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Artificial Intelligence in skin disease therapeutics: from drug discovery to personalized treatment pathways

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Disclosure of interests

None to declare.

Abstract

Artificial intelligence (AI) comprises computational methods capable of tasks associated with human cognition, and includes specialized subfields such as machine learning, deep learning, convolutional neural networks for image analysis, and large language models for text-based workflows. In dermatology, these methods are increasingly used across research and clinical practice, supporting drug discovery, diagnosis, decision-making, and personalized treatment. In drug discovery, AI can accelerate target identification, support in silico compound design, and predict the effectiveness and safety profiles of compounds. It also offers opportunities for drug repurposing, helping identify candidates for conditions with limited treatment options. In clinical practice, AI enhances teledermatology and imaging-based assessment, providing consistent lesion analysis, severity evaluation, and triage support across malignant, inflammatory, and infectious skin diseases. Beyond diagnosis, AI is beginning to play a significant role in supporting therapeutic decision-making. Clinical decision-support systems and multimodal AI tools assist clinicians by organizing information, suggesting management strategies, monitoring disease progression, and helping align treatment choices with current guidelines. AI models can further estimate treatment response, durability, and the likelihood of therapy adjustment, creating a basis for more individualized care. Despite these advances, significant challenges remain. Bias in training data, limited real-world validation, unclear regulatory frameworks, concerns over interpretability, and the need for patient and clinician trust remain ongoing barriers. This review aims to provide an up-to-date overview of the emerging application domains of AI in dermatology.

Keywords: artificial intelligence, drug discovery, diagnosis, decision support, personalized treatment, review

1. Introduction

Artificial intelligence (AI) refers to a broad class of computational systems designed to perform tasks that typically require human intelligence, including pattern recognition, prediction, reasoning, and language understanding. Over time, AI has evolved into multiple specialized subfields, many of which are already being actively applied in medical research and clinical practice [1].

Within the AI framework, machine learning (ML) represents a core approach in which systems learn directly from data rather than relying on explicitly programmed, rule-based logic. In ML, algorithms are trained on example data to identify statistical relationships between inputs and outputs, allowing them to generate predictions or classifications when presented with new, previously unseen data [2, 3].

A major class of ML methods is artificial neural networks, which are computational models loosely inspired by the structure of biological neural systems. Neural networks consist of interconnected processing units ("neurons") that transform input data through weighted connections and nonlinear activation functions. During training, these weights are iteratively adjusted to minimize prediction error, enabling the network to learn increasingly accurate representations of the data [3].

Deep learning (DL) refers to neural network-based methods that contain multiple stacked layers, allowing the model to progressively transform raw inputs into more complex, task-relevant patterns. Compared with shallow neural networks, DL models are capable of capturing highly complex, non-linear relationships and are particularly effective for high-dimensional data such as images, signals, and text [3].

Within DL, convolutional neural networks (CNNs) are a specialized neural network architecture designed for image analysis. CNNs process images by applying trainable convolutional filters to local regions, enabling the model to detect simple visual features such as edges and textures in early layers and more complex structures in deeper layers. By preserving spatial relationships within the image, CNNs are well-suited for dermatologic imaging tasks and have become the dominant approach for lesion classification, dermoscopy, and histopathologic image analysis [3].

In parallel, large language models (LLMs) represent another specialized class of DL models designed to process and generate human language. These models are trained on large-scale textual datasets and learn contextual relationships between words, sentences, and concepts, enabling them to capture meaning beyond isolated terms. As a result, LLMs can perform a wide range of language-based tasks, including text generation, summarization, information extraction, and support for clinical documentation. Whereas CNNs primarily operate on visual data, LLMs extend AI applications to text-driven clinical and research workflows [4] (***Figure 1***).

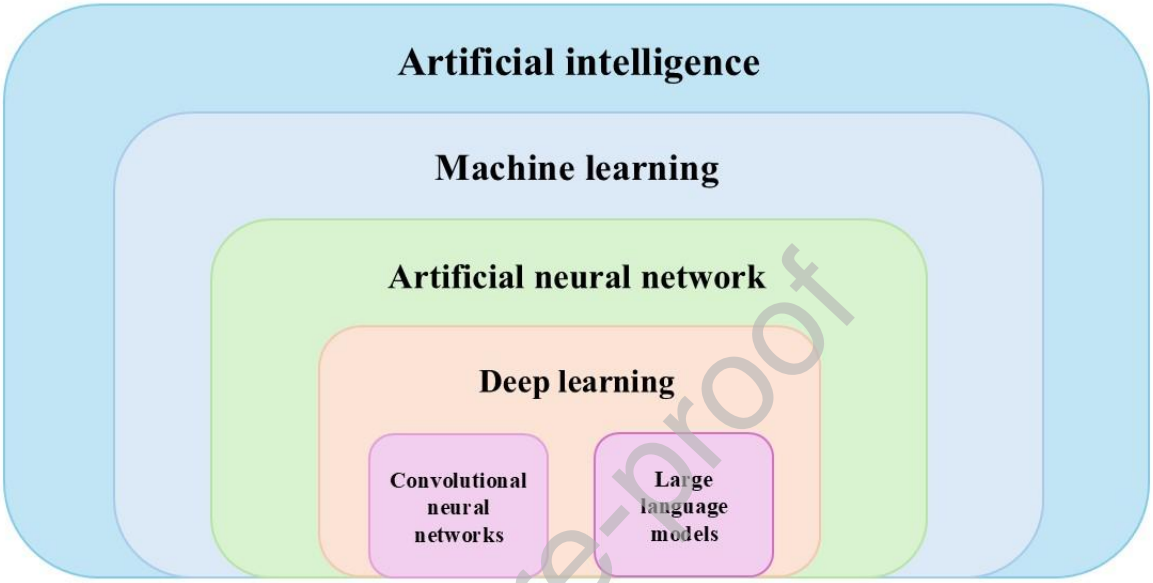

Figure 1. Conceptual hierarchy of artificial intelligence [1-3].

