Research Article

Phytochemical Screening and in-Silico Drug-Likeness Properties of Phytocompounds of Ixora Coccinea Against Common Gynaecological Pathogens

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ABSTRACT:

Medicinal plants continue to serve as an important source of bioactive compounds for the development of novel therapeutic agents. Ixora coccinea a member of the family Rubiaceae has been traditionally used in herbal medicine because of its diverse pharmacological properties. However, comprehensive investigations integrating phytochemical screening with computational drug discovery approaches against microbial targets associated with gynecological infections remain limited. The present study aimed to evaluate the phytochemical composition of Ixora coccinea leaf extracts and investigate the drug-likeness, pharmacokinetic properties, toxicity profile and molecular interactions of selected phytochemicals using In-silico approaches. Fresh leaves of Ixora coccinea were extracted separately using ethanol and distilled water and subjected to qualitative phytochemical screening. Phytochemicals reported in previous literature were further evaluated using SwissADME and pkCSM to determine physicochemical characteristics, drug-likeness and ADMET properties. Selected compounds were docked against six microbial target proteins associated with common gynecological pathogens using the HDOCK server. Physicochemical analysis identified seven compounds that satisfied the selected drug-likeness criteria and were retained for further investigation. ADMET prediction demonstrated favorable absorption, distribution, metabolism and excretion characteristics for most compounds, with no predicted hepatotoxicity or cardiotoxicity. Although two compounds showed predicted AMES mutagenicity and a few exhibited possible skin sensitization, the overall safety profile remained encouraging. Molecular docking analysis demonstrated that trans, trans-9,12-octadecadienoic acid exhibited the strongest binding affinity towards multiple microbial target proteins suggesting promising therapeutic potential. The findings indicate that Ixora coccinea leaves constitute a valuable source of bioactive phytochemicals with potential antimicrobial activity against pathogens associated with gynecological infections.

KEYWORDS: Phytochemical screening; ADMET profiling; SwissADME; pkCSM; Molecular docking; HDOCK; Gynecological infections; Natural products; Drug discovery.

INTRODUCTION:

Natural products remain one of the most important sources of therapeutic molecules for modern drug discovery. Despite remarkable advances in synthetic chemistry a significant proportion of clinically approved drugs are either directly derived from plants or developed from naturally occurring compounds. Medicinal plants possess structurally diverse secondary metabolites that exhibit a wide range of biological activities, including antimicrobial, antioxidant, anti-inflammatory, anticancer and immunomodulatory properties. As antimicrobial resistance continues to emerge worldwide, the identification of novel plant-derived bioactive compounds has become an important research priority. Ixora coccinea commonly known as Jungle Geranium or Flame of the Woods, belongs to the family Rubiaceae and is widely distributed throughout tropical and subtropical regions of Asia. The plant has long been utilized in traditional systems of medicine, including Ayurveda, for the management of gastrointestinal disorders, skin diseases, inflammatory conditions, fever, and wound healing. Besides its ornamental value, increasing scientific evidence has demonstrated that different parts of Ixora coccinea contain numerous biologically active constituents responsible for its pharmacological activities[3].

Previous phytochemical investigations have reported the presence of flavonoids, alkaloids, tannins, terpenoids, phenolic compounds, glycosides, saponins, coumarins, steroids and anthraquinones in different extracts of I. coccinea. These metabolites have attracted considerable attention because of their ability to inhibit microbial growth, reduce oxidative stress, and regulate inflammatory pathways. Recent chromatographic studies employing GC–MS and HPLC have further identified several low-molecular-weight bioactive compounds with promising pharmaceutical potential. The rapid development of computational biology has significantly accelerated the early stages of drug discovery. In-silico techniques such as molecular docking and ADMET prediction enable rapid screening of candidate molecules before costly laboratory experiments. Drug-likeness evaluation using SwissADME together with pharmacokinetic and toxicity prediction

