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Network pharmacology analysis of bioactive compounds and potential targets of Basella alba for psoriasis treatment

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Abstract

Psoriasis is a chronic inflammatory skin disease characterized by a complex and multifaceted pathophysiology. Due to its persistent and recurrent nature, it poses significant global health challenges, including increased risks of medication resistance, adverse side effects, and systemic comorbidities. Consequently, there is ongoing research into the use of various medicinal plants for its treatment. This research aims to investigate the bioactive compounds of *Basella alba* and their potential in treating psoriasis. A network pharmacology analysis was conducted to elucidate the relationship between the bioactive compounds of *Basella alba* and psoriasis. The Lipinski Rules of Five were followed for screening *Basella alba* compounds in order to find secondary metabolite compounds that met the established criteria. Swiss Target Prediction was used to predict the target protein, while Gene Cards was used to identify psoriasis-related proteins. Venny was used to perform the intersection of these findings. A network pharmacology analysis was conducted using String-DB, and the results were subsequently enriched through the Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway. The selection results identified 22 *Basella alba* active compounds, 11 of which fulfilled Lipinski's Rule of Five. Gene Cards identified 632 psoriasis-related proteins. Predictions showed that *Basella alba* bioactive compounds interact with 1,179 proteins, with 241 overlapping. *Basella alba* treats psoriasis by targeting TP53, AKT1, TNF, EGFR, IL6, STAT3, IL1B, GAPDH, BCL2, and MYC. Bioactive compounds in *Basella alba*, including beta-carotene, acacetin, kaempferol, bioflavonoid (rutin), *Basella* saponin C, and stigmasterol glucoside, may have antipsoriatic effects through apoptotic pathways and inflammation. This research suggests that the bioactive compounds of *Basella alba* have the potential to be effective natural treatments for psoriasis.

Keywords: Basella alba, Bioactive compounds, Network pharmacology, Potential targets, Psoriasis.

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1. Introduction

Psoriasis is a chronic inflammatory autoimmune skin disease triggered by lifestyle, environmental, genetic, or a combination of factors [1]. Keratinocyte hyperproliferation and enhanced migration of immature cells to the stratum corneum are characteristic of psoriasis, a T-cell-mediated disease. Trauma or antigens are considered to activate T-cells in genetically susceptible individuals, resulting in cytokine production and the development of the psoriatic phenotype [2]. Psoriasis affects about 2% of the world's population and is equally common in males and females. It can start at any age, although two peaks have been observed: 20–30 and 50–60 [3]. Psoriasis prevalence in adults was estimated to be between 0.51% and 11.43%, whereas in children it was between 0% and 1.37% [4]. Psoriasis decreases the quality of life and is associated with metabolic syndrome, which includes obesity, dyslipidemia, diabetes, and hypertension [5]. Understanding immune activity in psoriasis, which is regulated by the innate and adaptive immune systems, has made it easier to manage this complicated disease that affects people beyond their skin [6].

The current pharmacological management for psoriasis includes topical, oral, systemic, increasingly biologic, and ultraviolet phototherapy [2]. Due to its persistence, psoriasis treatment should last a long time to reduce its severity and improve patient care, especially regarding the patient's health-related quality of life (HRQOL) and chronic disease management [7]. No treatment exists for psoriasis; it can only be used to control symptoms and reduce comorbidities [8]. Due to the continual and complex nature of the disease, additional research is needed to create more effective treatments. The ability of natural products to bind and modulate disease-related cellular targets makes them essential in medicine. Medicinal plants contain several bioactive compounds that can heal many disorders. Traditional treatments may benefit from their low side effects, affordability, and accessibility [9].

Basella alba, often known as Malabar spinach or Indian spinach, is a plant that has therapeutic properties, particularly for skin conditions. *Basella alba* has been traditionally used in herbal therapy, and it may be effective in the treatment of psoriasis symptoms, despite a lack of scientific studies on psoriasis. *Basella alba L. (Synonym: Basella rubra Roxb.)* is a member of the *Basellaceae* family [9]. *Basella sp.*, native to tropical Southern Asia, grows throughout tropical Asia and Africa, from India to Indonesia [10]. The two species of *Basella* that Carl Linnaeus identified are *Basella rubra* L. and *Basella alba* L. The traits of their leaves and stem colors allow *Basella rubra* L. and *Basella alba* L. to be distinguished from one another [9]. *Basella alba* is a plant with promising pharmacological and medicinal properties. Although scientific research on psoriasis is limited, herbal medicine has historically employed *Basella alba* for its anti-inflammatory, antioxidant, and wound-healing properties, which could potentially help in alleviating psoriasis symptoms. The bioactive compounds, potential targets, and mechanisms of action of *Basella alba* for psoriasis treatment are not yet well understood. Biomedical research is focused on identifying pharmacological targets from the active compounds of medicinal plants to develop novel medicines. The advancement of network pharmacology has provided new insights into the complex bioactive compounds found in various medicinal plants [11].

The purpose of this investigation is to evaluate the potential therapeutic properties of *Basella alba*'s bioactive compounds in the treatment of psoriasis. A network of interactions was subsequently established between potential *Basella alba* targets and well-documented psoriasis-related targets. A comprehensive enrichment analysis was conducted to examine the mechanisms of action of *Basella alba*. The findings of this study could enhance our comprehension of the bioactive compounds, potential targets, and underlying mechanisms of *Basella alba*, which may be beneficial for the development of new therapies for psoriasis.

2. Materials and Methods

2.1. Screening of potentially bioactive compounds of Basella alba

The PubChem database (https://pubchem.ncbi.nlm.nih.gov/) searches for SMILE (simplified molecular-input line-entry system) and bioactive structures in Basella alba based on literature studies, such as Kumar, et al. [12] and Deshmukh and Gaikwad[13]. The following Google searches were done https://powo.science.kew.org/taxon/urn:lsid:ipni.org:names:164286-1; and also https://www.fgcu.edu/cas/communityimpact/foodforest/files/malabarspinach-ada.pdf. The SMILE is a simple pattern that describes the structural features of a compound. It is very important in in silico research, especially for figuring out what the molecule is meant to do and which protein it will bind to based on structural similarities. Because there was little information about the organism in databases, probable components were examined through literature using Google with the keyword "*Basella alba* compounds, components, and substances". Following the removal of duplicates, the solubility and gastrointestinal (GI) absorption statistics were generated using the SwissADME (http://www.swissadme.ch/) database [14] and the chemical information for each compound was gathered using the PubChem (https://pubchem.ncbi.nlm.nih.gov/) database [15].

2.2. Prediction of Basella alba bioactive compound activity using Quantitative Structure-Activity Relationship (QSAR) Approach

The Structure-Activity Relationship (SAR) approach is used in the Way2Drug web portal's PASS (Prediction of Activity Spectra for Substances) online database to predict the biological activity of compounds. The WAY2DRUG PASS prediction tool (http://www.pharmaexpert.ru/passonline/predict.php) evaluates bioactive compounds of *Basella alba* as potential anti-psoriatic agents. WAY2DRUG PASS Prediction uses SAR (Structure-Activity Relationship) analysis to compare the input compound of *Basella alba* with compounds that are already known to have certain potentials. The higher the predictive value that may be derived, the more similar the compounds' structures are. High similarity compounds typically have similar potentials. The Pa value (Probability to be active) is a predictive value from WAY2DRUG PASS that describes the potential of a tested compound, with a score range of 0-1. The Pa value shows the precision of the acquired prediction function; the higher the Pa value of a function, the better its accuracy. If the Pa value is greater than 0.7, it indicates that the compound is predicted to have high potential as an anti-inflammatory, for example, because it has a high similarity to compounds in the database. A score of 0.5 is recommended as the cut-off score. The Pa value provides the accuracy of the obtained prediction function; the higher the Pa value of a function, the better the accuracy [16].

