Investigational
Medicinal Chemistry & Pharmacology

Research Article Open Access

Chemical profiling, molecular docking, and ADMET evaluation of *Bougainvillea formosa* stem and root barks essential oils

Oluwakayode Olubunmi Odeja[1], Israel Azogor Ekoro[2]*, Michael Gabriel Ibok[3], Ejike Onwudiegwu Okpala[4], Christiana Ene Ogwuche[1], Honesty Bamidele Akpeji[1], Caleb Ohirhian[1]

Abstract

Background: Essential oils have been recognized for their pharmaceutical applications as natural antioxidants. A combination of experimental and theoretical analyses was conducted on *Bougainvillea formosa* (*B. formosa*) stem and root barks essential oils.

Methods: The essential oils obtained through hydro-distillation were identified and quantified using gas chromatography–mass spectrometry (GC-MS) and were found to exhibit different compositions. The antioxidant capacity of the essential oils was determined through 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging assay at different concentrations (10, 50, 100, and 150 µg/mL). Five (5) major constituents from each essential oil were subjected to molecular docking analysis using the PDB: 1HD2 as a protein target to determine the molecular basis of the antioxidant activity. Drug-likeness and pharmacokinetic predictions indicated that the oils had favorable profiles.

Results: The stem bark oil contained aliphatic alcohols and long-chain hydrocarbons. In contrast, the root oil contained a large proportion of sesquiterpenoids. The calculated IC_{50} values for the root and stem bark oil were 10.22 µg/mL and 13.46 µg/mL, respectively. The positive control, ascorbic acid (2.05 µg/mL), exhibited higher scavenging activity than oils. The binding affinities of the stem bark oil compounds were determined as −4.2 to −5.6 Kcal/mol, and the root oil compounds had higher binding affinities −4.8 to −5.0 Kcal/mol.

Conclusion: Further safety evaluation is needed to justify the antioxidant potential of the oils.

Keywords: ADMET, Antioxidant Activity, *Bougainvillea formosa*; Essential Oils; Molecular Docking.

*Correspondence: Tel.: +2348062183532; E-mail address: israelekoro@gmail.com (Israel Azogor Ekoro)

[1]Department of Chemistry, Federal University of Petroleum Resources, Effurun, Delta State, Nigeria; [2]Department of Chemistry, Federal University of Medical and Health Sciences, Kwale, Delta State, Nigeria; [3]Department of Chemistry, University of Ibadan, Ibadan, Oyo State, Nigeria; [4]Department of Chemistry, Federal University Lokoja, Kogi State, Nigeria

Other authors
Email: odeja.oluwakayode@fupre.edu.ng (Oluwakayode Olubunmi Odeja); Email: michaelibok08@gmail.com (Michael Gabriel Ibok); Email: ejike.okpala@fulokoja.edu.ng (Ejike Onwudiegwu Okpala); Email: ogwuche.christiana@fupre.edu.ng (Christiana Ene Ogwuche); Email: akpeji.honesty@fupre.edu.ng (Honesty Bamidele Akpeji); Email: ohirhiancaleb693@gmail.com (Caleb Ohirhian).

Citation on this article: Odeja OO, Ekoro IA, Ibok MG, Okpala EO, Ogwuche CE, Akpeji HB, Ohirhian C. Chemical Profiling, Molecular Docking, and ADMET Evaluation of Bougainvillea formosa Stem and Root Barks Essential Oils. Investigational Medicinal Chemistry and Pharmacology (2026) 9(1):124; Doi: https://dx.doi.org/10.31183/imcp.2026.00124

Background

The high efficacy of herbal products in the treatment of different health conditions has attracted considerable interest. Essential oils (EOs) are complex mixtures of volatile organic compounds derived from plants, widely recognized for their diverse biological activities [1]. Essential oils (EOs) are gaining a lot of interest as natural substitutes, especially in medicine and the food industry [2]. EOs consists of various constituents. The compounds in EOs, which are characterized by antioxidant activities, constitute a large percentage and are often mentioned as good potential candidates to develop new bioactive agents that can be used in pharmaceuticals, cosmetics, and other industries [3]. The oils and their constituents have been assessed as possible alternatives to synthetic antioxidants in food processing, which shows their health-friendly effects. The curative value of aromatic and medicinal plants, along with their action against pathogenic microorganisms, is not a recent finding [2]. The secondary metabolites produced by EOs also exhibit insecticidal activity, which accounts for the progress in the development of biological pest management strategies [4-5]. Antioxidants protect biological systems against the harmful effects of free radicals, unstable molecules that can react with other molecules to achieve stability [6]. The imbalance of reactive oxygen species (ROS), coupled with an insufficiency of mechanisms to counteract their effects, can lead to cellular damage and ailments such as diabetes, heart disease, and cancer [7]. Essential oils (EOs) help mitigate this cellular damage by neutralizing free radicals, protecting against the oxidative stress of cells, and preventing lipid oxidation. This action explains the potent antioxidant abilities of EOs [8]. The range of chemicals in EOs provides a remarkable synergistic effect for the antioxidant function [9]. *Bougainvillea Formosa* (Willd. ex Schult. & Schult.f.) Holttum & Standl. (Nyctaginaceae), a cultivated variety of *Bougainvillea glabra* (Figure 1), belongs to the Nyctaginaceae family and is extensively grown as an ornamental plant due to its strikingly colorful bracts and prolonged blooming period. Although primarily appreciated for its decorative appeal, recent research has highlighted its potential in medicinal and nutritional contexts. Chemical studies of its foliage and blossoms have identified bioactive compounds, including flavonoids, phenolics, and betalains, which are known to support antioxidant, antimicrobial, and anti-inflammatory functions [10]. Traditionally, the plant has been used to address respiratory and digestive health issues. Extracts derived from *Bougainvillea* species have shown diverse therapeutic properties, including blood lipid regulation, anti-diabetic effects, pain relief, and cytotoxicity. Beyond its health-related uses, the plant's floral pigments and polyphenolic compounds have applications in the food sector, where they serve as natural coloring agents [11,12]. *In silico* studies, ADMET (absorption, distribution, metabolism, excretion, and toxicity) and molecular docking predictions, are important in modern drug discovery for assessing and optimizing lead compounds for pharmacokinetics and toxicology [13]. These methods determine the binding orientation and strength of small molecules, including certain phytochemicals and components of essential oils, to particular molecular targets [14]. They also reduce the chances of failure in drug development [15]. As part of our continued study of bioactive compounds of Nigerian medicinal plants, this paper presents an in-depth study of the essential oils extracted from the stem and root barks of *Bougainvillea formosa*. This study reports on the chemical composition of these essential oils. Antioxidant activities were determined *in vitro*, and *in silico* studies involving ADMET and molecular docking were conducted to predict the pharmacokinetics and the binding score.

