Available online at
www.heca-analitika.com/malacca_pharmaceutics

**Malacca Pharmaceutics**

Vol. 4, No. 2, 2026

# Mapping In Silico Strategies for Natural Product-Derived Candidates in Atopic Dermatitis: A Bibliometric Analysis and Methodological Review

**Mauly Rahadatul Aisya [1], Khalijah Awang [2], Khairan Khairan [3,4], Trina Ekawati Tallei [5], and Rinaldi Idroes [3,4,*]**

[1] Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia; maulyaisya@gmail.com (M.R.A.)
[2] Department of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur 50603, Malaysia; khalijah@um.edu.my (K.A.)
[3] School of Mathematics and Applied Sciences, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia; khairankhairan@usk.ac.id (K.K.); rinaldi.idroes@usk.ac.id (R.I.)
[4] Department of Pharmacy, Faculty of Mathematics and Natural Sciences, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia
[5] Department of Biology, Faculty of Mathematics and Natural Sciences, Universitas Sam Ratulangi, Manado 95115, Indonesia; trina_tallei@unsrat.ac.id (T.E.T.)

* Correspondence: rinaldi.idroes@usk.ac.id

**Article History**

Received 2 August 2026
Revised 6 September 2026
Accepted 14 September 2026
Available Online 25 September 2026

**Keywords**:
Atopic dermatitis
Bibliometric
In silico
Methodological review
Natural products

**Abstract**

Atopic dermatitis (AD) is a chronic inflammatory skin disease with a complex pathogenesis involving multiple molecular targets and biological pathways. The multicomponent nature of natural products broadens the range of potential compound-target interactions, supporting the use of in silico approaches to identify and prioritize therapeutic candidates. This review aimed to map the development of in silico strategies used to prioritize natural product-derived candidates for AD and to evaluate how these strategies have been applied across the literature. A bibliometric analysis and a methodological review were conducted on 70 articles retrieved from Scopus up to August 2026. Although no publication-year restriction was applied, the earliest article meeting the inclusion criteria was published in 2020, with publication output increasing over time. Molecular docking was employed in 57 studies (81.4%), network pharmacology in 53 studies (75.7%), molecular dynamics in 18 studies (25.7%), and dedicated ADMET screening in 11 studies (15.7%). The methodological review revealed variations in analytical workflow, ranging from candidate selection using databases or chemical profiling to target prioritization and evaluation of molecular interactions. Differences were also observed in data sources, selection criteria, analytical parameters, protocol validation, and the degree of methodological integration. These findings indicate substantial methodological diversity and highlight the need to align methods with study objectives, report analytical parameters more clearly, and strengthen connections between successive stages of analysis.



## 1. Introduction

Atopic dermatitis (AD) is a chronic and relapsing inflammatory skin disease that significantly impacts patients' quality of life by causing constant itching, recurring skin lesions, sleep disturbances, and a heavy psychological toll [1–5]. AD pathogenesis involves complex interactions among epidermal barrier dysfunction, immune dysregulation, and the activation of multiple interconnected inflammatory mediators and

pathways [6–8]. Advances in understanding these mechanisms have led to more targeted therapies, including biologics and Janus kinase (JAK) inhibitors. However, disease heterogeneity and variation in treatment response among individuals remain important considerations in the long-term management of AD [4, 9–13]. These considerations have encouraged continued exploration of other sources of therapeutic candidates, including natural products.

Natural products are widely investigated due to their diverse bioactive compounds, which may influence AD-relevant biological processes, such as inflammation, type 2 immune responses, oxidative stress, pruritus, and epidermal barrier function [4, 14, 15]. However, the multicomponent composition of natural products increases the complexity of drug candidate discovery. A single plant extract or herbal formulation may contain numerous compounds with diverse chemical characteristics, pharmacokinetic properties, and potential biological targets [16]. At the same time, AD also involves multiple interacting proteins and biological pathways [6, 7, 17, 18]. This complexity makes it harder to identify and prioritize candidates when compounds and targets are considered individually.

In silico approaches have become increasingly relevant for addressing this problem by facilitating candidate screening and prioritization at various stages of drug discovery. Physicochemical and pharmacokinetic predictions provide information on candidate properties, while target identification and network pharmacology explore compound-target relationships and associated biological pathways. Molecular docking and molecular dynamics provide additional insight into candidate-target interactions at structural and dynamic levels [17–23]. These approaches provide complementary information and can be applied according to the objectives and analytical stages of a study. In natural product research, where numerous compounds and potential targets are often involved, computational approaches can help reduce the number of candidates that require further evaluation.

Previous reviews have examined specific aspects of in silico research relevant to atopic dermatitis. Singab et al. [24] reviewed molecular docking studies of herbal candidates across several skin disorders, whereas Xu et al. [25] focused specifically on network pharmacology and molecular docking of artemisinin and its derivatives for AD. More recently, Wu et al. [26] reviewed broader in silico modeling approaches for AD, including computational and machine-learning strategies. However, these reviews did not specifically examine, at the field level, how natural product-derived candidates for AD are selected and progressively evaluated through ADMET assessment, target prediction, network pharmacology, molecular docking, molecular dynamics, and related validation stages.

However, the increasingly widespread use of in silico approaches raises questions about how these methods are applied in natural product research for AD. In silico methods can have different objectives, data sources, parameters, and levels of analysis [20, 21, 24, 27]. Therefore, using one or more of these methods does not indicate how the overall candidate prioritization process is conducted. Because individual studies generally focus on specific natural products, compounds, targets, or mechanisms, it is difficult to understand the field's development and methodological patterns when studies are considered separately. Consequently, it remains unclear how candidate selection, target prioritization, structural evaluation, and validation connect across studies in prioritizing natural product-derived candidates for AD. This is particularly relevant to AD drug discovery, where insufficiently reported selection criteria or inadequately validated computational protocols may reduce confidence in candidate prioritization and complicate subsequent experimental evaluation.

This study aimed to map the development of *in silico* strategies for natural product-derived candidates in AD using bibliometric analysis and to evaluate their application through a methodological review. The bibliometric analysis characterized the field's development, thematic structure, and influential works, but could not capture how computational methods were implemented, reported, or linked within individual studies. Conversely, the methodological review examined these study-level features but could not situate them within broader patterns of publication growth and knowledge structure. Integrating both analyses therefore provides a more comprehensive view of the field and the methodological variation in prioritizing natural product-derived candidates for AD.

## 2. Materials and Methods

### *2.1. Review Design and Literature Search*

This study combined bibliometric analysis with a methodological review to examine the field's development and the application of *in silico* strategies in natural product research for AD. The literature search was conducted in Scopus using the TITLE-ABS-KEY field, with no restriction on publication year, and covered records indexed through August 2026. Scopus filters were applied to retain records classified as articles and published in English. Scopus was selected because its

multidisciplinary coverage suited the interdisciplinary scope of this review, spanning biomedical, natural-product, chemical, and computational research [28], while also providing the standardized bibliographic and citation metadata required for bibliometric analysis. Using a single database also ensured consistency in the bibliographic metadata across the review's bibliometric and methodological components.

The search strategy centered on three main concept groups: atopic dermatitis, natural products, and *in silico* approaches. Terms within each concept group were combined using the Boolean operator OR, whereas the three concept groups were connected using AND. The search was conducted in titles, abstracts, and keywords using the following search string: TITLE-ABS-KEY ("atopic dermatitis" OR "atopic eczema") AND ("natural product*" OR "natural compound*" OR phytochemical* OR "plant-derived" OR "medicinal plant*" OR herbal OR botanical* OR "plant extract*" OR "herbal extract*" OR "botanical extract*" OR "natural extract*" OR "traditional medicine" OR "traditional Chinese medicine") AND ("in silico" OR computational OR "network pharmacology" OR "systems pharmacology" OR "molecular docking" OR "molecular dynamic*" OR ADMET OR "drug-likeness" OR "target prediction" OR "virtual screening" OR "computer-aided drug design").

All retrieved records were exported in CSV format together with the bibliographic metadata required for subsequent analyses. The identification and selection process was documented using a PRISMA 2020 flow diagram to present the number of records at the identification, screening, eligibility assessment, and inclusion stages [29].

*2.2. Eligibility and Study Selection*

Articles were included if they: (1) were original research articles; (2) specifically addressed AD or used an AD disease model; (3) evaluated natural products, extracts, naturally occurring compounds, phytochemicals, medicinal plants, herbal preparations, or other candidates derived from natural sources; and (4) applied at least one *in silico* approach relevant to candidate identification or prioritization, including drug-likeness or ADMET prediction, target prediction, network pharmacology, biological pathway analysis, molecular docking, molecular dynamics, or virtual screening. Articles were excluded if they were not primary research, did not specifically evaluate AD, did not investigate candidates derived from natural sources, or did not apply a relevant *in silico* approach.

Articles that met the inclusion criteria and had adequate bibliographic metadata were included in the bibliometric corpus. All articles in the final corpus were subsequently assessed at the full-text level to obtain the methodological information required for the methodological review. Thus, the same 70 eligible articles were included in both the bibliometric analysis and the methodological review. Study screening and data extraction were conducted by one reviewer according to the predefined eligibility criteria. Eligibility decisions and extracted information were subsequently rechecked against the source articles to ensure consistency.

*2.3. Bibliometric Analysis*

Bibliometric analysis was performed to characterize the development and structure of research on natural product-based *in silico* drug discovery for AD. The analysis included performance analysis to assess publication growth and research contributions, as well as science mapping to examine the field's conceptual and intellectual structure [30].

Bibliographic data were analyzed using bibliometrix/Biblioshiny and VOSviewer. Bibliometrix/Biblioshiny processed bibliographic metadata and analyzed publication productivity, publication sources, geographical distribution, citation patterns, and thematic development [31]. VOSviewer was used to construct and visualize author-keyword co-occurrence and cited-reference co-citation networks [32].

The initial analysis covered the corpus's general characteristics, annual and cumulative publication growth, publication sources, geographical distribution by author affiliation, and document citation patterns. Geographical distribution was calculated based on author affiliations using full counting, whereas citation patterns were evaluated using total citations (TC) and total citations per year (TCY). The conceptual structure of the field was assessed through author-keyword co-occurrence analysis using full counting with a minimum threshold of two keyword occurrences. Temporal changes in keywords were examined using overlay visualization based on the average publication year.

Thematic development was further analyzed using thematic evolution and thematic mapping by dividing the publication period into 2020–2024 and 2025–2026. This division was used to compare themes from the earlier and more recent publication periods while maintaining broadly comparable document volumes. Because the second period included records only through August 2026, differences between the two periods were interpreted descriptively rather than as definitive evidence of theme emergence or disappearance.

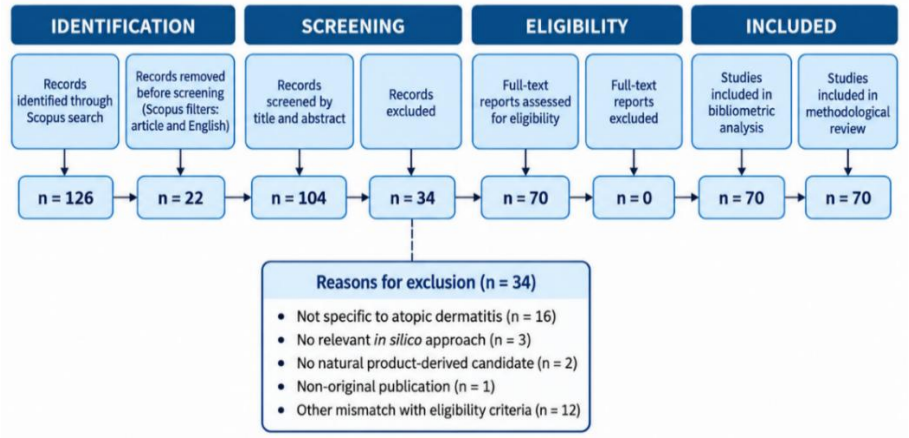



**Figure 1.** PRISMA flow diagram of the study selection process.

The intellectual structure of the field was examined using cited-reference co-citation analysis. Before network construction, author keywords were harmonized conservatively by normalizing spelling and case variants, merging clear synonyms and direct naming variants, and removing within-record duplicates. Distinct concepts were retained separately. Duplicate cited-reference variants referring to the same source were standardized to a single reference form. The co-citation network included the 40 cited references with the highest total link strength (TLS) in VOSviewer, and the resulting clusters were interpreted according to the characteristics of the references within each group.

*2.4. Methodological Review and Data Extraction*

The methodological review included all 70 articles in the final corpus and evaluated the application of *in silico* approaches in natural product research for AD. The review focused on the main computational methods used, the sequence of analyses, relationships between analytical stages, and variation in methodological procedures and reporting during candidate prioritization.

