IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

A Review Article On Ai Assisted Formulation Design In Cosmetic And Nutraceutical Industries

[1]Nusratfatema K. Shaikh, [2]Prof. Varsharani R. Avhad, [3]Arya A. Shaligram, [4]Shravan K. Yadav, [5]Aarati B. Shinde

[1, 3, 4,5]Students, [2]Professor

Department Of Pharmaceutics

Arihant College of Pharmacy, Ahilyanagar, India-414005

ABSTRACT:

Artificial Intelligence (AI) has revolutionized traditional formulation design procedures in the cosmetic and nutraceutical industries, allowing for more rapid and precise and economical product creation. Formulation research used to rely on trial-and-error experimentation, which required a lot of time and resources. Scientists can now examine large datasets, find the best ingredient combinations, and forecast the physical, chemical, and biological performance of formulations thanks to artificial intelligence (AI) and sophisticated computer models like machine learning (ML) and deep learning (DL). By examining consumer data, skin type, environmental factors, and ingredient interactions, artificial intelligence (AI) helps create customized skincare, hair care, and makeup solutions. Customized solutions with enhanced safety and efficacy characteristics result from this. Similar to this, AI is employed in the nutraceutical industry to create functional foods and supplements that target particular medical conditions by forecasting the stability, bioavailability, and synergistic effects of active ingredients. Furthermore, AI-powered simulation and predictive analytics solutions promote regulatory compliance; improve product stability, and lower formulation failures. Formulators can speed up innovation and sustainability objectives by combining cheminformatics, digital twins, and virtual screening. Notwithstanding its many benefits, issues including data quality, standardization, and ethical concerns persist. All things considered, AI-assisted formulation design is a paradigm shift toward intelligent, customized, and science-driven innovation in the nutraceutical and cosmetic industries, opening the door for the next generation of clever, customer-focused goods. In line with sustainability and green chemistry objectives, the use of AI-enabled digital twins, virtual formulation labs, and in silico simulations dramatically lowers formulation failures and lessens the need for physical trials. AI also helps with supply-chain optimization, real-time shelf-life prediction, regulatory paperwork, and quality-by-design (QbD) frameworks. Innovation and discovery are further accelerated by emerging technologies as autonomous robotic formulation systems, generative AI, and omics-driven data modeling. Not with standing these developments, problems still exist, such as inconsistent data quality, a dearth of standardized datasets, a lack of legal rules for AI-based formulation, and ethical issues with data privacy. All things considered, AI-assisted formulation design is a revolutionary step toward intelligent, customized, and sustainable innovation in nutraceuticals and cosmetics, setting a new standard for consumer-focused product development and precision formulation research.

KEYWORDS: Artificial intelligence, cosmetic, nutraceuticals, data collection, Ai-formulation

INTRODUCTION:

Healthcare, medicines, cosmetics, and nutraceuticals are just a few of the scientific fields where artificial intelligence (AI) has become a game-changing technology in recent years. AI is being used more and more to improve product design, formulation development, safety evaluation, and personalization in the nutraceutical and cosmetic industries, which are undergoing a digital revolution. Researchers are investigating AI-based methods for quicker and more precise formulation development in response to the increased consumer demand for safe, efficient, and tailored products. [1]

Formulation design has historically relied on empirical techniques and trial-and-error tests, which are frequently expensive, time-consuming, and labor-intensive. This method entails testing a variety of constituent combinations, assessing their chemical and physical stability, and then refining the finished product through several rounds.With data-driven modeling, predictive analytics, and machine learning algorithms that can realistically simulate and optimize formulations prior to laboratory testing, AI technologies now offer an effective substitute.AI helps create customized skincare and haircare products for the cosmetics business. To suggest appropriate formulations, machine learning models examine genetic data, lifestyle characteristics, and skin imaging data. For instance, AI can calculate the ideal concentration of active compounds for hydration or anti-aging, or it can forecast how specific ingredients will interact with a person's skin microbiota. Cosmetic companies are also using AI-powered virtual skin analysis technologies to provide tailored solutions based on real-time image analysis.AI is essential to the development of functional foods, dietary supplements, and herbal items with improved bioavailability, stability, and efficacy in the nutraceutical industry. AI can forecast ingredient compatibility, nutritional interactions, and their effects on human metabolism by examining massive biochemical and clinical datasets. Additionally, machine learning models aid in the discovery of new bioactive substances and the enhancement of delivery methods like liposomes, nanoparticles, or emulsions for better absorption.