While AI has begun to occupy an increasingly prominent role in medicine, dermatology is particularly well-suited for AI-driven innovation owing to its data-rich and visually oriented nature. Over the past decade, AI applications in dermatology have evolved from experimental

2. AI in drug discovery for skin disease

AI is currently being researched and implemented across several stages of drug discovery. ***Figure 2*** presents a conceptual pipeline demonstrating where AI methods are incorporated within these processes.

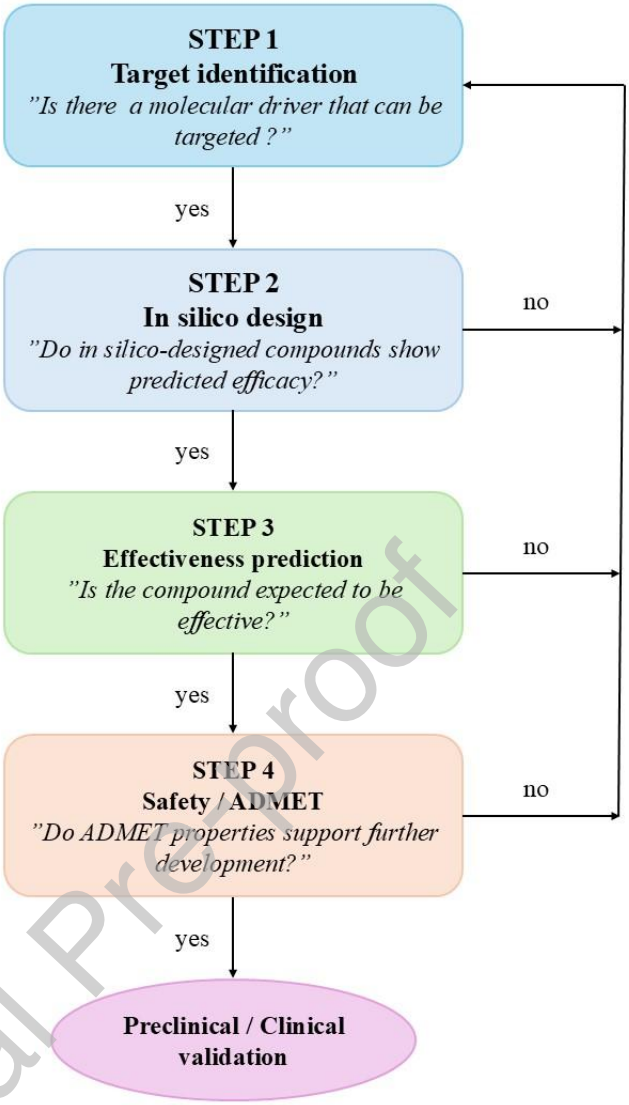

Figure 2. AI-augmented drug discovery pipeline.

2.1. Target identification

Target identification aims to recognize disease-relevant molecular entities, such as receptors, enzymes, or signaling proteins, that play a key role in pathogenesis and are amenable to therapeutic modulation. AI has opened new opportunities to discover novel molecular targets by making the analysis of large databases more efficient. Sakai *et al*. developed an ML-based system that mines the FDA Adverse Event Reporting System (FAERS) to identify drugs with potentially preventive effects on psoriasis and then links these candidate drugs to target proteins using large chemical structure databases. This big data-driven pipeline highlighted antiparkinsonian agents, particularly dopamine D2 receptor agonists, as candidates. In an imiquimod-induced psoriasis-like mouse model, the DRD2 agonist quinpirole improved the disease. This effect was associated with downregulation of IL-17 pathway-related mRNA expression in the skin and reduced serum levels of TNF-α and IL-10 [5].

AI has also shown promising results in identifying master regulators as potential therapeutic targets in primary cutaneous melanoma. Song *et al*. used bulk and single-cell transcriptomic datasets to construct gene co-expression networks that integrate tumor-intrinsic and microenvironmental signals. Linking network modules to survival and to estimates of the immune and stromal infiltrate, two biological axes were identified: an immune-dominant module in which the myosin gene *MYO1F* emerged as a key hub associated with favorable prognosis, and a pro-tumorigenic, poor-prognosis axis centered on the transcription factor ZNF180. Knockdown experiments in melanoma cell lines and xenograft models supported a driver role for ZNF180 in melanoma, highlighting this regulator as a candidate therapeutic target [6].

AI-based analysis of large-scale transcriptomic datasets can also contribute to target identification in a more indirect manner by delineating pathogenic pathways and immunological endotypes, which help prioritize therapeutic axes in atopic dermatitis (AD). For instance, in AD, AI has yielded promising results in mapping cutaneous gene expression patterns into clinically meaningful metagenes. RNA-sequencing data from skin biopsies in a cohort of 951 patients were decomposed into 29 metagenes (SKITm1-29) using an unsupervised decomposition approach, non-negative matrix factorization. These metagenes were then separated into disease-related clusters (psoriasis, AD, and healthy skin) with automated clustering methods. Statistical and ML-based models were used to examine how the metagenes correlate with local skin phenotypes (erythema, induration, excoriation, lichenification), rarer chronic forms of disease, global disease severity scores, and circulating cytokine levels. As a practical implication, metagene profiles derived from a single RNA-seq experiment can be used to estimate local skin manifestations and overall disease severity and infer the underlying immunological endotype [7].

2.2. *In silico* design & optimization

AI has transformed the modelling of drug molecules and their targets, enabling this to be performed not only *in vitro* and *in vivo*, but also and often more efficiently *in silico*.

Selective JAK1 inhibitors are small-molecule therapies used in the treatment of immune-mediated diseases, such as ulcerative colitis and AD. Using a deep neural network, Zixiao Wang *et al*. virtually screened large compound libraries, and the resulting hits were layered with structure-based pharmacophore models. Through subsequent molecular docking, molecular dynamics simulations, and in vitro JAK1 kinase inhibition assays, they identified 13 potential JAK1 inhibitor hits, four of which demonstrated significant inhibitory activity. This work established an integrated silico screening pipeline that delivered novel JAK1-directed hit compounds, which can serve as starting points for the development of new JAK1-targeted therapies [8].