Data were extracted using a structured matrix that covered the source and method of candidate compound selection; drug-likeness and ADMET assessment; target prediction and prioritization; network pharmacology, protein-protein interaction (PPI), Gene Ontology (GO), and pathway enrichment analyses; molecular docking; and molecular dynamics and binding-energy analyses when reported. Information on databases, computational resources, software, selection criteria, thresholds, analytical parameters, and protocol validation was also recorded when explicitly reported in the source articles.

In this review, dedicated ADMET screening was defined as the explicit evaluation of pharmacokinetic and/or toxicity properties beyond routine screening variables such as oral bioavailability and drug-likeness, using dedicated ADMET platforms or analyses. Routine oral bioavailability and drug-likeness values available in phytochemical databases were therefore not considered dedicated ADMET screening. Methodological information that was not explicitly stated in the articles was categorized as *not reported* and was not interpreted as evidence that the corresponding procedure had not been performed.

The extracted data were synthesized comparatively to identify patterns of method use, methodological variation, reporting practices, and the integration of computational approaches across studies. Method combinations were also examined at the study level to identify recurring linkages among candidate selection, target prioritization, network pharmacology, molecular docking, and molecular dynamics. The degree of integration reflected differences in the extent of computational analysis and was not treated as a direct indicator of study quality because method selection could vary according to the objectives of individual studies. Accordingly, this review was descriptive and comparative in scope and did not constitute a formal assessment of methodological quality or risk of bias.

## 3. Results and Discussion

*3.1. Bibliometric Landscape and Research Trends*

The Scopus search identified 126 records. After application of the article-type and English-language filters, 22 records were removed, leaving 104 records for title-and-abstract screening. Thirty-four records were excluded during screening, and the remaining 70 articles proceeded to full-text eligibility assessment. No articles were excluded at the full-text stage; therefore, all 70 eligible articles were included in both the bibliometric analysis and the methodological review (Figure 1).

**Table 1.** Main characteristics of the bibliometric dataset on natural product-based in silico research for AD, 2020–2026.

| Characteristic | Description | Value |
|---|---|---|
| Main dataset information | | |
| Time span | Publication period covered by the dataset | 2020–2026 |
| Documents | Number of articles meeting the inclusion criteria and analyzed | 70 |
| Sources | Number of journals/publication sources represented in the corpus | 43 |
| Annual growth rate | Average annual publication growth rate over the analysis period | 49.13% |
| Average document age | Average publication age at the time of analysis | 1.59 years |
| Average citations per document | Average number of citations received per article | 7.50 |
| **Document contents** | | |
| Index keywords | Number of unique terms recorded as Scopus Index Keywords | 1,472 |
| Author keywords | Number of unique keywords assigned by authors | 229 |
| **Authors** | | |
| Authors | Number of unique authors based on Scopus Author ID | **564** |
| Authors of single-authored documents | Number of authors publishing individually | 3 |
| **Author collaboration** | | |
| Single-authored documents | Number of articles with only one author | 3 |
| Co-authors per document | Average number of authors involved per article | 8.46 |
| International co-authorship | Percentage of articles involving affiliations from more than one country | 15.71% |

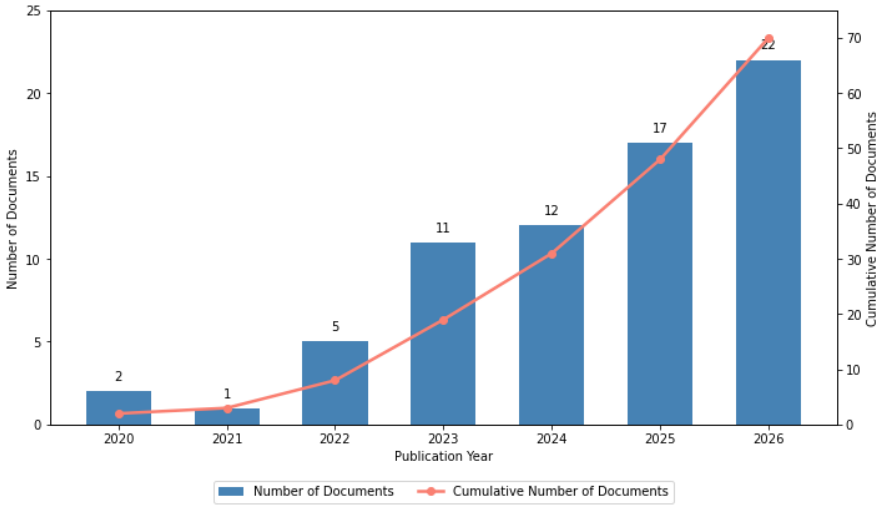



**Figure 2.** Annual scientific production and cumulative publication growth, 2020–2026. The 2026 data represent an incomplete year of publications.

These 70 articles were published across 43 sources between 2020 and 2026. Although the unrestricted search retrieved four records published before 2020, none met the predefined eligibility criteria. Two records did not apply a relevant *in silico* approach, while the other two did not specifically evaluate AD. Thus, the 2020 starting point of the final corpus reflects the eligibility criteria rather than a publication-year restriction. Overall, the characteristics summarized in Table 1 indicate that research on the *in silico* identification of natural product-derived candidates for atopic dermatitis is relatively recent.

The mean document age was 1.59 years, with an annual publication growth rate of 49.13%. Because the 2026 data cover only January through August, the annual growth rate of 49.13% should be interpreted cautiously and does not represent a complete-year comparison. This pattern indicates that much of the corpus was published within the past few years and that the concepts, methods, and research directions in this field remain dynamic and may continue to evolve as new studies emerge. The corpus included contributions from 564 authors, with an average of 8.46 co-authors per document, whereas only three articles were single-authored. International co-authorship accounted for 15.71% of the corpus. The corpus also contained 229 author keywords and 1,472 index keywords, reflecting considerable terminological diversity and providing a basis for examining the structure and evolution of research themes.

*3.1.1. Publication Growth and Landscape*

Annual scientific production increased over the period from 2020 through August 2026 (Figure 2). Publication output was initially low, with two articles in 2020 and one

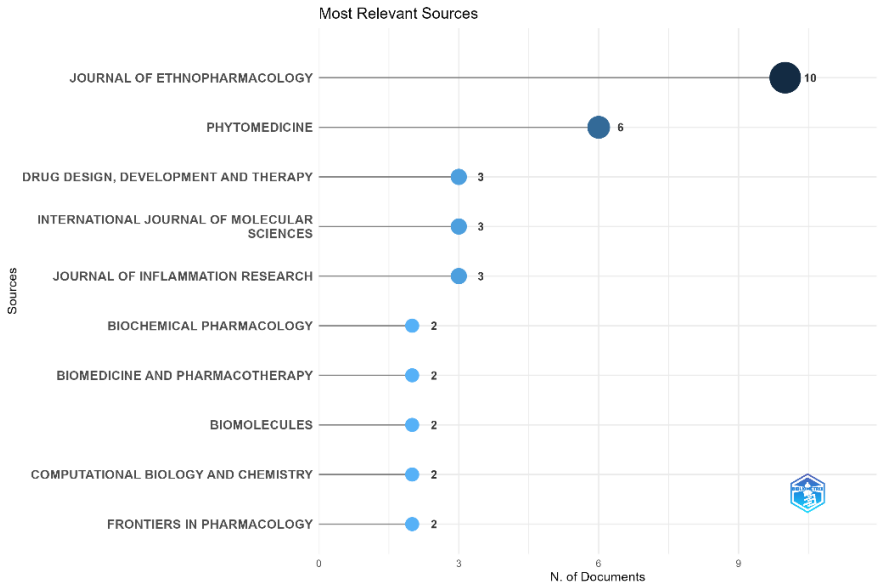



**Figure 3.** Top 10 most relevant publication sources based on the number of documents.

in 2021, before increasing to five articles in 2022. Growth became more evident from 2023 onwards, with 11 articles in 2023, 12 in 2024, 17 in 2025, and 22 by August 2026. In parallel, the cumulative number of publications increased from two articles in 2020 to eight in 2022, 19 in 2023, 31 in 2024, 48 in 2025, and 70 in 2026. The increasingly steep cumulative curve after 2022 indicates that most articles in the corpus were published in recent years. Although 2026 already had the highest publication count within the observation period, the year was incomplete at the time of analysis, and the total may therefore continue to increase by the end of the year. Overall, this pattern indicates growing research activity in the *in silico* discovery of natural product-derived candidates for AD, particularly since 2023.

*3.1.2. Sources and Geographical Distribution*

The distribution of publication sources showed that the corpus was not concentrated in a single journal (Figure 3). *Journal of Ethnopharmacology* was the most prolific source, with ten articles, followed by *Phytomedicine* with six. *Drug Design, Development and Therapy*, *International Journal of Molecular Sciences*, and *Journal of Inflammation Research* each published three articles. *Biochemical Pharmacology*, *Biomedicine and Pharmacotherapy*, *Biomolecules*, *Computational Biology and Chemistry*, and *Frontiers in Pharmacology* each contributed two articles. Collectively, these ten sources accounted for half of the corpus, comprising 35 of 70 articles, whereas the remaining 35 articles were distributed across 33 different sources. Thus, although *Journal of Ethnopharmacology* and *Phytomedicine* were the leading publication venues, the literature was broadly dispersed across other journals. This distribution reflects the field's multidisciplinary character, spanning natural products and pharmacology as well as molecular biology, inflammation, and computational research.

A different pattern emerged when the geographical distribution of research contributions was examined (Figure 4). In contrast to the relatively broad distribution of publication sources, research contributions by author affiliation were strongly concentrated in several Asian countries. Under the full-counting approach used by Biblioshiny, the counting unit represented country occurrences in the author-affiliation data rather than unique documents. Consequently, a single publication could contribute multiple country-affiliation occurrences, and the resulting country-production frequencies totaled 251 across the 70-document corpus. China had the highest frequency, with 171 contributions (68.1% of the total country-production frequency), followed by South Korea with 34 (13.5%), Italy with 13 (5.2%), Indonesia with 8 (3.2%), Bangladesh and Japan with 5 each (2.0%), and Malaysia and Qatar with 3 each (1.2%). The remaining countries together accounted for 9 contributions (3.6%). These findings indicate that the country-production frequency was strongly concentrated in China.

China's dominant contribution may partly reflect the strong representation of Traditional Chinese Medicine (TCM)-based research in the corpus, in which natural products and herbal formulations are frequently used as sources of candidates for computational investigation [16, 27]. This pattern may also have been influenced by the coverage of Scopus and the English-language restriction applied in this review. It should therefore not be interpreted as a complete representation of global research activity. Nevertheless, continued advances in

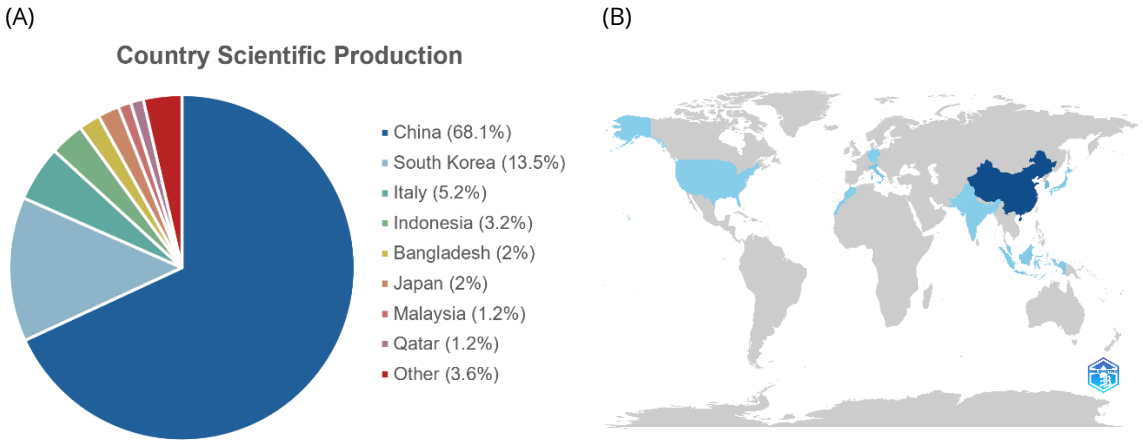



**Figure 4.** Geographical distribution of scientific production based on author affiliations. (A) Country-level scientific production; (B) global distribution of publication contributions.

