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In Silico Screening and Molecular Docking of Potential Bioactive Compounds of Gynura divaricata as Eczema Drug Candidates

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ABSTRACT

Eczema is a chronic inflammatory skin disorder characterized by impaired skin barrier function, itching, and increased susceptibility to allergens and irritants. Medicinal plants are widely explored as complementary therapeutic sources, including *Gynura divaricata*, which has traditionally been used for skin-related conditions. This study aimed to evaluate the anti-eczema potential of bioactive compounds derived from *G. divaricata* through an in silico approach. A total of 24 reported compounds were retrieved from chemical databases, and 10 of them met the PASS prediction threshold (Pa > 0.3). These compounds were further assessed for drug-likeness (Lipinski's criteria), ADME properties, and skin permeation using SwissADME. Molecular docking was performed against two eczema-related target proteins, IL-25 and HRH1. The results showed that all 10 compounds passed multiple screening parameters, with several compounds exhibiting favourable binding affinity and stabilising interactions with the target proteins. Alpha-Farnesene and Alpha-Cubebene demonstrated the highest predicted biological activity based on PASS analysis, while Naphthalene and Alpha-Cubebene showed strong binding affinity in the docking simulations. These findings suggest that bioactive compounds from *Gynura divaricata* have promising potential as candidates for eczema therapy and warrant further experimental investigation.

ABSTRAK

Eksim merupakan gangguan kulit inflamatori kronis yang ditandai oleh kerusakan fungsi sawar kulit, rasa gatal, serta peningkatan kerentanan terhadap alergen dan iritan. Tanaman obat banyak dieksplorasi sebagai sumber terapi komplementer, termasuk Gynura divaricata yang secara tradisional digunakan untuk perawatan kulit. Penelitian ini bertujuan mengevaluasi potensi anti-eksim senyawa bioaktif dari G. divaricata menggunakan pendekatan in silico. Sebanyak 24 senyawa diperoleh dari basis data kimia, dan 10 di antaranya memenuhi ambang prediksi PASS (Pa > 0,3). Senyawa-senyawa tersebut kemudian dianalisis untuk drug-likeness (kriteria Lipinski), sifat ADME, serta permeasi kulit menggunakan SwissADME. Molecular docking dilakukan terhadap dua protein target terkait eksim, yaitu IL-25 dan HRH1. Hasil penelitian menunjukkan bahwa seluruh 10 senyawa lolos beberapa parameter penyaringan, dengan beberapa senyawa menunjukkan afinitas ikatan yang baik serta interaksi stabil dengan protein target. Alpha-Farnesene dan Alpha-Cubebene memiliki aktivitas biologis tertinggi berdasarkan prediksi PASS, sedangkan Naphthalene dan Alpha-Cubebene menunjukkan afinitas pengikatan yang kuat pada simulasi docking. Temuan ini mengindikasikan bahwa senyawa bioaktif dari Gynura divaricata memiliki potensi menjanjikan sebagai kandidat terapi eksim dan layak untuk diteliti lebih lanjut melalui studi in vitro maupun in vivo.

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INTRODUCTION

Eczema, particularly atopic eczema, is a chronic inflammatory skin disorder characterized by impaired skin barrier function, recurrent itching, and susceptibility to allergens and irritants (Tsakok et al., 2019). This condition is common worldwide, with a prevalence reaching 15-30% in children and 2-10% in adults, especially in developed countries (Lee et al., 2016). DistruptiFon of the epidermal barrier often leads to transepidermal water loss and facilitates the penetration of Irritants and pathogens, thereby worsening clinical symptoms.

One of the key molecular factors involved in eczema pathogenesis is the decreased expression of filaggrin, a structural protein essential for forming the cornified envelope in the stratum corneum (Drislane & Irvine, 2020). Reduced filaggrin expression can weaken the skin barrier, increasing the risk of inflammation and irritation (Tsakok et al., 2019). Filaggrin gene expression can also be suppressed by interleukin-25 (IL-25), a cytokine that promotes Th2-mediated allergic inflammation (Hvid et al., 2011). In addition, the histamine H1 receptor (HRH1) plays a central role in mediating itch, vasodilation, and inflammatory responses in allergic skin disorders (Ohsawa &

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Hirasawa, 2014). Because IL-25 and HRH1 contribute significantly to eczema-related inflammatory pathways, these proteins represent promising molecular targets for therapeutic intervention.