Tyrosinase is a central enzyme in melanin production and a promising therapeutic target, and tyrosinase inhibitory peptides are being studied as safer depigmenting agents for conditions such as melasma and post-inflammatory hyperpigmentation. Charoenkwan *et al.* developed a sequence-based computational tool for the in-silico identification of tyrosinase-inhibitory peptides (TIPs). Using a curated set of experimentally validated TIPs together with carefully selected non-TIP peptides, they trained multiple ML models and combined their outputs into an integrated predictor, which achieved high accuracy on independent test data [9].

AI also supports the discovery of dermatologically relevant antimicrobial agents. In a particular study, the concept of "molecular de-extinction" was used [10]. This means proteomes from extinct species were mined for peptide sequences with potential antibiotic activity. They utilized a deep-learning framework that combines a peptide-sequence encoder with neural network heads to predict species-specific minimal inhibitory concentration (MIC) values across multiple bacterial pathogens. From this screen, 69 peptides were synthesized, many of which showed antimicrobial activity against ESKAPEE (*Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa, and Enterobacter spp., Escherichia coli*) pathogens. Lead peptides were also effective in vivo in mouse skin abscess models, demonstrating anti-infective activity. These AI-designed peptides may help expand the therapeutic arsenal against multidrug-resistant pathogens and could contribute to tackling antibiotic resistance. Beyond antibacterial discovery, ML approaches have also yielded advances in antifungal drug design. De Souza *et al*. used physicochemical descriptors of compounds with known activity against *Candida albicans* to train ML models, including a Random Forest classifier, which they then applied to the eMolecules® library for virtual screening. Of 17 top-ranked candidates selected for experimental testing, 11 proved active against Candida albicans [11].

2.3. Effectiveness prediction

ML models have also shown promise in predicting treatment effectiveness and durability. In psoriasis, biologic therapies are generally effective; however, many patients discontinue treatment within a few years due to loss of efficacy or other reasons. Du *et al*. compared a conventional risk factor-based statistical model with several ML algorithms for predicting the 5-year risk of treatment discontinuation, using data from the Danish DERMBIO biologics registry. The traditional Cox regression model, built from hazard ratios for individual predictors, showed only modest discrimination (AUC (area under curve) = 0.61). By contrast, the best-performing machine-learning model, a gradient boosted decision tree trained on just ten routinely collected clinical variables, achieved an AUC of 0.85, highlighting the potential of ML-based tools to support biologic selection and patient counselling in routine psoriasis care [12].

Some patients with AD respond poorly or not at all to dupilumab, despite its overall high efficacy. In a retrospective study, Murphy *et al.* analyzed pretreatment lesional skin biopsies from 70 patients treated with dupilumab (53 responders and 17 non-responders). As model inputs, they selected seven biopsy-derived variables, comprising histopathological features and semi-quantitative immunohistochemical scores for key inflammatory cytokines, capturing the local immunopathological profile before therapy. Using a logistic regression classifier with two outcome categories (responder vs non-responder), the model achieved a sensitivity of 88% for predicting non-response and an overall accuracy of 95.7% in distinguishing non-responders from responders, indicating that even relatively simple machine-learning approaches can effectively flag patients unlikely to benefit from dupilumab [13].

2.4. Safety, sensitization & absorption, distribution, metabolism, excretion, and toxicity (ADMET)

With current AI technologies, in silico safety assessment has progressed far beyond classical quantitative structure-activity relationships. Modern models can handle multiple toxicity

endpoints and ADMET parameters in parallel, providing an integrated prediction of a compound's overall safety profile [14].

Some explainable ML models can now classify the acute dermal toxicity of chemicals with AUC values around 0.8, effectively distinguishing between high- and low-risk compounds. Lou *et al*. compiled a large acute dermal toxicity dataset by integrating 1735 rabbit and 1679 rat LD_{50} experiments and used these data to build machine-learning and deep-learning classification models of dermal toxicity. Based on dermal LD_{50} values, chemicals were grouped into toxicity categories, and this classification task was used to train the models. The authors also released a standalone, user-friendly software tool that enables rapid estimation of the acute dermal toxicity risk of new compounds, providing an in-silico alternative that could support efforts to reduce reliance on traditional LD_{50} testing in rabbit and rat models [15].

2.5. AI-enabled repurposing

Already approved drugs may have therapeutic effects in other diseases, and drug repurposing means identifying these new uses for them. Huang *et al.* recognized a gap: most AI drug repurposing tools focus on diseases that already have approved treatments. To identify new drug candidates for diseases without existing therapies, they developed a graph foundation model for zero-shot drug repurposing, known as TxGNN. It ranks drugs as potential indications or contraindications for 17,080 diseases. TxGNN is trained on a large medical knowledge graph and combines a graph neural network with a metric-learning module. Compared with strong baseline models, it improved prediction accuracy for indications by 49.2% and for contraindications by 35.1% in benchmark tests. Many of the model's predictions match real-world off-label prescribing patterns [16]. TxGNN illustrates how large graph-based models can systematically explore repurposing opportunities, including diseases that currently lack approved therapies.

3. AI in diagnosis

3.1. AI in teledermatology and teletriage

Teledermatology delivers dermatological care remotely by connecting patients and clinicians through telecommunication technologies [17]. One of its most common applications is teletriage, enabling up to 70% of patient inquiries to be managed without the need for an in-person visit [18]. It is often enhanced with AI tools to improve diagnostic consistency, making it a promising technology for facilitating timely and reliable care worldwide [19]. Moreover, AI is transitioning from a purely diagnostic adjunct to a broader therapeutic decision-support tool, with emerging applications in personalized medicine and automated disease monitoring [20].