**Table 2.** Top 10 globally cited documents in the bibliometric corpus.

| Rank | Reference | Title | Source | TC | TCY |
|---|---|---|---|---|---|
| 1 | [33] | Cornus officinalis ethanolic extract with potential anti-allergic, anti-inflammatory, and antioxidant activities | Nutrients | 65 | 9.3 |
| 2 | [34] | Dictamnine ameliorates chronic itch in DNFB-induced atopic dermatitis mice via inhibiting MrgprA3 | Biochemical Pharmacology | 35 | 8.8 |
| 3 | [35] | Molecular Mechanisms of Luteolin Against Atopic Dermatitis Based on Network Pharmacology and in vivo Experimental Validation | Drug Design, Development and Therapy | 31 | 6.2 |
| 4 | [36] | Network pharmacology and molecular docking-based prediction of active compounds and mechanisms of action of Cnidii Fructus in treating atopic dermatitis | BMC Complementary Medicine and Therapies | 29 | 5.8 |
| 5 | [37] | The active compounds and therapeutic mechanisms of pentaherbs formula for oral and topical treatment of atopic dermatitis based on network pharmacology | Plants | 25 | 3.6 |
| 6 | [38] | Jiu-Wei-Yong-An Formula suppresses JAK1/STAT3 and MAPK signaling alleviates atopic dermatitis-like skin lesions | Journal of Ethnopharmacology | 25 | 5.0 |
| 7 | [39] | Network pharmacology-based analysis to explore the therapeutic mechanism of Cortex Dictamni on atopic dermatitis | Journal of Ethnopharmacology | 25 | 6.2 |
| 8 | [40] | Compound traditional Chinese medicine dermatitis ointment ameliorates inflammatory responses and dysregulation of itch-related molecules in atopic dermatitis | Chinese Medicine (United Kingdom) | 22 | 4.4 |
| 9 | [41] | Anti-inflammatory and antioxidant properties of Camellia sinensis L. extract as a potential therapeutic for atopic dermatitis through NF-κB pathway inhibition | Scientific Reports | 21 | 10.5 |
| 10 | [42] | Phytochemical Composition, Anti-Inflammatory Property, and Anti-Atopic Effect of Chaetomorpha linum Extract | Marine Drugs | 21 | 7.0 |

Note: TC = Total Citations; TCY = Total citations per year

computational methods and the availability of biological and chemical databases may provide greater opportunities for other countries to explore their own plant resources and natural products as sources of therapeutic candidates.

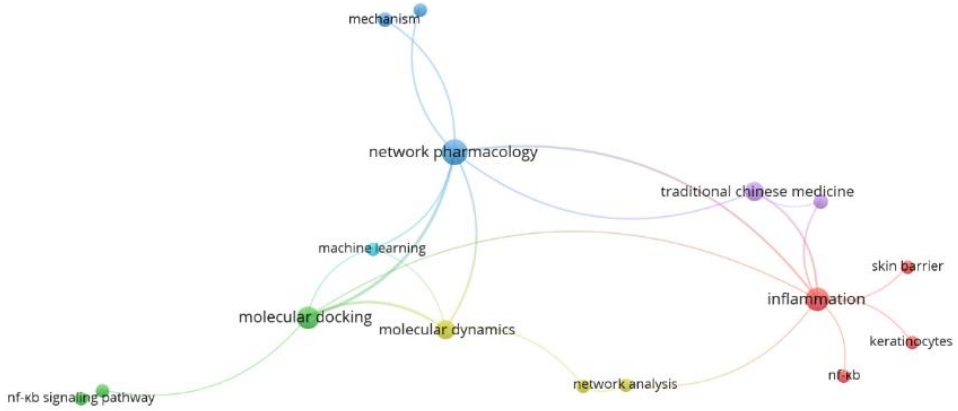
*3.1.3. Citation Impact and Influential Documents*

Beyond publication volume and distribution, citation analysis was used to identify the most frequently cited documents in the corpus (Table 2).

Quah et al. [33] had the highest total citation count, with 65 citations, followed by Yang et al. [34] with 35 and Tang et al. [35] with 31. When citation impact was considered on a per-year basis, however, Kim et al. [41] had the highest TCY value (10.5) despite accumulating only 21 total citations. This difference likely reflects the longer time available for earlier publications to accrue citations. Considering TC and TCY together therefore provides a more balanced view of citation patterns across studies.

The ten most highly cited articles also encompassed a range of natural products and methodological approaches. Some studies evaluated plant extracts and herbal formulations for their anti-inflammatory effects or their ability to improve AD-related symptoms. In contrast,

(A)




(B)

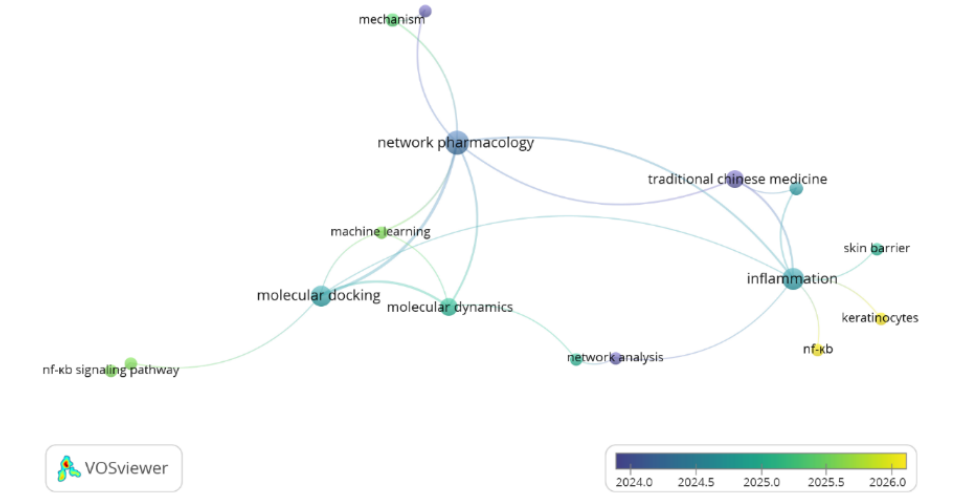



**Figure 5.** Conceptual and temporal structure of author keywords. (A) Keyword co-occurrence network; (B) overlay visualization based on average publication year. Node size reflects keyword occurrence, links indicate co-occurrence relationships, cluster colors in panel A represent groups of related keywords, and overlay colors in panel B indicate the average publication year.

others integrated network pharmacology, molecular docking, pathway analysis, and experimental validation to investigate molecular targets and mechanisms of action. For example, Tang et al. [35] combined network pharmacology with *in vivo* validation, while Khan et al. [36] used network pharmacology and molecular docking to predict active compounds and their mechanisms. These studies indicate that influential work in the corpus extends beyond assessing biological activity to investigating the molecular targets and mechanisms underlying the observed effects.

*3.1.4. Conceptual Structure and Research Trends*

After examining publication growth and distribution, the analysis extended to the evolution of research topics and methodological approaches within the corpus. The conceptual structure was assessed through author-keyword co-occurrence to identify frequently used terms, relationships among terms, and changes in research focus over time (Figure 5). This analysis provides an overview of the major themes and approaches shaping the development of natural product research on AD using *in silico* methods.

In the co-occurrence network shown in Figure 5A, network pharmacology was the most frequent methodological term, appearing 21 times, followed by molecular docking (13 occurrences) and molecular dynamics (7). Among non-methodological terms, inflammation was also prominent, appearing 14 times, while TCM appeared seven times. This pattern suggests that the connection between computational analysis and inflammatory mechanisms strongly characterizes natural product research on AD in the corpus. These frequencies reflect terms supplied by authors as author keywords and should not be interpreted as direct measures of how frequently each method was used in the included studies. Frequencies of actual method use were evaluated separately in the methodological review.

**Table 3.** Leading author keywords in the co-occurrence network.

| Author keyword | Occurrences | Links | Total link strength (TLS) |
|---|---|---|---|
| Network pharmacology | 21 | 7 | 20 |
| Inflammation | 14 | 8 | 13 |
| Molecular docking | 13 | 5 | 13 |
| Molecular dynamics | 7 | 4 | 9 |
| Traditional Chinese medicine | 7 | 3 | 6 |

Note: TLS = total link strength; links indicate the number of distinct connections with other author keywords.

Network pharmacology's prominence was also reflected in its total link strength (TLS), which reached 20, with seven links to other keywords. This indicates that network pharmacology is strongly connected to multiple themes within the network. Its association with molecular docking suggests that the two approaches frequently co-occur in the corpus, linking compound-target mapping with the evaluation of molecular interactions. In contrast, inflammation had the most links, with eight connections and a TLS of 13, indicating a strong relationship between inflammatory processes and other themes in the corpus. The appearance of terms such as *skin barrier*, *skin barrier function*, *keratinocytes*, and *NF-κB* further indicates increasing attention to more specific biological mechanisms relevant to AD. The presence of TCM is also consistent with the large contribution from China observed in the geographical analysis. The occurrence, number of links, and TLS values of the leading author keywords are summarized in Table 3.

The overlay visualization in Figure 5B further illustrates temporal changes in research focus. TCM and network pharmacology tended to be associated with earlier publication years, whereas molecular dynamics became more prominent around 2025. Keywords such as machine learning, single-cell RNA sequencing, NF-κB signaling pathway, keratinocytes, and NF-κB appeared more recently, particularly during 2025–2026. Although these terms occurred relatively infrequently, their emergence suggests a shift from compound-target mapping toward more specific investigations of disease mechanisms, molecular interaction stability, and a wider range of computational approaches.

Changes in research themes between 2020–2024 and 2025–2026 were further examined through thematic evolution and thematic mapping (Figure 6). The 2020–2024 and 2025–2026 periods contained 31 and 39 documents, respectively.

As shown in Figure 6A, network pharmacology remained present in both periods, while other themes changed their connections between the earlier and later periods. This pattern suggests that the field has developed through the expansion and recombination of established themes with newer approaches. A similar shift is evident in the thematic maps shown in Figure 6B. During 2020–2024, network pharmacology was a basic theme, while inflammation, TCM, and skin barrier function appeared as niche themes. In 2025–2026, network pharmacology remained a basic theme and became grouped with molecular docking and molecular dynamics, indicating increasing connections among these approaches in natural product research for AD. During the same period, the NF-κB signaling pathway and single-cell RNA sequencing emerged as more specific themes, suggesting a shift toward molecular and biological mechanisms of disease. Overall, the changing position and connectivity of these themes indicate that the field is evolving not only through a broader range of computational methods but also through increasingly specific biological questions [6, 7].

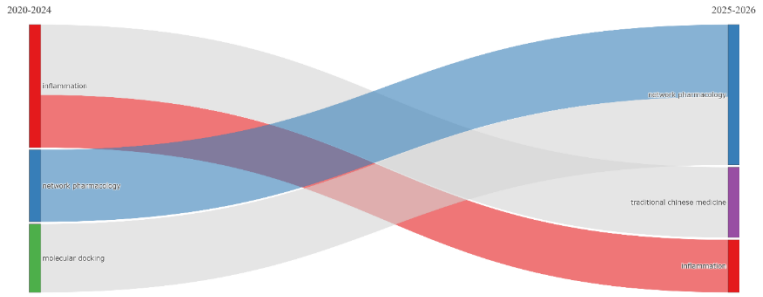
*3.1.5. Intellectual Structure*

After analyzing thematic development, the field's intellectual foundations were examined through cited-reference co-citation analysis. The 40 references with the strongest connections formed four major interlinked clusters (Figure 7). Node size represents the citation frequency of a reference within the corpus, whereas links indicate co-citation relationships, or how frequently two references were cited together.

The four clusters were not visually isolated but showed substantial interconnection among references. This pattern suggests that natural product research for AD using *in silico* approaches has developed through interactions among multiple knowledge domains spanning AD, natural products, databases, and computational methods. References related to target prediction and bioinformatics resources occupied central positions in the network, highlighting their role in connecting computational foundations with literature focused more directly on AD and its treatment.

Table 4 shows that the two largest clusters each contained 13 references, with one centered on computational methods and the other on AD therapeutics and natural product-based network pharmacology. A third cluster was centered on target prediction, molecular docking, and bioinformatics resources, indicating that databases and computational

(A)




(B)


**Figure 6.** Thematic evolution and thematic structure of author keywords across two publication periods. (A) Thematic evolution between 2020–2024 and 2025–2026; (B) thematic maps for 2020–2024 and 2025–2026 based on centrality and density.

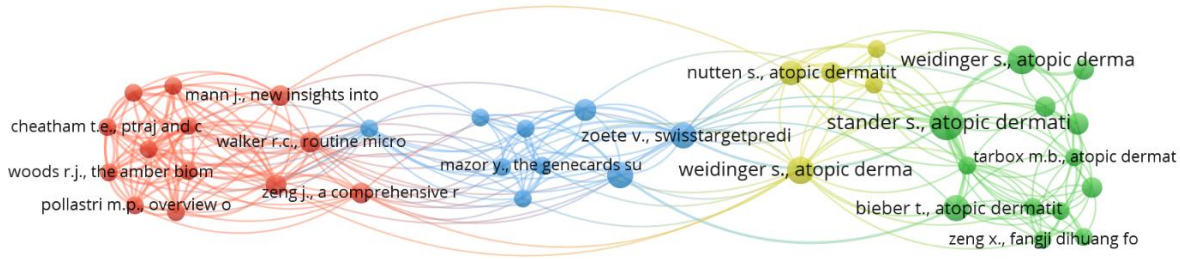



**Figure 7.** Cited-reference co-citation network of the 40 most strongly connected references. Node size reflects citation frequency, links indicate co-citation relationships, and colors represent the identified clusters.