Medicinal plants are widely explored as alternative therapeutic sources due to their abundance of bioactive compounds with anti-inflammatory, antimicrobial, and antioxidant properties. One such plant is *Gynura divaricata*, traditionally used in Indonesia and China for wound healing and skin treatments (Aaron et al., 2016; Kantawong et al., 2021). Previous phytochemical investigations have identified more than 24 bioactive constituents in *G. divaricata*, including alkaloids, flavonoids, terpenoids, and phenolic compounds, exhibit biological activities potentially relevant to skin disorders relevant to skin disorders (Xu & Zhang, 2017). However, despite its traditional use, the molecular interactions between these phytochemicals and eczema-related proteins target have not yet been elucidated.

This gap highlights the need for computational exploration to identify potential bioactive compounds capable of modulating IL-25 and HRH1. In silico methods—such as biological activity prediction, ADME evaluation, skin permeation analysis, and molecular docking—offer efficient tools for early-stage drug discovery by predicting compound–protein interactions prior to experimental validation.

Therefore, this study aims to investigate the anti-eczema potential of bioactive compounds from *Gynura divaricata* using a series of in silico approaches targeting IL-25 and HRH1. The findings are expected to provide preliminary theoretical insights into the therapeutic potential of *G. divaricata* and support future in vitro and in vivo studies.

METHODS

The search for ligands was carried out by reviewing the literature on bioactive compounds of the *Gynura divaricata* plant. Data on these compounds were retrieved from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). and subsequently analyzed using the PASS Online webserver (https://www.way2drug.com/PASSOnline/predict.php) to determine the biological potential of each compound. Ten bioactive compounds with the highest *Pa* values for anti-eczema and anti-inflammatory activities were selected for further evaluation. These compounds were then subjected to ADME (absorption, distribution, metabolism, and excretion) prediction using SwissADME (http://www.swissadme.ch/) and assessed based on Lipinski's Rule of Five (http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp).

Target proteins were obtained from the Protein Data Bank (https://www.rcsb.org/), specifically the interleukin-25 (IL-25; PDB ID: 7UWJ) and histamine H1 receptor (HRH1; PDB ID: 3RZE), both of which play significant roles in the physiological mechanisms of eczema. These protein data were further analyzed using the STITCH webserver (http://stitch.embl.de/) to investigate their biological interactions within the human body.

Preparation of ligands and proteins was performed using PyMOL software. Ligands in SDF format were converted into PDB format, while the 3D structures of the target proteins were refined by removing water molecules and co-crystallized ligands attached to their surfaces. The ligands were then subjected to energy minimization and converted into PDBQT format using PyRx version 0.8. The prepared ligands and proteins were subsequently processed for molecular docking using the same software.

The molecular docking process was performed in PyRx version 0.8 employing the AutoDock Vina program integrated within the application. Blind docking was conducted by arranging the grid to cover the entire surface of the target protein. The resulting docking complexes were then visualized using PyMOL software and the ProteinPlus webserver (https://proteins.plus/) to identify and analyze the types of interactions formed between the ligands and the target proteins.

RESULTS AND DISCUSSIONS

A total of 24 bioactive compounds from Gynura divaricata were identified from the literature (Xu & Zhang, 2017), consisting of alkaloid, flavonoid, triterpenoid, steroidal, nucleoside, ester, long-chain aliphatic hydrocarbon, ceramide acid, and phenolic groups. All compounds were retrieved from the PubChem database, and their three-dimensional molecular structures along with those of the IL-25 and HRH1 target proteins—were prepared and visualised as the basis for subsequent computational analyses (Figure 1).

