectively extracted and retained in the methanol fraction, possibly due to its polarity, which favors the solubilization of flavonoids, tannins, alkaloids, and other antimicrobial phytoconstituents. The antimicrobial activity observed in this study supports earlier ethnobotanical reports where these plants have long been utilized to treat fevers, skin conditions, and gastrointestinal problems [32]. Particularly, *Oxalis corniculata* is known among indigenous groups such as the Chakma and Marma for its use in dysentery and diarrhea treatment, which correlates well with the observed antimicrobial action against Salmonella species and E. coli, two intestinal pathogens [33]. Even though the plant isolates' inhibitory zones were lower than those of common antibiotics like griseofulvin and ciprofloxacin, the activity was still significant ($p < 0.05$), especially considering the crude nature of the extracts. This underlines the possibility of using these plants as a source of lead compounds to create new antimicrobial drugs, especially in light of the growing resistance to antibiotics. The antifungal screening also revealed that both plants possess moderate antifungal activity, with MMEOC showing superior inhibition against *Candida albicans* and *Saccharomyces cerevisiae*. This aligns with previous reports on the antifungal efficacy of flavonoids and phenolic acids, both of which are likely to be present in these extracts [34].

The ADMET profiling suggested acceptable drug-likeness for most of the selected compounds, with Arucadiol emerging as a promising candidate due to its favorable predicted pharmacokinetic profile. This diterpenoid's high predicted absorption and clean toxicity profile indicate its potential as a lead candidate for dual antioxidant-antimicrobial development. Diosmetin-7-O-β-D-glucopyranoside and Quercetin showed strong CBR-1 binding (−9.4 kcal/mol), which may be attributed to their polyphenolic structures capable of forming stable hydrogen bonds and π–π interactions within the active site, demonstrating binding affinities comparable to β-carotene rather than definitively surpassing it. Swertisin and Luteolin also exhibited favorable binding tendencies, further supporting the potential role of flavonoids from *Oxalis corniculata* as CBR-1 modulators. Arucadiol's equivalent −9.4 kcal/mol binding from *Premna obtusifolia* suggests diterpenoids as potential antioxidant scaffolds, consistent with literature describing plant phenolics in oxidative stress modulation via carbonyl reductase inhibition. Swertisin demonstrated a notable −10.0 kcal/mol affinity against DHFR, representing one of the strongest docking scores observed in this study; however, it should be noted that docking scores are approximations of binding affinity and do not account for entropic contributions, protein flexibility, or solvent dynamics. The predicted binding pose indicates potential occupancy of the NADPH-binding pocket involved in bacterial folate synthesis. The comparable binding tendencies of Acacetin, Vitexin, and 5,7-dimethoxy-3,3′,4′-

trihydroxyflavone further highlight *Oxalis corniculata* as a flavone-rich source with antibacterial potential. Arucadiol and Royleanone from *Premna obtusifolia* similarly broaden the phytochemical relevance of this plant.

Recent studies integrating *in vitro* bioassays with molecular docking and molecular dynamics simulations have similarly demonstrated the importance of flavonoid scaffolds in antioxidant and antibacterial mechanisms [35,36]. In particular, flavonoids exhibiting multiple hydroxyl substitutions often show favorable hydrogen bonding interactions within enzyme active sites, contributing to enhanced predicted binding stability. Additionally, network pharmacology combined with docking approaches has been increasingly used to elucidate multi-target phytochemical interactions [37]. In agreement with these contemporary studies, the present findings suggest that flavonoid derivatives such as Swertisin **(14)** and Quercetin **(13)** may act as promising antioxidant-antimicrobial scaffolds under computational evaluation. Although molecular docking studies on flavonoids and diterpenoids have been widely reported in various plant systems, the present study distinguishes itself through a structured cross-validation strategy that integrates experimental antioxidant and antimicrobial assays with target-based docking and ADMET profiling [35,36,38]. Rather than emphasizing structural novelty, this work prioritizes the rational selection of bioactive scaffolds derived from locally available ethnomedicinal plants. Such an integrative framework strengthens the translational relevance of the findings and offers a practical, reproducible model for phytochemical-driven drug discovery, particularly in resource-limited research settings. The computational results align with existing phytochemical literature documenting antioxidant and antimicrobial activities of flavonoids and diterpenoids from these species. However, the observed binding affinities should be regarded as preliminary predictive indicators rather than conclusive evidence of superior inhibitory activity. As with all docking-based screening approaches, the possibility of false-positive predictions remains, and further experimental validation is necessary to confirm the biological relevance of these interactions. While the results are encouraging, experimental validation through DPPH/ABTS assays for antioxidant activity, MIC/MBC determination for antimicrobial activity, and *in vivo* pharmacokinetic studies remains essential. Structural optimization of selected lead candidates (e.g., Arucadiol and Swertisin) may further improve potency and bioavailability for potential therapeutic development. Overall, these findings provide a rational basis for continued investigation of *Oxalis corniculata* and *Premna obtusifolia* within natural product-based drug discovery frameworks.

Overall, the study confirms that *Premna obtusifolia* and *Oxalis corniculata* L. possess valuable antioxidant and antimicrobial activities, likely due to their high phenolic content and rich phytochemical profiles. The results validate their traditional medicinal use and highlight their capacity to serve as organic sources of substances with biological activity. To pinpoint the precise active ingredients and clarify their modes of action, more phytochemical isolation, structural characterization, and *in vivo* pharmacological research are necessary.

Despite the promising *in vitro* and *in silico* findings, several methodological limitations should be acknowledged. The present study did not evaluate potential synergistic interactions between different solvent fractions or individual phytoconstituents. Such combinatorial assessments may provide additional insight into the overall antimicrobial efficacy of the crude extracts and warrant future investigation. Molecular docking provides an estimation of binding affinity based on static protein structures and does not account for protein flexibility, solvent dynamics, or entropic contributions. The absence of redocking validation and free-energy rescoring (e.g., MM-GBSA) may limit pose reliability. Additionally, ADMET predictions are computational approximations and require experimental pharmacokinetic validation. Therefore, the identified lead candidates should be considered as preliminary hits pending further biochemical and *in vivo* confirmation.

5. Conclusions

This study provides a comparative *in vitro* and *in silico* evaluation of *Premna obtusifolia* and *Oxalis corniculata*, two ethnomedicinal plants belonging to distinct botanical families but traditionally used for similar therapeutic indications in Bangladesh. The methanolic extracts demonstrated notable antioxidant activity and moderate antimicrobial effects, supporting their traditional applications. Computational docking of previously reported phytochemicals identified Swertisin **(14)** and Arucadiol **(8)** as compounds with favorable predicted binding affinities toward CBR-1 and DHFR targets under the applied docking conditions. However, these findings represent preliminary computational predictions and do not constitute confirmation of biological efficacy. Overall, this work contributes updated scientific evidence supporting ethnopharmacological use and provides a rational framework for prioritizing bioactive candidates for future quantitative antimicrobial testing, molecular dynamics simulations, and *in vivo* validation.

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