2.3. Prediction of Absorption, Distribution, Metabolism, and Excretion of Basella Alba Bioactive Compounds

The ADMET Lab database [17] is used to predict the toxicity of compounds and the potential for compounds to be absorbed based on the Lipinski rule of five (Rule of five/RO5/Drug likeness). The Lipinski rule of five is used to predict the physicochemical properties of a compound when administered orally. The following are the RO5 parameters: The log P coefficient must not be greater than 5, the molecular weight must not be greater than 500 Da, and the hydrogen bond donors and acceptors must not exceed five or ten. Meanwhile, the bioavailability data is obtained from the Swiss ADME database (http://www.swissadme.ch/) [14]. The selected compound is a compound with predictive potential values as an anti-psoriatic therapy that passes Lipinski's rule of five and has good bioavailability.

2.4. Target Association Analysis and Target Protein Prediction

The bioactive's target prediction was analyzed using the Comparative Toxicogenomic Database (https://ctdbase.org/) and the Similarity Ensemble Approach (https://sea.bkslab.org/) (prediction score > 0.3; p value <0.05) (Computer based). Targets for psoriasis were gathered from the Human Gene Database Genecards (https://www.genecards.org/) [18] Disgenet (https://www.disgenet.com) [19] and Open Target (https://platform.opentargets.org/) [20]. The disease and herbal targets were then mapped using a Venn diagram to determine their overlap. The tools InteractiVenn (www.interactivenn.net) [21] are used to visualize data as Venn diagrams. The Swiss Target Prediction database (http://www.swisstargetprediction.ch/) predicted the protein targets of the active compounds [22]. The target protein information, which encompassed names and IDs, was standardized using UniProt. (http://www.uniprot.org/) [23].

2.5. Pharmacology Network Analysis

The STRING DB V.12.0 database (https://string-db.org/) was utilized to analyze the intersection targets in stage 3 for protein-protein interactions (PPI) [24] with the following parameters organism: Homo sapiens; Network type is full STRING network, Required core: medium confidence (0.4), and FDR stringency medium 5 percent. The data format TSV from STRING was then further processed using CytoScape V.10.0 for network analysis. Cytoscape [25] program was used to visualize interaction data and to perform network analysis with a centrality analysis approach. Therefore, if such a protein is targeted, it can influence other proteins, or it can be referred to as a hub protein.

2.6. Functional Annotation

To perform enrichment analysis on GO (Gene Ontology), specifically on biological processes, cellular components, and molecular functions, and to determine the functionalities of the genes identified in the Venn intersection diagram, the Database for Annotation, Visualization, and Integrated Discovery (DAVID) (https://david.ncifcrf.gov/) is utilized [26]. Terminology with a False Discovery Rate value of less than 0.05 will be discussed further. The annotations used refer to the Gene Ontology (https://geneontology.org/). Annotation, visualization, and integrated discovery databases are employed to conduct Gene Ontology (GO) analyses of biological processes, cell components, and molecular functions [27]. GO functions and KEGG pathways with significant modifications ($P < 0.05$) were identified for further research. We investigated the enrichment of shared target genes for *Basella alba* and psoriasis.

3. Results and Discussion

3.1. Screening of Potentially Bioactive Compounds of Basella alba

This study identified 22 bioactive components of *Basella alba* as potential compounds, which were subsequently linked to relevant target proteins. Table 1 indicates that investigations into the bioactive components of *Basella alba* revealed potential treatments for psoriasis. According to this study, it shows that niacin exhibits the lowest molecular weight (Figure 1), measured at 123.11 g/mol. This indicates that a substance's absorption ability escalates as its molecular weight diminishes [28].

Table 1.
Profile of Bioactive Compounds of Basella alba.

Sample	Compound	Formulation	PubChem ID	MW (g/mol)
1	Gallic acid	C7H6O5	370	170.12
2	Salicylic acid	C7H6O3	338	138.12
3	Ferulic acid	C10H10O4	445858	194.18
4	Betacyanin	C24H26N2O13	6324775	550.5
5	Acacetin	C16H12O5	5280442	284.26
6	Anthraquinone	C14H8O2	6780	208.21
7	Basellasaponin A	C47H70O21	101720817	971
8	Basellasaponin B	C47H68O21	101720818	969
9	Basellasaponin C	C47H68O22	101720819	985
10	Basellasaponin D	C47H68O22	101720820	985
11	Beta sitosterol	C29H50O	222284	414.7
12	Beta-carotene	C40H56	5280489	536.9
13	Bioflavonoid (Rutin)	C27H30O16	5280805	610.5
14	Gomphrenin I	C24H26N2O13	90658633	550.5
15	Gomphrenin III	C34H34N2O16	101105498	726.6
16	Kaempherol	C15H10O6	5280863	286.24
17	Linoleic acid	C18H32O2	5280450	280.4
18	Lupeol	C30H50O	259846	426.7
19	Momordin II C	C47H74O18	14162557	927.1
20	Niacin	C6H5NO2	938	123.11
21	Stigmasterol glucoside	C35H58O6	6602508	574.8
22	Syringic acid	C9H10O5	10742	198.17

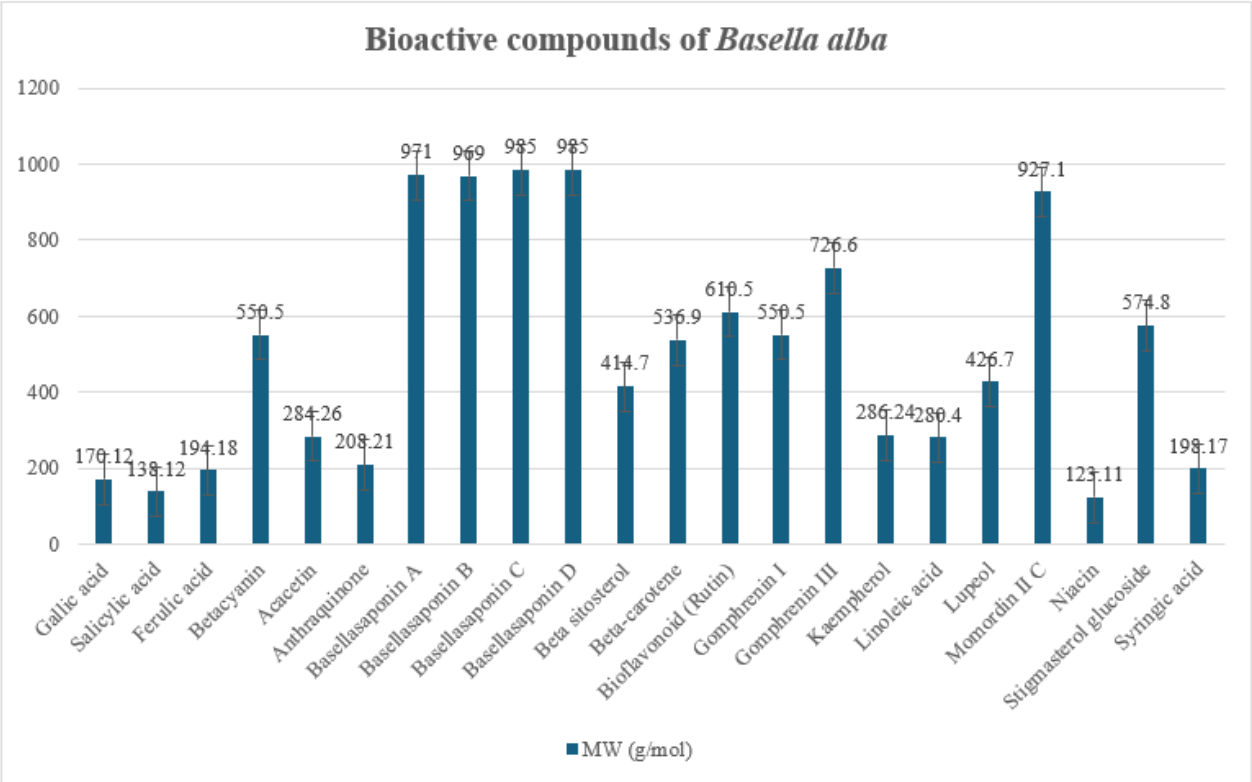

Figure 1.
The bioactive compounds of *Basella alba* as potential treatment of psoriasis related to its molecular weight.