**Table 4.** Characteristics and interpretation of cited-reference co-citation clusters.

| Cluster | n | Interpretive label | Representative intellectual basis |
|---|---|---|---|
| 1 | 13 | Computational pharmacology, ADMET, and molecular simulation foundations | Cheatham; Cooper; Crippen; Hou; Liu; Pollastri; Walker; Woods; Yeoh; Zoete (SwissADME). |
| 2 | 13 | Atopic dermatitis therapeutics and natural product-based network pharmacology | Bieber; Gudjonsson; Lin; Paller; Ständer; Tarbox; Wang; Weidinger; Williams; Zeng; Zhang; Zhao. |
| 3 | 9 | Target prediction, molecular docking, and bioinformatics resources | Protein Data Bank; AutoDock Vina; GeneCards; PubChem; SwissTargetPrediction; TCMSP; ligand-target pharmacology references. |
| 4 | 5 | Clinical, epidemiological, and diagnostic foundations of atopic dermatitis | Nutten; Ormerod; Ring; Weidinger; Williams. |

Note: Representative references indicate selected intellectual bases of each cluster and do not constitute the complete list of cited references within the cluster.

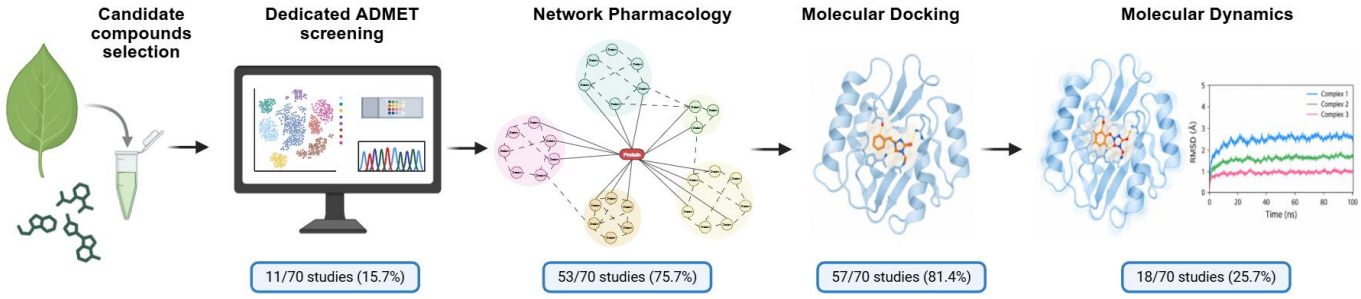



**Figure 8.** Main in silico approaches identified across the 70 reviewed studies.

tools form an important component of candidate identification and evaluation. A cluster focused on the clinical, epidemiological, and diagnostic foundations of AD further indicates that the field's intellectual structure is shaped not only by methodological references but also by literature that supports understanding of the disease. Overall, these clusters show that the field is built on the intersection of biological and clinical knowledge of AD with computational approaches used to identify and evaluate natural product-derived candidates.

Overall, the bibliometric analysis shows that research on natural products for AD using in silico approaches has expanded over the past several years. Network pharmacology and molecular docking were the most frequently represented computational approaches in the keyword analysis, alongside the growing presence of molecular dynamics and more specific biological themes. Bibliometric analysis, however, primarily characterizes growth patterns, thematic relationships, and knowledge structure. The following section therefore examines in greater detail how candidates were selected, targets were prioritized, computational methods were applied, and different analytical stages were linked within individual studies.

*3.2. Methodological Review of In Silico Strategies for Natural Product-Derived Candidates in Atopic Dermatitis*

Across the 70 articles reviewed, *in silico* research on natural products for atopic dermatitis employed a diverse range of computational methods (Figure 8). Molecular docking was the most frequently used approach, appearing in 57 of 70 studies [17, 19–23, 33–83], followed by network pharmacology in 53 studies [19, 20, 22, 23, 35–39, 43–50, 52, 54–56, 62, 63, 66–81, 83–96], molecular dynamics (MD) in 18 studies [20–23, 45, 51, 56, 57, 59, 60, 63–65, 73–75, 78, 81], and dedicated ADMET screening in 11 studies [21, 23, 44, 45, 54, 57, 59, 60, 65, 66, 86]. These differences in frequency reflect variation in study objectives and analytical depth. Consequently, the use of a larger number of methods should not be interpreted as evidence of higher study quality; rather, each method should be considered in relation to its intended function and how its output informs subsequent analytical stages.

The first major variation arose at the candidate compound selection stage. Database-driven candidate selection was widely applied across studies using herbal formulations, medicinal plants, and isolated natural compounds. Candidate compounds were generally retrieved from phytochemical or traditional medicine databases and subsequently evaluated through drug-likeness screening, target prediction, network pharmacology, or molecular docking [22, 35–39, 43, 46–48, 54, 63, 78, 84, 85]. This approach allows efficient screening of large numbers of compounds and links them to physicochemical properties, drug-likeness, and predicted targets. However, the presence of a compound in a database does not necessarily establish that it is present in the specific biological material or sample examined in a given study.

Other studies performed chemical profiling using analytical platforms such as UHPLC-MS/MS, GC-MS, LC-MS/MS, or UPLC-MS/MS before subjecting the detected compounds to *in silico* analysis. This approach provides a more direct connection between computational candidates and the composition of the material actually analyzed. Nevertheless, analytical detection alone does not establish that a detected compound is the most active or biologically relevant component. Several studies in the corpus followed this analytically anchored strategy by characterizing the chemical constituents of the investigated material before or alongside subsequent computational evaluation [17, 33, 41, 42, 44, 53, 91]. Database-driven selection therefore offers broad and efficient candidate exploration, whereas chemical profiling provides closer correspondence between computational candidates and the measured composition of the sample. Either strategy may be appropriate depending on the study objective and characteristics of the natural product under investigation.

After identifying candidate compounds, some studies used drug-likeness, pharmacokinetic, and toxicity assessments to prioritize candidates further [23, 54, 65]. Dedicated ADMET screening was clearly identified in 11 of 70 studies (15.7%), making it less frequent than network pharmacology or molecular docking. This lower frequency should not automatically be seen as a methodological weakness because the relevance of ADMET assessment depends on the study's purpose. When the objective is to prioritize candidates for further development, information on physicochemical properties, absorption, distribution, metabolism, excretion, and toxicity can help narrow the candidate set before target-based analyses.

Several studies also tailored screening parameters to the intended route of administration [97]. Mohammad et al. [22], for example, used oral bioavailability and drug-likeness in selecting *Panax ginseng* candidates while retaining compounds with lower oral bioavailability for possible topical use. In contrast, El Bouamri et al. [65] evaluated *Aloe vera* compounds using skin-related parameters such as skin permeability, dermal absorption, and skin irritation. These examples indicate that ADMET assessment is more informative when the selected parameters align with the intended route of administration. This consideration is particularly relevant in AD, where candidates may be developed for either oral or topical administration. The databases and computational resources used for candidate identification and screening are summarized in Table 5.

After candidate selection, most studies mapped targets potentially associated with AD. Network pharmacology was used in 53 of 70 studies (75.7%) and represented one of the principal computational approaches in the corpus. This frequent use aligns with both the multicomponent nature of natural products and the involvement of multiple proteins and biological pathways in AD pathogenesis. A typical workflow involved compound-target prediction, collection of disease-associated targets, identification of overlapping targets, construction of protein-protein interaction (PPI) networks, and Gene Ontology (GO) and pathway enrichment analyses [22, 36, 43]. This sequence narrows large numbers of potential compound-target relationships into more focused sets of targets and pathways. The databases and computational resources supporting these stages are summarized in Table 6.

Each stage of network pharmacology contributes a different type of information. Intersection analysis identifies targets associated with both candidate compounds and the disease, whereas PPI analysis examines relationships among targets and helps identify proteins occupying influential positions within the network. GO and pathway enrichment analyses then provide biological context for the resulting target set. These analytical stages allow network pharmacology to function primarily as a hypothesis-generation and target-prioritization framework for organizing multicomponent and multitarget relationships.

However, targets prioritized through network pharmacology should be interpreted cautiously [27]. A protein may be prioritized because it appears in an intersection set or has high degree, betweenness, or centrality values; however, its apparent importance remains dependent on the databases, selection criteria, and network parameters used. The same consideration applies to GO and pathway enrichment analyses, whose results depend on the target set submitted for analysis. Accordingly, interpretation should consider not only which targets rank highest but also how those targets were selected and reported.

Among the 53 studies using network pharmacology, 47 (88.7%) explicitly combined candidate- or compound-target sources with disease-target sources, whereas two (3.8%) reported candidate-target sources only, one (1.9%) reported a disease-target source only, and three (5.7%) did not explicitly identify either source category. This distribution illustrates that target sets were commonly generated by combining information from multiple public databases and prediction resources. However, overlap among database-derived targets does not by itself establish biological specificity to AD because database content, prediction algorithms, and inclusion thresholds may differ across resources. Downstream experimental and/or clinical follow-up was identified in 41 of the 53 studies (77.4%), whereas 12 (22.6%) remained computational only. Under a stricter criterion requiring an explicit link between a network-prioritized target or pathway and subsequent experimental confirmation, only 16 studies (30.2%) met this criterion. Thus, experimental or clinical follow-up should not be interpreted as evidence that every network-predicted target or pathway was independently confirmed.

More recent studies also incorporated data-driven approaches to complement conventional database-based target prioritization. Machine learning was used in four studies (5.7%) to refine key gene or target selection. In comparison, single-cell RNA sequencing was reported in five studies (7.1%) to provide cell-level gene-expression information [43, 56, 69, 70, 94]. Spatial transcriptomics was identified in only one study (1.4%) and was integrated

**Table 5.** Databases and computational resources used for compound retrieval, preliminary screening, and dedicated ADMET evaluation.

| Database/ resource | Main purpose | Use in corpus, n (%) | Representative source articles |
|---|---|---|---|
| TCMSP | Retrieval and preliminary screening of herbal compounds, including OB/DL information | 35/70 (50.0%) | [22, 36, 37] |
| HERB | Retrieval of herbal ingredients, targets, and TCM-related information | 17/70 (24.3%) | [38, 44, 70] |
| SwissADME | Drug-likeness, physicochemical, and pharmacokinetic prediction | 10/70 (14.3%) | [54, 59, 65] |
| pkCSM | Prediction of pharmacokinetic and toxicity properties | 4/70 (5.7%) | [54, 59, 65] |
| PreADMET | ADME/toxicity prediction, including skin-related parameters | 1/70 (1.4%) | [65] |
| ADMETlab | Integrated ADMET prediction | 1/70 (1.4%) | [23] |
| QikProp | Prediction of drug-like and pharmacokinetic descriptors | 1/70 (1.4%) | [57] |
| ProTox-II/III | In silico toxicity prediction | 1/70 (1.4%) | [60] |

Note: Resource-use counts are not mutually exclusive because individual studies may use more than one ADMET resource.

**Table 6.** Main databases and computational resources used for target mapping, network pharmacology, and pathway analysis.

| Database/ resource | Main purpose | Use in corpus, n (%) | Representative source articles |
|---|---|---|---|
| SwissTargetPrediction | Prediction of potential compound targets | 28/70 (40.0%) | [22, 36, 54] |
| DrugBank | Drug-target and target-related information | 9/70 (12.9%) | [37, 42, 85] |
| PharmMapper | Pharmacophore-based target prediction | 4/70 (5.7%) | [62, 66, 71] |
| GeneCards | Retrieval of AD-associated genes/targets | 36/70 (51.4%) | [22, 36, 37] |
| OMIM | Retrieval of disease-associated genes | 22/70 (31.4%) | [22, 37, 69] |
| DisGeNET | Disease-gene association retrieval | 17/70 (24.3%) | [22, 43, 44] |
| TTD | Therapeutic target retrieval | 14/70 (20.0%) | [35, 47, 84] |
| GEO | Gene-expression datasets for transcriptomic/bioinformatic integration | 10/70 (14.3%) | [54, 56, 81] |
| STRING | Construction of protein-protein interaction networks | 45/70 (64.3%) | [22, 36, 43] |
| Cytoscape | Network visualization and hub-target analysis | 43/70 (61.4%) | [22, 36, 44] |
| DAVID | GO and pathway enrichment analysis | 32/70 (45.7%) | [22, 36, 37] |
| Metascape | Functional enrichment and pathway/network interpretation | 8/70 (11.4%) | [49, 52, 81] |

with single-cell analysis [74]. Given their limited use in the current corpus, these approaches should be regarded as emerging strategies rather than evidence of a field-wide methodological transition.