Methods

Collection and preparation of the plant materials

Bougainvillea formosa stem and root barks were collected from the Botanical Garden located at the University of Ibadan, Ibadan, Oyo State, in February 2025. Identification and authentication were completed at the Forestry Research Institute of Nigeria, Oyo State, Nigeria. The specimen was deposited to the herbarium, which was registered with the accession number FHI 114212. The collected samples were then cut into smaller sizes.

Isolation of essential oils

A total of 610.15 g each of chopped stem and root bark sample from *Bougainvillea formosa* were subjected to hydrodistillation for three (3) hours using a fully glass Clevenger-type apparatus equipped with a temperature-controlled heating mantle, following procedures described by Odeja et al. [16] and Ibok et al. [17] following British Pharmacopia [18]. The distillate, comprising the volatile constituents, was collected in the receiver arm containing distilled water and analytical-grade n-hexane, which served as the solvent for the essential oil. The resulting oil-hexane mixture was transferred into labelled sample bottles. For preservation, the essential oils were sealed in glass vials and refrigerated at 4 °C prior to GC-MS characterization and biological evaluations. The oil yield (%) was subsequently calculated using the formula provided below (Equation 1).

$$\% \text{ Yield } = \frac{\text{Weight of essential oil}}{\text{Weight of fresh sample}} \times 100$$

Equation (1)

Gas chromatography-mass spectrometry (GC-MS) analysis and identification of the essential oil constituents

Stem and root barks essential oils of *Bougainvillea formosa* were subjected to GC-MS analysis on an Agilent 7809A gas chromatograph hyphenated with an Agilent mass detector having split/splitless injector interfaced to a mass selective detector operating at 70eV. Other experimental parameters were as follows: the ion source temperature was set at 200ºC within a mass spectral range of m/z 50-700 at a 1428amu/sec scan rate. The GC column was equipped with an HP-5MS column with a length of 30m, an internal diameter of 0.25mm and a film thickness of 0.25µm. The oven temperature was controlled: initial temperature of 80ºC for 2min, increased at 10ºC/min to 240ºC for 6 min. The carrier gas, Helium, was set at a 1mL/min flow rate. Injection volume, linear velocity and pressure were adjusted at 1.0 µL, 362 cm/s and 56.2 KPa. The oven temperature was 60ºC, held for 1 min to 180ºC for 3 min at 10ºC /min, the final temperature was 280ºC for 2 min at 10ºC /min. Both injector and detector temperatures were set at 250ºC.

The essential oil components were identified based on their retention indices, determined according to a homologous series of normal alkanes. Identifications were made by comparing the mass spectral fragmentation patterns (NIST data/base/Chemstation data system) with the data previously reported in the literature [16].

DPPH Radical Scavenging Method

The antioxidant activity assay was performed with modifications based on the method described by Odeja *et al*. [16] and Ibok *et al*. [17]. A 0.004 g quantity of DPPH reagent was dissolved in 100 mL of methanol to prepare the working solution. Test samples were serially diluted to obtain concentrations ranging from 10 to 150 µg/mL. In a 96-well microplate, 50 µL of each sample concentration was mixed with 150 µL of the DPPH solution. The reaction mixtures were incubated in the dark at ambient temperature for 30 minutes. Absorbance values were subsequently recorded at 595 nm. Ascorbic acid served as the reference standard across matching concentration ranges (10–150 µg/mL), while methanol was employed as the negative control. All experimental conditions—including sample, standard, and control—were conducted in triplicate. The percentage of free radical inhibition was determined using the formula below.

$$\% \text{ Inhibition } = \frac{\text{Control Absorbance} - \text{Sample Absorbance}}{\text{Control Absorbance}} \times 100$$

Equation (2)

Molecular Docking Protocol

Molecular docking analysis was performed to study the binding and interactions between the constituents of the essential oils and a target protein of antioxidant interest. Five (5) compounds each from the stem and root EOs, representing the highest percentage abundance, were selected as ligands. The ligands were obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) as 3D SDF files with assigned CID (chemical identifier). The ligands were further subjected to geometry optimization in the Avogadro 1.2 molecular program (http://avogadro.cc/) [19]. The MMFF94 (Merck Molecular Force Field 94) force field was employed to extract stable, low-energy geometries [20]. The 3D structure of the target protein (PDB: 1HD2) was retrieved from the RCSB database. The structure of the target protein was prepared for docking analysis by removing water molecules and heteroatoms. Molecular docking simulations were performed with the web server, CB-Dock2 (https://cadd.labshare.cn/cb-dock2/). . The blind docking option was selected, which utilized every region of the protein to find all potential binding sites [6]. LigPlot + tool used for post-docking analysis to identify and visualize the hydrogen and hydrophobic interactions between the ligands and the protein [21-22]. The docking outcome of the oil constituents was assessed and analyzed based on the binding affinity scores and interaction profiles.

ADMET and Drug-Likeness Evaluation

In silico prediction tools were used to estimate the potential bioactivity and pharmacokinetic and drug-likeness properties of the essential oils' constituents. The drug-likeness predictions were obtained from the Swiss-ADME online tool (https://www.swissadme.ch/). The SMILES (Simplified Molecular Input Line Entry System) representations of the compounds were entered into the server to obtain results for some physicochemical parameters, such as molecular weight (MW), lipophilicity (LogP), the number of hydrogen bond donors (nHB) and acceptors (nHA) [23]. Lipinski's Rule of Five was applied to the compounds to estimate the oral drug-likeness, based on established threshold values and compliance obtained [24]. The compounds that had none or very few violations were positively drug-like. The essential oil constituents' ADMET properties prediction was evaluated from the Deep-PK web server (https://biosig.lab.uq.edu.au/deeppk/). The optimized chemical structures of the compounds were generated and saved as appropriate (SMILES) and submitted to the server. When compared to the reference compound (Ascorbic acid), human intestinal absorption (HIA), blood–brain barrier (BBB), inhibition of CYP3A4, clearance values and carcinogenicity potential parameters were analyzed for the stem and root essential oils constituents.