using pkCSM provides valuable information regarding the absorption, distribution, metabolism, excretion, and safety of phytochemicals. Molecular docking further predicts the interaction between ligands and disease-associated proteins, allowing the identification of compounds with favourable binding characteristics. [13, 14] Gynecological infections remain a major public health concern worldwide. Opportunistic fungal pathogens such as Candida albicans and bacterial pathogens including Escherichia coli and Staphylococcus aureus are frequently implicated in reproductive tract infections. The increasing prevalence of antimicrobial resistance has highlighted the urgent need to discover safer and more effective therapeutic alternatives. Plant-derived phytochemicals have emerged as promising candidates because of their structural diversity and multiple mechanisms of antimicrobial action. Although several studies have reported the phytochemical composition and pharmacological activities of I. coccinea only limited investigations have combined qualitative phytochemical screening with comprehensive computational evaluation against microbial targets involved in gynecological infections. Integrating phytochemical analysis with drug-likeness prediction, ADMET assessment and molecular docking provides a systematic strategy for identifying promising lead compounds before experimental validation.

MATERIALS AND METHODS

Plant Material Collection: Fresh and healthy leaves of Ixora coccinea L. were collected from a local nursery located in Chandangaon, Chhindwara District, Madhya Pradesh, India. The plant was identified based on its characteristic morphological features and floral characteristics. Only mature, disease-free leaves were selected to minimize contamination and ensure sample uniformity. Immediately after collection, the leaves were transported to the laboratory for further processing.



Plant Drying leaves Leaf powder

Fig.1. Sample Collection and preparation

Preparation of Plant Extracts: The collected leaves were thoroughly washed with distilled water to remove adhering dust and other foreign materials. The cleaned leaves were shade-dried at room temperature (25–28°C) for 7–8 days. After complete drying, the leaves were pulverized using a mechanical grinder to obtain a fine powder and stored in an airtight glass container. For extraction, 10 g of the powdered leaf sample was transferred separately into two sterile conical flasks containing 100 mL of ethanol and 100 mL of distilled water, respectively. The mixtures were kept at room temperature for 24 h to facilitate solvent penetration and extraction of phytochemical constituents. The extracts were subsequently filtered through Whatman No. 1 filter paper, and the clear filtrates were collected as ethanol and aqueous extracts for qualitative phytochemical analysis [12].

Qualitative Phytochemical Screening: Phytochemical screening of the Ethanol and Aqueous leaf extracts of Ixora coccinea was carried out using standard qualitative procedures to identify various bioactive phytochemical constituents like Alkaloids, Amino Acid ,Glycosides, Saponins, Steroids, Terpenoids , Tannins , Flavonoids, Anthraquinones, Coumarin, Phenolic compounds.





Ethanol extract Aqueous extract

Fig.2. Phytochemical screenining of Ethanol and Aqueous leaf extract of Ixora coccinea

Selection of Phytochemicals for Computational Analysis: Bioactive compounds previously reported from Ixora coccinea were collected through an extensive review of published literature. Initially, twelve phytochemicals were shortlisted based on their reported occurrence in the plant. These compounds were subsequently evaluated for their physicochemical characteristics and drug-likeness properties [8, 14].

Retrieval of Chemical Structures:The chemical structures of the selected phytochemicals were retrieved from the PubChem database in the form of Simplified Molecular Input Line Entry System (SMILES) notation. Molecular formula, molecular weight, and PubChem Compound Identification (CID) numbers were also recorded. The retrieved SMILES strings served as input for subsequent drug-likeness, ADMET, and molecular docking analysis [14].

Physicochemical and Drug-Likeness Evaluation: The physicochemical properties of the selected phytochemicals were evaluated using the SwissADME web server. Parameters including molecular weight, lipophilicity (Log P), topological polar surface area (TPSA), hydrogen bond donors, hydrogen bond acceptors, number of rotatable bonds, and bioavailability score were analysed. Drug-likeness was assessed according to Lipinski's Rule of Five and other accepted medicinal chemistry criteria. Compounds satisfying the predefined selection criteria were retained for further computational analyses [14].