AI-based formulation design involves several core technologies:

1. Machine Learning (ML): Predicts stability, viscosity, and texture properties of formulations.
2. Deep Learning (DL): Identifies complex patterns and nonlinear relationships between ingredients and outcomes.
3. Natural Language Processing (NLP): Extracts insights from scientific literature and consumer feedback.
4. Predictive Modeling and Simulation: Reduces experimental workload by predicting formulation outcomes.[2]

There are several benefits of incorporating AI into formulation design, such as decreased time and expense, increased product safety, better personalization, and sustainable development. By reducing material waste and anticipating toxicity and allergenicity prior to human trials, it promotes green chemistry and makes regulatory compliance easier.Full-scale adoption is still hampered by issues including the scarcity of standardized datasets, high processing costs, and the requirement for multidisciplinary knowledge. Despite these obstacles, AI is nevertheless transforming formulation science and propelling the creation of next-generation, evidence-based, environmentally friendly, and customized cosmetic and nutraceutical products.[1]

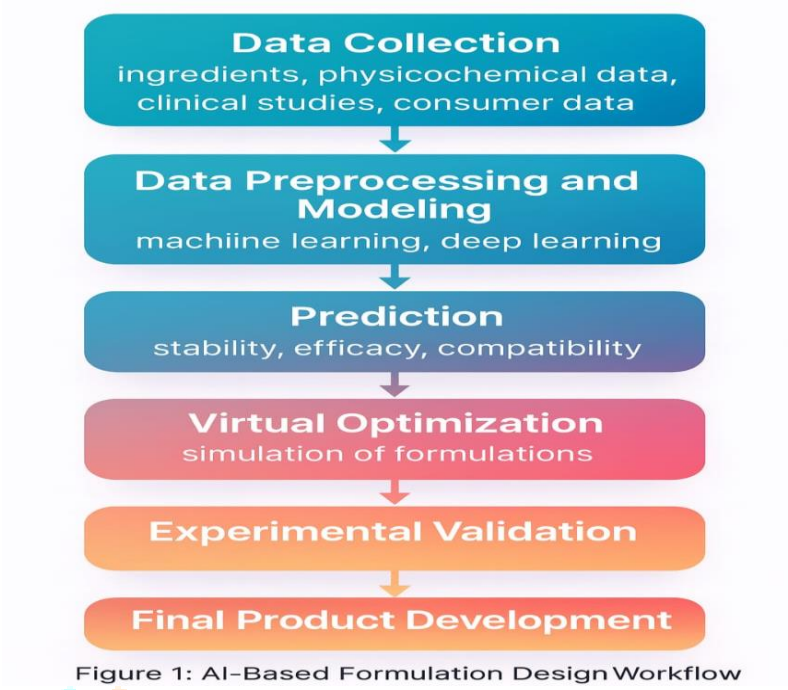


Figure 1: AI-Based Formulation Design Workflow

ROLE OF AI IN COSMETICS:

In the cosmetics sector, artificial intelligence (AI) has emerged as a game-changing technology that is changing how products are created, tested, customized, and marketed. AI facilitates quicker formulation development, improved product performance, increased safety assurance, and customized customer experiences by fusing data-driven modeling, machine learning algorithms, computer vision, and sophisticated analytics. The current role of AI throughout the lifecycle of cosmetic products is explained in depth in the note that follows.