Within this context, automated image-based classification of skin lesions is inherently challenging due to the fine-grained variability in lesion morphology [21]. CNNs, however, effectively manage these complex and highly variable tasks across numerous fine-grained object categories [22]. Consequently, extensive research has directly compared the diagnostic performance of AI with that of dermatologists. A notable example is the work by Esteva *et al*., who evaluated a single CNN trained on 129,450 clinical images representing 2,032 skin diseases. When tested against 21 board-certified dermatologists in the diagnosis of skin cancers, the CNN demonstrated accuracy comparable to, or in some cases exceeding that of expert clinicians, highlighting its potential as an autonomous classifier [23].

Moreover, human-AI collaboration can further enhance diagnostic reliability, promoting equitable access to high-quality care. Tschandl *et al.* demonstrated that human-AI collaboration surpasses the performance of either humans or AI alone, with the most pronounced benefits seen among less experienced clinicians, supporting the use of AI for simulating second opinions and telemedicine triage. Nonetheless, the study also highlighted that faulty AI outputs can mislead clinicians irrespective of experience level, underscoring the need for rigorous validation and human oversight [19].

Beyond diagnosis, AI-enhanced teledermatology platforms are beginning to influence therapeutics. Automated risk stratification determines which lesions require urgent excision, biopsy, or treatment initiation, while longitudinal telemonitoring allows therapy adjustments based on image-based severity indices. Such systems may ultimately reduce delays to treatment initiation, a key determinant of outcomes in conditions such as melanoma and inflammatory dermatoses [20, 24, 25].

3.2. AI in dermatopathology and skin imaging techniques

3.2.1. Dermatopathology

AI is increasingly used in dermatopathology to enhance diagnostic accuracy, analyze whole-slide images, and identify prognostic biomarkers. DL models demonstrate high performance in detecting skin malignancies, often nearing expert-level interpretation. These systems can also accurately predict prognosis while improving efficiency by automating tasks such as detecting margins, highlighting regions of interest, and quantifying immunohistochemical markers. AI systems can further support prognostic assessment and personalized oncology by identifying high-risk histological features predictive of recurrence and anticipating treatment response.

Despite these advances, challenges remain related to dataset quality, reliance on subjective "ground truth" and interpretability [26].

3.2.2. Dermoscopy

AI systems trained on dermoscopic images demonstrate high diagnostic accuracy for skin cancer detection. A validation study from the International Skin Imaging Collaboration (ISIC) showed that CNNs can reliably classify melanocytic and non-melanocytic lesions across large, diverse datasets, often matching or surpassing the performance of dermatologists in controlled settings. However, they found that even the best-performing model achieved markedly lower balanced accuracy on clinically realistic datasets. When compared with 18 dermatologists, algorithms outperformed experts for most trained categories but performed far worse for diagnoses not included in their training data, highlighting the importance of real-world validation [27].

3.2.3. Whole-body skin imaging

Total body photography (TBP) enhanced with AI tools is emerging as a key innovation for melanoma surveillance, particularly in high-risk populations. Marchetti *et al*. demonstrated that simple image-processing algorithms based on features such as size, color variation, and border irregularity can sensitively detect new or changing melanocytic lesions and can accurately distinguish melanoma from other lesions. These tools may support triage, surveillance, and prioritization of high-risk lesions, especially in patients with numerous nevi. However, the authors highlight the risk of overdiagnosis, underscoring the need for larger and more representative datasets before clinical adoption [28].

3.2.4. Other non-invasive imaging techniques

Emerging imaging modalities such as line-field confocal optical coherence tomography (LC-OCT), dermoscopy-guided high-frequency ultrasound (DG-HFUS), reflectance confocal microscopy (RCM), and thermal imaging provide new datasets suitable for AI-driven interpretation. DL applied to 3D LC-OCT images enables non-invasive assessment of cellular atypia, aiding clinical decision-making without biopsy [29]. Additionally, AI-assisted LC-OCT interpretation may facilitate broader adoption of LC-OCT in routine clinical practice [30]. In DG-HFUS, AI enables automatic lesion segmentation, aiding non-expert users to interpret sonographic findings [31]. AI also enhances RCM interpretation by improving image quality, automating delineation of key structures, and classifying skin lesions with reduced subjectivity and greater diagnostic consistency. ML tools can further assist less experienced readers, and improve tumor detection [32]. Thermal imaging combined with AI shows early promise for identifying microcirculatory changes, suggesting potential applications in vascular or inflammatory skin disorders [33].

Beyond these structural imaging methods, AI is being increasingly applied to optical and spectrally resolved techniques that capture biochemical and metabolic information, rather than morphology alone. Lihacova *et al*. showed that a multi-class CNN trained on limited multispectral and autofluorescence datasets can classify skin lesions by leveraging chromophore and fluorophore distribution patterns, supporting the feasibility of non-invasive optical AI diagnostics [34].

In parallel, autofluorescence photobleaching kinetics in basal cell carcinoma (BCC) have emerged as a functional imaging biomarker. Time-series autofluorescence imaging under 405

nm excitation reveals characteristic decay signatures linked to chromophore content, metabolic activity, and reactive oxygen species. These kinetic profiles delineate BCC lesion margins and enable ML models trained on autofluorescence decay parameters for automated lesion classification, suggesting a pathway toward robust non-invasive diagnostics capable of distinguishing BCC from benign and malignant lesions [35].

3.3. AI in the diagnosis and therapeutic management of key skin diseases

3.3.1. Psoriasis, atopic dermatitis

AI is transforming the management of chronic inflammatory dermatoses, including psoriasis and AD, by enabling automated lesion detection, differential diagnosis, subtype classification, and objective severity scoring. CNNs demonstrate high accuracy in segmenting lesions and quantifying disease burden, while AI-based predictive models support personalized therapeutic decision-making by forecasting treatment responses, including the selection of the optimal biologic agent in psoriasis and disease trajectory in AD. AI-enhanced TBP facilitates semi-automated PASI scoring for routine monitoring, and emerging tools, such as smart phototherapy devices, digital twin models, and algorithm-guided biologic optimization, further improve treatment precision and safety. In AD, AI integrates imaging, genomic, microbiome, and clinical data to inform individualized care and may streamline clinical trials through automated scoring and adherence tracking. Digital self-management platforms, mobile health applications, and telemedicine systems extend AI's role into continuous patient support (24, 36, 37).