Following target prioritization, molecular docking was the most widely used approach in the corpus, appearing in 57 of 70 studies (81.4%). Docking adds a structural layer of information by evaluating compound-target relationships identified through prediction or network analysis at the molecular level. Commonly reported outputs included binding affinity, binding pose, and amino acid residues interacting within the protein binding site [24]. Molecular docking therefore serves as an important bridge between target prioritization and the evaluation of potential molecular interactions.

Docking protocols varied considerably in implementation and reporting across studies. Among the 57 docking studies, the docking software was explicitly reported in 39 (68.4%), PDB identifiers in 29 (50.9%), grid or binding-site information in 24 (42.1%), and the use of a native or co-crystallized ligand in 9 (15.8%). Six studies (10.5%) explicitly reported RMSD-based validation against a native, co-crystallized, or original ligand. Four of these six studies explicitly described the validation procedure as redocking, whereas the remaining two reported RMSD-based protocol validation without explicitly using the term redocking. El Bouamri et al. [65], for example, redocked the native ligand and reported an RMSD below 2 Å, whereas Suleman et al. [59] reported an RMSD of 0.073 Å for redocking against COX-2. These validation procedures provide additional information on a docking protocol's ability to reproduce a known ligand position.

The limited explicit reporting of validation does not necessarily indicate that docking protocols in the remaining studies were invalid, because methodological details may not have been fully reported. Rather, this finding highlights an opportunity to improve consistency in reporting docking parameters and validation procedures. More complete reporting would provide a clearer methodological basis for interpreting and comparing binding affinities and interaction patterns across studies. This is particularly important because docking scores and poses are influenced by receptor and ligand preparation, protonation states, binding-site definition, docking parameters, scoring procedures, and protocol validation. Consequently, binding affinities reported without sufficient information on these

methodological elements should be interpreted as computational estimates rather than directly comparable measures of binding strength across studies.

Some studies subsequently evaluated docking-prioritized candidates using molecular dynamics. MD was used in 18 of 70 studies (25.7%), and 13 of these studies also reported binding-energy or free-energy analyses. Whereas docking captures interactions in one or a limited number of poses, MD allows changes in compound-protein complexes to be followed throughout a simulation trajectory. Parameters such as RMSD, RMSF, radius of gyration, hydrogen-bond counts, and changes in intermolecular interactions can be used to assess a complex from several complementary perspectives [20–22, 57]. Some studies also incorporated MM/PBSA or MM/GBSA calculations to estimate binding energy.

MD is therefore better regarded as a refinement stage that extends the information obtained from molecular docking. Its less frequent use than docking should not necessarily be considered a limitation, because not all research questions require additional simulation, and MD is substantially more computationally demanding. More important is whether the simulation design fits the research question. Variation in simulation duration, force field, system conditions, and analytical parameters further indicates that MD results should be interpreted in the context of the overall simulation design rather than based on a single metric such as RMSD.

When the methods were considered together, substantial variation was evident in the depth of computational integration. Network pharmacology and molecular docking were used together in 40 of 70 studies (57.1%). In these studies, network pharmacology generally served to prioritize candidate targets, which were subsequently evaluated through molecular docking. Eleven studies (15.7%) extended this combination to molecular dynamics to further evaluate the behavior and stability of selected compound-target complexes. Only two studies (2.9%) additionally incorporated dedicated ADMET screening alongside network pharmacology, molecular docking, and molecular dynamics. These patterns indicate that the most frequently observed linkage connected target prioritization with structural interaction assessment, while MD and dedicated ADMET evaluation were incorporated less consistently.

However, the presence of multiple methods within the same study does not necessarily indicate a fully connected analytical workflow or higher study quality. A study using only molecular docking may still provide relevant information when the research question specifically concerns a candidate's interaction with a defined target, and MD does not need to be included in every study. Methodological integration is therefore better assessed by whether the selected approaches fit the study objectives and whether the output of one analytical stage logically informs the next.

Overall, the methodological review showed that the main strength of *in silico* approaches in natural product research for AD lies in their ability to progressively narrow the analytical space. ADMET assessment provides information on candidate suitability, network pharmacology helps simplify complex multicomponent and multitarget relationships, molecular docking evaluates potential interactions at the structural level, and MD extends the analysis to the dynamics of candidate-target complexes. Each approach therefore serves a distinct function and can complement the others. The key issue is not the number of methods applied, but aligning each method with the study objective, ensuring transparent criteria, and maintaining continuity of information across analytical stages.

### *3.3. Methodological Considerations and Future Directions*

Based on the patterns identified, future research does not necessarily need to incorporate every *in silico* approach into a single pipeline. A more appropriate strategy is to align computational stages with the study's specific objective. Studies in early candidate exploration may place greater emphasis on compound screening, ADMET assessment, and target prediction. In contrast, studies with predefined targets may focus more directly on molecular docking. MD can then be applied selectively when further evaluation of key candidate-target complex dynamics is required. This approach gives each method a clear purpose and avoids adding analytical steps simply because they are available. Computational predictions should be interpreted as evidence for candidate and target prioritization and molecular interaction assessment, not as equivalent to experimentally validated biological activity. Where experimental evidence was reported, it was treated as supporting evidence rather than part of the review's primary methodological comparison.

Another area that could be strengthened is the transparency and consistency of methodological reporting. For ADMET assessment, the parameters and thresholds used should be clearly stated and aligned with the intended route of administration. In network pharmacology, database sources, intersection criteria, PPI parameters, and the basis for hub-target selection should be explicitly reported. For molecular docking, protein and ligand preparation, binding-site definition,

docking parameters, and validation procedures should be reported to improve reproducibility. Similarly, MD studies should report simulation duration, force field, system conditions, and analytical parameters comprehensively.

Advances in machine learning, transcriptomics, single-cell analysis, and other bioinformatics approaches also create opportunities to expand strategies for candidate and target prioritization. However, their use should remain guided by the research question and the type of information required. Overall, the field may benefit from more purpose-driven *in silico* strategies, clearer reporting of methods and parameters, and more explicit connections between analytical stages. Future methodological development should therefore focus not simply on adding more computational methods, but on more clearly defining each method's role in prioritizing natural product-derived candidates for AD.

### *3.4. Limitations*

Several limitations should be considered when interpreting this review. The corpus was retrieved exclusively from Scopus and restricted to articles published in English. Consequently, potentially relevant studies published in other languages may not have been captured. In addition, the 2026 data reflect an incomplete publication year, while citation counts may change depending on the date of data collection. Methodological comparisons also relied on information explicitly reported in individual articles; therefore, parameters categorized as *not reported* should not be interpreted as procedures that were necessarily omitted. Differences in study objectives and designs should also be considered when comparing the use of computational methods across studies.

## 4. Conclusions

Natural product-based *in silico* drug discovery for atopic dermatitis is a relatively recent research field. Although the literature search was not restricted by publication year, the earliest article meeting the inclusion criteria in the corpus was published in 2020. Since then, publication activity has increased, and approaches have expanded from compound-target mapping to a broader range of computational analyses, including assessment of candidate properties, target prioritization, molecular interaction analysis, and complex dynamics.

The methodological review shows that the studies in this field have not followed a single standardized workflow. Differences in candidate sources, databases, selection criteria, analytical parameters, and method combinations reflect the diversity of computational strategies used to address different research objectives. Accordingly, using more methods does not necessarily indicate a better approach. Greater importance should be placed on a clear rationale for candidate and target selection, alignment of methods with study objectives, transparent reporting of analytical parameters, and logical continuity between successive analytical stages. These findings should be interpreted within the limitations of a Scopus-only, English-language corpus, the incomplete 2026 observation period, and methodological comparisons based on information explicitly reported in the included studies; therefore, information categorized as *not reported* should not be interpreted as evidence that the corresponding procedure was not performed. For future studies, greater consistency in reporting the basis for candidate and target prioritization, key analytical parameters, docking validation, and MD settings where applicable would improve transparency and reproducibility.

**Author Contributions:** Conceptualization, M.R.A., K.K., and R.I.; methodology, M.R.A., K.K., and R.I.; validation, M.R.A., K.A., K.K., T.E.T., and R.I.; formal analysis, M.R.A. and R.I.; investigation, M.R.A.; data curation, M.R.A. and K.K.; writing—original draft preparation, M.R.A.; writing—review and editing, M.R.A., K.A., K.K., T.E.T., and R.I.; visualization, M.R.A.; supervision, K.A., K.K., T.E.T., and R.I.; project administration, K.K. and R.I. All authors have read and agreed to the published version of the manuscript.

**Funding:** This work was supported by the Ministry of Higher Education, Science, and Technology of the Republic of Indonesia through the Program Magister Menuju Doktor untuk Sarjana Unggul (PMDSU), Grant No. 323/C3/DT.05.00/PL/PMDSU/2026.

**Ethical Clearance:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** The bibliographic data analyzed in this study were obtained from the Scopus database and are subject to its access and licensing policies. The processed bibliometric dataset and methodological extraction matrix are available from the corresponding author upon reasonable request.

**Conflicts of Interest:** All the authors declare no conflicts of interest.

## References

1. Silverberg, J. I., Gelfand, J. M., Margolis, D. J., Boguniewicz, M., Fonacier, L., Grayson, M. H., Simpson, E. L., Ong, P. Y., and Chiesa Fuxench, Z. C. (2018). Patient Burden and Quality of Life in Atopic Dermatitis in US Adults: A Population-Based Cross-Sectional Study, *Annals of Allergy, Asthma and Immunology*, Vol. 121, No. 3, 340–347. doi:10.1016/j.anai.2018.07.006.

2. Eyerich, K., Gooderham, M. J., Silvestre, J. F., Shumack, S. P., Mendes-Bastos, P., Aoki, V., Ortoncelli, M., Silverberg, J. I., Teixeira, H. D., Chen, S. H., Calimlim, B. M., Takemoto, S., Sancho, C., Fritz, B., and Irvine, A. D. (2024). Real-World Clinical, Psychosocial and Economic Burden of Atopic Dermatitis:

Results from a Multicountry Study, *Journal of the European Academy of Dermatology and Venereology*, Vol. 38, No. 2, 340–353. doi:10.1111/jdv.19500.

3. Andersen, L., Nyeland, M. E., and Nyberg, F. (2020). Increasing Severity of Atopic Dermatitis Is Associated with a Negative Impact on Work Productivity among Adults with Atopic Dermatitis in France, Germany, the U.K. and the U.S.A., *British Journal of Dermatology*, Vol. 182, No. 4, 1007–1016. doi:10.1111/bjd.18296.

4. Gkalpakiotis, S., Kannenberg, S., Kingo, K., Nada, H. R., Rakhmatulina, M. R., Lesiak, A., Nicolescu, A. C., Darlenski, R., Masri, A., Zhou, L., Albuquerque, T., Hammad, S., and Almasry, I. (2024). Real-World Clinical, Psychosocial, and Economic Burden of Atopic Dermatitis: Results From the ESSENTIAL AD Multicountry Study, *Dermatology and Therapy*, Vol. 14, No. 5, 1173–1187. doi:10.1007/s13555-024-01146-8.

5. Abdel-Mageed, H. M. (2025). Atopic Dermatitis: A Comprehensive Updated Review of This Intriguing Disease with Futuristic Insights, *Inflammopharmacology*, Vol. 33, No. 3, 1161–1187. doi:10.1007/s10787-025-01642-z.

6. Fukushima-Nomura, A., Kawasaki, H., Yashiro, K., Obata, S., Tanese, K., Ebihara, T., Saeki, H., Etoh, T., Hasegawa, T., Yazaki, J., Seita, J., Ohara, O., Sekita, A., Miyai, T., Ashizaki, K., Koseki, H., Sakurada, K., Kawakami, E., and Amagai, M. (2025). An Unbiased Tissue Transcriptome Analysis Identifies Potential Markers for Skin Phenotypes and Therapeutic Responses in Atopic Dermatitis, *Nature Communications* , Vol. 16, No. 1, 1–22. doi:10.1038/s41467-025-59340-x.

7. D'Avino, P., Kim, J., Li, M., Gessner, P., Westermann, P., Pat, Y., Beha, C., Traidl-Hoffmann, C., Bost, J., Gaudenzio, N., Messner, C. B., Akdis, C. A., and Mitamura, Y. (2026). Distinct Roles of IL-4, IL-13, and IL-22 in Human Skin Barrier Dysfunction and Atopic Dermatitis, *Allergy: European Journal of Allergy and Clinical Immunology*, Vol. 81, No. 2, 480–497. doi:10.1111/all.70060.

8. Ma, J., Fang, Y., Hu, J., Li, S., Zeng, L., Chen, S., Li, Z., Meng, R., Yang, X., Zhang, F., Ji, G., Liao, P., Chen, L., and Wu, W. (2025). Innovative Microbial Strategies in Atopic Dermatitis, *Frontiers in Immunology*, Vol. 16, 1–11. doi:10.3389/fimmu.2025.1605434.