The biological activity of these compounds was evaluated using the PASS Online webserver. Ten compounds exhibited antieczema and anti-inflammatory Pa values greater than 0.3, indicating predicted biological activity (Table 1). Among these, Alpha-Farnesene (Pa = 0.928) and Alpha-Cubebene (Pa = 0.888) showed the highest predicted antieczema and anti-inflammatory activity, respectively. A higher Pa value reflects closer structural similarity to known active molecules and thus greater likelihood of exhibiting the predicted activity (Filimonov et

al., 2014). Although all ten compounds are predicted to possess biological activity, Alpha-Farnesene and Alpha-Cubebene were emphasised due to their superior Pa values.

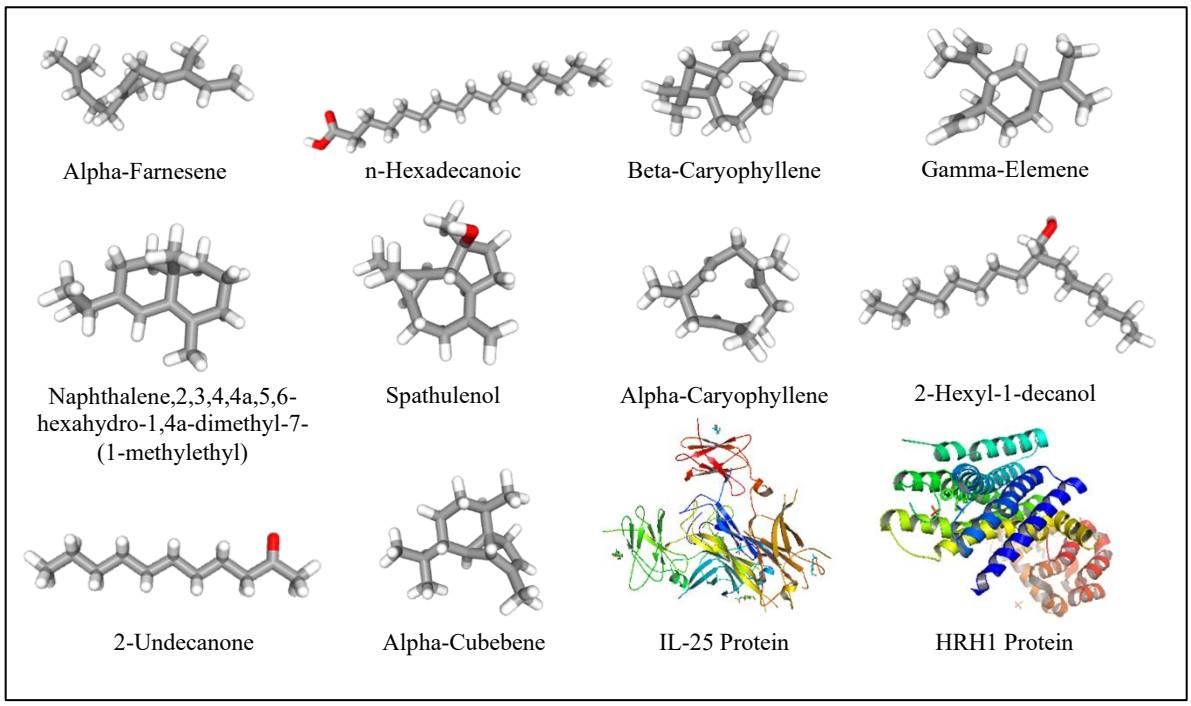

Table 1. PASS Online analysis results of *Gynura divaricata* bioactive compounds

Number	Compounds	CID	PASS Online Pa Value	
			Antieczema	Antiinflamatory
1.	Alpha-Farnesene	5281516	0.928	0.669
2.	n-Hexadecanoic	985	0.920	0.647
3.	Beta-Caryophyllene	5281515	0.897	0.745
4.	Gamma-Elemene	6432312	0.888	0.754
5.	Naphthalene,2,3,4,4a,5,6-hexahydro-1,4a-dimethyl-7-(1-methylethyl)	520383	0.840	0.505
6.	Spathulenol	92231	0.826	0.521
7.	Alpha-Caryophyllene	5281520	0.819	0.741
8.	1-Decanol,2-hexyl	95337	0.750	0.543
9.	2-Undecanone	8163	0.737	0.602
10.	Alpha-Cubebene	442359	0.737	0.888