1. **Ai in cosmetic formulation design :**

- Ingredient compatability and stability prediction:

AI models examine an ingredient's chemical structure, log P, HLB values, and functional characteristics to forecast:

- Probability of phase separation
- Stability of emulsions
- Changes in viscosity
- Degradation mechanisms and shelf life

Machine learning methods reduce laboratory trial-and-error by quickly screening thousands of constituent combinations.[3]

2. **Texture, rheology, and sensory prediction:**

Creams, lotions, gels, and foundations are examples of cosmetic products that rely significantly on sensory characteristics such as:

- Spreadability
- Stickiness
- Greasiness
- Time of absorption
- Smoothness

AI models that have been trained using rheology data and assessments from sensory panels can:Estimate the sensory experience based on the composition of the formulationMake suggestions for changes to oils, emulsifiers, or polymersHelp create items that are in line with consumer preferencesThe number of physical sensory trials required is greatly decreased as a result.Machine learning methods reduce laboratory trial-and-error by quickly screening thousands of constituent combinations.[3]

Ai in cosmetic product personalization

- Ai powered skin analysis

Using computer vision, deep learning models analyze:

i. Skin tone
ii. Pores size
iii. Acne
iv. Wrinkles
v. Hyperpigmentation
vi. Redness and texture

Smart mirrors and apps (like L'Oréal and Olay Skin Advisor) scan the skin and offer tailored suggestions for:

1. Moisturizers
2. Serums
3. Cleaners
4. Sunscreen
5. Products that prevent aging

- Personalized formulation development

AI is used by some businesses to create unique formulas based on:

1. Type of skin
2. Environmental elements (UV index, humidity)
3. Skin issues
4. Diet and way of life

This signifies a significant change from mass manufacturing to customized beauty.[3]

3. Ai in cosmetic safety and assessment

In traditional toxicology, testing is expensive, time-consuming, and frequently involves animal experiments. AI helps with in silico toxicity by forecasting:

- inflammation of the skin
- Allergenicity
- Phototoxicity
- Potential for endocrine disruption
- Risk of cancer

Early detection of potentially hazardous compounds is aided by models like QSAR (Quantitative Structure–Activity Relationships).This is particularly crucial as animal testing for cosmetics is becoming restricted or outlawed in many nations.[4]

4. Ai in marketing, consumer insights and trend prediction

AI aids businesses in comprehending customer behavior by:

- Analytical prediction
- Social media sentiment analysis
- Forecasting beauty trends
- Prediction of product performance
- Businesses are able to quickly adjust to what customers desire, such as vegan products, clean beauty, or particular ingredients.[4]

5. Ai in manufacturing and quality control

5.1 Smart manufacturing

1. Automation powered by AI guarantees
2. Regular homogenization and mixing
3. Heat cycles that are optimized
4. Viscosity, pH, and texture monitoring in real time

5.2 Quality assurance

1. Defects in packaging
2. Product discoloration
3. Inconsistencies in texture
4. Contamination by foreign particles[4]

6. Ai in dermatology and cosmeceuticals

AI assists dermatologists and cosmetic chemists by:

6.1 Identifying skin diseases

6.2 Recommending cosmeceutical treatments

6.3 Tracking treatment progress

6.4 Predicting therapeutic outcomes

This bridges the gap between medical dermatology and cosmetic science. [4]

7. Ai-driven innovation in cosmetic product development

7.1 Generative Ai for new ingredients

1. Innovative emollients
2. Novel antioxidants
3. UV filters
4. Anti-aging peptides

7.2 Predicting product performance before manufacturing

1. Active compound penetration of the skin
2. SPF efficacy
3. Curves of moisturization
4. Anti-aging effectiveness

As a result, expenses are decreased and product development cycles are shortened. [3]

ROLE OF AI IN NUTRACEUTICALS:

The nutraceutical sector, which focuses on creating food-derived products that offer health advantages beyond basic nutrition, is fast changing due to artificial intelligence (AI). In the past, clinical trials and labor-intensive testing were used in nutraceutical research to assess the safety and effectiveness of formulations. Through sophisticated computational modeling, predictive analytics, and bioinformatics, AI now makes it possible to design nutraceuticals more quickly, data-driven, and precisely.