Results

Hydrodistillation of fresh stems and roots of *Bougainvillea formosa* (610.15 g each) yielded 2.61 g of colorless stem oil (0.4278% w/w) and 5.03 g of pale-yellow root oil (0.8244% w/w), calculated on a fresh weight basis. The chemical constituents of these oils are presented in Table 1 and Figures 2 and 3. Gas chromatography–mass spectrometry (GC-MS) analysis identified twenty (20) compounds in the stem oil, representing 89.81% of its total composition, and ten (10) compounds in the root oil, accounting 100% of the total oil composition. The predominant compounds in the stem essential oil were 2-Nonen-1-ol (9.98%), Tetracosane (9.00%), E-2-Tetradecen-1-ol (7.25%) and Phytol (7.23%). In contrast, the root oil was primarily composed of Ar-tumerone (38.11%), α-Tumerone (20.50%) and β-Tumerone (19.37%) (Table 1). The antioxidant capacity of *Bougainvillea formosa* essential oils was evaluated using the DPPH free radical scavenging assay. Percentage inhibition relative to a reference standard was determined across a concentration range of 10.0–150.0 µg/mL, as presented in Table 2. The stem essential oil exhibited inhibition activities ranging from 24.38% to 32.17%, while the root essential oil showed higher inhibition values, ranging from 29.79% to 38.18%, indicating a concentration-dependent increase in radical scavenging activity. The binding affinity scores of the stem and root EOs are presented in Table 3. Figure 4a-e, Figure 5a-d, and Figure 6 represent binding interactions of the stem EOs, root EOs, and Ascorbic acid respectively. Table 4-5 presents ADMET and Drug-likeness properties of the essential oil compounds

Discussion

The essential oil extracted from the roots of *Bougainvillea formosa* was found to be predominantly composed of sesquiterpenoids characterized by the bisabolene skeleton, with Ar-turmerone (38.11%), α-Turmerone (20.50%), and β-Turmerone (19.37%) as the major constituents. These compounds are renowned for their diverse pharmacological potential, including antioxidants activities [25]. Interestingly, this profile mirrors the chemical constituents found in turmeric essential oil—derived from the rhizomes of *Curcuma longa,* where turmerones are also the principal bioactive agents contributing to turmeric's distinctive aromatic flavor and scent [26].

Notably, the root oil of *B. formosa* exhibits compositional similarities to turmeric essential oil, reinforcing its potential as an alternative source of bioactive terpenoids. In addition to the dominant sesquiterpenes, a range of terpenoid compounds, such as monoterpenes and lesser-known sesquiterpenes like α-Curcumene, *p*-Cymene, β-Sesquiphellandrene, (E)-Atlantone and Emery 2216, were identified in trace amounts. Despite their lower concentrations, these molecules are acknowledged for their remarkable pharmacological properties, expanding the scope of *B. formosa* as a valuable candidate in therapeutic and nutraceutical applications [27].

The essential oil extracted from the plant's stem was predominantly composed of 2-Nonen-1-ol, accounting for 9.98% of its chemical profile. This compound is well-established in the flavoring industry due to its ability to produce distinct melon-like, fatty and sweet notes, making it a key ingredient in enhancing the flavor of vegetables, melons, cucumbers, and various tropical fruits. While detailed medicinal uses aren't noted, its extensive application in food products indicates promising potential within the food and beverage industry as a natural flavor enhancer [28]. Additionally, the stem oil contained Tetracosane, which exhibited cytotoxic activity against several cell lines, including AGS, MDA-MB-231, HT-29, and NIH 3T3, with IC_{50} values ranging from 128.7μM to over 250μM [29], suggesting possible bioactive properties worth further exploration. Another notable compound, Phytol, was identified in both stem and root oils in varying concentrations, contributing to the biological profile of the plant. The stem essential oil also includes other pharmacologically active molecules that collectively support its broader therapeutic potential. The antioxidant potential of *Bougainvillea formosa* essential oils, as assessed by the DPPH free radical scavenging assay, reveals meaningful biological activity, with both stem and root oils demonstrating concentration-dependent inhibition. Specifically, the stem essential oil exhibited moderate scavenging efficiency, with inhibition values spanning from 24.38% at the lowest concentration to 32.17% at the highest. In contrast, the root essential oil consistently outperformed its stem counterpart, recording higher inhibition values between 29.79% and 38.18%. This suggests that the root essential oil possesses a stronger antioxidant profile, which could be attributed to the presence of higher concentrations of active phytochemicals. The observed increase in inhibition with rising concentrations across both samples affirms a dose-dependent relationship, supporting the potential utility of these oils in natural antioxidant applications. Such findings not only highlight their relevance in the formulation of health-promoting food and cosmetic products but also point toward their possible role in managing oxidative stress-related conditions when further pharmacological validation is conducted.

The molecular docking investigation was conducted with the major constituents (5) of *Bougainvillea formosa* stem and root essential oil in order to provide a molecular insight into their antioxidant effects through the interaction of the molecules with the target protein (PDB ID: 1HD2) [30]. The five constituents that were the most abundant in the GC-MS analysis of the stem and root essential oils were selected. The binding affinity values of the elements of the essential oil of the stem were in the range of -4.2 to -5.0kcal/mol (Table 3), as they reflected the interaction with the active site of the protein. Phytol exhibited the highest binding affinity among the constituents of the stem oil, with a docking score of -5.0kcal/mol, and there were hydrogen bond interactions with Gly17 and Leu96 residues (Figure 4d). These interactions implied that a constant binding orientation could be adapted to aid antioxidant activity. Resorcinol dimethyl ether had a binding affinity of -4.7kcal/mol in the absence of hydrogen bond formation, suggesting that hydrophobic interactions were probably the strongest force affecting its binding. E-2-tetradecen-1-ol was found to have a docking score of -4.5kcal/mol and formed a hydrogen bond with Arg86 residue (Figure 4c). 2-nonen-1-ol which corresponds to CID 61896 had the lowest binding affinity of -4.2 kcal/mol, but displayed hydrogen bond interactions with Ala90, Gly92, and Val94 residues (Figure 4a). Essential oil components from the root exhibited more significant binding scores (−4.8 to −5.6kcal/mol), showing a higher affinity against the antioxidant-related protein. β-Turmerone and α-Turmerone showed the most significant binding affinities, with a docking score of −5.6 kcal/mol for both compounds (Table 3, Figure 5b-c). Ar-Turmerone had a predicted binding affinity of −5.5 kcal/mol with hydrogen bonding to the Leu96 residue (Figure 5a). The interaction visualization of phytol in the stem essential oil was already shown in Figure 4d and is therefore not included in Figure 5 to avoid repetition. N-hexadecanoic acid had the lowest binding score of −4.8 kcal/mol and interacted through hydrogen bonds with the residues Lys93 and Val94 (Figure 5d). The strongest binding affinity, with a docking score of −5.8kcal/mol, was found with the reference compound ascorbic acid, which bound to Arg86, Val94, and Leu96 residues through multiple hydrogen bonds (Figure 6). Ascorbic acid is a well-known antioxidant, and its interaction profile was strongly established; therefore, the docking protocol confirmed the relevance of the chosen binding site to antioxidant activity. It was observed that some root essential oil constituents, such as turmerone isomers, exhibited binding affinities close to that of the reference compound. This indicates that they are strong antioxidant agents.