This study found a 22-bioactive compound component-target network of *Basella alba* with 241 overlapping targets related to psoriasis. Some *Basella alba* chemicals may have synergistic effects due to similar targets [12, 29]. Various in vivo and in vitro studies have demonstrated that *Basella alba* is rich in bioactive compounds with therapeutic properties, which enables the identification of numerous related targets. For instance, a study by Sushila et al. [30] evaluated the cytotoxic activity of the whole plant methanolic extract of *Basella alba*. Another study by Arokoyo et al. [31] focused on

the modulation of inflammatory cytokines by the aqueous extract of *Basella alba* in streptozotocin-induced diabetic rats. Phenolic compounds were indicated to be responsible for the antioxidant activity and antidiabetic properties, indicating great potential for further development of functional foods for disease prevention [32].

3.2. Prediction of Bioactive Compound Activity using Structure-Activity Relationship (SAR) Approach

The WAY2DRUG Pass Prediction tool uses Structure-Activity Relationship (SAR) analysis to compare input compounds with known compounds that have specific potential. The greater the similarity of the structure of the compounds, the higher the prediction value obtained. Compounds with similar structures can be predicted to have similar potential. The Pa value (Probability of being Active) is the output prediction value of the WAY2DRUG PASS, which describes the potential of a tested compound.

Based on SAR analysis using the WAY2DRUG PASS prediction tool, the bioactive compounds in *Basella alba* have good potential as an apoptosis agonist (0.585), anti-inflammatory (0.573), antioxidant (0.470), proliferative disease treatment (0.431), antipsoriatic (0.415), JAK2 expression inhibitor (0.375), TNF expression inhibitor (0.260), transcription factor NF-κB inhibitor (0.248), NF-E2-related factor 2 stimulant (0.250), interleukin 6 antagonist (0.122), and VEGF expression inhibitor (0.062) as seen in Figure 2.

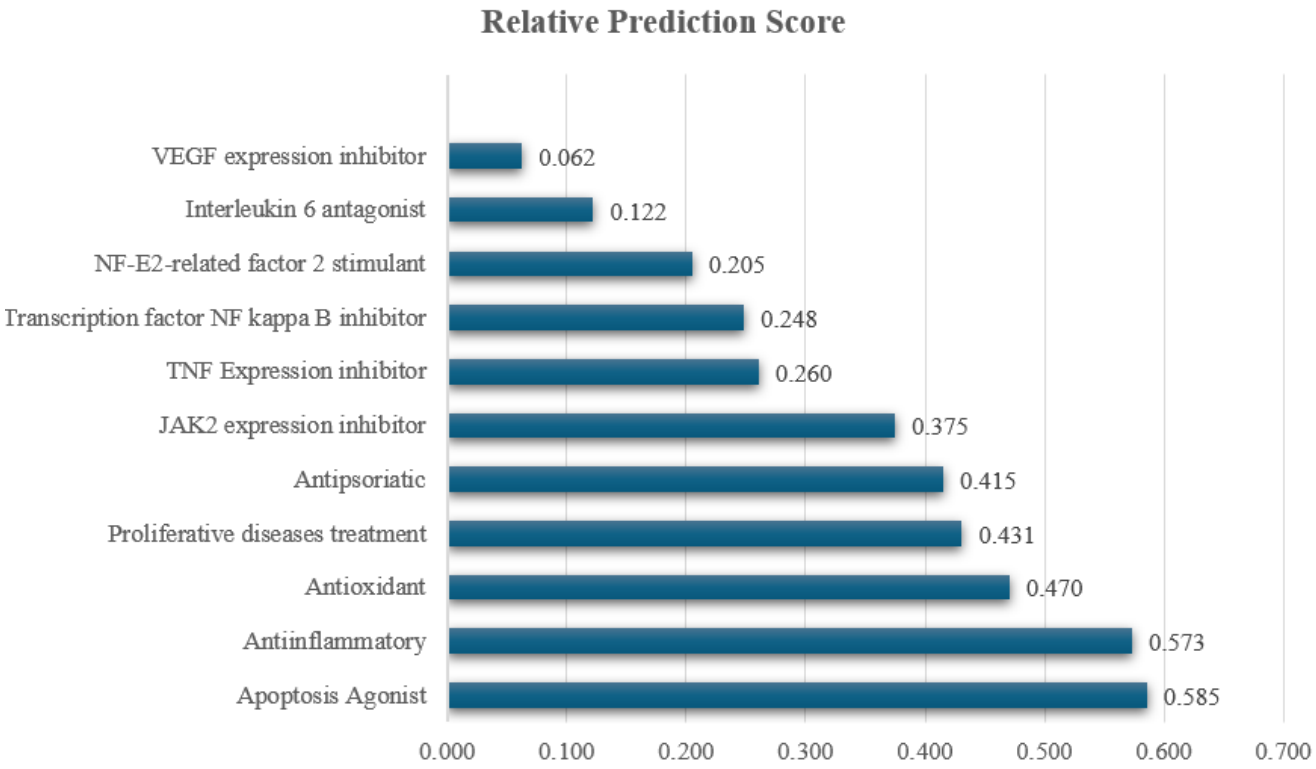

Figure 2.
Prediction of Bioactivity of *Basella alba* as an antipsoriatic treatment based on the SAR-WAY2DRUG PASS Online approach

A score of 0.5 is recommended as the cut-off score. The Pa value provides the accuracy of the obtained prediction function; the higher the Pa value of a function, the better the accuracy. The most promising compounds of *Basella alba* for additional research based on the WAY2DRUG PASS Online approach are those that have an average activity value over 0.4 for apoptotic agonists, anti-inflammatory, antioxidant, proliferative disease treatment, and antipsoriatic. The parameters of apoptosis agonist, anti-inflammatory, antioxidant, proliferative disease treatment, antipsoriatic, JAK2 expression inhibitor, TNF expression inhibitor, transcription factor NF-κβ inhibitor, NF-E2-related factor 2 stimulant, IL-6 antagonist, and VEGF expression inhibitor are used to assess the potential as antipsoriatic based on the hallmarks of psoriasis. *Basella alba* has the highest potential as an apoptosis agonist and anti-inflammatory. Compounds with relatively high potential values (> 0.4) include beta-carotene, ferulic acid, acacetin, kaempferol, gallic acid, rutin, momordin II C, syringic acid, linoleic acid, lupeol, bellasaponin C, and salicylic acid (Figure 3).