Drug-likeness evaluation was then performed using Lipinski's Rule of Five and SwissADME (Table 2). All ten selected compounds had molecular weights below 500 g/mol, suggesting favourable membrane permeability (Lipinski, 2004). Only one compound—Naphthalene,2,3,4,4a,5,6-hexahydro-1,4a-dimethyl-7-(1-methylethyl)—exceeded the HBD threshold with a value of 5. Four compounds displayed LogP values greater than 5, indicating reduced permeability due to increased lipophilicity. For molar refractivity, only n-Hexadecanoic did not meet the <130 criterion, as it had a value greater than 130. Overall, all ten compounds satisfied at least two Lipinski parameters, supporting their suitability as drug-like molecules.

Table 2. PASS Online analysis results of *Gynura divaricata* bioactive compounds

Number	Compound Name	Lipinski Rules of Five					SwissADME
		Molecule Weight (<500 g/mol)	HBD (<5)	HBA (<10)	LogP (<5)	Molar Refractivity (40<x<130)	Skin permeation (cm/s)
1.	Alpha-Farnesene	204.35	0	0	5.20	70.99	-3.20
2.	Beta-Caryophyllene	204.35	0	0	4.73	66.74	-4.44
3.	Gamma-Elemene	204.35	0	0	4.89	68.83	-3.75
4.	n-Hexadecanoic	256.42	1	2	5.55	174.67	-2.77
5.	Naphthalene,2,3,4,4a,5,6-hexahydro-1,4a-dimethyl-7-(1-methylethyl)	204.35	5	6	-0.05	77.15	-4.49
6.	Spathulenol	220.35	1	1	3.39	65.97	-5.44
7.	Alpha-Caryophyllene	204.35	0	0	5.04	68.90	-4.32
8.	1-Decanol,2-hexyl	242.44	0	2	6.09	115.85	-2.81
9.	2-Undecanone	170.29	0	1	4.21	62.38	-4.43
10.	Alpha-Cubebene	204.35	0	0	4.27	64.51	-4.37

Further evaluation of skin permeation was conducted using SwissADME LogKp predictions. According to SwissADME criteria, compounds with LogKp values closer to zero or in the positive range exhibit greater skin permeability. Among the analysed compounds, n-Hexadecanoic and 1-Decanol,2-hexyl showed the most positive LogKp values, indicating the highest predicted capability to penetrate the epidermal layer (Demir & Istifli, 2022). This characteristic is relevant to topical formulations aimed at delivering active compounds into deeper skin tissues (Chang et al., 2012).