The molecular docking result was well correlated with the *in vitro* antioxidant result, and it showed that the root essential oil displayed a better antioxidant activity than the leaf essential oil. The binding affinities and favorable interaction patterns found for the constituents of the root justified their experimental results. This aligns with other research where compounds like cis-verbenyl acetate showed favorable binding affinities to protein targets related to colorectal cancer [31], and isoflavans exhibited antibacterial and antioxidant activity through interactions with DNA gyrase and human peroxiredoxin [32]. The correlation of the molecular docking result with *in vitro* antioxidant activity provided evidence for the validity of the computational approach and revealed that the increase in antioxidant activity of root essential oil was mainly due to its major bioactive constituents.

The ADMET evaluation of essential oils (EOs) from *B. formosa* stem and root indicated some concerning safety-related discrepancies when compared to the reference compound ascorbic acid (Table 4). However, the stem and root EOs were predicted to have similar relative pharmacokinetic properties. The ascorbic acid and EO compounds were predicted to be absorbed and well assimilated in the human gastrointestinal tract [33]. However, ascorbic acid was predicted to have a low chance of crossing the blood-brain barrier (BBB), while all EO components showed predicted permeability across the BBB [34]. As regards metabolism, it was predicted that none of the EO constituents would act as a CYP3A4 inhibitor, indicating a low chance for metabolic drug-drug interactions to occur [35]. Ascorbic acid showed similar non-inhibitory behavior, indicating metabolic compatibility, as observed with the essential oils. The stem EO compounds had positive values for clearance, which predicted that they were eliminated faster and more efficiently [36]. All clearance values for root EO constituents were also positive overall, except for N-hexadecanoic acid. The predictions on toxicity differed among the essential oil constituents and the reference compound. Most stem essential oil constituents were predicted to be non-carcinogenic and thus labeled "safe" except for the predicted "toxic" resorcinol dimethyl ether. The constituents of the root essential oil such as Ar-turmerone, β-turmerone, and α-turmerone were predicted to be carcinogenic as well, despite their favorable docking scores (Table 3). Hence, a strong binding affinity does not guarantee safety. Other root essential oils such as phytol and N-hexadecanoic acid were also labeled as "safe".

The drug-likeness of the stem and root essential oil compounds of *B. formosa* was determined using Lipinski's Rules of Five [37]. According to the rule, a compound is most likely to be orally bioavailable when it has a molecular weight of less than 500

Da, a lipophilicity (LogP) within the range of 0-5, fewer than five (5) hydrogen bond donors, and zero or fewer than ten (10) hydrogen bond acceptors, with no more than one exception [37]. The stem essential oil compounds (Table 5), 2-nonen-1-ol, E-2-tetradecen-1-ol, and resorcinol dimethyl ether, showed no violations, therefore, exhibiting positive prospects of having appropriate physicochemical profiles. Phytol was in compliance with Lipinski's rule, despite having a single violation of the LogP (5.25). Excessive lipophilicity was violated in tetracosane (8.25), which might have a detrimental effect on oral bioavailability. It was observed that the root essential oil compounds (Table 4) exhibited better adherence to Lipinski's Rule of Five. All three turmerone isomers and N-hexadecanoic acid did not violate any of the criteria, which are indicative of excellent oral drug-likeness. The reference compound, ascorbic acid, did not meet the hydrogen bond donor criterion and was very hydrophilic. The essential oil compounds from *B. formosa* showed great drug-likeness profiles, which justify their potential as lead compounds in drug development.

Figure 1. Picture of *Bougainvillea formosa* plant.