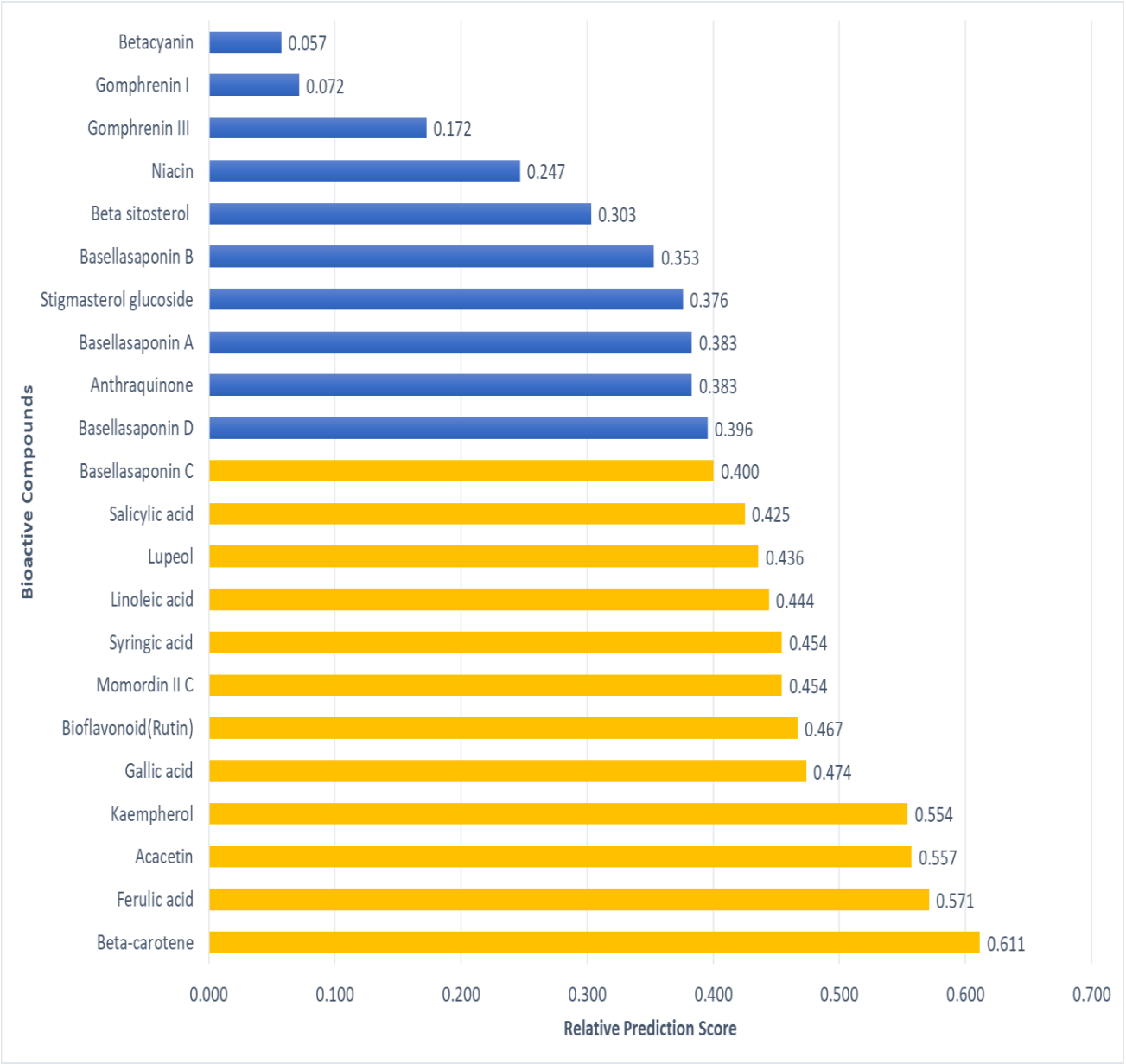

Figure 3.
Prediction of Bioactivity of *Basella alba* compounds based on the SAR approach using Way2Drug Pass Online.

Beta-carotene, ferulic acid, acacetin, kaempferol, rutin, and stigmasterol glucoside were identified in *Basella alba* and may affect numerous targets. For potential value (0.4) and confidence level 0.4, it is chosen from the range of 0 - 1 because with the similarity searching approach, the closer it gets to 1, the more similar the structure of the *Basella alba* compound is to the structure of the training set compound in the pass server database with certain potential. According to Filimonov et al. [16], it is stated that if we use a value above 0.3, we can find new novel compounds with certain activities [16].

This study employed an in silico analysis approach to evaluate potential bioactive compounds and to examine the bioactivity potential of *Basella alba* as a potential therapy for psoriasis, as seen in Table 2. The beta-carotene compound in *Basella alba* has the highest potential for bioactivity as an apoptosis agonist, with a probable activity (Pa) value of 0.943. This compound is predicted to have a high potential in both computational and laboratory tests. A Pa score of 0.3-0.7 indicates that the molecule is computationally capable of the action under investigation but has not been proven in laboratory experiments or has limited potential. Basella saponin C is the chemical that has the highest anti-inflammatory activity, utilizing a Pa value of 0.831. *Basella alba's* most potent antioxidant is bioflavonoid (rutin), with a Pa value of 0.923, while stigmasterol glucoside, with a Pa value of 0.959, has the most important antiproliferative role. The most active ingredient of *Basella alba* as an antipsoriatic is beta-carotene, which has a Pa value of 0.91 and also serves as an apoptosis agonist (Pa value of 0.943).

Table 2.
Basella alba bioactive compound related to its potencies.

No.	Active compounds	Apoptosis Agonist	Anti inflammatory	Antioxidant	Proliferative diseases treatment	Anti psoriatic	JAK2 expression inhibitor	TNF Expression inhibitor	Transcription factor NF kappa B inhibitor	NF-E2-related factor 2 stimulant	IL-6 antagonist	VEGF expression inhibitor	Relative Prediction Score
1	Betacyanin	0	0	0.326	0.191	0	0	0	0	0	0	0	0.057
2	Gomphrenin I	0	0	0.431	0.213	0	0	0	0	0	0	0	0.072
3	Gomphrenin III	0.301	0.281	0.475	0.314	0.181	0	0	0	0	0	0	0.172
4	Niacin	0	0.459	0	0.161	0.548	0.464	0.326	0.149	0.543	0.182	0.113	0.247
5	Beta sitosterol	0.558	0.467	0.178	0	0.643	0.463	0.317	0.101	0	0	0	0.303
6	Basellasaponin B	0.769	0.721	0.586	0.381	0.448	0	0	0.271	0	0	0	0.353
7	Stigmasterol glucoside	0.702	0.599	0.379	0.959	0.644	0	0	0.1	0	0	0	0.376
8	Basellasaponin A	0.814	0.816	0.598	0.449	0.498	0	0	0.271	0	0	0	0.383
9	Anthraquinone	0.584	0.41	0.189	0.263	0.318	0.816	0.47	0.192	0.586	0.236	0.205	0.383
10	Basellasaponin D	0.811	0.818	0.642	0.449	0.543	0	0	0.297	0	0	0	0.396
11	Basellasaponin C	0.826	0.831	0.611	0.449	0.497	0	0	0.389	0	0	0	0.400
12	Salicylic acid	0.392	0.713	0.318	0.268	0.491	0.759	0.503	0.242	0.487	0.185	0.14	0.425
13	Lupeol	0.883	0.708	0.28	0.462	0.546	0.532	0	0.51	0	0.214	0	0.436
14	Linoleic acid	0.545	0.73	0.314	0.519	0.536	0.465	0.751	0.137	0.311	0.182	0	0.444
15	Syringic acid	0.538	0.498	0.403	0.317	0.494	0.83	0.596	0.284	0.435	0.155	0.129	0.454
16	Momordin II C	0.85	0.83	0.68	0.675	0.478	0	0	0.577	0	0.219	0	0.454
17	Bioflavonoid (Rutin)	0.747	0.728	0.923	0.952	0.32	0.28	0	0.253	0	0.385	0	0.467
18	Gallic acid	0.562	0.548	0.52	0.324	0.571	0.786	0.56	0.265	0.506	0	0.128	0.474
19	Kaempherol	0.881	0.676	0.856	0.602	0.181	0.745	0.476	0.286	0.556	0.254	0.283	0.554
20	Acacetin	0.827	0.595	0.628	0.538	0.179	0.812	0.649	0.479	0.564	0.315	0.309	0.557
21	Ferulic acid	0.702	0.604	0.54	0.558	0.596	0.915	0.819	0.407	0.308	0.235	0	0.571
22	Beta-carotene	0.943	0.69	0.775	0.639	0.91	0.52	0.89	0.136	0.52	0	0	0.611
	Pa average	0.585	0.573	0.47	0.431	0.415	0.375	0.26	0.248	0.205	0.122	0.062	

The efficacy of herbal medicine is frequently the outcome of the interaction of numerous components, targets, and pathways [33]. By functioning as an antioxidant, beta-carotene, a precursor to vitamin A, has the potential to alleviate inflammation in the skin by neutralizing detrimental free radicals that are responsible for the rapid turnover of skin cells, which is a hallmark of psoriasis [34]. Research indicates that individuals with psoriasis may benefit from a diet that is abundant in beta-carotene; this could potentially contribute to the improvement of skin lesions [35].

Beta-carotene is a carotenoid that exhibits antioxidant and immunomodulatory properties. Beta-carotene's primary function is to act as an antioxidant, which can help prevent oxidative stress that contributes to the inflammatory process in psoriasis. According to evidence, beta-carotene may also influence angiogenesis, a critical process in the development of psoriasis. Beta-carotene has been shown to inhibit proangiogenic factors, such as vascular endothelial growth factor [36]. Beta-carotene's role as a vitamin A precursor suggests it may affect keratinocyte differentiation and epidermal growth. This may reveal its processes in psoriasis. Beta-carotene is a promising candidate for the management of psoriasis due to its combination of anti-inflammatory, antioxidant, and anti-angiogenic properties [37]. Consequently, additional research is required to establish the critical importance of basellasaponin C as an anti-inflammatory in psoriasis. Clinical trials are needed to confirm its efficacy, determine beneficial dosages, and clarify its function in psoriasis treatment. However, more extensive experimental and clinical studies are needed to prove that it works, is safe, and can be used most effectively in treating psoriasis.