ADMET Prediction: The pharmacokinetic and toxicity profiles of the selected phytochemicals were predicted using the pkCSM web server. The SMILES notation of each compound was submitted individually to estimate absorption, distribution, metabolism, excretion, and toxicity (ADMET) parameters. Predicted properties included intestinal absorption, Caco-2 permeability, volume of distribution, blood-brain barrier permeability, cytochrome P450 interactions, total clearance, AMES toxicity, hepatotoxicity, cardiotoxicity, skin sensitization, and acute oral toxicity. These predictions were used to evaluate the drug-likeness and safety of each phytochemical before molecular docking [14].

Selection of Target Proteins: Target proteins associated with common microbial pathogens responsible for gynecological infections were selected through an extensive literature survey. The selected proteins included Secreted Aspartyl Proteinase-3 (SAP3), Lanosterol 14-α-demethylase (CYP51), Agglutinin-like Sequence Protein-3 (ALS3), DNA gyrase from Escherichia coli, DNA gyrase from Staphylococcus aureus, and Sortase A from Staphylococcus aureus. Corresponding three-dimensional protein structures were obtained from the Protein Data Bank (PDB) using their respective PDB accession numbers [20].

Ligand Preparation: The SMILES structures of the selected phytochemicals were converted into Protein Data Bank (PDB) format using an online molecular conversion tool. The generated three-dimensional ligand structures were verified prior to docking to ensure structural compatibility with the selected receptor proteins.

Molecular Docking Analysis: Protein–ligand docking was performed using the HDOCK web server to investigate the binding interactions between the selected phytochemicals and target proteins. Three-dimensional structures of receptor proteins and ligand molecules were uploaded to the server in PDB format. Docking was carried out using the default server parameters. For each protein–ligand complex, docking score, confidence score, and ligand root mean square deviation (RMSD) were recorded. Lower docking scores indicated stronger predicted binding affinity, while higher confidence scores reflected increased reliability of the docking model. The resulting complexes were analysed to identify potential lead compounds exhibiting favourable interactions with microbial target proteins associated with gynaecological infections.

RESULTS: Qualitative phytochemical screening demonstrated the presence of several bioactive secondary metabolites in both ethanol and aqueous leaf extracts of Ixora coccinea (Table 1). The results indicated that the extraction solvent had a considerable influence on the phytochemical profile. Among the ten phytochemical groups evaluated, the ethanol extract showed positive reactions for coumarins, anthraquinones, terpenoids, tannins, phenolic compounds, glycosides, and amino acids, whereas the aqueous

extract exhibited positive reactions for coumarins, terpenoids, tannins, phenolic compounds, and glycosides. Flavonoids, alkaloids, saponins, and steroids were not detected in either extract under the experimental conditions employed.

Table.1. Phytochemical Screening of ethanol and aqueous extract of leaf extracts of Ixora coccinea

S.no.	Phytochemicals	Ethanol solution	Aqueous solution
1.	Coumarin	+	++
2.	Anthraquinones	+	-
3.	Terpenoids	+	-
4.	Steroids	-	-
5.	Flavanoids	-	-
6.	Tannins	++	++
7.	Alkaloids	-	-
8.	Phenols	++	++
9.	Glycosides	+	+
10.	Saponins	-	++
11.	Amino acids	+	-

(++) Strong Positive, (+) Positive, (-) Negative

Physicochemical Screening and Selection of Bioactive Compounds: Twelve phytochemicals previously reported from Ixora coccinea were initially shortlisted through an extensive literature survey. Their physicochemical properties were evaluated using the SwissADME web server to assess molecular characteristics associated with drug-likeness. The evaluation included molecular weight, lipophilicity (Log P), hydrogen bond donor and acceptor counts, topological polar surface area (TPSA), number of rotatable bonds, and bioavailability score. Based on these parameters, five compounds were excluded because they did not satisfy the selected physicochemical criteria. Consequently, seven phytochemicals - Gallic acid (C1), Caffeic acid (C2), n-Hexadecanoic acid (Palmitic acid) (C3), trans,trans-9,12-Octadecadienoic acid (C4), 1,5-Dimethylpyrazole (C5) , Dihydrobenzofuran (C6) and 1,3,5-Trimethylcyclohexane (C7) were selected for further computational analyses (Table 2).