1. AI in bioactive compound discovery:

- Novel bioactive chemicals from natural sources, including plants, herbs, marine species, and microorganisms, can be identified with the aid of AI techniques.
- To forecast possible health advantages, machine learning (ML) and deep learning (DL) models examine chemical structures, biological pathways, and pharmacological data.
- Molecular docking simulations and AI-driven virtual screening eliminate the need for lengthy laboratory screening, saving money and time.
- For instance, AI can forecast a natural molecule's potential for anti-inflammatory or antioxidant properties prior to experimental confirmation. [5]

2. Formulation design and optimization:

- AI analyzes constituent compatibility, solubility, bioavailability, and stability to help build nutraceutical formulations.
- For maximal absorption and effectiveness, it can forecast the best ingredient ratios and delivery methods (such as liposomes, emulsions, and nanoparticles).
- In order to guarantee product stability and safety, predictive models assess shelf life, taste masking, and the interaction of active substances with excipients.
- This results in better therapeutic outcomes and quicker product development. [5]

3. Personalized nutrition:

- Personalized nutrition, or the creation of dietary supplements based on an individual's health profile, is one of the most significant uses of AI in nutraceuticals.
- AI creates customized dietary regimens by analyzing data from microbiome investigations, metabolomics, genetics, and lifestyle choices.
- AI algorithms use these insights to suggest particular nutraceutical formulations for the treatment of ailments like diabetes, obesity, heart disease, and vitamin deficiencies.
- For instance, based on gut microbiota analysis, AI systems can suggest vitamin or probiotic combinations.[5]

4. **Predictive analytics for efficacy and safety:**

- AI systems use data-driven models to forecast the pharmacokinetics, toxicity, and biological effects of nutraceutical components.
- By simulating metabolic processes and interactions between nutrients and biological systems, these instruments guarantee the safety of products.
- AI can also improve pharmacovigilance and regulatory compliance by identifying any adverse effects or contraindications prior to market release.[6]

5. **Quality control and manufacturing:**

- AI in manufacturing guarantees the quality, uniformity, and standardization of nutraceutical products.
- AI-driven sensors keep an eye on the quality of raw materials, identify contaminants, and maintain exact process conditions.
- Automation and predictive maintenance technologies boost productivity and lower production costs, encouraging sustainable manufacturing.[6]

6. **Market analysis and consumer insights:**

- AI uses market demands, consumer behavior, and health trends to inform product creation.
- To find popular substances or unmet health needs, Natural Language Processing (NLP) algorithms examine scientific publications, patents, and internet reviews.
- This makes it possible for businesses to create focused, scientifically supported nutraceutical products.[6]

INTEGRATION OF AI IN COSMECEUTICALS:

In cosmetic science, AI—especially machine learning—represents a paradigm-shifting approach that has the potential to completely change how goods are created, tested, customized, and governed. The wider ramifications of AI go much beyond technical optimization, even though early applications have mostly concentrated on predictive modeling for efficacy and safety. Practically speaking, AI greatly improves formulation processes' speed, cost-effectiveness, and reproducibility, in stark contrast to the "trial-and-error" approach.[8]