3.3. Prediction of Absorption, Distribution, Metabolism and Excretion of Basella Alba Bioactive Compounds

A well-balanced combination of safety, pharmacokinetics, and biochemical activity is necessary for a medication to be effective. For a drug candidate to be successful, an ideal absorption, distribution, metabolism, excretion, and toxicity (ADMET) profile is just as important as high potency and selectivity [38]. ADMETlab is used to predict whether a bioactive compound has similarities to orally consumed drugs through the RO5 approach or drug-likeness [29]. In this study, we used ADMETlab 2.0, a completely redesigned version of the widely used ADMETlab web server (https://admetmesh.scbdd.com/) for the predictions of pharmacokinetics and toxicity properties of chemicals [39]. Compounds that do not pass Lipinski's rules are likely to have difficulty reaching blood circulation, as evidenced by the additional bioavailability score (Table 3). Physical characteristics can optimize bioavailability or permeability in specific substances. There is no consensus on bioavailability-related physical features. Although lipophilicity is thought to promote bioavailability, at least one study found that hydrophobicity decreases cell penetration. Others have stressed the need to minimize hydrogen bonding or polar surface area. A transporter with structure-activity correlations may be needed in various circumstances [30].

A Bioavailability Score (ABS) measures the probability that a drug will have >10% bioavailability in rats or detectable Caco-2 permeability. ABS = 0.11 for anions with PSA >150 Å2, 0.56 for 75-150 Å2, and 0.85 for <75 A. For remaining compounds, ABS is 0.55 if passing the rule-of-five and 0.17 otherwise ABS also finds poorly- and well-absorbed chemicals in human. The bioavailability of compounds depending on their predominant charge at biological pH. The fraction of anions with >10% F falls from 85% if the polar surface area (PSA) is ≤ 75 Å2, to 56% if 75 < PSA < 150 Å2, to 11% if PSA is ≥ 150 Å2. Compounds with a molecular weight greater than 500 are generally less permeable and tend to have lower bioavailability. The Abbot Bioavailability Score is similar but seeks to predict the probability of a compound having at least 10% oral bioavailability in rats or measurable Caco-2 permeability. This semi-quantitative rule-based score, relying on total charge, TPSA, and violations of the Lipinski filter, defines four classes of compounds with probabilities of 11%, 17%, 56%, or 85%. Like the other methods in this section, it primarily focuses on the fast screening of chemical libraries to select the best molecules to be purchased, synthesized, or promoted at a further stage of a medicinal chemistry project [14, 30].

Table 3.
Predictions of ADME of *Basella alba* compound according to Lipinski.

No	Compounds	nHD	nHA	MW	LogP	Number of violations	Bioavailability Score	Lipinski
1	Gallic acid	4	5	170.02	0.645	0	0.56	Accepted
2	Salicylic acid	2	3	138.03	2.221	0	0.85	Accepted
3	Ferulic acid	2	4	194.06	1.803	0	0.85	Accepted
4	Betacyanin	7	15	550.14	2.599	3	0.11	Rejected
5	Acacetin	2	5	284.07	3.645	0	0.55	Accepted
6	Anthraquinone	0	2	208.05	3.414	0	0.55	Accepted
7	Basellasaponin A	10	21	970.44	2.003	3	0.55	Rejected
8	Basellasaponin B	9	21	968.43	1.848	3	0.11	Rejected
9	Basellasaponin C	10	22	984.42	2.046	3	0.11	Rejected
10	Basellasaponin D	10	22	984.42	2.038	3	0.11	Rejected
11	Beta sitosterol	1	1	414.39	7.663	1	0.55	Accepted
12	Beta-carotene	0	0	536.44	11.15	2	0.17	Rejected
13	Bioflavonoid (Rutin)	10	16	610.15	0.763	3	0.17	Rejected
14	Gomphrenin I	9	15	550.14	1.131	3	0.11	Rejected
15	Gomphrenin III	9	18	726.19	0.681	3	0.11	Rejected
16	Kaempherol	4	6	286.05	2.656	0	0.55	Accepted
17	Linoleic acid	1	2	280.24	6.652	0	0.85	Accepted
18	Lupeol	1	1	426.39	7.291	0	0.55	Accepted
19	Momordin II C	10	18	926.49	2.414	3	0.11	Rejected
20	Niacin	1	3	123.03	0.405	0	0.85	Accepted
21	Stigmasterol glucoside	4	6	574.42	5.738	2	0.55	Rejected
22	Syringic acid	2	5	198.05	1.212	0	0.56	Accepted

According to this study, out of the 22 compounds tested, 11 compounds were eliminated because they did not comply with Lipinski's rule of 5 and had low bioavailability values Lipinski's rule states that a biologically active molecule needs to fulfil the following conditions before being evaluated for use as an orally delivered drug; otherwise, it will display inadequate penetration or absorption: (1) Not more than five hydrogen bond donors (nitrogen or oxygen atoms paired with one or more hydrogen atoms) (nHD <5). (2) No more than ten hydrogen bond acceptors (nitrogen or oxygen atoms) (nHA<10). (3) A molecular weight of fewer than 500 daltons (DA) (MW<500). (4) An octanol-water partition coefficient log P of not more than five (LogP<5). If the component does not belong to that group, it is difficult to absorb, enter the bloodstream, and reach the target [31]. The standard for accepting and rejecting, as shown in Table 2, does not meet all the requirements of Lipinski's rule, but actually allows up to 1 violation. Based on Table 2, it is found that Beta sitosterol, although it has a logP >5, is still accepted because it is the only violation. So if there are zero or one violation of Lipinski's rule, the compound still meets the criteria for acceptance. Therefore, an "Accepted" compound must have a violation number of 0 or 1, and a compound with >1 must be "Rejected". The bioavailability score (range 0 – 1) is a depiction of the extent to which a compound can be absorbed and enter the bloodstream when administered orally [14]. The 11 compounds that were approved for this study are ideal drugs in terms of absorption because their bioavailability scores are all greater than or equal to 0.55 [32]. On the other hand, if a drug's bioavailability score is less than 0.55, it is deemed to have low bioavailability and is rejected. The fact that the *Basella alba*'s active ingredient was rejected due to its low bioavailability score does not rule out its potential. The issue then becomes that the chemical needs more work to be absorbed when taken orally. Drug formulation into liposomes, niosomes, phytosomes, solid lipid nanoparticles, polymer nanoparticles and microparticles, self-contained micro-emulsifying drug delivery systems, and microemulsions can increase the bioavailability of medications with low absorption [40].

3.4. Target Association Analysis & Target Protein Prediction

Data mining through a union global data exploration via the Comparative Toxicogenomic Database (https://ctdbase.org) and the Similarity Ensemble Approach database (https://sea.bkslab.org) shows that 1,179 target proteins can be targeted by *Basella alba*. The difference between the two databases is that the Similarity Ensemble Approach lists the similarity of protein structures and includes related scoring, while the Comparative Toxicogenomic Database does not have a score because this database is based on data from research that has been carried out previously, and then the data is collected. The combination of these two databases will produce a more complete analysis.

When related to psoriasis, out of 632 proteins data associated with psoriasis, the Venn diagram (Figure 4) shows 241 proteins that are linked to psoriasis but are also targeted by compounds in Basella alba after the target genes of the active components of Basella alba were matched with the target genes linked to psoriasis directly. In the STRING database, a PPI network with 241 overlapping targets was constructed at a 0.4 confidence level. To determine the hub proteins in the network, the Analyze Network tools in Cytoscape were used to assess the created network.

Figure 4.
Venn diagram of intersection proteins associated with psoriasis and bioactive targets of *Basella alba*.