3.3.2. Skin cancer

As discussed previously, AI's impact on skin cancer diagnosis, including teletriage, melanoma surveillance and dermatopathology is extensive and continues to expand. Recent evidence shows that AI systems can reach high diagnostic accuracy across multiple skin cancer types, with CNNs achieving strong sensitivity and specificity, particularly in distinguishing melanoma from benign or melanocytic lesions [38]. An additional review reported that although some models exceed 90% sensitivity and specificity in focused diagnostic tasks, their performance declines when applied in real-world settings. Notably, the review found that AI tends to benefit non-specialists more than experts, narrowing the diagnostic gap in primary care and telemedicine contexts, provided these systems are calibrated and deployed with appropriate oversight [39]. Although AI systems can achieve similarly high, or even higher diagnostic accuracy than dermatologists, their real-world performance depends heavily on clinical context, dataset diversity, and model robustness [23,40]. Advances in architectures, including reinforcement learning and enhanced training strategies, have enhanced model calibration, reduced overconfidence, and aligned algorithmic outputs more closely with clinician reasoning, supporting safer integration into clinical workflows [41]. These developments illustrate both the potential and limitations of AI in skin cancer care, highlighting the importance of rigorous validation and context-sensitive deployment.

3.3.3. Sexually transmitted infections and anogenital dermatoses

AI models show strong potential for detecting STIs and anogenital dermatoses, as demonstrated in a recent meta-analysis by Soe *et al*. Their study reported high pooled sensitivity and specificity across several conditions, including monkeypox, herpes simplex, genital warts, psoriasis, and scabies. Most available studies, however, remain at the proof-of-concept stage, with limited external validation and inadequate representation of clinically relevant

differentials, constraining real-world applicability. Nonetheless, these findings suggest that AI could offer valuable clinical support in sexual health care by aiding screening, triage, and early therapeutic decision-making, particularly in settings with limited specialist expertise [42].

3.4. Cosmetic dermatology and skin quality assessment

AI has significant implications for esthetic dermatology by enabling objective quantification of skin quality attributes such as texture, pigmentation, pore size, and wrinkle depth. These quantitative metrics reduce interobserver variability and allow consistent tracking of treatment outcomes. Integrated AI systems can recommend personalized cosmetic treatments by analyzing demographic and environmental factors, facilitating individualized care. Such data-driven approaches are increasingly used to evaluate interventions, such as resurfacing, pigmentation treatments, and injectable therapies [43].

3.5. Large language models

LLMs represent a special category within AI-based diagnostic tools, owing to their widespread adoption and high level of accessibility. These systems are actively being investigated across multiple healthcare applications; however, their most prominent use to date has been in diagnostic support. ***Figure 3*** illustrates a conceptual workflow of large language models [44]. Unlike many clinical AI tools that are restricted to professional environments, widely available LLM-based platforms such as ChatGPT can also be accessed by the general public, enabling lay users to engage in preliminary health-related information seeking and self-assessment. Boostani *et al*. conducted several studies investigating these systems, demonstrating that these openly available web-based platforms (ChatGPT-4o - OpenAI, Gemini 2.0 Flash - Google, Claude 3.7 Sonnet - Anthropic) are capable not only of processing textual information, but also of evaluating clinical and dermoscopic images [45-48]. Based on their findings, the performance of these AI-based models in detecting skin tumors often approaches, and in certain cases matches, the diagnostic accuracy of dermatologists [47,48]. Similarly promising results were observed in inflammatory skin diseases (e.g. acne, rosacea, hidradenitis suppurativa) [45, 46]. In one such study, 71 images from 44 patients with hidradenitis suppurativa were evaluated by the three LLMs. Diagnostic accuracy was 87.3% (95% CI: 77.6%-93.2%) for ChatGPT-4o, 77.5% for Claude Sonnet, and 32.4% for Gemini. They also looked at Hurley staging, which was the most accurate with Gemini, while ChatGPT provided the most appropriate therapeutic recommendations (88.7%) [46].

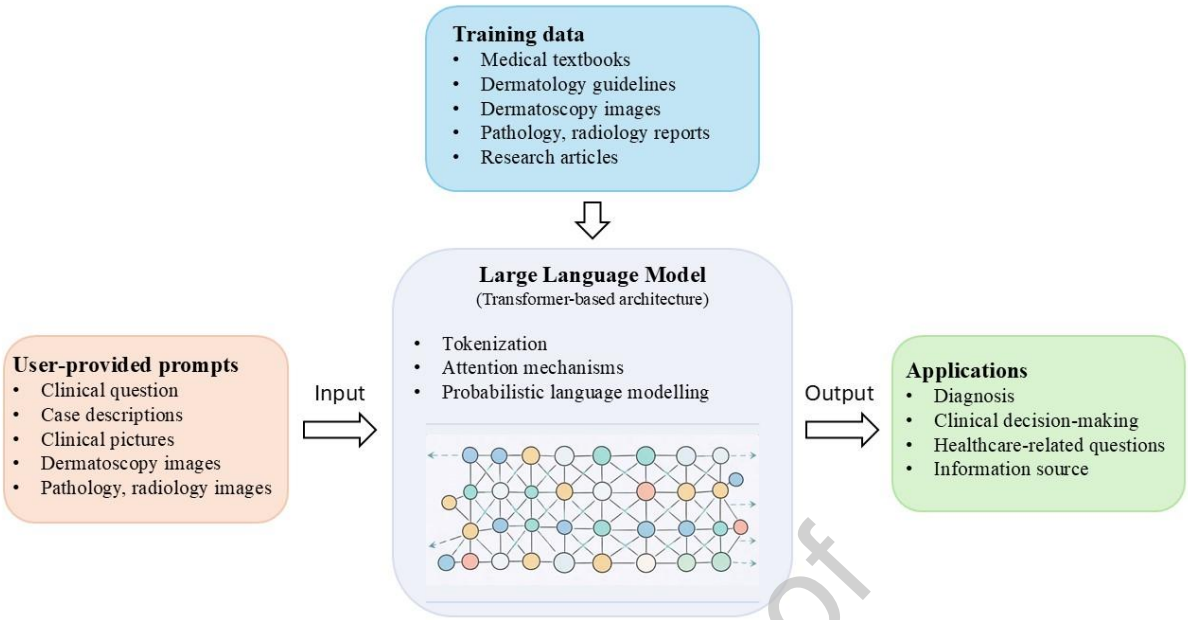

Figure 3. Workflow of large language models in dermatology [44,49].