9. Wollenberg A, Howell MD, Guttman-Yassky E Silverberg JI, Kell C, Ranade K, Moate R, and Merwe Rene van der. (2019). Treatment of Atopic Dermatitis with Tralokinumab, an Anti-IL-13 MAb, *Journal of Allergy and Clinical Immunology*, Vol. 143, No. 1, 135–141. doi:10.1016/j.jaci.2018.05.029.

10. Guttman-Yassky, E., Bissonnette, R., Ungar, B., Suárez-Fariñas, M., Ardeleanu, M., Esaki, H., Suprun, M., Estrada, Y., Xu, H., Peng, X., Silverberg, J. I., Menter, A., Krueger, J. G., Zhang, R., Chaudhry, U., Swanson, B., Graham, N. M. H., Pirozzi, G., Yancopoulos, G. D., et al. (2019). Dupilumab Progressively Improves Systemic and Cutaneous Abnormalities in Patients with Atopic Dermatitis, *Journal of Allergy and Clinical Immunology*, Vol. 143, No. 1, 155–172. doi:10.1016/j.jaci.2018.08.022.

11. Guttman-Yassky, E., Thaçi, D., Pangan, A. L., Hong, H. C. ho, Papp, K. A., Reich, K., Beck, L. A., Mohamed, M. E. F., Othman, A. A., Anderson, J. K., Gu, Y., Teixeira, H. D., and Silverberg, J. I. (2020). Upadacitinib in Adults with Moderate to Severe Atopic Dermatitis: 16-Week Results from a Randomized, Placebo-Controlled Trial, *Journal of Allergy and Clinical Immunology*, Vol. 145, No. 3, 877–884. doi:10.1016/j.jaci.2019.11.025.

12. Simpson, E. L., Bieber, T., Guttman-Yassky, E., Beck, L. A., Blauvelt, A., Cork, M. J., Silverberg, J. I., Deleuran, M., Kataoka, Y., Lacour, J.-P., Kingo, K., Worm, M., Poulin, Y., Wollenberg, A., Soo, Y., Graham, N. M. H., Pirozzi, G., Akinlade, B., Staudinger, H., et al. (2016). Two Phase 3 Trials of Dupilumab versus Placebo in Atopic Dermatitis, *New England Journal of Medicine*, Vol. 375, No. 24, 2335–2348. doi:10.1056/nejmoa1610020.

13. Bieber, T., Simpson, E. L., Silverberg, J. I., Thaçi, D., Paul, C., Pink, A. E., Kataoka, Y., Chu, C.-Y., DiBonaventura, M., Rojo, R., Antinew, J., Ionita, I., Sinclair, R., Forman, S., Zdybski, J., Biswas, P., Malhotra, B., Zhang, F., and Valdez, H. (2021). Abrocitinib versus Placebo or Dupilumab for Atopic Dermatitis, *New England Journal of Medicine*, Vol. 384, No. 12, 1101–1112. doi:10.1056/nejmoa2019380.

14. Silverberg, J. I., Guttman-Yassky, E., Gadkari, A., Kuznik, A., Mallya, U. G., Mastey, V., Zhang, H., Chen, Z., Chen, C., Korotzer, A., Sierka, D., Fenton, M. C., Kaur, M., and Jalbert, J. J. (2021). Real-World Persistence with Dupilumab among Adults with Atopic Dermatitis, *Annals of Allergy, Asthma and Immunology*, Vol. 126, No. 1, 40–45. doi:10.1016/j.anai.2020.07.026.

15. Zhang, J., Boesjes, C. M., Loman, L., Kamphuis, E., Romeijn, M. L. E., Spekhorst, L. S., Haeck, I., van der Gang, L. F., Dekkers, C. C., van der Rijst, L. P., Oosting, A. J., van Lumig, P., van Lynden-van Nes, A. M. T., Tupker, R. A., Nijssen, A., Flinterman, A., Politiek, K., Touwslager, W. R. H., Christoffers, W. A., et al. (2024). Dupilumab Provides Sustained Effectiveness on Patient-Reported Outcomes and Favorable Safety in Patients with Moderate-to-Severe Atopic Dermatitis: Up to 5-Year Results from the Daily Practice BioDay Registry, *Journal of the American Academy of Dermatology*, Vol. 91, No. 2, 300–311. doi:10.1016/j.jaad.2024.04.026.

16. Hua, H., Tang, J. Y., Zhao, J. N., Wang, T., Zhang, J. H., Yu, J. Y., Yang, C. M., Ai, Y. L., and Luo, Q. X. (2025). From Traditional Medicine to Modern Medicine: The Importance of TCM Regulatory Science (TCMRS) as an Emerging Discipline, *Chinese Medicine (United Kingdom)*, Vol. 20, No. 1, 1–18. doi:10.1186/s13020-025-01152-8.

17. Xu, X., Yan, S., Zhang, Y., Cao, L., Chen, T., Yang, X. W., Liu, G. F., Meng, J., Ren, S., Wang, D. M., Liu, X., and Pan, Y. (2024). Comparison of the Chemical Constituents of Saposhnikoviae Radix Associated with Three Different Growth Patterns and Its Therapeutic Effect against Atopic Dermatitis, *Journal of Ethnopharmacology*, Vol. 333, 118417. doi:10.1016/j.jep.2024.118417.

18. Hayati, R., Lukitaningsih, E., Earlia, N., El-Shazly, M., and Idroes, R. (2025). Molecular Insights into Atopic Dermatitis Treatment: Investigating Bioactive Compounds in Aceh's Traditional Fermented Coconut Oil, *Journal of Biomolecular Structure and Dynamics*, 1–16. doi:10.1080/07391102.2025.2487195.

19. Liu, C., Shu, S., Xia, Z., Chen, G., and Xu, Y. (2022). Exploring the Latent Mechanism of Huanglian Jiedu Decoction Formula for Anti-Atopic Dermatitis by Systems Pharmacology, *Combinatorial Chemistry & High Throughput Screening*, Vol. 26, No. 3, 610–629. doi:10.2174/1386207325666220531091324.

20. Pandaleke, T. A., Handono, K., Widasmara, D., and Susianti, H. (2024). The Immunomodulatory Activity of Orthosiphon Aristatus against Atopic Dermatitis: Evidence-Based on Network Pharmacology and Molecular Simulations, *Journal of Taibah University Medical Sciences*, Vol. 19, No. 1, 164–174. doi:10.1016/j.jtumed.2023.10.005.

21. Suleman, M., Moltrasio, C., Tricarico, P. M., Marzano, A. V., and Crovella, S. (2024). Natural Compounds Targeting Thymic Stromal Lymphopoietin (TSLP): A Promising Therapeutic Strategy for Atopic Dermatitis, *Biomolecules*, Vol. 14, No. 12, 1–17. doi:10.3390/biom14121521.

22. Mohammad, S., Karim, M. R., Iqbal, S., Samad, A., Awais, M., Mathiyalagan, R., Kim, Y. J., Yang, D. U., and Yang, D. C. (2025). Network Pharmacology and Molecular Docking Approach to Predict the Oral and Topical Therapeutic Mechanisms of Panax Ginseng's Active Compounds on Atopic Dermatitis, *Journal of Biomolecular Structure and Dynamics*, Vol. 43, No. 18, 11146–11161. doi:10.1080/07391102.2025.2497467.

23. Soriano, L. M., Youn, K., and Jun, M. (2025). In Silico Integrated Systems Biology Analysis of Gut-Derived Metabolites from Philippine Medicinal Plants Against Atopic Dermatitis, *International Journal of Molecular Sciences*, Vol. 26, No. 21, 1–42. doi:10.3390/ijms262110731.

24. Singab, A. N. B., Mostafa, N. M., Fawzy, I. M., Bhatia, D., Suryawanshi, P. T., and Kabra, A. (2022). Herbal Arsenal against Skin Ailments: A Review Supported by In Silico Molecular Docking Studies, *Molecules*, Vol. 27, No. 19, 1–38. doi:10.3390/molecules27196207.

25. Xu, W., Zhu, Q., Chen, J., He, J., Yuan, A., Cao, P., and Zhang, L. (2025). Exploring the Mechanisms of Artemisinin and Its Derivatives in the Treatment of Atopic Dermatitis Based on Network Pharmacology and Molecular Docking: A Review, *Medicine (United States)*, Vol. 104, No. 19, e42287. doi:10.1097/MD.0000000000042287.

26. Wu, H. L. A., Le Floch, P., Duverdier, A., Irvine, A. D., Dubrac, S., and Tanaka, R. J. (2026). Current Research Landscape and Future Prospects of in Silico Modeling Approaches for Atopic Dermatitis, *JID Innovations*, Vol. 6, No. 5, 1–12. doi:10.1016/j.xjidi.2026.100513.

27. Zhao, W., Wang, B., and Li, S. (2024). Network Pharmacology for Traditional Chinese Medicine in Era of Artificial Intelligence, *Chinese Herbal Medicines*, Vol. 16, No. 4, 558–560. doi:10.1016/j.chmed.2024.08.004.

28. Gusenbauer, M. (2022). *Search Where You Will Find Most: Comparing the Disciplinary Coverage of 56 Bibliographic Databases*, *Scientometrics* (Vol. 127). doi:10.1007/s11192-022-04289-7.

29. Page, M. J., McKenzie, J. E., Bossuyt, P. M., Boutron, I., Hoffmann, T. C., Mulrow, C. D., Shamseer, L., Tetzlaff, J. M., Akl, E. A., Brennan, S. E., Chou, R., Glanville, J., Grimshaw, J. M., Hróbjartsson, A., Lalu, M. M., Li, T., Loder, E. W., Mayo-Wilson, E., McDonald, S., et al. (2021). The PRISMA 2020 Statement: An Updated Guideline for Reporting Systematic Reviews, *BMJ*, n71. doi:10.1136/bmj.n71.

30. Donthu, N., Kumar, S., Mukherjee, D., Pandey, N., and Lim, W. M. (2021). How to Conduct a Bibliometric Analysis: An Overview and Guidelines, *Journal of Business Research*, Vol. 133, 285–296. doi:10.1016/j.jbusres.2021.04.070.

31. Aria, M., and Cuccurullo, C. (2017). Bibliometrix: An R-Tool for Comprehensive Science Mapping Analysis, *Journal of Informetrics*, Vol. 11, No. 4, 959–975. doi:10.1016/j.joi.2017.08.007.

32. van Eck, N. J., and Waltman, L. (2010). Software Survey: VOSviewer, a Computer Program for Bibliometric Mapping, *Scientometrics*, Vol. 84, No. 2, 523–538. doi:10.1007/s11192-009-0146-3.

33. Quah, Y., Lee, S. J., Lee, E. B., Birhanu, B. T., Ali, M. S., Abbas, M. A., Boby, N., Im, Z. E., and Park, S. C. (2020). Cornus Officinalis Ethanolic Extract with Potential Anti-Allergic, Anti-Inflammatory, and Antioxidant Activities, *Nutrients*, Vol. 12, No. 11, 1–13. doi:10.3390/nu12113317.

34. Yang, N., Shao, H., Deng, J., Yang, Y., Tang, Z., Wu, G., and Liu, Y. (2023). Dictamnine Ameliorates Chronic Itch in DNFB-Induced Atopic Dermatitis Mice via Inhibiting MrgprA3, *Biochemical Pharmacology*, Vol. 208. doi:10.1016/j.bcp.2022.115368.

35. Tang, L., Gao, J., Li, X., Cao, X., and Zhou, B. (2022). Molecular Mechanisms of Luteolin Against Atopic Dermatitis Based on Network Pharmacology and in Vivo Experimental Validation, *Drug Design, Development and Therapy*, Vol. 16, 4205–4221. doi:10.2147/DDDT.S387893.

36. Khan, S. A., Wu, Y., Li, A. S. M., Fu, X. Q., and Yu, Z. L. (2022). Network Pharmacology and Molecular Docking-Based Prediction of Active Compounds and Mechanisms of Action of Cnidii Fructus in Treating Atopic Dermatitis, *BMC Complementary Medicine and Therapies*, Vol. 22, No. 1, 1–14. doi:10.1186/s12906-022-03734-7.

37. Chu, M., Tsang, M. S. M., He, R., Lam, C. W. K., Quan, Z. B., and Wong, C. K. (2020). The Active Compounds and Therapeutic Mechanisms of Pentaherbs Formula for Oral and Topical Treatment of Atopic Dermatitis Based on Network Pharmacology, *Plants*, Vol. 9, No. 9, 1–19. doi:10.3390/plants9091166.

38. Qinwufeng, G., Jiacheng, L., Xiaoling, L., Tingru, C., Yunyang, W., and Yanlong, Y. (2022). Jiu-Wei-Yong-An Formula Suppresses JAK1/STAT3 and MAPK Signaling Alleviates Atopic Dermatitis-like Skin Lesions, *Journal of Ethnopharmacology*, Vol. 295. doi:10.1016/j.jep.2022.115428.