Table 2. Drug Likeness Properties of majour retrieved compounds of I. coccinea

S.no.	Compound Denotation	Molecular weight	H-bond acceptors	H-bond donors	No. of rotatory bonds	Total Surface area	Lipinski
1	C1	170.12	4	1	4	67.135	Yes
2	C2	180.16	3	3	2	74.381	Yes
3	C3	256.42	1	1	14	113.169	Yes
4	C4	276.41	1	1	10	123.897	Yes
5	C5	96.13	2	0	0	42.769	Yes
6	C6	120.15	1	0	0	54.269	Yes
7	C7	126.24	0	0	0	58.653	Yes

Drug-Likeness and ADMET Prediction: The selected phytochemicals were further analysed using the pkCSM web server to predict their pharmacokinetic and toxicity characteristics.

Absorption: Predicted intestinal absorption varied among the selected compounds. 1,5-Dimethylpyrazole exhibited the highest predicted human intestinal absorption, followed closely by Dihydrobenzofuran. Caco-2 permeability analysis also demonstrated favourable absorption characteristics for these compounds, suggesting efficient gastrointestinal uptake following oral administration (Table 3).

Table 3. Absorption Properties of major retrieved compounds of I. coccinea

S.no.	Absorption Parameters	C1	C2	C3	C4	C5	C6	C7
1	Water solubility (mol/L)	-2.56	-2.762	-5.562	-5.455	0.019	-1.753	-4.042
2	Caco2 permeability (cm/s)	-0.081	1.964	1.558	1.597	1.657	1.39	1.402
3	Intestinal absorption (human) (%)	43.374	86.536	92.004	94.942	100	96.926	94.834
4	Skin Permeability (log Kp)	-2.735	-2.735	-2.717	-2.717	-2.632	-1.995	-1.347
5	P-glycoprotein substrate	No	No	No	No	Yes	No	No
6	P-glycoprotein I inhibitor	No	No	No	No	No	No	No
7	P-glycoprotein II inhibitor	No	No	No	No	No	No	No

Distribution: Distribution analysis revealed considerable variation in the pharmacokinetic behaviour of the selected phytochemicals. Predicted volume of distribution (VDss) ranged from low to moderate values, indicating differences in tissue penetration. Dihydrobenzofuran and 1,3,5-Trimethylcyclohexane exhibited comparatively better tissue distribution, while Gallic acid demonstrated limited distribution. Blood-brain barrier permeability predictions suggested that Dihydrobenzofuran and 1,3,5-Trimethylcyclohexane possess relatively greater ability to cross the blood-brain barrier than the remaining compounds (Table 4).

Table 4. Distribution Properties of major retrieved compounds of I. coccinea

S. no.	Distribution Parameters	C1	C2	C3	C4	C5	C6	C7
1	VDss (human) (log L/kg)	-1.855	0.011	-0.543	-0.703	-0.153	0.236	0.389
2	Fraction unbound (human) (Fu)	0.617	0.556	0.101	0.071	0.669	0.381	0.4
3	BBB permeability (log BB)	-1.102	0.059	-0.111	-0.038	-0.024	0.452	0.74
4	CNS permeability (log PS)	-3.74	-3.323	-1.816	-1.387	-2.686	-1.901	-1.74

Metabolism: Cytochrome P450 interaction analysis indicated that most selected phytochemicals neither acted as substrates nor inhibitors of the major CYP450 enzymes. Only trans,trans-9,12-Octadecadienoic acid demonstrated interaction with CYP3A4, whereas the remaining compounds showed comparatively favourable metabolic profiles, suggesting a lower probability of clinically significant drug-drug interactions (Table 5).