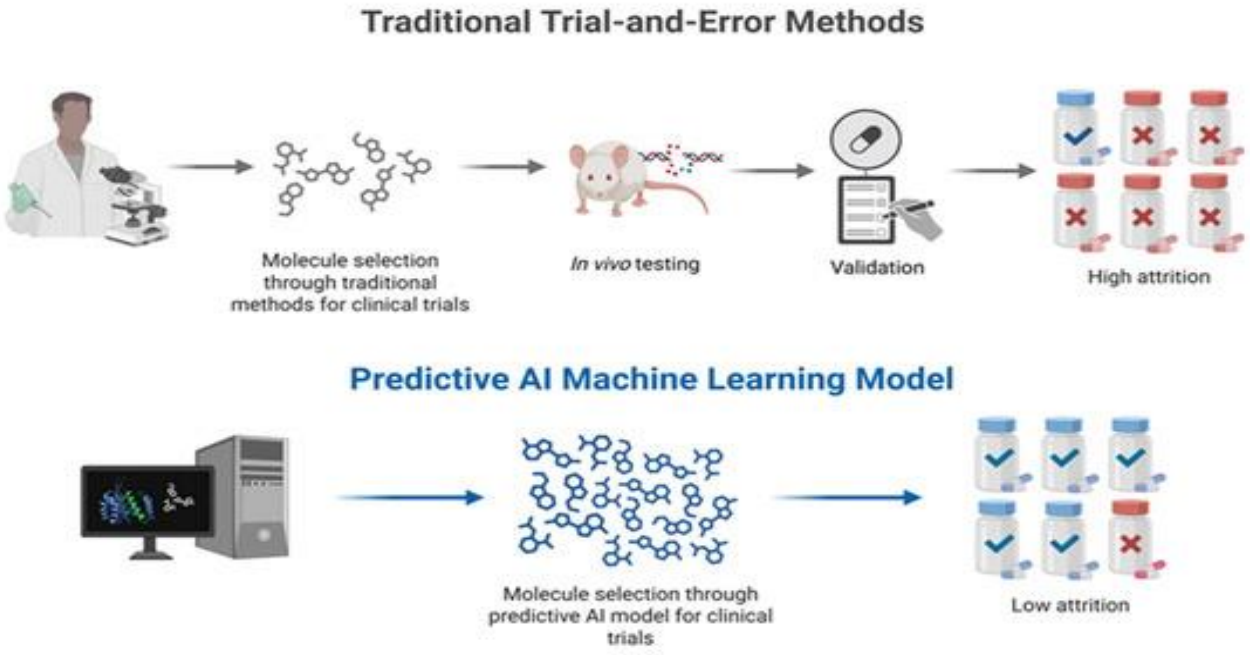


Figure 2: Predictive Ai machine learning model [9]

For example, deep learning techniques can forecast solubility and emulsification potential or identify synergistic combinations of active ingredients by analyzing complex datasets. This could reduce product development time and costs while simultaneously improving formulation precision and reproducibility. Furthermore, AI has the potential to revolutionize the evaluation of product tolerability, which is especially important for cosmetics meant for frequent or extended usage [10]. By enabling in silico screening of components and prediction of crucial formulation properties (such as solubility, stability, rheology, and texture), data-driven models lessen the need for iterative, trial-and-error trials. These techniques facilitate a "fail fast" strategy, which saves time and costs by eliminating less-than-ideal candidates early in the

pipeline.Additionally, AI can speed up the search for safer, more sustainable chemicals, helping to shift away from synthetic additives and contentious preservatives and toward more environmentally friendly substitutes like biomimetic peptides, biodegradable polymers, and low-impact surfactants. This is in line with the ideas of sustainable development and the growing demands of consumers for cosmetics made responsibly. [9]

Risk reduction and safety evaluation are two other important benefits of AI. Even though they are usually less severe than those seen in pharmaceutical settings, adverse responses can have a big impact on product viability and customer satisfaction. These days, skin irritation, allergic reactions, and photosensitivity can be accurately predicted using machine learning algorithms based on clinical or genetic data and post-marketing surveillance. In complete accordance with EU regulations, predictive toxicology models that have been trained on past datasets and verified against regulatory standards provide a workable substitute for animal testing. These technologies, when combined with developments in wearable biosensors and digital dermatology, also make it easier to monitor tolerability in real-time during post-marketing stages, allowing for transparent and repeatable safety assessments and encouraging adherence to data protection and ethical standards.[9]

Official indications on AI-driven predictive models in the cosmetological setting are still lacking, despite the fact that regulatory organizations (like the European Commission and the U.S. Food and Drug Administration) are already actively investigating the validation and standardization of in silico models in toxicology. The widespread use of AI technologies may be hampered by unclear regulatory procedures, especially when it comes to risk assessment and product claims. In order to establish best practices, guarantee algorithmic decision-making openness, and verify model performance across a range of demographics and use cases, cooperative projects including business, academia, and regulatory bodies are crucial. [9]

There are a lot of opportunities and obstacles associated with integrating artificial intelligence into the field of cosmetic science. On the one hand, AI presents revolutionary possibilities for the creation of customized formulas by predicting product performance, tolerability, and customer happiness with previously unheard-of accuracy. This technical capability enables skincare to be customized depending on factors including age, hormone state, lifestyle, ethnicity, and even microbiome makeup, in addition to skin type or personal concerns. The potential use of AI and ML in dermocosmetic product development for patients with skin conditions like psoriasis and atopic dermatitis that have a substantial clinical and psychological impact is also very important.[10]