3.5. Pharmacology Network Analysis

PPI networks are now a crucial tool for understanding biological processes because they can predict high-throughput data, including protein function, developmental regulation formation, disease candidate gene identification, and therapeutic target identification, as well as large-scale gene expression data [24]. Based on the degree centrality analysis, the proteins that have the most interactors with other psoriasis proteins include TP53, AKT1, TNF, EGFR, IL6, STAT3, IL1B, GADPH, BCL2 and MYC (Figure 5). It is predicted that *Basella alba* active compounds are thought to regulate psoriasis pathogenesis through various pathways.

The purpose of this investigation is to establish a gene-pathway network that will facilitate the investigation of the primary target genes of *Basella alba* in the context of psoriasis. According to the results of the degree centrality analysis, the top five genes—TP53, AKT1, TNF, EGFR, and IL6—were chosen as the primary target genes. The remaining genes were STAT3, IL1B, GADPH, BCL2, and MYC, which are the psoriasis proteins with the greatest number of interactors. TP53 is a tumor suppressor gene responsible for the synthesis of the p53 protein. The p53 protein inhibits excessive cellular growth and division, modulating cell proliferation. It is positively expressed in various inflammatory skin disorders, such as psoriasis and chronic dermatitis. A study by Baran et al. found that P53-positive cells were predominantly in the basal layer of healthy skin and non-lesional psoriatic skin. In lesional psoriatic skin, they were present in all epidermal layers. P53 appears crucial in psoriasis pathogenesis [41]. The phosphatidylinositol 3-kinase (PI3K) and protein kinase B (AKT) signaling pathway is integral to various physiological activities, including cell proliferation and survival. The accelerated turnover of keratinocytes in psoriasis is directly linked to the activation of the PI3K-AKT pathway, which triggers downstream signaling cascades leading to enhanced cell proliferation and survival, and a significant component of the transcriptional and apoptotic program that is regulated by this pathway is p53 (TP53) [42]. The epidermal growth factor receptor (EGFR) is a well-studied tyrosine kinase receptor that plays a variety of key roles during cell development, including cellular homeostasis, proliferation, division, differentiation, and apoptosis. The active epidermal lesions of psoriasis have been shown to overexpress EGFR and its endogenous ligands [43]. Patients with psoriasis have higher levels of the pleiotropic pro-inflammatory cytokine IL-6 in their blood and skin lesions. IL-6 plays a crucial role in the development of Th17 cells, a specific type of T cell that is significantly involved in psoriasis pathogenesis [44].

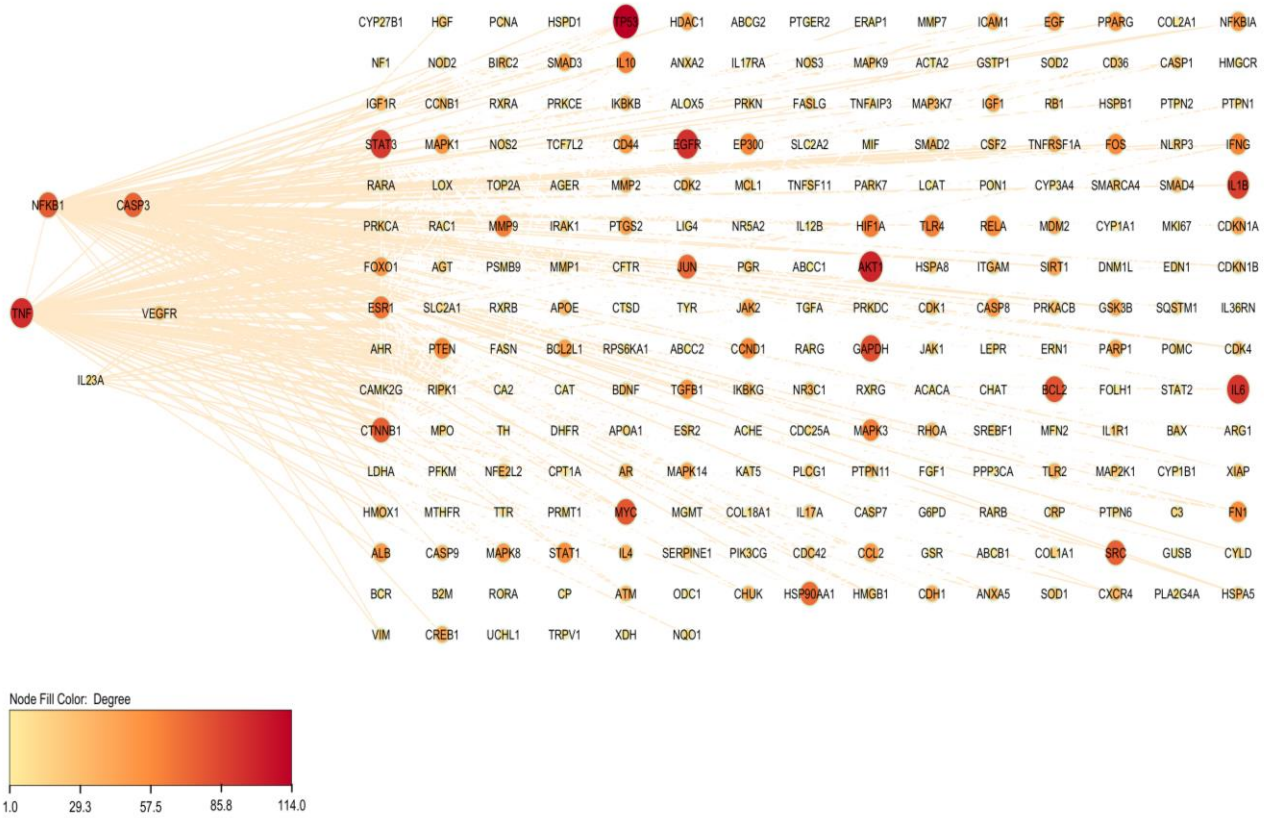

Figure 5.
Protein-Protein Interaction Target Bioactive of *Basella alba* in Psoriasis.

The degree centrality study identifies TP53, AKT1, TNF, EGFR, IL6, STAT3, IL1B, GAPDH, BCL2, and MYC as the psoriasis proteins with the highest number of interactors, as seen in Table 4 which may be the main genes that *Basella alba* targets for psoriasis and crucial proteins with a specific role in promoting psoriasis.

Table 4.
TOP 10 Degree Interactor Proteins.

Name	Degree	Closeness Centrality
TP53	114	0.65
AKT1	100	0.62
TNF	96	0.61
EGFR	94	0.61
IL6	92	0.60
STAT3	90	0.59
IL1B	88	0.59
GAPDH	82	0.59
BCL2	80	0.58
MYC	79	0.58