39. Yang, N., Shao, H., Deng, J., and Liu, Y. (2023). Network Pharmacology-Based Analysis to Explore the Therapeutic Mechanism of Cortex Dictamni on Atopic Dermatitis, *Journal of Ethnopharmacology*, Vol. 304. doi:10.1016/j.jep.2022.116023.

40. Zhang, R., Zhang, H., Shao, S., Shen, Y., Xiao, F., Sun, J., Piao, S., Zhao, D., Li, G., and Yan, M. (2022). Compound Traditional Chinese Medicine Dermatitis Ointment Ameliorates Inflammatory Responses and Dysregulation of Itch-Related Molecules in Atopic Dermatitis, *Chinese Medicine (United Kingdom)*, Vol. 17, No. 1, 1–19. doi:10.1186/s13020-021-00555-7.

41. Kim, M. J., Yang, Y. J., Min, G. Y., Heo, J. W., Son, J. D., You, Y. Z., Kim, H. H., Kim, G. S., Lee, H. J., Yang, J. H., and Park, K. Il. (2025). Anti-Inflammatory and Antioxidant Properties of Camellia Sinensis L. Extract as a Potential Therapeutic for Atopic Dermatitis through NF-KB Pathway Inhibition, *Scientific Reports*, Vol. 15, No. 1, 1–14. doi:10.1038/s41598-025-86678-5.

42. Frusciante, L., Geminiani, M., Trezza, A., Olmastroni, T., Mastroeni, P., Salvini, L., Lamponi, S., Bernini, A., Grasso, D., Dreassi, E., Spiga, O., and Santucci, A. (2024). Phytochemical Composition, Anti-Inflammatory Property, and Anti-Atopic Effect of Chaetomorpha Linum Extract, *Marine Drugs*, Vol. 22, No. 5, 1–26. doi:10.3390/md22050226.

43. Xia, T., Liang, X., Liu, C. S., Hu, Y. N., Luo, Z. Y., and Tan, X. M. (2022). Network Pharmacology Integrated with Transcriptomics Analysis Reveals Ermiao Wan Alleviates Atopic Dermatitis via Suppressing MAPK and Activating the EGFR/AKT Signaling, *Drug Design, Development and Therapy*, Vol. 16, 4325–4341. doi:10.2147/DDDT.S384927.

44. Li, X., Feng, L., Zhong, T., Mo, X., Wang, D., Gu, J., Chen, D., Zeng, X., and Yan, F. (2023). Gu-Ben-Hua-Shi (AESS) Formula Ameliorates Atopic Dermatitis via Regulating NLRP3 Signaling Pathways, *Saudi Pharmaceutical Journal*, Vol. 31, No. 11, 101792. doi:10.1016/j.jsps.2023.101792.

45. Jin, J., Chowdhury, M. H. U., Das, T., Biswas, S., Wang, K., Rahman, M. H., Choi, K. Y., and Adnan, M. (2023). Chemico-Biological Interaction Unraveled the Potential Mechanistic Pathway of Ixeridium Dentatum Compounds against Atopic Dermatitis, *Computational Biology and Chemistry*, Vol. 106, No. July, 107933. doi:10.1016/j.compbiolchem.2023.107933.

46. Ren, Y., Wu, Q., Liu, C., Zhang, J., Wang, Z., Li, Y., and Zhang, Y. (2023). Discovery of a Traditional Chinese Herbal Combination for the Treatment of Atopic Dermatitis: Saposhnikoviae Radix, Astragali Radix and Cnidium Monnieri, *Archives of Dermatological Research*, Vol. 315, No. 7, 1953–1970. doi:10.1007/s00403-023-02575-9.

47. Liu, J., Tao, Y., Zou, X., Liu, Q., Meng, X., Zhang, Y., and Su, J. (2023). In Vitro and in Vivo Exploration of the Anti-Atopic Dermatitis Mechanism of Action of Tibetan Medicine Qi-Sai-Er-Sang-Dang-Song Decoction, *Journal of Ethnopharmacology*, Vol. 306. doi:10.1016/j.jep.2023.116155.

48. Zhao, W., Jiang, H., Gu, Y., Zhang, W., Bao, S., Dai, M., Dong, B., Yang, Y., Li, K., Qin, L., and Zeng, X. (2023). Fangji Dihuang Formulation Ameliorated DNCB-Induced Atopic Dermatitis-like Skin Lesions by IL-17 Signaling Pathway: Integrating Network Analysis and Experimental Validation, *Frontiers in Pharmacology*, Vol. 14, 1–15. doi:10.3389/fphar.2023.1220945.

49. Yang, M., Zhao, M., Xia, T., Chen, Y., Li, W., Zhang, H., Peng, M., Li, C., Cao, X., Liang, L., Yue, Y., Zhong, L., Du, J., Li, J., Wang, Y., and Shu, Z. (2023). Physalis Alkekengi L. Var. Franchetii Combined with Hormone Therapy for Atopic Dermatitis, *Biomedicine and Pharmacotherapy*, Vol. 162. doi:10.1016/j.biopha.2023.114622.

50. Zhong, Y., Zhao, Y., Meng, X., Wang, F., and Zhou, L. (2024). Unveiling the Mechanism of Liangxue Siwu Decoction in Treating Rosacea Through Network Pharmacology and In-Vitro Experimental Validation, *Journal of Inflammation Research*, Vol. 17, 5685–5699. doi:10.2147/JIR.S471097.

51. Zeng, C., Weng, L., Song, Y., Huang, Y., Xiang, W., Ye, Z., Yu, C., Lai, Z., Song, Y., Yang, H., Zhang, L., and Liu, B. (2024). N-Butanol

Extract of Broussonetia Papyrifera (L.) L'Hér. Ex Vent Root Bark Alleviates Atopic Dermatitis by Targeting E3 Ubiquitin Ligase WWP1 to Promote NLRP3 Degradation, *Biomedicine and Pharmacotherapy*, Vol. 180. doi:10.1016/j.biopha.2024.117561.

52. Nie, J., Jiang, X., Wang, G., Xu, Y., Pan, R., Yu, W., Li, Y., and Wang, J. (2024). Yu-Ping-Feng-San Alleviates Inflammation in Atopic Dermatitis Mice by TLR4/MyD88/NF-KB Pathway, *Journal of Ethnopharmacology*, Vol. 329. doi:10.1016/j.jep.2024.118092.

53. Ouyang, X. L., Yuan, Z. L., Chen, X. B., Gan, H. W., Guo, S. H., Cai, J., and Zhong, J. J. (2024). Can Aged Camellia Oleifera Abel Oil Truly Be Used to Treat Atopic Dermatitis?, *Frontiers in Pharmacology*, Vol. 15, 1–10. doi:10.3389/fphar.2024.1449994.

54. Pratama, Y. A., Marhaeny, H. D., Winarto, S., Palmado, I. A., Widyananda, M. H., Rahmadi, M., Taher, M., Hasan, A. A., and Kleuser, B. K. (2025). Network Pharmacology and Molecular Docking Investigation of Curcuma Xanthorrhiza Roxb. Rhizome with the Mechanisms Underlying as the Potential Drug of Eczema Treatment, *Journal of Advanced Pharmaceutical Technology & Research*, Vol. 16, No. 4, 219–226. doi:10.4103/JAPTR.JAPTR_117_25.

55. Chen, F., Liu, J., Yu, X., Jia, H., Yang, C., and Zhao, B. (2025). Aspergillus Oryzae Fermented Plumula Nelumbinis Against Atopic Dermatitis Through AKT/MTOR and Jun Pathways, *Pharmaceuticals*, Vol. 18, No. 1. doi:10.3390/ph18010020.

56. Li, S., Jiang, Y., Hu, C., Ding, Y., Fu, X., Xing, S., and Zeng, L. (2025). Elucidating the Mechanisms of Chrysanthemum Action on Atopic Dermatitis via Network Pharmacology and Machine Learning, *International Journal of Molecular Sciences*, Vol. 26, No. 23, 1–21. doi:10.3390/ijms262311262.

57. Zhang, S., Chen, N., Wu, F., Xu, X., Zheng, X., Cheng, Z., Wang, M., Wu, Y., Jiang, S., Liu, Q., Liu, C., Zhang, F., and Han, B. (2025). Discovery of Therapeutic Promising Natural Products to Target Kv1.3 Channel, a Transmembrane Protein Regulating Immune Disorders, through Multidimensional Virtual Screening, Molecular Dynamics Simulations and Biological Validation, *International Journal of Biological Macromolecules*, Vol. 308. doi:10.1016/j.ijbiomac.2025.142636.

58. Kim, H. J., Park, M., Jang, S., Song, H. K., Lee, S. K., and Kim, T. (2025). Pulsatilla Koreana Nakai Extract Attenuates Atopic Dermatitis-like Symptoms by Regulating Skin Barrier Factors and Inhibiting the JAK/STAT Pathway, *International Journal of Molecular Sciences*, Vol. 26, No. 7. doi:10.3390/ijms26072994.

59. Suleman, M., Sayaf, A. M., Moltrasio, C., Tricarico, P. M., Giambuzzi, F., Rimondi, E., Melloni, E., Secchiero, P., Marcuzzi, A., Marzano, A. V., and Crovella, S. (2025). Phytocompounds in Precision Dermatology: COX-2 Inhibitors as a Therapeutic Target in Atopic-Prone Skin, *Biomolecules*, Vol. 15, No. 7, 1–22. doi:10.3390/biom15070998.

60. Sarkar, D., Pramanik, A., Majumdar, S., Das, D., Mahato, M., Pramanik, A., and Bhattacharyya, S. (2025). Dihydromyricetin, the Active Component of Rattan Tea Alleviates Symptoms of Systemic Sclerosis and Atopic Dermatitis through Modulation of RORγt and IL17A Production in T Cells, *Journal of Nutritional Biochemistry*, Vol. 144. doi:10.1016/j.jnutbio.2025.110000.

61. Kato, K., Akamatsu, M., Kakimaru, S., Koreishi, M., Takagi, M., Miyashita, M., Murata, Y., Nakamura, Y., Satoh, A., and Tsujino, Y. (2025). Fraglide-1 from Traditional Chinese Aromatic Vinegar: A Natural AhR Antagonist for Atopic Dermatitis, *Food and Chemical Toxicology*, Vol. 197. doi:10.1016/j.fct.2025.115301.

62. Liu, X., Chen, L., Sun, P., Jiang, X., Li, P., Xu, Z., Zhan, Z., and Wang, J. (2025). Network Pharmacology and Experimental Verification: Phellodendri Chinensis Cortex-Cnidii Fructus Herb Pair Alleviates Atopic Dermatitis by Regulating the TLR4/NF-KB Pathway, *Drug Design, Development and Therapy*, Vol. 19, 1451–1474. doi:10.2147/DDDT.S505248.

63. Khan, S. A. (2025). Network Pharmacology and in Silico Analysis Reveal Kochiae Fructus as a Potential Therapeutic against Atopic Dermatitis through Immunomodulatory Pathway Interactions, *PLoS ONE*, Vol. 20, No. 4, 1–32. doi:10.1371/journal.pone.0320818.

64. Ru, N., Guo, M. Z., Xu, H., Wu, Y. P., Li, Z. X., Wang, R., Ouyang, S. H., Cao, Y. F., Sun, W. Y., Tan, H. L., Wang, H. J., Kurihara, H., Liang, L., Li, Y. F., Yang, Q., Huang, Q. L., Ning, N., Zheng, X. F., Wu, Y. P., et al. (2026). Oral Chinese Patent Medicine Alleviates Atopic Dermatitis by Regulating ALOX15-Derived Oxylipins Disorder, *Phytomedicine*, Vol. 159. doi:10.1016/j.phymed.2026.158524.

65. El Bouamri, L., Bouribab, A., Bouachrine, M., and Chtita, S. (2026). In Silico Investigation of Aloe Vera Phytoconstituents Targeting Key Proteins Involved in Atopic Dermatitis Progression, *Biotechnologia*, Vol. 107, No. 2, 121–136. doi:10.5114/bta/216302.

66. Sun, P., Zhao, X., Lin, Y., Xu, Z., Jia, Y., Wang, J., Wang, J., and Zhan, Z. (2026). Combining Metabolomics and Network Pharmacology to Clarify the Mechanism of Angelica Sinensis-Sophora Flavescens Pills in Treating Atopic Dermatitis through the Sweet-Bitter Harmonization Theory, *Journal of Ethnopharmacology*, Vol. 355. doi:10.1016/j.jep.2025.120570.

67. Chen, X., Shen, Q., Zhou, R., Lin, Y., Zhou, T., Chen, K., Wang, P., Chen, Y., Liu, H., and Yang, A. (2026). Screening of Active Constituents in Camellia Oil against Atopic Dermatitis via Molecular Docking and Experimental Validation: Elucidation of the Underlying Molecular Mechanism, *Inflammopharmacology*, Vol. 34, No. 2, 1301–1314. doi:10.1007/s10787-026-02118-4.