However, it is important to consider the ethical and societal ramifications of AI. Proactive governance is required due to algorithmic biases and privacy issues. Strict aesthetic standards have long been promoted by the cosmetics business, which favors younger people and phototypes with lighter skin. AI has the potential to mimic and even magnify these biases if left unchecked. However, AI may also give an opportunity: developers may create more inclusive and equitable systems by putting measures like dataset diversity, algorithmic fairness techniques, and adherence to evolving regulatory frameworks into practice. Last but not least, the utilization of consumer data—often obtained via wearables, social media, and mobile apps—raises important concerns around consent, privacy, and openness.To guarantee that these technologies continue to be reliable and customer-focused, ethical stewardship in data governance is crucial. In order to guarantee that AI applications benefit a variety of people and promote just and transparent decision-making, it is imperative to address these issues.[10]

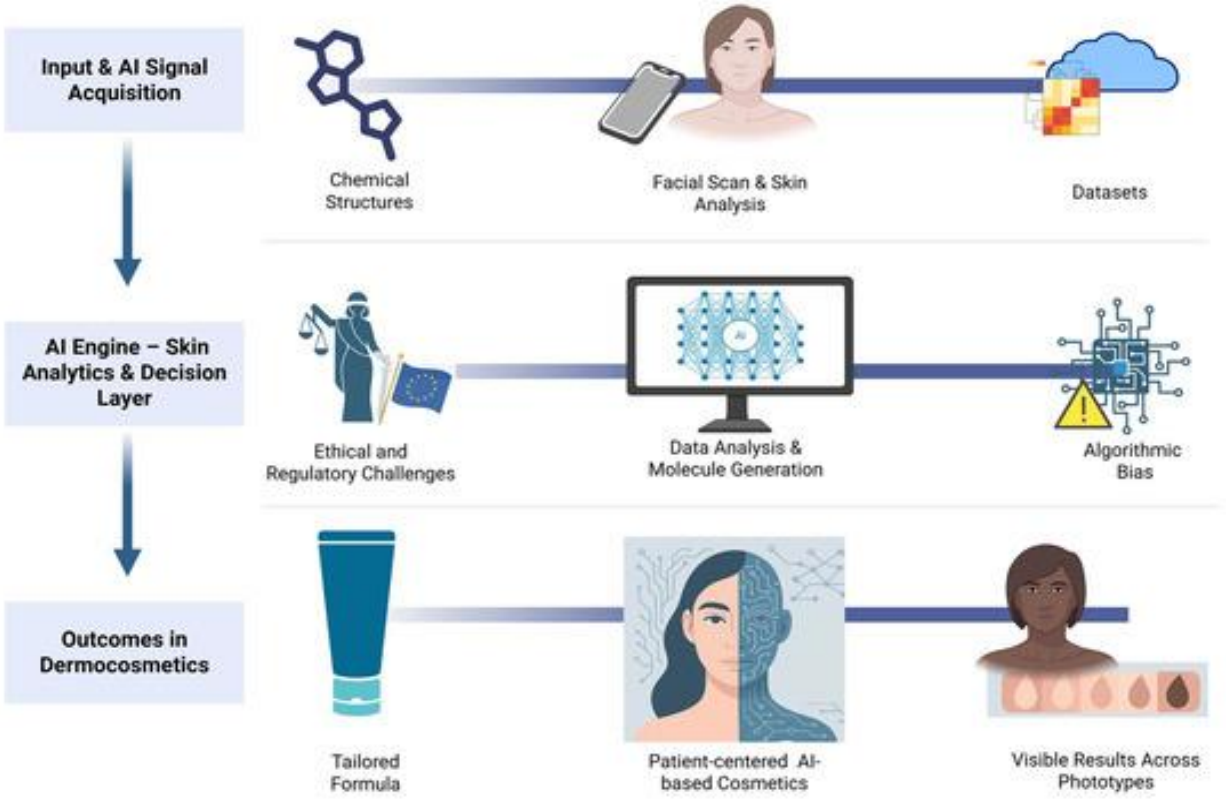
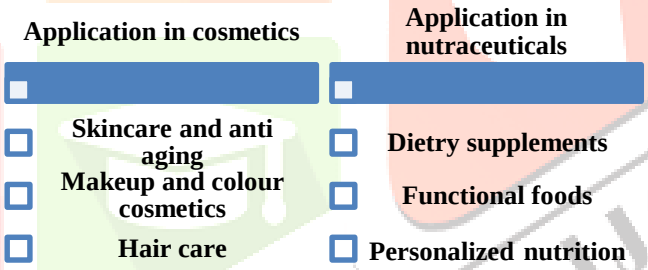


Figure 3: Schematic Representation of Ai driven model [10]

APPLICATIONS:



1. Application in cosmetics:

1.1 Skincare and anti aging:

AI predicts the anti-wrinkle efficacy of serums made with peptides and hyaluronic acid. For instance, by mimicking skin permeation, L'Oréal's AI platform has created goods like UV-protective lotions.

