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Application of AI in the Design of Novel Peptide-based Ingredients for Skincare Products

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Abstract: This review provides a systematic review of the current applications and developmental trends of artificial intelligence (AI) in the design of novel peptide-based cosmetic ingredients. With rapid advancements in computational biology and artificial intelligence algorithms, the development paradigm for peptide-based skincare products is undergoing a revolutionary shift—from traditional trial-and-error screening to intelligent, precision-driven design. By leveraging machine learning algorithms, deep learning models, and molecular simulation techniques, artificial intelligence has significantly enhanced the efficiency and success rate of peptide ingredient development while reducing associated costs. The review highlights breakthroughs in artificial intelligence applications for peptide molecular design, stability optimization, transdermal delivery prediction, and efficacy evaluation. It also explores the integration of artificial intelligence with interdisciplinary fields such as synthetic biology and nanotechnology, and offers insights into current challenges and future development directions.

Keywords: Artificial intelligence; Peptides; Skincare

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1. Introduction

Peptide compounds, known for their high activity, strong specificity, and excellent safety profile, have become a key focus in the development of anti-aging skincare ingredients. Traditional peptide development has largely relied on trial-and-error screening, a process that is time-consuming, costly, and inefficient—typically taking 3 to 5 years to bring a new peptide ingredient to market. With the rapid advancement of computational biology and artificial intelligence (AI), the development of peptide ingredients has entered a new era of digitalization and intelligence. By leveraging machine learning algorithms, molecular simulations, and big data analytics, researchers can now rapidly predict the relationship between peptide structures and their biological activities, enabling the precise design of active peptides that target key pathways involved in skin aging [1].

2. Core technologies of AI-assisted peptide design

The application of AI technology in peptide design primarily relies on machine learning, molecular docking, and big data analysis. Machine learning builds predictive models by analyzing vast datasets of known peptides, including their sequences, structures, and biological activities. Commonly used algorithms include convolutional neural networks (CNN), recurrent neural networks (RNN), and generative adversarial networks (GAN). Molecular docking simulates, through computational methods, the interactions between peptides and target proteins—such as collagen, elastin, or inflammatory factors—to predict binding affinity and biological activity. Big data analysis involves advanced tools and techniques to process and interpret large-scale datasets, enabling the design and optimization of peptide structures. For instance, Dong et al. leveraged AI-assisted design to develop an antimicrobial peptide that demonstrated potent and selective inhibition against *Cutibacterium acnes*, achieving a minimum inhibitory concentration (MIC) of 2–4 μg/mL. These designed peptides show strong potential as promising candidates for acne treatment [2].

3. Application of AI in the development of peptide-based ingredients for skincare products

3.1. Target discovery and molecular design

AI technology can analyze vast biomedical databases to identify key targets and pathways involved in skin aging, enabling the design of targeted peptide molecules. WIS's R&D team has integrated AI-driven design with automated synthesis platforms to establish a triad system for cyclic peptide discovery—virtual screening, intelligent synthesis, and activity validation. By leveraging machine learning algorithms to simulate tens of thousands of peptide folding pathways, this system dramatically enhances the efficiency of candidate molecule selection. The Aging Science Innovation Research Center at Zhejiang Tsinghua Yangtze River Delta Research Institute utilized a computational biology platform to uncover HMGB1, a critical target in inflammatory aging, and subsequently designed cIY-8, a cyclic peptide that specifically targets inflammatory aging—the first such cyclic peptide molecule to directly address this aging mechanism [3].

3.2. Stability optimization

Peptide stability is a critical factor limiting its efficacy in practical applications. By leveraging molecular modifications and structural optimization, AI-driven approaches have effectively addressed these challenges. Cyclic peptides, with their closed-loop molecular architecture, offer enhanced stability in theory. Utilizing ADCP docking technology combined with the ADFR suite, Yang et al. identified a series of novel cyclic peptides targeting JAK1, Keap1, and TGF-β proteins. Among them, MKC1 demonstrated the most promising anti-aging activity. At a concentration of just 0.001%, MKC1 achieved a 20% reactive oxygen species (ROS) clearance rate and significantly upregulated the expression of type I collagen and elastin genes [4].