3.6. Functional Annotation

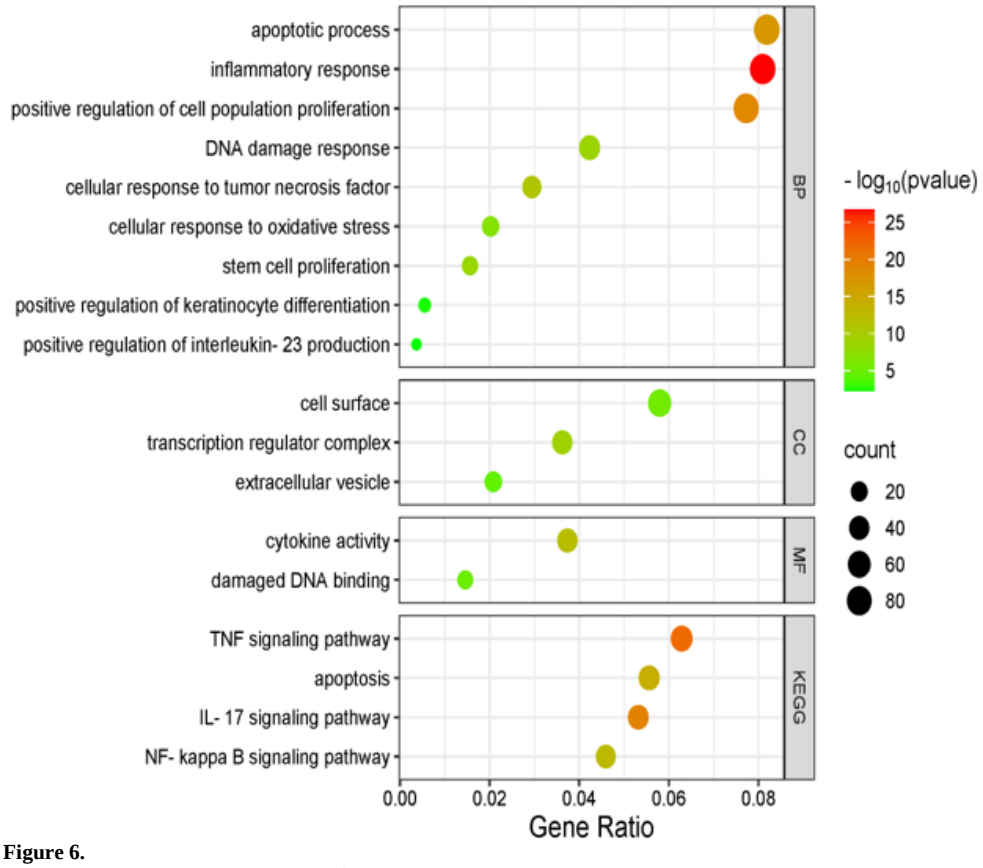

Figure 6.
Functional Analysis Target Bioactive of Basella alba.

According to functional analysis, the quantity of highly enriched GO and KEGG keywords indicates the bioactive target of *Basella alba* (Figure 6). Pathways with P-value <0.05 significant changes were found. The circle's size indicates the number of genes, and its color indicates the P-value. While the functional annotation analysis target of *Basella alba* as shown in Table 5.

GO Enrichment Analysis. The David database analyzed and enriched 241 common targets, yielding 752 in total, comprising 388 biological processes (BP), 127 cellular components (CC), and 57 molecular functions (MF). The number of genes in the route increases with the size of the circle. The apoptotic process, inflammatory reaction, positive regulation of cell population growth, DNA damage response, cellular response to tumor necrosis factor, and cellular response to oxidative stress are the most important biological processes (BP). The highly enriched GO terms in Cellular Components (CC) included cell surface, *transcription* regulator complex, and extracellular vesicle. Molecular Function (MF) analysis mainly includes cytokine activity and damaged DNA binding. Bioinformatics was performed on 241 targets to determine *Basella alba*'s psoriasis-fighting mechanism. *Basella alba* molecular function, cellular constitution, and biological processes have been improved by GO enrichment analysis. The results showed that the principal targets were considerably enriched in apoptosis, inflammatory response, positive cell population growth regulation, DNA damage response, tumor necrosis factor response, and oxidative stress response. The GO keywords extracellular vesicle, transcription regulator complex, and cell surface were highly abundant in Cellular Components (CC). Molecular function (MF) investigation focuses on cytokine activity and DNA binding defects.

KEGG Pathway Enrichment Analysis. A total of 180 pathways were obtained through KEGG pathway enrichment analysis. Cytoscape is used to reinforce the disease-pathway-target-compound-drug network. TNF signaling, apoptosis, IL-17 signaling, and NF-k signaling are the primary ones, according to the KEGG pathway enrichment study. According to the KEGG target enrichment data, *Basella alba* might be a viable therapeutic target for psoriasis. To find the potential targets for psoriasis, the PPI network of *Basella alba* putative targets was integrated with the existing network. Based on the enrichment analysis results, which were supported by existing literature, literature was retrieved and GO and KEGG enrichment studies were conducted on key target genes. Analytical data for future discussions can be obtained by searching the literature that has been validated by high-throughput tests and research using murine models.

Table 5.
Functional Annotation Analysis Target of Basella alba.

Terms	Count	Category	Genes
Inflammatory response	88	BP	CXCL8, TNFAIP3, IL27, PARK7, HMGB1, TNF, CXCL2, PIK3CG, LTB4R, CX3CL1, POLB, PYCARD, IKBKB, CYP26B1, RPS6KA5, IL18RAP, FFAR4, FFAR3, AKT1, IKBKG, RAC1, LGALS9, MAP3K7, PTGIR, CERS6, CHUK, IL1R1, SPHK1, PLA2G4B, PLA2G4C, IL18, FOS, MIF, IL17RC, IL17RA, TNFRSF1A, IL1A, IL23A, IL1B, TLR9, TLR4, CD44, MGLL, TLR2, PTGER4, CRP, PTGFR, CEBPB, PTGER2, PTGER3, ALOX15, CXCR4, NOD1, AGER, RELA, C3, HRH1, CNR2, TBXA2R, IRAK2, CCL5, CCL2, NLRP3, RIPK1, S1PR3, CD14, NLRP1, TGFB1, FKRP, VCAM1, NOS2, PLA2G2A, STAT3, NR1H4, SELE, NFKB1, NFATC4, SELP, CXCL10, BMP2, IL6, IL5, FASN, NOX4, IL17B, IL17A, NFE2L2, NFKBIB
Positive regulation of cell population proliferation	84	BP	VIPR1, RARG, CDKN1B, CSF2, IRS1, PTEN, FASLG, FGF1, FGF2, HOXC10, CX3CL1, IGF1R, CAPNS1, MYC, KDR, SOX9, TIMP1, CAPN1, JAK2, IL13RA1, IL11, TRPC5, EDN1, CNOT6L, SPHK2, PRMT1, SPHK1, FSHB, MIR21, CCDC117, MIF, TMEM250, SIRT1, CDC25B, AR, IFNG, ALDH1A2, IL1B, TRAF5, RARA, PTGFR, PRKAA1, HDAC1, CHRNA7, ODC1, TGFA, TNFRSF11A, EGFR, RELA, S1PR3, S1PR2, SLAMF1, XBP1, TGFB1, KDM4C, TSLP, EGF, INSR, FN1, AKR1C3, AKR1C2, IGF1, MEIS3, IL2, SMARCA4, VEGFA, ACER2, BMP4, TJP1, IL4, CXCL10, BMP2, IL6, CNOT7, GDNF, IL7, CDK4, LEP, CDK2, BCL2, MDM2, CTNNB1, PTPN6, IL7R
Apoptotic process	89	BP	APP, RARG, PTEN, TNFAIP3, CGB3, FASLG, AHR, NR3C1, BBC3, PYCARD, CASP9, CASP7, CASP8, KAT5, OPA1, CASP3, CHEK1, CASP1, EP300, IKBKG, JAK2, MAP3K7, TP63, PARP1, DAPK1, IGFBP3, PRKCE, DAPK3, MMP9, RHOB, TRAIP, TNFRSF1A, IL1A, SLC5A8, IFNG, IL1B, TRAF5, TAX1BP1, RARB, TMBIM6, GAPDH, SQSTM1, TP53, BIRC2, PPID, TLR2, PPARD, BECN1, KMT2A, PRUNE2, CXCR4, HTT, NOD1, FOXO1, BCL2L11, MFN2, MAPK1, NLRP3, RIPK1, CD14, FADD, NLRP1, RFFL, MAPK3, XBP1, GADD45B, BAD, GADD45A, NEK6, CFLAR, NSG1, MAPK14, NFKB1, SOD1, VEGFA, NFKBIA, STK17A, STK17B, PMP22, BCL2, CDK1, MDM2, PDCD4, CYCS, BAX, TAF6, IL17A, BCL2L1, TP73
Cellular response to tumor necrosis factor	32	BP	MIR20B, ASAH1, CXCL8, RORA, SLC2A4, RELA, CX3CL1, IKBKB, PYCARD, CCL5, CYP1B1, CCL2, AKT1, MAPK1, RIPK1, PCK1, MAP3K7, MAPK3, PCK2, EDN1, VCAM1, CHUK, TRPV1, FOS, MAPK14, GFER, SIRT1, NFKB1, NFKBIA, COL1A1, FABP4, NFE2L2
DNA damage response	46	BP	H2AX, TOP2A, BRSK1, CDKN1A, MIR34A, PRKDC, OGG1, XIAP, FOXO1, BBC3, CASP9, POLB, NUAK1, CCND1, KAT5, CHEK2, MYC, CASP3, CHEK1, ABL1, DGCR8, MAPK1, IKBKG, POLK, TP63, MCL1, MAPK3, BARD1, PARP1, PRMT1, GADD45A, SIRT1, TRAIP, ACER2, RAD51, TAOK1, TRAF6, DDIT3, BCL2, CDK1, ATM, MAPT, CLOCK, TP53, ATR, TP73
Stem cell proliferation	17	BP	RARG, TGFB1, CDKN2C, ABCB1, LIG4, FGF2, RUNX2, GLI2, KDR, NF1, CTNNB1, RARB, SFN, SOX9, NES, TP53, TP63
Cellular response to oxidative stress	22	BP	PRKN, NQO1, XBP1, ABCC1, G6PD, PRKAA1, GPX1, PARP1, STAU2, GSR, ARNT, PARK7, FOXO3, SOD2, HIF1A, FOXO1, MAPK8, ABL1, PPARGC1A, HSPA1A, NFE2L2, SNCA
Positive regulation of keratinocyte differentiation	6	BP	IL20, PRKCH, NUMA1, MIR125B1, VDR, NCOA3