1.2 Makeup and colour cosmetics:

For longevity and shade matching, algorithms maximize pigment dispersion. AI is used by companies like Fenty Beauty to create inclusive shade ranges based on data on skin tones worldwide.

1.3 Hair care :

Shampoos that repair damage without sulfates are the result of predictive models that evaluate the stability of ingredients under heat or humidity.[7]

2.Application in nutraceuticals:

2.1 Dietrysuppliments:

AI creates vitamin blends to improve absorption; for example, it combines vitamin D with lipids to increase absorption. AI is used by DSM Nutritional Products to create omega-3 supplements that are more stable.

2.2 Functional food :

AI predicts fermentation results and optimizes probiotic strains for gut health in goods like enriched yogurts.

2.3 Personalized nutrition :

Websites like Habit employ user data analysis to suggest formulations, such metabolism-specific caffeine-free energy pills.[7]

CHALLENGES AND LIMITATION

Formulation science is changing as a result of artificial intelligence (AI), which makes personalization, virtual simulation, and predictive modeling possible. Nevertheless, despite tremendous advancements, a number of obstacles prevent AI from being fully integrated into the creation of cosmetic and nutraceutical formulations. Data quality, technology limitations, regulatory concerns, and industry readiness are the causes of these restrictions.

1. Limited and Non-Standardized Data Availability
2. Complexity of Biological and Chemical Interactions
3. High Cost of AI Infrastructure and Expertise
4. Limited Regulatory Frameworks for AI-Driven Formulations
5. Data Privacy and Ethical Concerns (Especially in Personalized Products)[11]
6. Difficulty in Interpreting AI Models
7. Lack of Integration Between AI Tools and Traditional R&D Workflows
8. Variability in Natural Ingredients (Nutraceuticals)
9. Limited Validation of AI Models
10. Risk of Over-Reliance on AI[12]

FUTURE PROSPECTIVE:

Over the next ten years, artificial intelligence is predicted to change how cosmetics and nutraceuticals are formulated. AI will be crucial to design, testing, and regulatory compliance as companies move toward personalization, sustainability, and quick innovation.

1. **Hyper- personalized products at scale:**

Personalized skincare and customized nutraceutical mixes (e.g., formulas adapted to skin phenotype, microbiota, diet, or vitamin demands) provided either as bespoke finished products or personalized recommendation engines will be made possible by AI + computer vision + consumer data. In its early stages, this is already commercial and will grow.

2. **Faster R and D and fewer experiments:**

By simulating texture, stability, solubility, and release profiles and reducing the number of physical tests required to attain a target formula, predictive models (ML and physics-informed models) will decrease cycle times and save costs. Draft formulations and experimental designs will also benefit from the use of Large Language Models (LLMs).

3. **In-silico safety and reduced animal testing :**

ML models for toxicity, irritation, and sensitization will enable early safety screening and help supplement or replace costly lab assays and animal testing, expediting safety evaluation and regulatory submission preparation.

4. **Generative formulation & optimization:**

Innovative constituent combinations and concentrations that satisfy multi-objective goals (efficacy, stability, cost, and green metrics) will be suggested by generative models. Competing constraints will be automatically traded off via optimization methods.

5. **Supply-chain and sustainability gains:**

AI can support customer desire for sustainable beauty and nutraceutical products by optimizing ingredient source, suggesting less harmful alternatives, and forecasting shelf life to cut waste.