3.3. Optimization of transdermal delivery

AI enables the prediction and design of peptide molecules with enhanced skin barrier penetration through high-throughput screening, molecular simulation, and bioinformatics analysis. Furthermore, AI can simulate the distribution and transport behavior of peptides within the skin, guiding researchers in refining key physicochemical properties—such as solubility, permeability, and stability—to improve transdermal efficiency and bioavailability. For instance, Shandong Jitai Peptide Biotechnology Co., Ltd. has developed dendritic spherical peptides using an

AI-powered computational biology platform. These peptides feature a three-dimensional "tree-like" or protein-mimicking globular structure, designed to strengthen affinity with the skin's stratum corneum and significantly enhance skin penetration.

3.4. Formulation design and synergistic efficacy

AI technology is not only applied in the design of individual peptide ingredients but also plays a pivotal role in developing peptide combinations. By analyzing synergistic interactions among different peptides, AI enables optimization of formulation ratios to maximize efficacy. Studies have shown that the combination of acetyl dipeptide-1 cetyl ester, acetyl tetrapeptide-2, and Pseudoalteromonas ferment extract significantly enhances the mRNA expression of Col-I, LOXL-1, Elastin, Fibrillin-1, Fibulin-5, and TGF-β in HFF-1 cells, demonstrating strong anti-aging activity through synergistic effects [5].

4. Challenges and limitations

Although AI technology shows great promise in the design of peptide-based cosmetic ingredients, it still faces several challenges. Training AI models requires large volumes of high-quality, standardized data. However, the cosmetics industry currently lacks a unified standard for peptide activity data, and differences in testing methods and reporting practices across laboratories can compromise the accuracy and reliability of AI models. Many deep learning models function like "black boxes"—while their predictions may be accurate, they often fail to provide biologically meaningful explanations, making it difficult for researchers to fully trust AI-generated designs. This limits the broader application of AI in peptide development. Although AI can significantly shorten the initial design phase, experimental validation of peptide candidates still demands extensive in vitro and in vivo testing, which remains time-consuming and costly. Moreover, novel peptide ingredients designed by AI may encounter regulatory hurdles, especially when their mechanisms of action differ substantially from traditional ingredients, necessitating the establishment of new safety and efficacy evaluation criteria. Skin aging involves multiple signaling pathways and molecular targets, and peptides may exert effects through diverse mechanisms. This complexity makes it challenging for AI models to fully capture all relevant biological factors [6].

5. Future development directions

With continuous technological advancements, the application of AI in the design of peptide-based skincare ingredients is evolving toward the integration of multi-omics technologies, automation, high-throughput processing, personalized customization, sustainability, and cross-disciplinary technological convergence. By integrating multi-omics data—such as genomics, proteomics, and metabolomics—more comprehensive biological models of skin aging can be constructed, providing AI with a richer and more robust data foundation. When combined with automated synthesis and high-throughput screening, AI-driven design enables a closed-loop development system. Leveraging individual skin characteristics, gene expression profiles, and environmental factors, AI can tailor personalized peptide formulations. Deep integration of AI with cutting-edge fields like synthetic biology and genetic engineering will drive cosmetic ingredient innovation from single-function solutions into an era of "precision customization." Furthermore, AI can help design greener, more sustainable peptide production processes, minimizing chemical usage and energy consumption, aligning with the beauty industry's growing emphasis on environmental responsibility [7].

6. Summary and prospect

The application of AI in the design of novel peptide-based cosmetic ingredients is fundamentally transforming the research paradigm and accelerating innovation within the beauty industry. By leveraging machine learning algorithms, molecular simulations, and big data analytics, AI enables the efficient development of peptide molecules with high bioactivity, stability, and skin permeability—significantly shortening development timelines and reducing costs. Several AI-designed anti-aging peptides have already been commercialized, including dendritic sphere peptides, recombinant humanized type V collagen, and cyclic decapeptides, which demonstrate remarkable efficacy in targeted anti-aging, emotional skincare, hydration, and skin barrier repair. Nevertheless, challenges remain in data quality, algorithm interpretability, and the complex mechanisms underlying peptide functionality. Looking ahead, as multi-omics integration, automated experimental platforms, and personalized formulation strategies continue to advance, AI will play an increasingly pivotal role in cosmetic peptide development. Meanwhile, the industry must establish unified data standards, validation protocols, and regulatory frameworks to ensure the safety, effectiveness, and reliability of AI-designed ingredients. The deep integration of AI with cosmetic raw material development will drive the industry's evolution from "manufacturing" to "intelligent creation", delivering more effective, precise, and safer anti-aging solutions to consumers.

Disclosure statement

The authors declare no conflict of interest.

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