Table 5. Metabolism Properties of major retrieved compounds of I. coccinea

S.no.	Metabolism Parameters	C1	C2	C3	C4	C5	C6	C7
1	CYP2D6 substrate	No	No	No	No	No	No	No

2	CYP3A4 substrate	No	No	Yes	Yes	No	No	No
3	CYP1A2 inhibitior	No	No	No	Yes	No	No	No
4	CYP2C19 inhibitior	No	No	No	No	No	No	No
5	CYP2C9 inhibitior	No	No	No	No	No	No	No
6	CYP2D6 inhibitior	No	No	No	No	No	No	No
7	CYP3A4 inhibitior	No	No	No	Yes	No	No	No

Excretion: Predicted total clearance values indicated variability in elimination rates among the selected phytochemicals. Trans,trans-9,12-Octadecadienoic acid and n-Hexadecanoic aci demonstrated relatively rapid predicted clearance, whereas Caffeic acid showed comparatively slower elimination (Table 6).

Table 6. Excretion Properties of major retrieved compounds of I. coccinea

S.no.	Excretion Parameters	C1	C2	C3	C4	C5	C6	C7
1	Total Clearance	0.518	-7.098	1.763	1.792	0.622	0.26	0.116
2	Renal OCT2 substrate	No	No	No	No	No	No	No

Toxicity: Toxicity prediction demonstrated encouraging safety profiles for most phytochemicals. No compound was predicted to exhibit hepatotoxicity or hERG-mediated cardiotoxicity. However, Caffeic acid and Dihydrobenzofuran displayed predicted AMES mutagenicity, while several compounds showed possible skin sensitization. Overall, the majority of the selected phytochemicals exhibited acceptable pharmacokinetic and toxicity characteristics, supporting their suitability for subsequent molecular docking studies (Table 7).

Table 7. Toxicity Properties of major retrieved compounds of I. coccinea

S.no.	Toxicity Parameters	C1	C2	C3	C4	C5	C6	C7
1	AMES toxicity	No	Yes	No	No	No	Yes	No
2	Max. tolerated dose (human)	0.7	0.674	-0.708	-0.873	1.067	0.907	0.588
3	hERG I inhibitor	No	No	No	No	No	No	No
4	hERG II inhibitor	No	No	No	No	No	No	No
5	Oral Rat Acute Toxicity (LD50)	2.218	2.482	1.44	1.456	2.274	1.887	1.637
6	Oral Rat Chronic Toxicity (LOAEL)	3.06	3.668	3.181	2.838	1.509	1.907	2.325
7	Hepatotoxicity	No	No	No	No	No	No	No
8	Skin Sensitivity	No	No	Yes	Yes	Yes	Yes	No

9	T.Pyriformis toxicity	0.285	0.285	0.84	0.764	-0.451	0.236	0.201
10	Minnow toxicity	3.188	5.509	-1.083	-0.82	2.299	1.59	1.069

Molecular Docking Analysis: Protein-ligand docking was performed against six microbial target proteins associated with common gynecological infections using the HDOCK server. The docking analysis demonstrated that binding affinities differed among the selected phytochemicals depending on the receptor protein. Among all investigated compounds, trans,trans-9,12-Octadecadienoic acid consistently exhibited the strongest predicted binding affinity towards most target proteins, including SAP3, CYP51, ALS3, DNA gyrase of Escherichia coli, DNA gyrase of Staphylococcus aureus, and Sortase A. Gallic acid and Caffeic acid also demonstrated favourable docking interactions with several receptors but generally exhibited lower binding affinities than trans,trans-9,12-Octadecadienoic acid. The docking scores, confidence values, and RMSD values collectively suggested stable protein-ligand interactions, supporting the potential antimicrobial activity of the selected phytochemicals (Table 8).

Table 8. Interaction of retrieved compounds with target proteins.