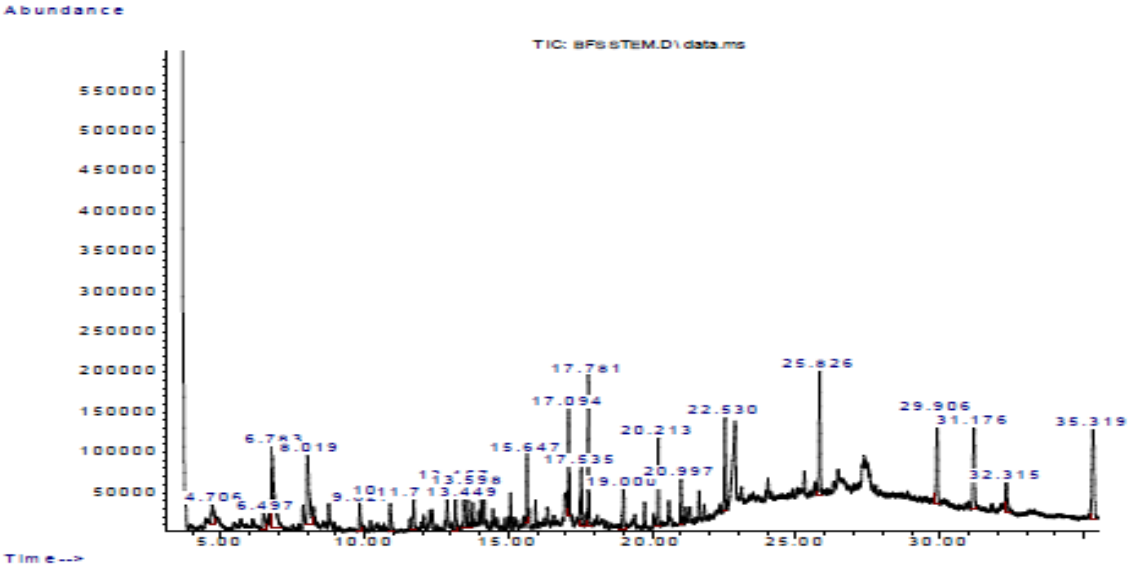

Figure 2. GC-MS chromatogram of the Stem essential oil of *B. formosa*

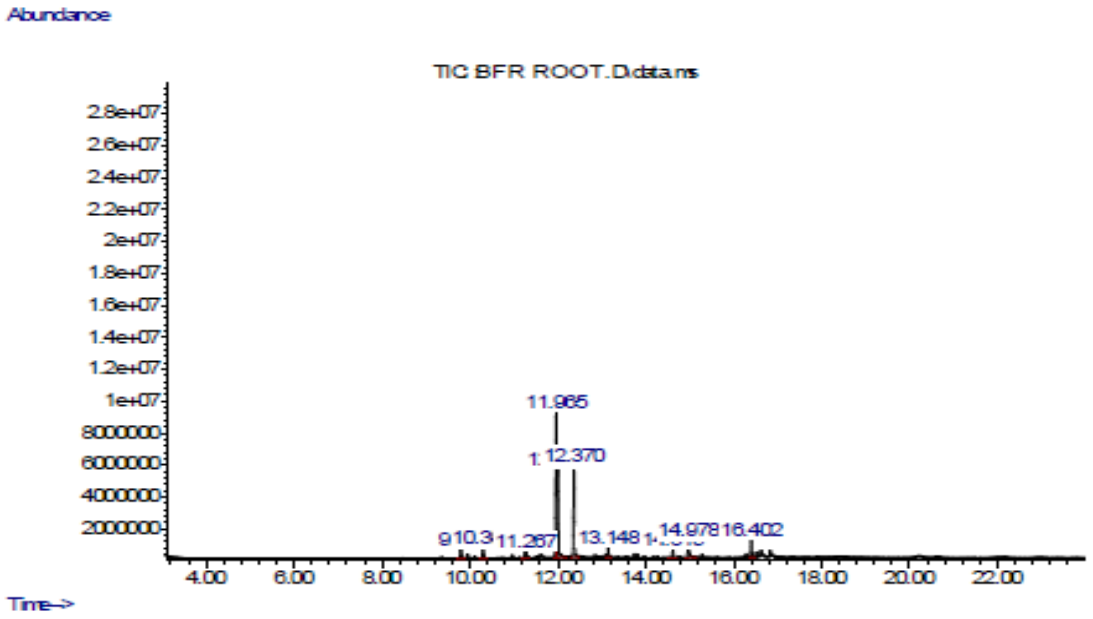

Figure 3. GC-MS chromatogram of the Root essential oil of *B. formosa*

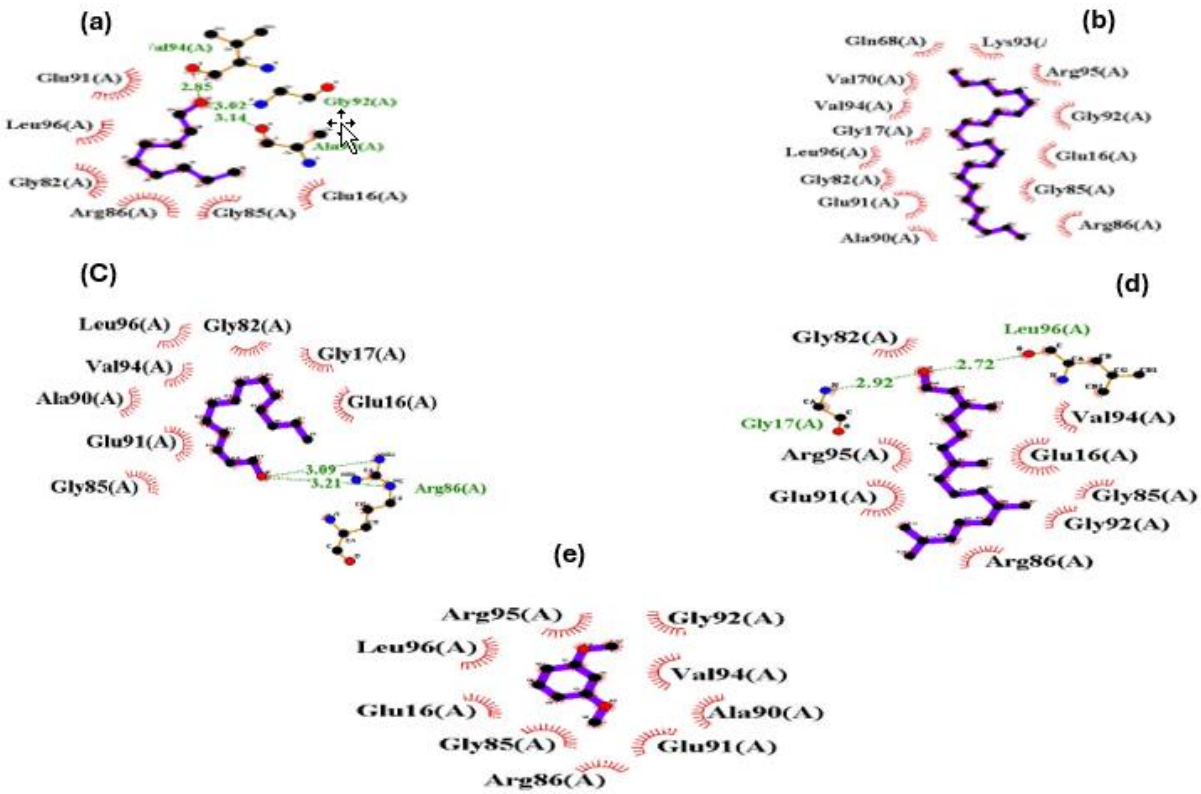

Figure 4. Docking Interactions of PDB: 1HD2 and *B. formosa* Stem Essential Oils (a) 2-Nonen-1-ol (b) Tetracosane (c) E-2-Tetradecen-1-ol (d) Phytol (e) Resorcinol dimethyl ether