68. Zhang, X., Wang, Y., Zhao, D., Yin, C., Wu, H., Zeng, J., Shi, X., He, M., Feng, G., Wang, Y., Liu, J., Huang, W., and Tian, H. (2026). Unveiling the Pharmacological Basis of Rhodiola Crenulata for Atopic Dermatitis: A Multi-Model Approach Combining Zebrafish, Mouse Studies, and Intelligent Computational Analysis, *Phytomedicine*, Vol. 159, 1–19. doi:10.1016/j.phymed.2026.158498.

69. Jia, Y., Ma, L., Chen, Q., Yang, Y., Min, W., and Luo, D. (2026). Integrating Network Pharmacology, Machine Learning, and Molecular Docking to Explore the Therapeutic Mechanisms of Huangqin in Atopic Dermatitis: A STROBE-Compliant Observational Study, *Medicine*, Vol. 105, No. 30, e49911. doi:10.1097/MD.0000000000049911.

70. Luo, L. (2026). Exploration of the Potential Mechanisms of Yinqiao Powder in Treating Atopic Dermatitis: Integrating Network Pharmacology, Single-Cell, and Bulk RNA Sequencing, *Journal of Asthma and Allergy*, Vol. 19, 1–25. doi:10.2147/JAA.S592593.

71. Ye, C., Liu, Y., Li, Y., Li, Z., Sui, L., Cui, J., Jiang, Z., Li, J., Song, J., and Liu, J. (2026). The Stem of Schisandra Chinensis and Schisandrin B Alleviated DNCB-Induced Atopic Dermatitis in Mice by Inhibiting the NF-KB Pathway, *Frontiers in Immunology*, Vol. 17, 1–16. doi:10.3389/fimmu.2026.1725312.

72. Li, J., Liu, C., Liu, J., He, J., Wang, C., Ma, P., Li, L., and Li, H. (2026). Sappanone A Exerted Strong Anti-Inflammatory Effects in the Treatment of Atopic Dermatitis Through IL-21R-Mediated JAK1/STAT3 Pathway, *Phytotherapy Research*, Vol. 40, No. 1, 144–158. doi:10.1002/ptr.70123.

73. Yan, X., Cheng, L., Zhi, G., Che, M., Shen, H., Du, Z., Ma, X., Geng, F., and Li, B. (2026). Therapeutic Efficacy of Sanhuang Xiexin Decoction on Atopic Dermatitis via Suppressing STAT3 Signaling, *Journal of Ethnopharmacology*, Vol. 358. doi:10.1016/j.jep.2025.120993.

74. Ren, Y., Wu, M., Liu, K., Zhang, L., Zhang, Y., and Qin, W. (2026). Integrating Bioinformatics, Machine Learning and Molecular Biology to Elucidate the Anti-Allergic Mechanisms of Ginkgo Biloba Leaves, *Computational Biology and Chemistry*, Vol. 123. doi:10.1016/j.compbiolchem.2026.109017.

75. Song, R., Zhu, Y., Xue, K., Deng, X., Wang, R., Su, Y., Chen, X., and Yuan, H. (2026). A "Controlled Assembly" Strategy for Constructing Coptidis Rhizoma Self-Assembled Nanoparticles to Ameliorate Inflammatory Damage in Atopic Dermatitis,

*Bioactive Materials*, Vol. 56, 234–247. doi:10.1016/j.bioactmat.2025.10.010.

76. Du, H., Wang, N., Wang, C., Luo, S., Ji, X., Li, R., Wang, Y., Lai, X., Li, H., Ding, Y., and An, H. (2026). Genistein Alleviates Skin Inflammation in Atopic Dermatitis by Inhibiting Mast Cell Degranulation through Toll-like Receptor, *Phytomedicine*, Vol. 159, 158308. doi:10.1016/j.phymed.2026.158308.

77. Zhang, Y., Wang, J. A., Li, L. F., Chen, X. W., Gui, Q. F., He, C., Zhu, Y., Tao, Y., Meng, J. F., Song, M. R., Sun, R., Wang, J., Guo, J. S., Liu, S., and Zhang, Z. J. (2026). Micheliolide Directly Targets Keratinocyte Annexin A2 to Abrogate STAT3-Driven Inflammation and Pruritus in Atopic Dermatitis, *Phytomedicine*, Vol. 157, 1–16. doi:10.1016/j.phymed.2026.158303.

78. Yu, H. L., and Zhou, R. (2026). Potential Anti-Atopic Dermatitis Effects of Kochiae Fructus Revealed by Network Pharmacology and Preliminary in Vitro Validation, *South African Journal of Botany*, Vol. 196, 820–834. doi:10.1016/j.sajb.2026.06.056.

79. Tai, Y., Cao, S., Zhong, W., Li, S., Han, J., Liu, X., Cao, S., Wang, X., Jin, S., Liu, C., Shen, Y., Xing, Y., Li, M. Y., Zuo, H. X., Zhang, G., Ma, J., and Jin, X. (2026). Jingfang Granules Alleviate Atopic Dermatitis by Restoring Skin Barrier Function and Inhibiting NF-KB/NLRP3 Axis and JAK/STAT3 Axis, *Phytomedicine*, Vol. 155. doi:10.1016/j.phymed.2026.158187.

80. Xu, P., Wan, Y., Jin, X., Yuan, Y., Ma, H., Wang, Y., Wang, F., and Qu, L. (2026). Gardenia Jasminoides Fruit Extract Alleviates MC903-Induced Atopic Dermatitis and Reduces IL-4/IL-13-Induced Tight Junction Disruption and Inflammation by Regulating the Phosphorylation of STAT6, *Journal of Ethnopharmacology*, Vol. 360. doi:10.1016/j.jep.2025.121124.

81. Zhang, T., Cao, C., Zhang, L., Lina, J., Wang, Q., Qingli, L., Hu, J., Du, W., Xu, Y., Liu, J., Gao, Z., Kong, L., Li, Q., Yang, F., and Duan, X. (2026). Paeoniflorin Modulates MYC Protein to Restore Immune–Epithelial Balance and Delay the Progression of Atopic Eczema, *International Journal of Clinical Practice*, Vol. 2026, No. 1. doi:10.1155/ijcp/6215711.

82. Shi, Y., Jin, X., Zhang, B., Wei, D., Xie, B., Fu, S., Zhang, H., and Song, X. (2026). Targeting TRPV4 with Sclareol Ameliorates Atopic Dermatitis through by Suppression of Inflammatory Response and Oxidative Stress, *Biochemical Pharmacology*, Vol. 253, 118315. doi:10.1016/j.bcp.2026.118315.

83. Wang, X., Jia, N., Joo, H., Wang, S., Zhang, C., Chen, Q., and Jiang, W. (2026). Yin-Hua Li-Shi Formula Exerts Anti-Atopic Dermatitis Effects Through Luteolin Targeting AKT/MAPK-IL-6/IL-17 Axis, *Journal of Inflammation Research*, Vol. 19, 1–17. doi:10.2147/JIR.S594212.

84. Xu, Y. Bin. (2021). The Research on Huanglian Jiedu Decoction against Atopic Dermatitis, *Scientific Programming*, Vol. 2021. doi:10.1155/2021/5557908.

85. Wang, T., You, W., Zhao, L., Zhang, B., and Wang, H. (2023). Network Pharmacology Revealed the Mechanisms of Action of Lithospermum Erythrorhizon Sieb on Atopic Dermatitis, *Clinical, Cosmetic and Investigational Dermatology*, Vol. 16, 651–658. doi:10.2147/CCID.S403736.

86. Lee, S. H., Oh, Y., Bong, S. K., Lee, J. W., Park, N. J., Kim, Y. J., Park, H. B., Kim, Y. K., Kim, S. H., and Kim, S. N. (2023). Paedoksan Ameliorates Allergic Disease through Inhibition of the Phosphorylation of STAT6 in DNCB-Induced Atopic Dermatitis like Mice, *Applied Biological Chemistry*, Vol. 66, No. 1. doi:10.1186/s13765-023-00815-0.

87. Zhang, L., Chen, N., Liao, Y., Kong, Y., Yang, X., Zhan, M., Xu, W., Wang, Y., Zhu, S., and Hu, Y. (2024). Efficacy and Action Mechanisms of Compound Shen Chan Decoction on Experimental Models of Atopic Dermatitis, *International Immunopharmacology*, Vol. 137. doi:10.1016/j.intimp.2024.112479.

88. Lee, J., Seo, Y. S., Lee, A. Y., Nam, H. H., Ji, K. Y., Kim, T., Lee, S., Hyun, J. W., Moon, C., Cho, Y., Jung, B., Kim, J. S., and Chae, S. (2024). Anti-Atopic Effect of Scutellaria Baicalensis and Raphanus Sativus on Atopic Dermatitis-like Lesions in Mice by Experimental Verification and Compound-Target Prediction, *Pharmaceuticals*, Vol. 17, No. 3. doi:10.3390/ph17030269.

89. Meng, Y., Liu, Y., Guo, J., Guo, X., Han, X., and Zhang, L. (2024). Qing-Re-Chu-Shi Decoction Ameliorates 2,4-Dinitrochlorobenzene-Induced Atopic Dermatitis in NC/Nga Mice through Anti-Inflammation and Immunoregulatory Mechanisms, *Journal of Ethnopharmacology*, Vol. 323. doi:10.1016/j.jep.2024.117702.

90. Huang, Z., Fan, B., Mao, W., Kuai, L., Feng, J., Wang, Y., Zhou, M., and Miao, X. (2024). Topical Application of Artemisia Annua L. Essential Oil Ameliorates 2,4-Dintrochlorobenzene-Induced Atopic Dermatitis in Mice, *Journal of Ethnopharmacology*, Vol. 333. doi:10.1016/j.jep.2024.118439.

91. Wu, Y., Wu, J. Y., Bai, J. X., Wang, X. Q., Li, A. S. M., Fan, X. Y., Han, R. X., Wang, L., Dou, X., Fu, X. Q., and Yu, Z. L. (2025). Macrophage and Keratinocyte Cell Assays Suggest That the Supercritical CO2 Extract of Black Soybean Possesses Anti-Inflammatory and Skin Barrier-Protective Effects, *Food Research International*, Vol. 218. doi:10.1016/j.foodres.2025.116824.

92. Huang, K., Liu, Q., Zhang, R., Nian, H., Luo, Y., Luo, Y., Fei, X., Kuai, L., Li, B., Tan, Y., Li, S., and Ma, X. (2025). Preclinical and Clinical Studies on Qin-Zhu-Liang-Xue Decoction: Insights from Network Pharmacology and Implications for Atopic Dermatitis Treatment, *Frontiers of Medicine*, Vol. 19, No. 1, 134–148. doi:10.1007/s11684-024-1101-7.

93. Chen, Y., Tang, Z., Han, Z., Wang, M., Li, X., Lai, L., Zhou, P., Wang, F., and Li, F. (2025). A Topical Chinese Herbal Inhibits Pruritus and Skin Inflammation via Neural TRPM8 in Atopic Dermatitis, *Phytomedicine*, Vol. 139. doi:10.1016/j.phymed.2025.156524.

94. Feng, H., Zhou, Y., Ren, X., Zhu, X., Duan, X., Qu, S., Zhu, B., Li, Y., and Qin, Y. (2025). Kushe Tincture Ameliorates DNCB-Induced Atopic Dermatitis by Affecting NF-Kb/JAK-STAT3 Pathway: Bioinformatics Analysis and Animal Experiment Verification, *Journal of Inflammation Research*, Vol. 18, 15293–15308. doi:10.2147/JIR.S562462.

95. Kim, H. M., Kim, G. L., Gil, T. Y., Sim, H. Y., Lee, H., Lee, D. S., Lee, K. Y., and An, H. J. (2026). Topical Trichosanthis Radix Water Extract Attenuates Atopic Dermatitis-Like Skin Inflammation: Marker Standardization, Network Pharmacology, and Preclinical Validation, *Mediators of Inflammation*, Vol. 2026, No. 1. doi:10.1155/mi/8744885.

96. Wang, M., Cheng, G., Ma, X., Xu, H., Sun, S., Zhang, Y., Jiang, W., Chen, Q., Li, B., Li, D., Ma, X., and Song, J. (2026). Rutin Targets PD-L1 for the Treatment of Atopic Dermatitis: Network Pharmacological Analysis and Experimental Evidence, *International Immunopharmacology*, Vol. 179. doi:10.1016/j.intimp.2026.116570.

97. Hsiao, W. K., Herbig, M. E., Newsam, J. M., Gottwald, U., May, E., Winckle, G., and Birngruber, T. (2024). Opportunities of Topical Drug Products in a Changing Dermatological Landscape, *European Journal of Pharmaceutical Sciences*, Vol. 203. doi:10.1016/j.ejps.2024.106913.