S.No	Target Proteins	Compounds	Docking score	Confidence score	Ligand rmsd (Å)
1.	SAP3 (Candida albicans)	Gallic acid	-101.55	0.2751	65.69
		Caffeic acid	-103.87	0.2844	67.83
		Hexadecadanoic acid	-108.19	0.3023	58.49
		Octadecadanoic acid	-120.36	0.3560	63.28
		Dimethylpyrazole	-62.19	0.1473	67.94
		Dihydrobenzofuran	-74.03	0.1795	64.15
		Trimethylcyclohexane	-69.07	0.1654	62.50
2.	CYP51 (Candida albicans)	Gallic acid	-132.11	0.4115	31.19
		Caffeic acid	-128.67	0.3949	32.18
		Hexadecadanoic acid	-112.47	0.3207	30.04
		Octadecadanoic acid	-127.17	0.3878	35.51
		Dimethylpyrazole	-81.57	0.2028	34.11
		Dihydrobenzofuran	-90.65	0.2338	33.75
		Trimethylcyclohexane	-70.98	0.1707	31.98
3.	ALS3 (Candida albicans)	Gallic acid	-120.21	0.3553	171.13
		Caffeic acid	-132.09	0.4114	172.79
		Hexadecadanoic acid	-114.77	0.3308	172.34
		Octadecadanoic acid	-129.00	0.3965	169.69
		Dimethylpyrazole	-67.01	0.1598	171.69
		Dihydrobenzofuran	-86.40	0.2189	173.86
		Trimethylcyclohexane	-79.21	0.1953	170.72
4.	DNA Gyrase B (E.coli).	Gallic acid	-99.16	0.2657	38.55
		Caffeic acid	-103.68	0.2837	39.39
		Hexadecadanoic acid	-103.34	0.2823	35.49
		Octadecadanoic acid	-116.37	0.3379	39.92
		Dimethylpyrazole	-60.03	0.1419	38.95
		Dihydrobenzofuran	-68.39	0.1635	37.89
		Trimethylcyclohexane	-59.90\	0.1416	36.94
		Gallic acid	-126.67	0.3854	58.61

5.	DNA Gyrase B (E.coli.)	Caffeic acid	-126.40	0.3841	59.59
		Hexadecadanoic acid	-123.46	0.3703	57.33
		Octadecadanoic acid	-150.23	0.5011	57.60
		Dimethylpyrazole	-69.52	0.1666	57.47
		Dihydrobenzofuran	-89.84	0.2309	57.77
		Trimethylcyclohexane	-80.81	0.2004	55.36
6.	Sortase A (S.aureus)	Gallic acid	-94.00	0.2460	44.17
		Caffeic acid	-97.70	0.2600	42.28
		Hexadecadanoic acid	-94.26	0.2470	39.74
		Octadecadanoic acid	-109.05	0.3060	37.06
		Dimethylpyrazole	-64.20	0.1514	43.05
		Dihydrobenzofuran	-71.22	0.1714	43.37
		Trimethylcyclohexane	-60.70	0.1436	45.63

DISCUSSION

The present study revealed that the ethanolic extract of Ixora coccinea leaves contained a greater diversity of phytochemicals than the aqueous extract, indicating that ethanol is a more efficient solvent for extracting bioactive constituents. This finding agrees with previous studies, which reported that alcoholic solvents effectively extract both polar and moderately non-polar secondary metabolites due to their intermediate polarity (3,6). Similarly, Nakka et al. (2025) identified several bioactive compounds in the methanolic extract of Ixora coccinea supporting the suitability of organic solvents for phytochemical extraction. The presence of phenolic compounds, tannins, terpenoids, glycosides, and coumarins in both extracts suggests that these metabolites may contribute to the medicinal properties of I. coccinea. Phenolic compounds and tannins are known for their antioxidant and antimicrobial activities, whereas terpenoids and coumarins have been reported to exhibit anti-inflammatory and broad-spectrum antimicrobial effects (8,12). Anthraquinones and amino acids were detected only in the ethanolic extract, further highlighting the superior extraction capability of ethanol.

The absence of flavonoids, alkaloids, saponins, and steroids in the present study may be attributed to differences in extraction conditions, geographical origin, seasonal variation, or analytical methods. Similar variations in the phytochemical profile of I. coccinea have been reported previously (13). Overall, the qualitative phytochemical screening confirms that I. coccinea leaves are a rich source of bioactive constituents and provides a strong basis for subsequent ADMET profiling and molecular docking studies.