Positive regulation of interleukin-23 production	4	BP	CSF2, IFNG, IL17RA, IL17A
Transcription regulator complex	40	CC	ZNF771, ZNF254, RARG, PRKDC, NR1I2, AHR, RELA, SOX2, RXRB, RXRA, KAT5, EP300, SOX9, TEAD2, NCOA1, SMAD2, NCOA2, JUN, CREBBP, SMAD4, SMAD3, PARP1, STAT3, ARNT, ESR1, POU5F1, RUNX2, NFKB1, NFATC4, MED25, KLF5, CDK4, DDIT3, ZNF714, CDK2, RARA, CTNNB1, RARB, BMAL1, TP53
Cell surface	64	CC	ACHE, APP, SPARC, ITGAM, CTNND1, PTPRJ, IL27, PTPRK, HMGB1, TNF, CX3CL1, ICAM1, CDH5, MRC1, LIPG, CA4, CD36, HAVCR1, HSP90AA1, ABCC2, ANXA2, ADIPOQ, MIF, IL17RC, F3, TNFRSF1A, BACE1, IL1A, FOLH1, MET, TLR4, CFTR, CD44, TLR2, RTN2, ADCYAP1R1, ABCB1, LPAR1, CXCR4, LPAR2, TGFA, NOD2, AGER, EGFR, HSPD1, C3, DUOX1, GRIN2A, ADGRG2, IRAK1, CD59, PROM1, LDLR, HSPA8, TGFB1, VCAM1, HSPA5, NRDC, GRIN2B, IGF2R, VEGFA, BMP2, SDC1, FOLR1
Extracellular vesicle	23	CC	SLC12A2, CBR1, MIR30A, MIR20B, MIR17, MIR34A, MIR26B, MIR27B, APOA1, MIR29C, MIR22, MIR21, MIR30C1, MIR214, MIR100, MIR122, MIR125B1, MIR494, MIR185, MIR152, GNB1, APOE, SPTAN1
Cytokine activity	41	MF	CSF2, IL20, FASLG, IL27, HMGB1, FGF2, TNF, IL36A, IL36B, SPP1, IL12B, TNFSF11, IL36RN, TIMP1, IL10, IL32, IL11, IL33, WNT10B, EDN1, TGFB1, TSLP, ADIPOQ, IL18, IL36G, MIF, IL2, IL1F10, VEGFA, BMP4, IL4, IL1A, BMP2, IL6, IL5, IFNG, IL23A, IL7, IL1B, IL17B, IL17A
Damaged DNA binding	16	MF	H2AX, CREBBP, PCNA, PARP1, MPG, OGG1, XRCC1, HMGB1, POLB, RPA3, CRY2, EP300, POLK, NEIL1, TP63, POLH
TNF signaling pathway	52	KEGG	CSF2, TNFAIP3, TNF, CXCL2, CX3CL1, ICAM1, IKBKB, CASP7, RPS6KA5, CASP8, CASP3, AKT1, IKBKG, DNM1L, MAP3K7, MAP2K4, MAP2K1, EDN1, RIPK3, CHUK, FOS, MMP9, TNFRSF1A, CREB1, IL1B, TRAF5, BIRC2, CEBPB, XIAP, PIK3R1, NOD2, PTGS2, RELA, SOCS3, MAPK9, MAPK8, CCL5, CCL2, MAPK1, RIPK1, FADD, MAPK3, JUN, VCAM1, CFLAR, MAPK14, SELE, NFKB1, NFKBIA, CYLD, CXCL10, IL6
IL-17 signaling pathway	44	KEGG	GSK3B, CEBPB, CSF2, CXCL8, TNFAIP3, PTGS2, ELAVL1, TNF, CXCL2, RELA, IKBKB, MAPK9, MAPK8, CASP8, CASP3, CCL2, MAPK1, FADD, IKBKG, MAP3K7, MAPK3, JUN, HSP90AA1, CHUK, MMP1, FOS, MAPK14, IL17RC, MMP9, MUC5AC, IL17RB, NFKB1, IL17RA, IL4, NFKBIA, CXCL10, IL6, IL5, IFNG, TRAF6, IL1B, TRAF5, IL17B, IL17A
Apoptosis	46	KEGG	BCL2A1, XIAP, FASLG, PIK3R1, TNF, RELA, BBC3, CASP9, IKBKB, MAPK9, CASP7, MAPK8, CASP8, BCL2L11, CASP3, AKT1, MAPK1, RIPK1, FADD, IKBKG, CAPN1, CTSD, SPTAN1, MCL1, MAPK3, JUN, MAP2K1, GADD45B, PARP1, CHUK, GADD45A, BAD, CFLAR, FOS, NFKB1, TNFRSF1A, ERN1, NFKBIA, DDIT3, BCL2, BAX, CYCS, ATM, TP53, BIRC2, BCL2L1
NF-κβ signaling pathway	38	KEGG	CXCL8, BCL2A1, XIAP, TNFAIP3, TNFRSF11A, PTGS2, TNF, CXCL2, RELA, ICAM1, IKBKB, IRAK1, TNFSF11, RIPK1, IKBKG, PLCG1, CD14, MAP3K7, VCAM1, GADD45B, PARP1, CHUK, IL1R1, GADD45A, CFLAR, NFKB1, TNFRSF1A, NFKBIA, CYLD, CXCL12, TRAF6, IL1B, TRAF5, BCL2, ATM, TLR4, BIRC2, BCL2L1

Psoriasis is a chronic inflammatory dermatological illness caused by the immune system, including contributions from genetic and environmental factors. It illustrates the features of autoimmune disorders in relation to inflammation, when the two pathways converge and even intensify one another [45]. Apoptosis is a critical process for preventing autoimmunity within the system. Both excessive and insufficient activity can result in numerous diseases and disorders. As apoptotic processes diminish, the number of autoreactive cells in the periphery increases, as does their accumulation. This leads to the

onset of psoriasis, among other conditions [46]. Consequently, *Basella alba* may exert a regulatory influence in the etiology of psoriasis, act as an apoptotic agonist by intervening in various biological processes, and potentially impact certain cellular components and molecular activities in psoriasis treatment.

4. Conclusion

This study indicates that beta-carotene, ferulic acid, acacetin, and kaempferol in *Basella alba* could be promising treatments for psoriasis. The treatment of psoriasis involves factors such as an apoptotic agent, anti-inflammatory properties, and regulation of cell proliferation. The primary target genes in the *Basella alba* gene network for psoriasis include TP53, AKT1, TNF, EGFR, IL6, STAT3, IL1B, GADPH, BCL2, and MYC. The current study has the potential to stimulate and lead future research to confirm the molecular targets of *Basella alba* against psoriasis, as well as its therapeutic applicability. It is important to note the study's limitations. The results are based on network pharmacology analysis, which relies on computational predictions and may not fully capture the complexities of biological systems. Therefore, further experimental studies, including in vitro and in vivo experiments using mouse models of psoriasis, are necessary to validate these findings and provide more concrete evidence. This additional research will strengthen the evidence in the study and improve the understanding of *Basella alba*'s therapeutic potential and its active components.

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