The figure illustrates the conceptual workflow of large language models (LLMs) applied in dermatology. LLMs are pre-trained on large-scale text. During deployment, the model inference is initiated by user-provided prompts, which represent the clinical input supplied by users. Contemporary LLMs are predominantly built on transformer architecture, a neural network design that generates predictions by integrating information from all preceding tokens within a given context. This integration is achieved through a self-attention mechanism, which dynamically assigns importance to input elements based on their contextual relevance. The input text is tokenized and processed, and the model generates responses through probabilistic language modeling by predicting the most likely subsequent tokens based on patterns learned during pre-training (51).

Transformer: a neural network architecture composed of stacked attention-based layers that model relationships between all tokens in a sequence simultaneously, forming the computational backbone of modern LLMs. Tokenization: the process of splitting input text into small units (tokens) that are converted into numerical representations for model processing. Attention: a mechanism that allows the model to weigh the importance of different tokens relative to each other, enabling context-aware understanding of text. Probabilistic language modeling: the process by which a model estimates the probability of the next token in a sequence based on the preceding context (51)

4. AI in Decision Support

4.1. Clinical decision-support systems

Clinical decision-support systems (CDSS) are digital tools designed to provide clinicians with timely, filtered, and context-specific clinical information that supports diagnostic and therapeutic decision-making. This function has been repeatedly emphasized in dermatology-

focused CDSS evaluations, where such systems improve decision-making efficiency and streamline information retrieval. Products such as “Dermatoclic®” or “VisualDx ®” exemplify this model by offering structured differential diagnoses, photographic comparisons across skin types, and evidence-based management suggestions, further enhancing clinical workflow efficiency [50].

Evidence shows that dermatology-focused CDSS improve practice by offering quick access to recommendations, visual resources across all phototypes, confidence-building support, and shorter consultations, thereby enhancing usability and physician satisfaction [50]. Furthermore, CDSS use can significantly increase diagnostic accuracy; for instance, one feasibility study demonstrated a 34% relative improvement in diagnostic correctness when general practitioners used a visual dermatology CDSS instead of standard consultations [51].

ML-driven systems further extend these capabilities. Large-scale evaluations show that AI-enabled mobile applications, such as the “mHealth” app can accurately support diagnosis across a broad spectrum of dermatological diseases, including in patients with skin of color, demonstrating feasibility for point-of-care decision support and reducing disparities in access to dermatologic expertise. These mobile decision-support tools have proven to be feasible and effective in real-world clinical workflows, reinforcing their value for early triage and detection [52]. Another specialized melanoma CDSS platform integrates clinical, dermoscopic, and molecular data to assist with diagnosis, prognosis, and risk stratification, providing predicted diagnoses, survival estimations, and biomarker-based prognostic insights in an intuitive format [53].

4.2. AI-based risk prediction and early decision support

AI has become a key enabler of early diagnostic support in dermatology, particularly through DL systems capable of classifying skin lesions with high accuracy and supporting early recognition of malignancy. Evidence from a systematic review shows that ML performs exceptionally well in early melanoma detection, with many AI systems reaching AUC values above 90% in binary melanoma classification tasks and often matching or surpassing dermatologists in controlled evaluations [54].

Beyond malignancy detection, AI-based systems support early recognition of inflammatory and infectious conditions such as psoriasis, eczema, acne, or viral, bacterial, fungal, and parasitic skin infections, identifying subtle morphological cues that may be missed by non-specialists, thereby expanding early diagnostic support across a wider clinical spectrum [55].

AI-driven prognostic models further enhance early decision support by integrating demographic, serological, histopathological, and molecular data to estimate individualized probabilities of metastasis, recurrence, or survival. José Luis Díaz-Ramón *et al*. assessed a melanoma-specific CDSS that combines dermoscopic imaging with biomarker-based prognostic modules to generate personalized estimates of survival and recurrence risk, thereby assisting clinicians in the earliest stages of care planning [53]. Emerging evidence also suggests that AI can be utilized to predict treatment failure or suboptimal response, enabling clinicians to adjust therapies earlier in the management of chronic dermatologic diseases [56].

Some of these systems additionally support early decision-making by offering basic urgency assessments and clear explanations of symptom severity, which may encourage more timely care-seeking [57].

4.3. Treatment selection and optimization

AI integrates a variety of data types, including clinical features, imaging data, biomarker profiles, and assessments of disease severity, which aids clinicians in guiding the most appropriate interventions for their patients [58]. Research highlights that the integration of AI into clinical decision-making processes can refine treatment pathways, such as determining optimal follow-up intensities post-surgery [59, 60]. These tools align clinical assessments with established treatment guidelines, allowing for more precise therapy escalation or de-escalation. As such, AI contributes to a more systematic approach in managing chronic skin conditions, which often require nuanced treatment strategies [61].

Moreover, AI approaches are being developed to predict treatment responses, allowing clinicians to estimate which therapies, such as immunotherapy or combination regimens, are most likely to benefit patients [62, 63]. This novel capability reduces reliance on trial-and-error methods of prescribing, minimizing patient exposure to ineffective treatments while enhancing the likelihood of positive outcomes [64].

While many of these AI applications remain in early evaluation stages and necessitate further external validation to establish their efficacy and reliability in clinical settings, existing studies underscore the substantial potential of AI to refine therapeutic decision-making processes, improve patient outcomes, and enhance resource utilization in dermatological care [60, 65]. Continuous advancements in AI technologies promise to further integrate these systems into everyday clinical practice, making them indispensable tools for dermatologists [66].