Drug-Likeness and ADMET Profiling: Drug-likeness and ADMET profiling are essential steps in the early stages of drug discovery, as they help identify compounds with favourable pharmacokinetic properties before experimental validation. In the present study, seven phytochemicals selected from Ixora coccinea demonstrated acceptable physicochemical characteristics based on SwissADME analysis, suggesting their potential as drug candidates. Similar computational screening approaches have been widely adopted to prioritize bioactive plant compounds for pharmaceutical research (17).

The ADMET analysis predicted that most of the selected phytochemicals possessed favourable absorption and distribution profiles, indicating their potential for adequate oral bioavailability. In addition, none of the compounds showed predicted hepatotoxicity or hERG-mediated cardiotoxicity, suggesting a promising preliminary safety profile. However, Caffeic acid and Dihydrobenzofuran were predicted to exhibit AMES mutagenicity, while some compounds showed possible skin sensitization. These findings emphasize that although computational predictions are valuable for early screening, they require confirmation through in vitro and in vivo toxicological studies.

Overall, the ADMET results indicate that the majority of the selected phytochemicals possess acceptable pharmacokinetic and safety characteristics, supporting their further evaluation through molecular docking and biological assays. These findings are consistent with recent studies demonstrating that integrating ADMET prediction with phytochemical screening improves the efficiency of identifying promising lead molecules from medicinal plants while reducing the time and cost associated with conventional drug discovery (9,14).

Molecular Docking: Molecular docking was performed to evaluate the binding affinity of the selected phytochemicals against key microbial proteins associated with gynecological infections, including SAP3, CYP51,

ALS3, DNA gyrase B (Escherichia coli and Staphylococcus aureus) and Sortase A. The docking results revealed considerable variation in binding affinity among the selected compounds, indicating differences in their potential to interact with these therapeutic targets.

Among the investigated phytochemicals, trans,trans-9,12-octadecadienoic acid exhibited the strongest binding affinity towards most target proteins, suggesting its potential as a promising lead compound. Strong binding interactions with CYP51 and SAP3 may interfere with ergosterol biosynthesis and fungal virulence in Candida albicans whereas interactions with DNA gyrase and Sortase A indicate possible antibacterial activity against E. coli and S. aureus. Similar studies have demonstrated that phytochemicals with favourable docking scores against these proteins may inhibit microbial growth by disrupting essential cellular processes (4,16).

Gallic acid and caffeic acid also exhibited favourable binding interactions with several receptor proteins, supporting previous reports that phenolic compounds possess significant antimicrobial activity through interactions with multiple molecular targets. Although molecular docking provides valuable insights into protein–ligand interactions, it represents a predictive computational approach and does not confirm biological activity. Therefore, the promising docking results obtained in the present study should be validated through in vitro antimicrobial assays, enzyme inhibition studies, and in vivo investigations. Overall, the docking analysis supports the therapeutic potential of Ixora coccinea phytochemicals and highlights trans,trans-9,12-octadecadienoic acid as a promising candidate for further antimicrobial drug development.

CONCLUSION

The present study demonstrated that Ixora coccinea leaves are a valuable source of bioactive phytochemicals with promising pharmaceutical potential. Qualitative phytochemical screening revealed that the ethanolic extract contained a greater diversity of secondary metabolites than the aqueous extract, highlighting ethanol as a more efficient extraction solvent. These findings support the traditional medicinal use of I. coccinea and provide a scientific basis for its continued investigation. Computational evaluation using SwissADME and pkCSM indicated that most of the selected phytochemicals possessed favourable drug-likeness characteristics and acceptable pharmacokinetic profiles. The majority of the compounds were predicted to exhibit good absorption and low risks of hepatotoxicity and cardiotoxicity, although a few compounds showed possible mutagenicity or skin sensitization, emphasizing the need for further toxicological validation.

Molecular docking study identified trans,trans-9,12-octadecadienoic acid as the most promising phytochemical because of its consistently strong binding affinity toward multiple microbial target proteins associated with common gynecological pathogens. Gallic acid and caffeic acid also demonstrated favourable interactions, suggesting that multiple constituents of I. coccinea may contribute to its antimicrobial activity.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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