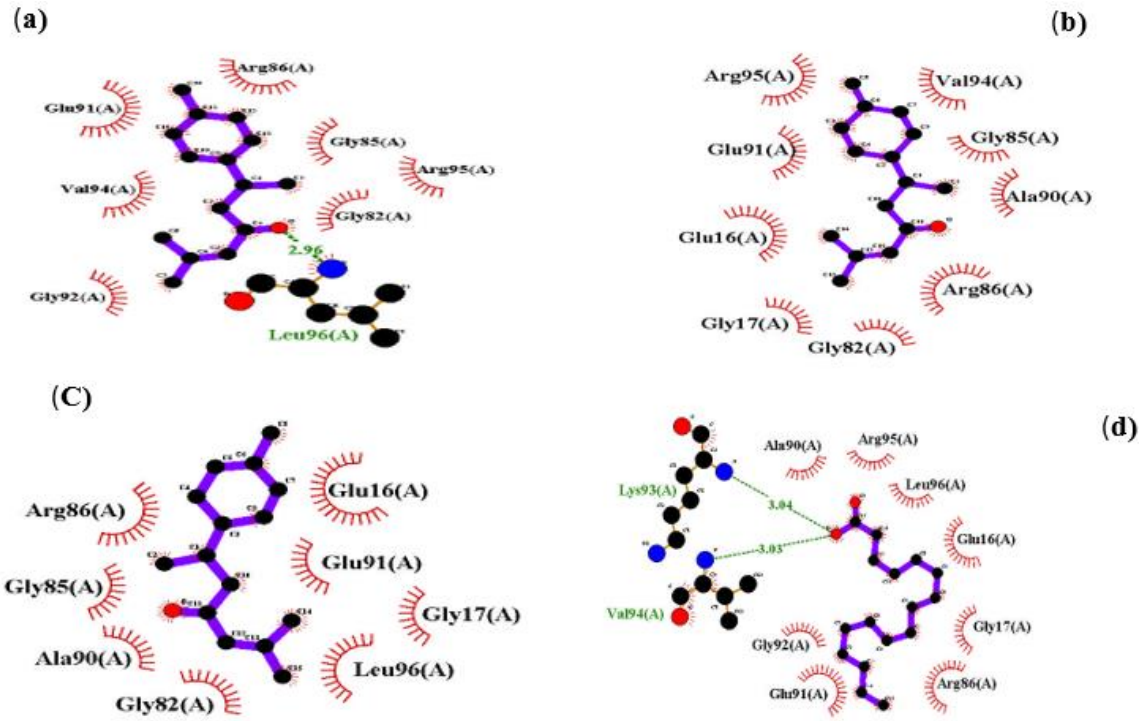

Figure 5. Docking Interactions of PDB: 1HD2 and *B. formosa* Root Essential Oils (a) Ar-tumerone (b) β-Turmerone (c) α-Turmerone (d) n-Hexadecanoic acid

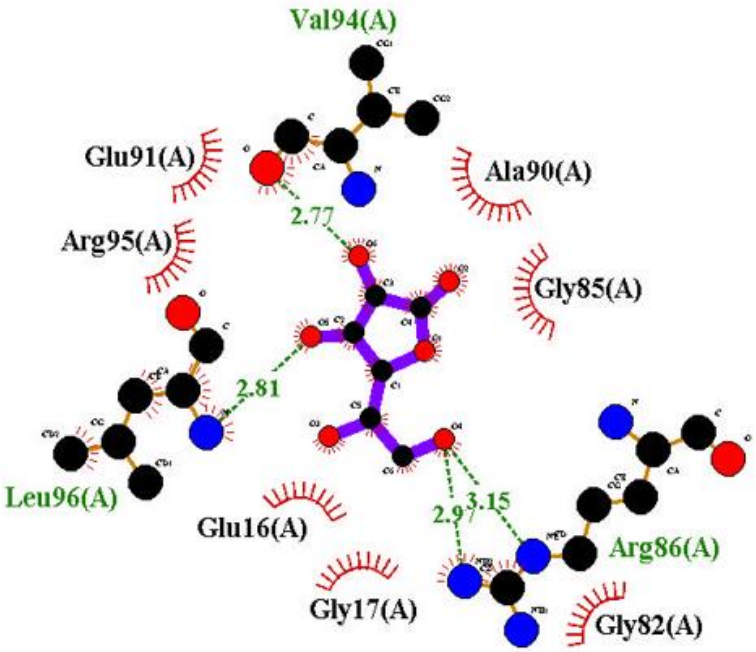

Figure 6. Docking Interactions of PDB: 1HD2 and Ascorbic acid

Table 1. Essential Oils Compositions of *B. formosa* Stems and Roots

Identified compounds	Retention indices	Stem essential oil	Roots essential oil	
2-Nonen-1-ol	1051	9.98	-	
Tetracosane	402.5	9.00	-	
E-2-Tetradecen-1-ol	1713	7.25	-	
Phytol	2122	7.23	3.72	
Resorcinol dimethyl ether	1147	6.99	-	
Kemamide O	2375	6.12	-	
E-14-Hexadecenal	2189	5.85	-	
Octacosane	442.42	5.47	-	
hexahydrofarnesylacetone	1838	4.57	-	
Carvone	1231	4.48	-	
Tridecanal	1510	2.82	-	
(3E)-3-Octadecene	1795	2.62	-	
Heptacosane	426	2.61	-	
cis-Geranylacetone	1434	2.58	-	
1,2-Dimethyl-2-cyclopentene	706	2.37	-	
(E,E)-2,4-Decadienal	1318	2.2	-	
(E)-2-Tridecenal	1982	2.1	-	
β-Barbatene	1451.6	1.9	-	
(Z)-Dec-2-enal	1280	1.84	-	
Cyclododecane	1338.3	1.83	-	
		89.81%	100%	TOTAL COMPOSITION
Ar-tumerone	1664	-	38.11	
β-Turmerone	1701	-	20.5	
α-Turmerone	1680.3	-	19.37	
n-Hexadecanoic acid	1964	-	6.16	
α-Curcumene	1483	-	2.81	
β-Sesquiphellandrene	1525	-	2.78	
p-Cymene	1023.06	-	2.61	
(E)-Atlantone	1785.1		2.03	
Emery 2216	1927	-	1.91	

Table 2. DPPH Free Radical Scavenging Activity of the Essential Oils of Stems and Roots *B. Formosa*

Concentration (µg/mL)	Scavenging activity (%)		
	BF Stems	BF Roots	Vitamin C
10.0	24.37931	29.79142	58.39124
20.0	25.3227	31.97613	89.72194
50.0	28.79838	31.62857	89.8709
100.0	30.53621	37.58686	90.21847
150.0	32.17474	38.18269	91.80734
IC_{50} (µg/mL)	13.4585	10.2197	2.0501

BF: *B. formosa*

Table 3. Binding Affinity Score for *B. formosa* EOs and PDB: 1HD2.

Compound	CID	Binding Affinity Score (Kcal/mol)	Hydrogen Bond Residues
Stem Essential Oil			
2-Nonen-1-ol	61896	-4.2	Ala 90 Gly 92 Val 94
Tetracosane	12592	-4.4	NIL
E-2-Tetradecen-1-ol	5353006	-4.5	Arg 86
Phytol	5280435	-5.0	Gly 17 Leu 96
Resorcinol dimethyl ether	9025	-4.7	NIL
Root Essential Oil			
Ar-tumerone	558221	-5.5	Leu 96
β-Turmerone	196216	-5.6	NIL
α-Turmerone	14632996	-5.6	NIL
n-Hexadecanoic acid	540086	-4.8	Lys 93 Val 94
Phytol	5280435	-5.0	Gly 17 Leu 96
Reference Control			
Ascorbic acid	54690394	-5.8	Arg 86 Val 94 Leu 96