4.4. Drug-drug and drug-disease interaction detection

AI has become an integral component of modern medication safety, particularly in detecting drug-drug (DDI) and drug-disease interactions. AI technologies leverage extensive pharmacological data, electronic health records (EHRs), molecular structures, and knowledge graphs to identify clinically meaningful and precise interactions [67].

Luo *et al*. described the KEDD framework, a multimodal system that integrates molecular structures, structured pharmacological knowledge graphs, and unstructured biomedical text to generate mechanistically informed and context-aware DDI predictions. This approach achieves state-of-the-art performance and provides clinically meaningful outputs that extend far beyond the capacity of rule-based systems. By capturing complex pharmacological relationships, AI holds significant promise for improving medication safety and reducing avoidable adverse events [67].

AI-driven models employ ML and DL architectures to identify clinically relevant DDIs, including previously unrecognized or rare interactions that traditional rule-based systems often fail to detect. Rohani and Eslahchi demonstrated that topological neural network models can uncover novel DDIs with higher predictive performance than earlier computational approaches, highlighting AI's capacity to detect subtle pharmacological relationships not evident from structured drug databases [68].

Advanced graph-based and molecular feature-driven systems further enhance this capability. Luo *et al*. demonstrated that AI models integrating EHRs, molecular structure embeddings, and knowledge-graph representations can generate clinically meaningful and highly precise interaction predictions, supporting safer prescribing workflows [67]. Moreover, studies on

clinician attitudes indicate that dermatologists expect AI to play an auxiliary but important role in improving treatment safety and reducing decision-making errors [69].

Integrating AI-derived interaction detection into CDSS has been proposed as a mechanism to enhance prescribing safety, reduce contraindicated drug combinations, and promote more consistent, evidence-based therapeutic decisions. Omiye *et al*. emphasize that AI systems are well-positioned to standardize medication-related decision processes and minimize preventable errors in dermatologic care [60].

Despite the promising potential of AI in this area, it is essential to remain cognizant of the current challenges, including the need for extensive external validation and integration into existing healthcare infrastructures [70]. Continued research is vital to quantify AI's effectiveness in improving clinical outcomes while ensuring these systems are adequately trained using diverse datasets to enhance reliability and applicability in real-world settings (10). As the adoption of AI in medication safety grows, the emphasis on education and training for healthcare professionals must also increase to leverage these advancements effectively [71].

4.5. AI-driven clinical guidelines and recommendation systems

Traditional methods for consulting clinical guidelines can be time-consuming and inconsistent, particularly in fast-paced clinical environments. AI-driven platforms enhance this process by integrating real-time patient data, including demographics, disease severity, comorbidities, laboratory results, and imaging findings, to generate personalized recommendations in line with best medical practices [72].

Natural Language Processing is essential in allowing AI systems to automatically extract and update guideline content, ensuring that new evidence is swiftly incorporated into clinical workflows [73]. In dermatology, these AI-enabled systems standardize treatment pathways for various conditions such as psoriasis, AD, and melanoma, while also adjusting recommendations based on the individual risk profiles and predicted treatment responses of patients [74]. This approach can lead to integrated decision pathways that support clinicians throughout patient care, from diagnosis to long-term management [26].

Although many AI-driven clinical guideline systems are still in early development stages, they represent a significant advancement toward achieving consistent, efficient, and personalized dermatologic care. As these technologies continue to evolve, their integration into clinical practice is expected to enhance decision-making processes, improve treatment outcomes, and ultimately elevate the quality of patient care in dermatology [75].

5. AI in personalized treatments for skin diseases

5.1. Predicting treatment response and therapy optimization

Beyond clinical decision support, AI also enables increasingly tailored therapeutic strategies. Tang *et al*. outlined a conceptual framework that describes how AI can implement precision medicine in inflammatory skin diseases. Their approach emphasized biological interpretation and the discovery of clinically meaningful subgroups. Using unsupervised learning methods, such as clustering and dimensionality reduction, they demonstrated how AI could uncover previously unrecognized endotypes reflecting molecular pathways, immune activation patterns, or barrier dysfunction signatures. These endotypes, in turn, formed the basis for identifying therapeutic phenotypes, defined as patient subsets with distinct response trajectories to systemic agents, biologics, or small-molecule treatments. By incorporating serial imaging, dynamic symptom monitoring, and time-resolved omics data, AI was shown to map transitions between disease states, predict flares, and adapt therapeutic strategies accordingly [76].

Poweleit *et al*. reviewed how ML enhanced therapeutic drug monitoring and model-informed precision dosing. They demonstrated that, while pharmacometrics had long supported individualized dosing, AI enabled the handling of high-dimensional, multimodal clinical data from EHRs, wearables, and laboratory measurements. Machine-learning models, such as "XGBoost," outperformed Bayesian approaches in drug exposure prediction with fewer sampling points, while decision-tree and random-forest models supported individualized dose optimization with performance comparable to expert dosing [77].

Schaffer *et al*. demonstrated how automated ML (AutoML) could enhance personalized care in dermatology by applying it to real-world data from 309 patients with psoriasis vulgaris or psoriatic arthritis to predict the need for therapy changes at 24 weeks. Hundreds of models were trained, with the best one achieving an AUC of 0.91. This indicated that the AutoML-selected model reliably distinguished between patients who later required therapy modification and those who did not, enabling the earlier identification of underlying treatment failure. The model identified several key predictors of therapy change, including initial systemic therapy, baseline CASPAR score, and longitudinal changes in quality of life. Additional analyses further illustrated how different therapies varied in their likelihood of switching, with methotrexate and certain biologics associated with lower probabilities of change, whereas infliximab combined with methotrexate was more frequently switched. Beyond predicting therapy switches, the authors also applied AutoML to model additional clinically relevant outcomes, including changes in the PASI score over 24 weeks and baseline Bath Ankylosing Spondylitis Disease Activity Index (BASDAI) score. For PASI change, a blended model achieved an AUC of 0.92, accurately differentiating patients likely to show significant clinical improvement from those who were not [78].