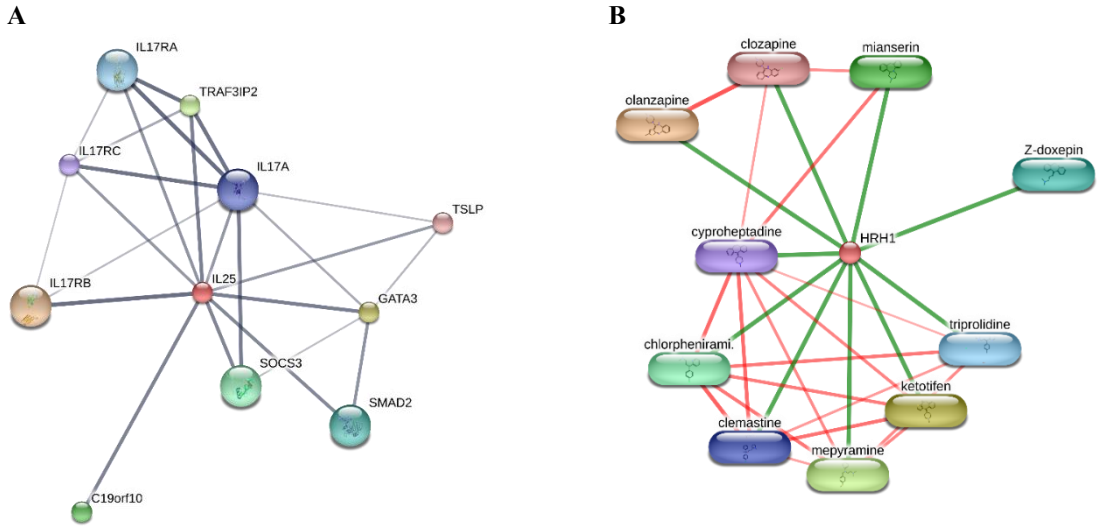

Figure 2. Results of target protein analysis using STITCH webserver. (A) IL-25; (B) HRH1

To confirm the relevance of the selected protein targets, STITCH analysis was performed (Figure 2). IL-25 is known to promote Th2-mediated proinflammatory signalling, contributing to eczema pathophysiology (Pandaleke & Pandaleke, 2014). Meanwhile, HRH1 regulates itch, vasodilation, and inflammatory responses typical of allergic skin reactions (Shimamura et al., 2012). Their involvement in eczema-associated pathways supports their suitability as molecular docking targets for examining the inhibitory potential of the *G. divaricata* compounds.

Molecular docking was performed using PyRx to predict ligand–protein binding affinity (Table 3). For IL-25, Naphthalene showed the most favourable binding affinity (–7.0 kcal/mol), outperforming the wild-type ligand (CID: NAG). For HRH1, Alpha-Cubebene demonstrated the lowest affinity (–7.1 kcal/mol), surpassing both wild ligands (CID: OLC and D7V). More negative affinity values indicate stronger and more stable binding interactions (Demir & Istifli, 2022). These results suggest that Naphthalene and Alpha-Cubebene may effectively interact with and potentially inhibit IL-25 and HRH1, respectively.

Table 3. Molecular docking results of *Gynura divaricata* bioactive compounds

Compounds	Binding Afinity (kcal/mol)	
	IL-25	HRH1
2-Hexyl-1-decanol	-5.1	-4.4
2-Undecanone	-4.7	-4.7
Alpha-Caryophyllene	-6.4	-6.2
Gamma-Elemene	-6	-6.3
Naphthalene	-7	-6.7
Spathulenol	-6.3	-6.3
Alpha-Cubebene	-6.5	-7.1
Alpha-Farnesene	-4,6	-4.8
Beta-Caryophyllene	-6.1	-6.3
n-Hexadecanoic	-5.4	-5.3
Wild Ligand of IL-25		
2-acetamido-2-deoxy-beta-D-glucopyranose (CID : NAG)	-6.2*	
Wild Ligand of HRH1		
(2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CID : OLC)		-4.6*
(3Z)-3-(dibenzo[b,e]oxepin-11(6H)-ylidene)-N,N-dimethylpropan-1-amine (CID : D7V)		-6.8*
(3E)-3-(dibenzo[b,e]oxepin-11(6H)-ylidene)-N,N-dimethylpropan-1-amine (CID : 5EH)		-7.2*