NIL: No Interaction

Table 4. ADMET Evaluation of *B. formosa* Stem and Root Essential Oils

Compounds	Absoprtion (HIA)	Distribution (BBB)	Metabolism (CYP3A4 Inhibitor)	Excretion (Clearance)	Toxicity (Carcinogenesis)
Stem Essential Oil					
2-Nonen-1-ol	Absorbed	Penetrable	Non-Inhibitor	8.29	Safe
Tetracosane	Absorbed	Penetrable	Non-Inhibitor	4.16	Safe
E-2-Tetradecen-1-ol	Absorbed	Penetrable	Non-Inhibitor	7.11	Safe
Phytol	Absorbed	Penetrable	Non-Inhibitor	9.29	Safe
Resorcinol dimethyl ether	Absorbed	Penetrable	Non-Inhibitor	6.43	Toxic
Root Essential Oil					
Ar-tumerone	Absorbed	Penetrable	Non-Inhibitor	8.21	Toxic
β-Turmerone	Absorbed	Penetrable	Non-Inhibitor	7.93	Toxic
α-Turmerone	Absorbed	Penetrable	Non-Inhibitor	7.06	Toxic
N-Hexadecanoic acid	Absorbed	Penetrable	Non-Inhibitor	-0.07	Safe
Phytol	Absorbed	Penetrable	Non-Inhibitor	9.29	Safe
Reference Control					
Ascorbic acid	Absorbed	Non-penetrable	Non-Inhibitor	3.11	Safe

Table 5. Drug-likeness properties of *B. formosa* EOs and Ascorbic acid

Compounds	MW	LogP	nHB	nHA
Stem Essential Oil				
2-Nonen-1-ol	142.24	2.49	1	1
Tetracosane	338.65	8.25	0	0
E-2-Tetradecen-1-ol	212.37	3.80	1	1
Phytol	296.53	5.25	1	1
Resorcinol dimethyl ether	138.16	1.48	2	0
Root Essential Oil				
Ar-tumerone	216.32	3.68	1	0
β-Turmerone	218.33	3.37	1	0
α-Turmerone	218.33	3.37	1	0
N-Hexadecanoic acid	256.42	4.19	2	1
Phytol	296.53	5.25	1	1
Reference Control				
Ascorbic acid	176.12	-2.60	6	4

Conclusion

This study demonstrated the antioxidant efficacy of *Bougainvillea formosa* stems and roots essential oils through experimental and theoretical methodologies. Characterization of the oils from the roots and stems indicated their composition through gas chromatography-mass spectrometry analysis. The total amount of sesquiterpenoid constituents in the oils from the roots was greater than that of the stem fraction. The in vitro free radical scavenging assay confirmed that radical scavenging was concentration dependent. The root essential oil also exhibited greater radical scavenging activity, with a half-maximal inhibitory concentration of 10.22µg/mL, than the stem oil, which had a value of 13.46µg/mL. Tümerone isomers in the root oil exhibited the highest binding affinity score (-5.6kcal/mol) in their molecular docking studies. The predicted ADMET profile indicated toxicity concerns for some of the metabolites, despite the high binding scores. These findings warrant the need to carry out the isolation of the different chemical entities from the oils. The *in vitro* as well as *in vivo* toxicity assessment of the metabolites is therefore recommended.

Abbreviations

ADMET: Absorption, Distribution, Metabolism, Excretion, and Toxicity
BBB: Blood Brain Barrier
CID: Chemical Identifier
DPPH: 2, 2-diphenyl-1-picrylhydrazyl
EO: Essential Oil
GC-MS: Gas Chromatography-Mass spectrometry
HIA: Human Intestinal Absorption
MMFF94: Merck Molecular Force Field 94
MW: Molecular Weight
nHA: Number of Hydrogen Bond Acceptors
nHB: Number of Hydrogen Bond Donors

Authors' Contribution

OOO: Conceptualization, Experiment and Supervision. IAE: Final draft, Theoretical Methodology, and Experiment. MGI: Analysis and Editing. EOO: Review. CEO: Analysis and Editing. HBA: Experiment. CO: Experiment and First draft

Acknowledgments

The authors acknowledge the anonymous reviewers

Conflict of interest

The authors declare no conflict of interest

Article history:

Received: 08 January 2026
Received in revised form: 24 February 2026
Accepted: 28 February 2026
Available online: 28 February 2026