6. **Integration with omics and clinical data for nutraceuticals:**

Evidence-based tailored nutrition formulations that target particular metabolic states or deficiencies will be made possible by combining genomes, metabolomics, microbiome, and lifestyle data with artificial intelligence.[13]

CONCLUSION:

In the nutraceutical and cosmetic industries, artificial intelligence (AI) is revolutionizing formulation science by replacing conventional trial-and-error techniques with data-driven, predictive, and incredibly effective methodologies. Formulators can optimize ingredient selection, improve stability, forecast safety, and more precisely develop high-performance goods by integrating machine learning, deep learning, predictive modeling, virtual screening, and digital twins. AI in cosmetics speeds up the development of customized skincare products, enhances rheological and sensory forecasts, lowers formulation errors, and promotes moral, non-animal safety testing. Similar to this, AI improves the discovery of bioactive compounds in nutraceuticals, forecasts bioavailability, facilitates customized nutrition, and fortifies quality assurance and legal compliance.Despite its transformative potential, AI-driven formulation faces challenges such as limited standardized datasets, model interpretability issues, regulatory ambiguities, and ethical concerns related to data privacy and algorithmic bias. Overcoming these limitations requires collaborative efforts between industry, academia, and regulatory agencies to establish clear guidelines, improve data governance, and ensure model transparency.All things considered, AI-assisted formulation design signifies a paradigm change toward sustainable, intelligent, and customized product development. The cosmetic and nutraceutical industries are about to enter a new era of innovation where goods are safer, more effective, environmentally conscious, and perfectly customized to individual needs thanks to the combination of cutting-edge computational techniques and scientific understanding. Consumer expectations will continue to be redefined by this progression, which will also establish new benchmarks for formulation research in the future.

REFERENCE:

1. Di Guardo, A., Trovato, F., Cantisani,C., Dattola,A., Niatico, SP., Pellacaini,G., and Paganelli,A. (2025) artificial intelligence in cosmetic formulation: predictive modeling for safety, tolerability, and regulatory perspective. Cosmetics, 12(4) 157
2. Franzol, A., Banin, T. M., Brazil, T. R., Rezende, M. C., & others (2025). Artificial Intelligence, Molecular Dynamics, and Beyond: Computational Insights in Cosmetics Research and Formulation Design. Wiley.
3. Wipro. (2025). AI in Cosmetics Drives New Standards in Beauty Innovation. Wipro Consumer Packaged Goods Insights.
4. Venkatesh, S., & Shankar, V. (2023). Applications of Artificial Intelligence, Machine Learning, and Deep Learning in Nutrition: A Systematic Review. Public Health Nutrition.
5. Bhupathyraaj, M., Vijaya Rani, K. R., &Essa, M. (Eds.) (2024).Artificial Intelligence in Pharmaceutical Sciences.CRC Press, pp. 1–460.
6. Ali, M., et al. (2021).AI-based Predictive Tools for Pharmaceutical and Nutraceutical Product Development.Computers in Biology and Medicine, 134, 104478, pp. 1–12.
7. Academic review: Rodrigues, T., et al. (2022). "AI in Formulation Design: A Review." Pharmaceutical Research, 39(10), 2345-2358. DOI: 10.1007/s11095-022-03345-6.
8. A review on artificial intelligence in cosmetic formulation: predictive modeling for safety, tolaribility, and regulatory perspective by Federica trovato and Carmen cantisani cosmetics 2025, 12(4), pg no 157.
9. Kenig, N.; Monton Echeverria, J.; Rubi, C. Ethics for AI in Plastic Surgery: Guidelines and Review. Aesthetic Plast. Surg. 2024, 48, 2204–2209. [Google Scholar] [CrossRef] [PubMed]
10. Yu, X.; Ong, K.G.; McGeehan, M.A. Skin Phototype Classification with Machine Learning Based on Broadband Optical Measurements. Sensors 2024, 24, 7397. [Google Scholar] [CrossRef] [PubMed]
11. Yucel, A., &Uysal, A. (2025). AI's Intelligence for Improving Food Safety: Only as Strong as the Data that Feeds It. Current Food Science & Technology Reports, 3, Article 15.
12. MDPI Authors. (2025). Artificial Intelligence (AI) in Pharmaceutical Formulation and Dosage Calculations. Pharmaceutics, 17(11), Article 1440.
13. Di Guardo, A. et al. (2025) — Artificial Intelligence in Cosmetic Formulation: Predictive Modeling for Safety, Tolerability, and Regulatory Perspectives — Cosmetics