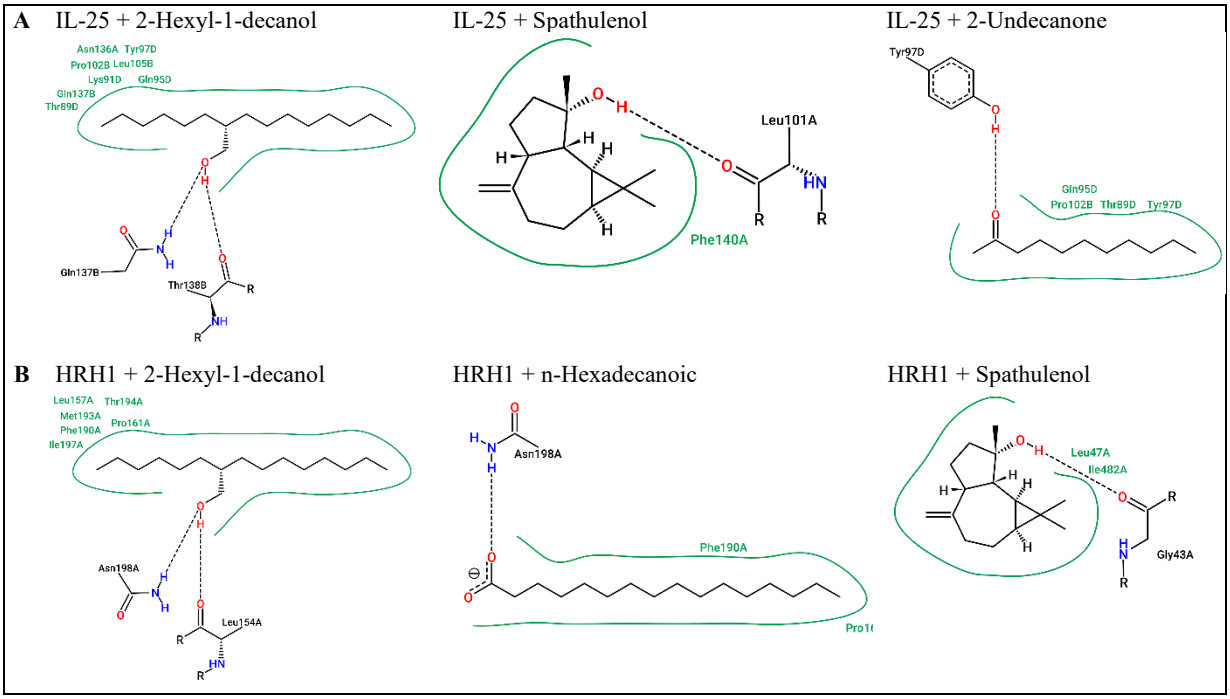

Figure 3. (A) Interaction between IL-25 and ligand; (B) Interaction between HRH1 and ligand. The dashed line is hydrogen bonding, and the green line is hydrophobicity

ProteinPlus visualisations revealed that ligand–protein interactions were stabilised by hydrogen bonds and hydrophobic contacts (Figure 3). Of all evaluated ligands, 2-Hexyl-1-decanol formed two hydrogen bonds with both IL-25 and HRH1, whereas the remaining ligands formed only one. Hydrogen bonding contributes to interaction specificity and stability, while hydrophobic interactions help anchor the ligand within the protein pocket (Frimayanti et al., 2021). The combined presence of these interactions strengthens the predicted binding stability and supports the docking outcomes. Overall, the findings indicate that several *Gynura divaricata* bioactive compounds demonstrate favourable physicochemical properties, predicted biological activity, and strong interaction potential with IL-25 and HRH1, supporting their promise as preliminary candidates for eczema therapy.

CONCLUSIONS

Gynura divaricata contains bioactive compounds with promising potential as candidates for eczema therapy. In this study, ten compounds were identified in silico as having predicted antieczema and anti-inflammatory activity based on PASS analysis (Pa > 0.3). These compounds also fulfilled key parameters of **Lipinski's Rule of Five** and **SwissADME**, supporting their drug-likeness profile and potential suitability for topical administration through adequate skin permeability. Molecular docking results further demonstrated that several compounds—particularly Naphthalene and Alpha-Cubebene—show strong predicted interactions with IL-25 and HRH1, involving stabilizing hydrophobic and hydrogen-bond interactions. Overall, these findings indicate that the bioactive compounds of *Gynura divaricata* show promise as preliminary candidates for eczema treatment. Nevertheless, further in vitro and in vivo studies are required to validate their biological efficacy and safety before clinical development can be considered.

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