References

1. Peng X, Ren W, Jia M, Zhou Q, Li B, Li G, Xie Y, Dai X, Cao H, Shi X. 2025. Multi-scale study on the volatility of essential oil and its modulation methods. *J Drug Deliv Sci Technol.* 29:107227.
2. Tit DM, Bungau SG. 2023. Antioxidant activity of essential oils. *Antioxidants.* 12:383.
3. Da Costa LS, de Moraes ÂAB, Cruz JN, Mali SN, Almeida LQ, do Nascimento LD, Ferreira OO, Varela ELP, Percário S, de Oliveira MS. 2022. First report on the chemical composition, antioxidant capacity, and preliminary toxicity to *Artemia salina* L. of *Croton campinarensis* Secco, A. Rosário & PE Berry (Euphorbiaceae) essential oil, and *in silico* study. *Antioxidants.* 11:2410.
4. Adeyemi MH. 2010. The potential of secondary metabolites in plant material as deterrents against insect pests: A review. *Afr J Pure Appl Chem.* 4:243–6.
5. Mssillou I, Saghrouchni H, Saber M, Zannou AJ, Balahbib A, Bouyahya A, Allali A, Lyoussi B, Derwich E. 2022. Efficacy and role of essential oils as bio-insecticide against the pulse beetle *Callosobruchus maculatus* (F.) in post-harvest crops. *Ind Crops Prod.* 189:115786.
6. Ekoro IA, Odeja OO, Osharode ME, Tade OO, Omadoko O, Caesar AT, Ehigiator S. 2025. Molecular docking, normal mode analysis and quantum chemical investigations of selected isoxazole-diphenylamine hybrids as potential antioxidants. *In Silico Res Biomed.* 30:100107.
7. Sah J, Singh I. 2025. Role of essential oils and antioxidants in the treatment of fibrosis. *Curr Drug Res Rev.* 17(1):76–89.
8. Chen X, Shang S, Yan F, Jiang H, Zhao G, Tian S, Chen R, Chen D, Dang Y. 2023. Antioxidant activities of essential oils and their major components in scavenging free radicals, inhibiting lipid oxidation and reducing cellular oxidative stress. *Molecules.* 28(11):4559.
9. Khodaei N, Nguyen MM, Mdimagh A, Bayen S, Karboune S. 2021. Compositional diversity and antioxidant properties of essential oils: Predictive models. *LWT.* 138:110684.
10. Mahey P, Sontakke M, Muchahary S, Gupta AK, Jha AK, Kandpal R, Kunwar T, Choudhary A. 2025. Transforming the therapeutic and nutritional benefits of *Bougainvillea* flowers for sustainable uses and food security. *Discover Food.* 5:156. doi:10.1007/s44187-025-00302-z.
11. Adebayo GI, Alabi OT, Owoyele BV, Soladoye AO. 2009. Anti-diabetic properties of the aqueous leaf extract of *Bougainvillea glabra* (Glory of the Garden) on alloxan-induced diabetic rats. *Rec Nat Prod.* 3(4):187.
12. Islam MZ, Hossain MT, Hossen F, Akter MS, Mokammel MA. 2016. In-vitro antioxidant and antimicrobial activity of *Bougainvillea glabra* flower. *Res J Med Plant.* 10(3):228–36.
13. Chavan SS, Shamkuwar PB, Damale MG. 2025. Computational ADMET, drug-likeness, QSPR and molecular docking analysis of phytochemicals from *Avicennia marina*. *Int J Environ Sci.* 11(6S):917–35.
14. Karim A, Marghich M, Amrani O, Addous A, Harit T, Beyi L, Mekhfi H, Aziz M. 2025. Effects of the *Thymus satureioides* essential oil on rodent intestinal smooth muscle: an in vitro and in silico studies. *J Ethnopharmacol.* 120316.
15. Murugan S, Moulishankar A, Palanivel S, Kumaradoss KM, Thirugnanasambandam S. 2025. Computational drug discovery of nitroimidazole compounds targeting Ddn protein of *Mycobacterium tuberculosis*: insights from QSAR modeling, ADMET, molecular docking, and molecular dynamics simulation studies. *Med Novel Technol Devices.* 100406.
16. Odeja O, Ibok M, Okpala E. 2021. Composition and biological assays of the leaf essential oil of *Asparagus flagellaris*. *Clin Phytosci.* 7(12):1–8.
17. Ibok MG, Odeja OO, Okpala EO, Eghwubare JE, Anifalaje EO. 2023. *Eremomastax speciosa* (Hochst.): GC/MS profiling, antioxidant and antimicrobial activities of stem essential oil. *Future J Pharm Sci.* EMID: eacc123fd99babb4..
18. British Pharmacopoeia**.** 1980. London: HM Stationery Office; 2:109.
19. Hanwell MD, Curtis DE, Lonie DC, Vandermeersch T, Zurek E, Hutchison GR. 2012. Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. *J Cheminform.* 4(1):17.
20. Zeinalipour-Yazdi CD. 2024. A computational study of H-bonded networks in cyclic water clusters, $(H_2O)_n$ (n = 3–12). *J Mol Model.* 30(3):58.
21. Laskowski RA, Swindells MB. 2011. LigPlot+: multiple ligand–protein interaction diagrams for drug discovery. *J Chem Inf Model.* 51:2778–86.
22. Riaz A, Kaleem A, Abdullah R, Iqtedar M, Hoessli DC, Aftab M. 2024. In silico approaches to study the human asparagine synthetase: an insight of the interaction between the enzyme active sites and its substrates. *PLoS One.* 19(8):e0307448.
23. Pathivada VS, Bandyopadhyay A, Chhabra R. 2025. Virtual screening and molecular dynamic simulation to identify the potent SOX2-inhibiting drugs. *Indian J Biochem Biophys.* 62(6):596–606.
24. Lohit N, Singh AK, Kumar A, Singh H, Yadav JP, Singh K, Kumar P. 2024. Description and in silico ADME studies of US-FDA approved drugs or drugs under clinical trial which violate the Lipinski's rule of 5. *Lett Drug De. Discov.* 21(8):1334–58.
25. Tossetta G, Fantone S, Giannubilo SR, Marzioni D. 2021. The multifaced actions of curcumin in pregnancy outcome. *Antioxidants (Basel).* 10(1):126.
26. Nair A, Amalraj A, Jacob J, Kunnumakkara AB, Gopi S. 2019. Non-curcuminoids from turmeric and their potential in cancer therapy and anticancer drug delivery formulations. *Biomolecules.* 9:13.
27. Luz JG, Lacerda DA, Corrêa EF, Araújo GF, Araújo RF, Chaves FC, Tavares-Dias M. 2025. *Zingiber officinale* (ginger), *Curcuma longa* (turmeric) and *Cymbopogon nardus* (lemon grass) essential oils have anti-dactylogyrideans potential in *Colossoma macropomum* Cuvier 1816 (tambaqui). *Aquac. Fish Fish.* 5(6):e70146.
28. Brkić Bubola K, Lukić I, Krapac M, Koprivnjak O. 2023. Exploring the connection between the occurrence and intensity of "grubby" defect and volatile composition of olive oil. *Foods.* 12(24):4473.
29. Uddin SJ, Grice D, Tiralongo E. 2012. Evaluation of cytotoxic activity of patriscabratine, tetracosane and various flavonoids isolated from the Bangladeshi medicinal plant *Acrostichum aureum*. *Pharm Biol.* 50(10):1276–80.
30. Namrata B, Sreenivasulu P, Devendra S. 2024. Identification of the novel drug target for the treatment of HIV by using the bioinformatics approach. *Res J Biotechnol.* 19:12.
31. Samah B, Lanez E, Benamor ML, Bekkar Y, Salah NN, Bourougaa L, Bouraoui R, Garzoli S, Lanez T. 2025. GC/MS analysis and computational evaluation of *C. cinerea* EO constituents for colorectal cancer: molecular docking, dynamics, and quantum chemical insights into cis-verbenyl acetate. *Comput Biol Chem.* 108754.
32. Hussein K, Eswaramoorthy R, Melaku Y, Annisa ME. 2021. Antibacterial and antioxidant activity of isoflavans from the roots of *Rhynchosia ferruginea* and in silico study on DNA gyrase and human peroxiredoxin. *Int J Secondary Metabolite.* 8(4):321–36.
33. Dascalu D, Isvoran A, Ianovici N. 2023. Predictions of the biological effects of several acyclic monoterpenes as chemical constituents of essential oils extracted from plants. *Molecules.* 28(12):4640.
34. Pujicic A, Popescu I, Dascalu D, Petreuș DE, Isvoran A. 2025. Predictions of the biological effects of the main components of tarragon essential oil. *Int J Mol Sci.* 26(5):1860.
35. Ding M, Zhu Q, Lu W, Zhu S. 2023. Design and synthesis of multivalent drug delivery system with CA IX inhibitors as ligands. *Bioorg Med Chem.* 93:117456.
36. Dulsat J, López-Nieto B, Estrada-Tejedor R, Borrell JI. 2023. Evaluation of free online ADMET tools for academic or small biotech environments. *Molecules.* 28(2):776.
37. Saritha K, Alivelu M, Mohammad M. 2024. Drug-likeness analysis, in silico ADMET profiling of compounds in *Kedrostis foetidissima* (Jacq.) Cogn, and antibacterial activity of the plant extract. *In Silico Pharmacol.* 12(2):67.