5.2. AI-enabled disease monitoring and patient follow-up

AI can further support personalized treatment by enhancing patient follow-up and enabling more precise monitoring of changes in disease severity, thereby allowing treatment strategies to be adjusted accordingly. In their study, Wongvibulsin *et al*. outlined how digital health technologies, such as mobile applications, teledermatology platforms, and wearable sensors, could serve as patient-generated data sources that enabled personalized dermatologic care. Through mobile health tools, professionals were able to capture both objective clinical signs

and patient-reported factors, helping to recognize disease fluctuations that were often missed during periodic clinical visits. AI algorithms were described as being able to interpret temporal patterns in symptoms, detect changes in disease activity, monitor treatment adherence, and identify lifestyle or behavioral factors that influenced treatment response [79].

Building on the previous article, the subsequent research provided continuation by examining not only diagnosis but also the assessment of disease severity. The study focused on how effectively AI models could grade the severity of various inflammatory skin diseases using clinical images. Cai ZR *et al*. reviewed studies published between 2017 and 2023, ultimately analyzing 45 studies comprehensively and including 19 of them in a meta-analysis. Their pooled results showed that AI models achieved an average sensitivity of 80.5% and a specificity of 96.2% in severity assessment. Performance varied across conditions; for example, AI reached a sensitivity of 91.8% in AD and approximately 80.7% in acne. These findings highlighted that AI systems were approaching dermatologist-level accuracy in severity grading, which was essential for enabling personalized treatments [80].

Another important application is psoriasis, in which disease severity assessment is often subjective and time-consuming. Breslavets *et al*. compared an automated AI system with dermatologists in assessing the body surface area (BSA) affected by psoriasis, using a ground-truth reference defined by consensus among expert dermatologists. They analyzed 35 anonymized full-body photographs of psoriasis patients, dividing the body into anatomical segments. The system's output showed stronger similarities with the verified data (e.g. high Pearson and Spearman correlation), and demonstrated fewer errors compared to the dermatologists' assessments [81]. In another study, Huang *et al*. developed a DL system to estimate PASI scores using 14,096 images from 2,367 patients with psoriasis. The model outperformed the mean performance of 43 experienced dermatologists, achieving a 33.2% improvement in overall PASI score accuracy [82].

6. Challenges of AI

Despite substantial progress, several challenges must be addressed before AI can be broadly and safely integrated into dermatologic practice.
Algorithmic bias remains one of the most critical limitations of current AI systems. Many dermatologic models are trained on datasets that inadequately represent diverse skin phototypes, age groups, and clinical settings, leading to reduced generalizability and the risk of perpetuating health disparities [83].

A further challenge concerns the clinical evaluation of AI systems. Dermatologic diagnosis is inherently multimodal, relying on patient history, symptom progression, physical examination, and contextual clinical judgement in addition to visual assessment. However, many studies evaluating CNNs rely on artificial experimental settings, such as isolated image classification tasks. Under these conditions, clinician performance may be systematically underestimated, as physicians are deprived of the contextual information fundamental to real-world decision-making [19]. Moreover, many AI systems lack prospective, real-world validation across diverse clinical workflows, raising concerns regarding performance drift, dataset shift, and robustness outside controlled research environments [84].

Interpretability and transparency are also central to clinical acceptance. While DL models can achieve high diagnostic accuracy, their opaque decision-making processes limit clinician confidence and complicate accountability. One solution is the use of explainable AI models [85].

Closely related to this issue are regulatory and legal challenges, as existing approval frameworks have not yet been fully adapted to continuously learning AI systems, and the responsibility for AI-assisted clinical decisions remains insufficiently defined [86].

Successful implementation further depends on patient trust and acceptance. In a scoping review, Sally *et al*. emphasized that patients are key stakeholders in the uptake of AI in health care and highlighted the importance of incorporating patient expectations into AI development in order to fully realize the potential benefits of AI systems [87].

7. Conclusion

This review provided a comprehensive synthesis of how AI is reshaping dermatology across the continuum from drug discovery to personalized clinical care. We demonstrated that AI is being actively researched and, in certain settings, is already being applied in drug discovery, diagnosis, and decision support, contributing to more personalized treatment approaches. Although there are still many remaining challenges and AI is not replacing dermatologists, it is gradually reshaping therapeutic workflows and supporting a shift toward more efficient, data-driven care, in which AI and dermatologists work together.

Abbreviations:

AD, atopic dermatitis; ADMET, absorption, distribution, metabolism, excretion, and toxicity; AI, artificial intelligence; AUC, area under curve; BASDAI, Bath Ankylosing Spondylitis Disease Activity Index; BCC, basal cell carcinoma; CDSS, clinical decision-support systems; CNN, convolutional neural network; DG-HFUS, dermoscopy-guided high-frequency ultrasound; DDI, drug-drug interaction; DL, deep learning; EHR, electronic health record; ESKAPEE, Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa, and Enterobacter spp., Escherichia coli; FAERS, FDA Adverse Event Reporting System; MIC, minimal inhibitory concentration; ML, machine learning; LC-OCT, line-field confocal optical coherence tomography; PASI, Psoriasis Area Severity Index; RCM, reflectance confocal microscopy; TBP, Total body photography; TIP, tyrosinase-inhibitory peptide

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CRediT roles

István Szondy - conceptualization, methodology, investigation, data curation, writing - original draft, visualization; Katalin Martyin - investigation, data curation, writing - review & editing; Gabriella Mohos - investigation, data curation, writing - review & editing; Tara Kiss - investigation, data curation, writing - review & editing; Katalin Szabó - investigation, data curation, writing - review & editing; András Bánvölgyi - conceptualization, investigation, data curation, writing - review & editing, Mehdi Boostani - writing - review & editing, supervision; Mohamad Goldust - writing - review & editing, supervision; Andrzej Grzybowsk - writing - review & editing, supervision; Norbert Kiss - conceptualization, methodology, writing - original draft, visualization, supervision, project administration

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: