INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

Review Article

Drug Repurposing in Psoriasis: Unlocking Therapeutic Insights Through Computational Methods

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ARTICLE INFO

Published: 14 Oct 2025
Keywords:
Psoriasis, Drug Repurposing, Computational approach, Omics technologies, Molecular docking, Network Pharmacology
DOI:
10.5281/zenodo.17352052

ABSTRACT

Psoriasis is an autoimmune inflammatory skin disease of chronic nature that heavily compromises the quality of life in patients, whose pathogenesis is based on the multifactorial interplay of genetic and environmental elements that are responsible for the varied clinical presentations and comorbidities. The conventional translation of research results into newly approved medicines continues to be a time-consuming and expensive process, which has seen Drug Repurposing as a revolutionary approach in contemporary drug discovery. By using already tested drugs on humans, Drug Repurposing saves time and investment needed to discover new therapeutic uses. Advances in computational tools like molecular docking, network pharmacology, and machine learning have further expedited this process, enabling the integration of biomedical information from chemical structures to clinical outcomes. Network strategies probe for biological interactions to uncover new therapeutic opportunity, whereas artificial intelligence and machine learning utilize sophisticated algorithms to uncover drug–disease relationships and predict efficacy across various datasets. Additionally, hybrid approaches that integrate omics information with conventional computational methods offer a richer paradigm for candidate prioritization and validation. In the case of psoriasis, where chronic unmet therapeutic needs persist, drug repurposing offers a promising alternative to traditional discovery pipelines, with the benefits of known safety profiles, accelerated clinical translation, and regulatory tractability.

INTRODUCTION

Psoriasis is a chronic, immune-mediated inflammatory skin disorder characterized by keratinocyte hyperproliferation, parakeratosis, abnormal angiogenesis, and infiltration of immune cells into the dermis and epidermis [1]. Its pathogenesis involves a multifactorial interplay between genetic susceptibility and environmental

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

triggers, making it one of the most common autoimmune disorders worldwide [2]. Clinically, psoriasis manifests as well-demarcated erythematous plaques with scaling, often affecting the elbows, knees, scalp, and other areas, and follows a chronic, relapsing course [3]. Globally, psoriasis affects approximately 125 million individuals, with prevalence rates ranging from 1.1% in high-income Southern Latin American countries to nearly 2% in East Asia and Western Europe [4,5]. Beyond skin involvement, psoriasis is associated with multiple comorbidities, including psoriatic arthritis, metabolic syndrome, cardiovascular diseases, and psychological disorders such as anxiety and depression [6].

The disease arises from complex interactions among keratinocytes, immune cells, and resident skin cells, with both innate and adaptive immunity playing central roles [7]. Dendritic cells (DCs), particularly plasmacytoid DCs (pDCs) and myeloid DCs (mDCs), are activated via antimicrobial peptides like LL37, which bind self-DNA or RNA and trigger TLR7/8/9 signaling, resulting in type I interferon and proinflammatory cytokine production [8]. This cascade drives Th1 and Th17 differentiation, sustaining keratinocyte hyperproliferation and chronic inflammation through cytokines such as IL-17, IL-21, IL-22, TNF-α, and IFN-γ [9–11]. Psoriasis presents in multiple clinical subtypes, including plaque, guttate, inverse, pustular, and erythrodermic forms [5].

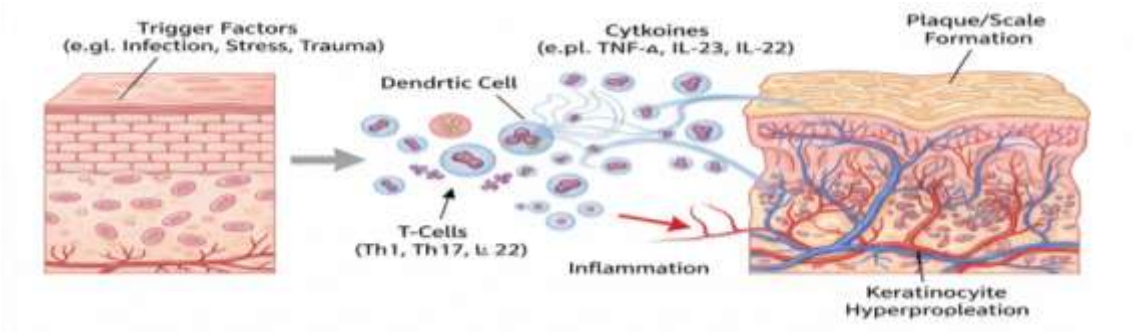

Fig 1. Pathophysiology of Psoriasis

2. CURRENT STRATEGIES FOR PSORIASIS MANAGEMENT

Psoriasis treatment aims to alleviate symptoms, improve quality of life, and prevent disease progression [12]. Conventional therapies include topical agents (Corticosteroids, vitamin D analogues, Retinoids, Calcineurin inhibitors, Keratolytics), which are effective for mild to moderate disease but limited by side effects such as skin atrophy, irritation, and poor compliance over large body surface areas [13,14]. Phototherapy, including narrow-band Ultraviolet B (UVB) and Psoralen + Ultraviolet A (PUVA), achieves significant lesion clearance but carries long-term safety risks like photoaging and carcinogenesis [14-16].

Systemic non-biologics, such as Methotrexate, Cyclosporine, and Acitretin, are standard for moderate-to-severe disease but require careful monitoring due to hepatotoxicity, nephrotoxicity, and teratogenicity [17,18].

Biologics targeting TNF-α, IL-12/23, IL-17, and IL-23 achieve high clinical responses (PASI-90/100) but are associated with infection risks and high costs, limiting accessibility [19,20]. Small-molecule oral drugs, including PDE4 inhibitors (Apremilast) and JAK/TYK2 inhibitors, offer

better tolerability and ease of administration but with slightly reduced efficacy [17,18,21].

Emerging strategies, such as nanocarrier formulations, natural product–derived compounds, and Stem cell–based therapies, are under investigation, highlighting the need for innovative, cost-efficient, and personalized solutions [22-24]. Despite these advances, the limitations of current therapies emphasize a persistent unmet need in psoriasis treatment.

Table. 1 Current Psoriasis therapies and their adverse effects

THERAPY TYPE	EXAMPLES	CLINICAL USE	LIMITATIONS	REF
Topical treatments	Corticosteroids, Vitamin D analogues, Retinoids, Calcineurin inhibitors, Keratolytics, Coal tar, Dithranol, Tapinarof, Roflumilast	First-line for mild to moderate psoriasis, localized lesions; proven effective.	Skin atrophy, irritation, tachyphylaxis poor compliance if >20% BSA affected.	[13]
Phototherapy	Narrow-band UVB, PUVA (psoralen + UVA), Excimer light	Effective for moderate psoriasis; significant lesion clearance.	Photoaging, carcinogenic not suitable for long-term use.	[14]
Systemic non-biologics	Methotrexate, Cyclosporine, Acitretin	Cornerstone for moderate-to-severe disease; useful when topicals/phototherapy fail.	Hepatotoxicity, nephrotoxicity, teratogenicity, metabolic abnormalities;	[18]
Biologics	TNF-α inhibitors; IL-12/23 inhibitor; IL-17 inhibitors; IL-23 inhibitors	Revolutionized moderate-to-severe psoriasis;	Risk of infections, malignancy; very high cost limits access.	[20]
Oral small-molecule drugs	Apremilast (PDE4 inhibitor), JAK inhibitors, TYK2 inhibitors	Convenient oral administration; good tolerability.	Slightly less efficacy compared to biologics.	[21]

3. DRUG REPURPOSING: AN ATTRACTIVE APPROACH

Conventional drug discovery is time-consuming, costly, and associated with high attrition rates, taking 12–18 years and over $2.6 billion per approved drug [25,26]. To overcome these challenges, drug repurposing also known as repositioning, reprofiling, or indication expansion—has emerged as a promising alternative [27,28]. This strategy seeks new therapeutic applications for drugs that are already approved, in development, or shelved for non-safety reasons. Repurposing offers several advantages: reduced development time and cost, established safety and pharmacokinetic profiles, and the potential to bypass early-phase preclinical or clinical trials [29,30]. Regulatory incentives, including tax credits and accelerated approval pathways, further enhance the attractiveness of repurposing, especially for rare or complex diseases [31,32]. Three main stakeholders drive drug repurposing efforts: Academia, Pharmaceutical firms, and Technology-focused companies. Academia typically contributes through basic research, in silico studies, and high-throughput screening, whereas technology companies provide innovative computational pipelines and screening platforms. Pharmaceutical firms focus on late-stage development, regulatory expertise, and lifecycle management. Collaborations among these stakeholders integrate scientific innovation

with regulatory and developmental capabilities, facilitating successful repurposing initiatives [33,34].

Drug repurposing is particularly relevant to psoriasis, as several approved drugs act on pathogenic pathways such as STAT3, NF-κB, Akt, and cytokine networks including IL-17/IL-23 [35-37]. Computational approaches can identify candidate drugs that modulate these pathways, accelerating the discovery of effective treatments for psoriasis with known safety profiles. This review focuses on computational strategies used for drug repurposing in psoriasis, including network-based, omics-based, structure-based, and machine learning approaches, highlighting their applications, strengths, limitations, and future potential.

4. COMPUTATIONAL APPROACHES - REVOLUTIONIZING DRUG REPURPOSING

Computational methods are transforming drug repurposing through the use of heterogeneous biomedical information, such as chemical structures, gene expression signatures, protein-protein interactions, and clinical data. The techniques forecast new drug-target associations, off-target side effects, and important molecular networks, revealing potential new therapeutic avenues. By being complemented with experiment validation, they streamline the discovery and optimization of repurposed medicines, offering an expedient and cost-saving option compared to conventional drug discovery [38–40]. In psoriasis, computational approaches such as Molecular Docking, Network Pharmacology, Machine Learning, and Systems Biology enable speedy screening of known drugs, synergistic combination identification, and lead prioritization for validation. Through multidimensional dataset analysis, these methods enable the discovery of drugs that fine-tune key inflammatory and immune mechanisms, providing effective avenues for the discovery of new psoriasis therapies [41]. The key computational methods employed in drug repurposing for psoriasis are described below.

4.1 Omics Approaches in Drug Repurposing for Psoriasis

Omics technologies have transformed our comprehension of intricate diseases, among them psoriasis. Genomic research has recognized several susceptibility loci for psoriasis, showing aspects of its genetic architecture. For example, the discovery of the IL23R gene variant has highlighted the contribution of the IL-23/Th17 pathway in the pathogenesis of psoriasis [42]. Transcriptomic studies have also shed further light on the molecular signatures of psoriasis, and have shown the upregulation of pro-inflammatory cytokines IL-17A, IL-22, and TNF-α within psoriatic lesions [43]. These studies have not only contributed to our knowledge of the disease, but have also opened the door to targeted therapies.

Proteomics, the investigation of proteins on a large scale, has also given us more insight into the pathophysiology of psoriasis. Research using mass spectrometry has found differentially expressed proteins in psoriatic skin, including those with a role in keratinocyte proliferation and immune response [44]. In addition, metabolomics has shown differences in the metabolic pathways in psoriasis patients that indicate possible biomarkers for severity of disease and response to treatment [45]. Together, these omics technologies have highlighted the complex nature of psoriasis and the possibility of drug repurposing strategies.

4.1.1 Genomics and Drug Repurposing

Genomic research has been pivotal to the discovery of critical pathways involved in

psoriasis, most notably the IL-23/Th17 pathway, which has driven the repurposing of drugs like ustekinumab, initially designed for Crohn's disease [46]. Genome-wide association studies (GWAS) identified psoriasis-associated variants that are enriched in immune signaling pathways such as JAK/STAT, NF-κB, and Wnt, thus facilitating the prediction of response to therapy and enabling personalized medicine strategies [47]. Chemogenomic profiling has added to these findings by suggesting druggable targets like IL13 and POLI, with compounds such as Hydrocortisone analogs, Rilonacept, and the non-toxic compound Pandel suggested for repurposing [48].

4.1.2 Transcriptomics and Drug Repurposing

Transcriptomic research has revealed psoriasis-specific gene expression signatures in psoriatic skin, offering a basis for the identification of drugs that can reverse them. Methotrexate and apremilast, for instance, suppress pro-inflammatory genes and continue to be a focus of repurposing strategies [49]. Systems biology techniques combining transcriptomic datasets with drug–gene interaction databases, such as Connectivity Map analyses, have identified new repositioning candidates like Pyroxamide, Droxinostat, and Ziprasidone, most of which were initially developed for cancer, cardiovascular, or neurological conditions [50,51].

4.1.3 Proteomics and Drug Repurposing

Proteomics has charted the protein profile of psoriatic skin, which contains overexpressed molecules like S100A8 and S100A9 that are associated with keratinocyte proliferation and immune cell activation [52]. The proteins are disease severity biomarkers as well as drug targets. Statins, for example, have shown promise in cutting down on inflammatory protein expression, and this makes them of interest for repurposing in psoriasis treatment [53].

4.1.4 Metabolomics and Drug Repurposing

Metabolomics has identified specific metabolic signatures in psoriasis, such as disturbances in lipid and amino acid metabolism [54]. These observations suggest that metabolic dysregulation is a causal force in disease pathogenesis. Therapeutic agents like metformin, classically utilized in diabetes, have been suggested as repurposing agents to normalize metabolic homeostasis in psoriatic subjects, highlighting the value of metabolomic information in therapeutic development [55].

4.1.5 Integrative Systems Approaches

Integrative frameworks combining genomics, transcriptomics, proteomics, and metabolomics have refined immune-specific mechanisms and prioritized druggable modules. The DIME framework, for example, incorporated single-cell RNA sequencing of 40 immune cell types, emphasizing the central roles of Th17 and dendritic cells and nominating druggable pathways within IL-17/IL-23 and NF-κB signaling [56]. Large-scale meta-analyses of a multi-ancestry GWAS of approximately half a million individuals found 76 druggable genes like IL12B and IL23A, with scoring systems adding Disulfiram and Doxylamine to the high-priority list [57]. Previous integrative studies validated the method by prioritizing IL1B and HMOX1, making methotrexate the top repurposed drug and Resveratrol an emerging anti-inflammatory candidate [58]. Together, these omics-guided pipelines merge into hybrid approaches that identify both known immunomodulators and new agents from multiple pharmacologic classes and thus hasten mechanism-based psoriasis drug

repurposing with improved translational potential [59,60].

4.2 NETWORK PHARMACOLOGY

The Network-driven approach leverages the complexity of biological networks by integrating gene, protein, pathway, and drug interaction networks to identify therapeutic opportunities beyond the traditional "one drug–one target" model [61–63]. Protein–Protein Interaction (PPI) networks, disease–gene associations, and drug–target databases are combined to pinpoint hub genes and signaling modules that serve as actionable intervention points for known drugs.

4.2.1 Early Applications in Psoriasis

Early implementations of network approaches in psoriasis mapped molecular landscapes by combining PPI networks, disease–gene associations, and pathway enrichment. Highly connected enzymes such as RUVBL2, PSMA2, ZAP70, IKBKE, and EGFR were systematically ranked, many of which have corresponding drugs in clinical use, suggesting repurposing potential [64].

Pathway-based analyses have also illustrated mechanistic insights. For example, the CDK4/6–EZH2 pathway induces psoriatic inflammation via STAT3 activation and IκBζ induction; inhibition using breast cancer drugs Abemaciclib and Palbociclib, or EZH2 inhibitors, reversed inflammation in murine models, highlighting pathway-targeted repurposing opportunities [65].

4.2.2 Machine Learning and Co-Expression Models

Intracellular PPI networks have been simulated to mimic signal transmission, with machine learning predicting drug–disease relationships capable of reprogramming pathological signaling toward healthy states [66]. Co-expression-based models, such as Cogena, group disease transcriptomes into modules and integrate pathway enrichment with Connectivity Map data to identify known psoriasis drugs (e.g., Cyclosporin, Methotrexate) and predict novel candidates [67].

4.2.3 Network Pharmacology for Apoptotic Regulation

Network pharmacology has been applied to apoptotic regulation in psoriasis. Psoriasis–apoptosis interaction networks revealed hub regulators such as RELA, MAPK1/3, MMP9, IL1B, AKT1, and STAT1, with repurposing candidates including Acetylcysteine, Arsenic trioxide, Bortezomib, and Curcumin, identified through network pharmacology, molecular docking, and molecular dynamics simulations [68].

4.2.4 Systems-Level and Multi-Omics Integration

Systems-level models integrating transcriptomic and PPI data in inflammatory skin diseases have ranked High-Priority Proteins (HPPs), exploring drug–gene interactions to uncover repurposing opportunities [69]. The general philosophy of network pharmacology emphasizes connectivity and network topology as key determinants of disease mechanisms and drug action [70].

4.2.5 Case Studies of Network-Based Repurposing in Psoriasis

- **Methotrexate:** Network analyses further elucidated its immune-modulatory actions [71].
- **Apremilast:** A PDE4 inhibitor repurposed for psoriasis, shown to impact multiple inflammatory pathways [72].
- **Thalidomide:** Originally a sedative, network studies revealed its role in cytokine modulation and immune cell function [73].

4.3 ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING (AI/ML) APPROACHES

AI and ML have emerged as pivotal tools in drug discovery, enabling the analysis of vast datasets to uncover novel drug-disease associations. The application of these technologies in drug repurposing is particularly relevant for complex diseases like psoriasis, where multiple pathways are involved. Various studies have demonstrated the efficacy of ML algorithms in predicting drug efficacy and safety profiles based on existing biological data [74].

4.3.1 Data-Driven Approaches

Data-driven methodologies form the backbone of AI/ML in drug repurposing. High-dimensional biological data, including genomic, transcriptomic, and proteomic information, can be utilized to train ML models. For instance, a study which employed a random forest algorithm to analyze gene expression profiles in psoriasis patients, successfully identifying existing drugs that could be repurposed for treatment. Their findings underscored the potential of integrating multi-omics data to enhance the predictive power of ML models in identifying novel therapeutic candidates [75].

4.3.2 Convolutional Neural Networks (CNNs)

CNNs have been employed for image-based analysis in dermatology, facilitating the identification of psoriasis lesions and the assessment of treatment responses. A study which demonstrated that CNNs could classify skin lesions with accuracy comparable to dermatologists, suggesting their potential utility in monitoring psoriasis and evaluating treatment efficacy. By integrating image data with clinical outcomes, CNNs can aid in the identification of existing drugs that may be effective for psoriasis management [76].

4.3.3 Recurrent Neural Networks (RNNs)

RNNs, particularly long short-term memory (LSTM) networks, have been utilized for sequence prediction tasks, such as drug response modeling. By analyzing temporal data related to psoriasis treatment outcomes, RNNs can uncover patterns that may inform repurposing strategies. For instance, the study which employed LSTMs to predict patient responses to existing therapies based on historical treatment data, providing insights into potential repurposing opportunities [77].

4.3.4 Case Studies of AI/ML and DL in Psoriasis Drug Repurposing

Several case studies illustrate the successful application of AI/ML and DL in identifying repurposing candidates for psoriasis. One notable example is the study which utilized a combination of ML algorithms and clinical data to identify the antihypertensive drug Amlodipine as a potential treatment for psoriasis. Their findings were validated through preclinical models, highlighting the robustness of AI-driven approaches in drug repurposing [78].

Another significant study which employed a DL framework to analyze electronic health records (EHRs) of psoriasis patients, identifying existing medications with potential efficacy in psoriasis management. Their approach demonstrated the feasibility of using real-world data to inform drug repurposing efforts, emphasizing the importance of integrating clinical datasets into AI models [79].

4.4 STRUCTURE BASED APPROACH

Structure-Based Drug Design (SBDD) is a computational approach utilizing the three-

dimensional macromolecular structures of biological molecules to identify putative therapeutic candidates [80]. By facilitating the rational design of molecules that bind to known targets, SBDD enhances the efficacy and selectivity of drug candidates and has been especially useful for repurposing drugs for new applications, such as psoriasis.

4.4.1 Molecular Docking

A key element of SBDD is molecular docking, where interactions between a ligand and a target protein are mimicked to predict binding affinity and ligand orientation in the active site [81,82]. Molecular docking has been used in several studies to identify FDA-approved compounds that can modulate psoriasis-associated pathways, including the IL-17 receptor, thus revealing potential repurposing candidates [83].

4.4.2 Virtual Screening

Virtual screening complements molecular docking by enabling rapid evaluation of large compound libraries against a target of interest [84]. It has been applied to discover compounds targeting the IL-23/IL-17 pathway, a central pathway in psoriasis pathogenesis [85].

4.4.3 Examples of Repurposed Drugs in Psoriasis

- **Apremilast:** An oral Phosphodiesterase 4 (PDE4) inhibitor originally for other inflammatory diseases, it suppresses pro-inflammatory cytokines and enhances anti-inflammatory mediators [86].
- **Topical Calcineurin Inhibitors** (Tacrolimus and Pimecrolimus): Initially created for other skin diseases, these drugs were later repurposed for localized psoriasis through immune modulation [87].

4.4.4 Recent computational studies emphasize multi-target SBDD approaches:

Screening ~2,000 FDA-approved compounds against fifteen validated psoriasis protein targets identified compounds—including antiviral and anticancer drugs—with stronger binding than reference ligands. Drugs, such as Nelarabine, Fludarabine, Clofarabine, Cladribine, Sofosbuvir, and Ganciclovir, were proposed as potential multi-target repurposing candidates [41].

Integrated methods combining molecular docking, one-class Support Vector Machine (SVM) algorithms, and molecular dynamics simulations identified drugs such as Pioglitazone, Trimipramine, and Dimetindene. Docking predicted strong binding affinities, SVM modeling suggested anti-psoriasis activity, and molecular dynamics simulations confirmed the stability of drug-target complexes [88].

4.5 HYBRID APPROACHES

The contemporary hybrid computational approach combines bioinformatics-driven multi-omics analysis with classical computational methods into a multi-perspective framework for systematic identification of therapeutic candidates.

4.5.1 Omics-Driven Candidate Identification

The approach typically begins with large-scale transcriptomic, genomic, or proteomic data mined from databases such as the Gene Expression Omnibus (GEO) to acquire disease-specific signatures [89]. Bioinformatics platforms, exemplified by the Connectivity Map (CMap), prioritize compounds capable of reversing these signatures, applying a systems-level filter to rank candidates for further mechanistic investigation [90].

4.5.2 Multi-Step Computational Validation

Candidate compounds are subsequently validated through a multi-step computational pipeline

- Ligand-based similarity searches against ChEMBL [91],
- High-confidence structure-based virtual screening against Protein Data Bank (PDB) targets [92],
- Network analysis using tools like Search Tool for the Retrieval of Interacting Genes/Proteins (STRING) to contextualize drug targets within larger disease networks. [93]

By cross-validating systems-level omics predictions with atom-level structural interactions, hybrid computational modeling enhances mechanistic insight and translational potential.

4.5.3 Applications in Psoriasis

Several studies illustrate the efficacy of this strategy in psoriasis

4.5.3.1 Metabolomics and Network Pharmacology: Untargeted plasma metabolomics with network pharmacology and pathway enrichment identified dysregulated pathways (amino acid/lipid metabolism, sphingolipid metabolism, mTOR signaling) and druggable proteins such as ESR1, OPRM1, and HSD11B1. Compounds like Tamoxifen showed repurposing potential [94].

4.5.3.2 Genomics-Informed Approaches: GWAS and Mendelian randomization analyses have highlighted therapeutic targets such as PPARG and indicated potential repurposable agonists including Pioglitazone, Rosiglitazone, Troglitazone, Fenofibric acid, and Bezafibrate [95,96].

4.5.3.3 Integrated Bioinformatics and Machine Learning: Hybrid methods combining bioinformatics, ML, and molecular verification identified hub genes (KIF4A, DLGAP5, NCAPG, CCNB1, CEP55) with predicted molecules like etoposide showing high target affinity and inhibition of disease markers [97].

4.5.3.4 Multi-Omics Strategies: Integration of Proteome-wide Mendelian randomization, Protein–Protein Interaction networks, druggability prediction, single-cell RNA sequencing, and Phenome-Wide Association studies revealed plasma proteins (IL23R, ERAP2, IFNLR1) as therapeutic targets, with Scopoletin and Esculetin as potential repurposable drugs [98].

4.5.3.5 Systems Biology with Deep Learning: Systems biology approaches combined with deep neural network–inferred drug-target interaction models and genome-wide microarray data identified key biomarkers (STAT3, CEBPB, NF-κB, FOXO1), enabling the prediction of drug candidates based on regulatory potential, toxicity, and sensitivity [99].

Table. 2 Various Computational approaches

Computational Approach	Data/ Input Source	Methodology / Key Tools	Validation	Ref
Omics-based	Transcriptomics (microarray, RNA-seq), Proteomics, Metabolomics	Differential expression analysis, gene set enrichment, connectivity mapping, LINCS, GEO datasets	*in vitro*, clinical datasets	[42-45]
Network-based	Protein–Protein Interaction (PPI) networks, Gene-Disease networks, signaling pathways	Network pharmacology, graph algorithms, topological analysis, Cytoscape	*in vitro, in vivo*	[61-63]

Machine Learning / AI-based	Multi-omics datasets, chemical descriptors, clinical data	Supervised/unsupervised learning, deep learning, QSAR models, predictive modeling	*in silico* prediction + validation	[74-77]
Structure-based / Molecular Docking	3D protein structures, drug libraries	Molecular docking, virtual screening	*in silico* + experimental validation	[81,82,84]
Hybrid Approaches	Combination of omics, network, and structural data	Multi-modal integration, AI-assisted network analysis	Multi-level validation	[89,90]

5. STRENGTHS

- **Efficiency:** Computational methods enable speedy screening of existing drugs, significantly reducing the time required for drug discovery compared to traditional methods.
- **Cost-effectiveness:** These approaches can save substantial costs associated with drug development, as they utilize already approved drugs with established safety profiles.
- **Comprehensive data integration:** Computational techniques leverage heterogeneous biomedical information, such as chemical structures, gene expression, and clinical data, to identify new drug-target associations and potential therapeutic avenues.
- **Identification of synergistic combinations:** Computational methods can help identify drug combinations that may work synergistically to enhance treatment efficacy.
- **Mechanism-based discovery:** By focusing on specific pathogenic pathways relevant to psoriasis, computational approaches can identify candidate drugs that modulate these pathways, potentially leading to more effective treatments.
- **Regulatory advantages:** Drug repurposing can benefit from regulatory incentives, such as tax credits and accelerated approval pathways, making it particularly attractive for complex diseases like psoriasis.

6. CHALLENGES

- **Dependence on data quality**: The effectiveness of computational methods relies heavily on the quality and completeness of the underlying data, which can sometimes be limited or biased.
- **Validation challenges:** While computational predictions can identify potential drug candidates, experimental validation is necessary to confirm their efficacy and safety, which can still be time-consuming and costly.
- **Complexity of biological systems:** The intricate nature of biological networks can make it challenging to accurately model interactions and predict outcomes, leading to potential oversights or inaccuracies in drug-target associations.
- **Limited understanding of off-target effects:** Computational methods may not fully account for off-target side effects, which can complicate the therapeutic profile of repurposed drugs.
- **Integration difficulties:** Combining various omics data and computational techniques can be complex and may require specialized expertise, which can limit accessibility for some researchers or institutions.
- **Potential for false positives:** The high dimensionality of data and the complexity of biological interactions can lead to false positives in drug predictions, necessitating

careful evaluation and prioritization of candidates.

7. FUTURE PERSPECTIVE

The future perspective of computational approaches in drug repurposing for psoriasis is promising and multifaceted. As technology continues to advance, the integration of more sophisticated computational methods, such as Machine Learning, Network Pharmacology, and Omics-based analyses, will enhance the ability to identify novel therapeutic candidates more efficiently. These approaches will likely lead to the discovery of drugs that target specific pathways involved in psoriasis, such as those related to inflammation and immune response.

Moreover, the combination of computational strategies with experimental validation will streamline the drug discovery process, reducing the time and costs associated with traditional drug development. The ability to analyze large datasets and identify common biomarkers will facilitate the prioritization of lead compounds for further investigation, ultimately leading to more effective treatments.

As regulatory frameworks evolve to support drug repurposing, including incentives for research in rare and complex diseases like psoriasis, the collaboration among academia, pharmaceutical companies, and technology firms will become increasingly vital. This collaborative environment will foster innovation and the rapid translation of computational findings into clinical applications.

Additionally, the ongoing exploration of multi-target drugs and the refinement of hybrid approaches that combine bioinformatics with traditional pharmacological strategies will open new avenues for treatment. As a result, computational approaches are expected to play a critical role in addressing the unmet needs in psoriasis management, leading to more personalized and effective therapeutic options in the future.

CONCLUSION

Drug repurposing represents a promising alternative to traditional drug discovery, particularly in the context of complex diseases like psoriasis. The integration of computational methods and omics technologies has the potential to significantly enhance the efficiency and effectiveness of drug repurposing efforts, paving the way for new therapeutic avenues and improved patient outcomes. As research continues to evolve, the application of these innovative strategies will likely yield valuable insights and facilitate the discovery of effective treatments for psoriasis and other challenging condition

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HOW TO CITE: R. Abirami, R. Indumathy, P. Vinodhini, V. Soundarya, Drug Repurposing in Psoriasis: Unlocking Therapeutic Insights Through Computational Methods, Int. J. of Pharm. Sci., 2025, Vol 3, Issue 10, 1470-1487. https://doi.org/10.5281/zenodo.17352052