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Review Article

A systematic structured review of artificial intelligence in essential oil study: Identification and classification

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Abstract

In recent years, the integration of Artificial Intelligence (AI) techniques into Essential Oil (EO) research has sparked significant interest, promising transformative advancements across various aspects of this field. However, a comprehensive, systematically structured synthesis of the existing literature on AI applications in EO studies remains limited. This systematic review addresses this gap by adhering to the Preferred Reporting Items for Systematic Reviews and Meta-Analysis (PRISMA) guidelines and employing advanced search methodologies using the Scopus and Web of Science (WoS) databases. The search strategy encompasses keywords related to AI, EOs, and their associated applications. Following predefined inclusion and exclusion criteria, relevant articles were screened, and data were extracted and synthesized. The synthesis is expected to provide insights into three overarching themes: (1) antimicrobial and antibiofilm activity of EOs, (2) classification and prediction of EO characteristics, and (3) identification and authentication of plant species. Notably, this study is a PRISMA-guided systematic review that comprehensively synthesizes AI and Machine Learning (ML) applications across identification, classification, and bioactivity-related domains in EO research. This addresses a gap that has not been systematically covered. Through the integration of AI techniques, studies within these themes are anticipated to demonstrate advancements in understanding the biological activities, chemical compositions, and botanical origins of EOs. In essence, this systematic review provides a comprehensive overview of the current state of AI utilization in EO research. It also identifies emerging trends, methodological advancements, and potential applications of AI in this field, paving the way for future investigations.

Keywords: artificial intelligence, essential oil, PRISMA, systematic review

Introduction

In recent years, the intersection of artificial intelligence (AI) and traditional scientific domains has led to unprecedented advancements, fostering innovative approaches and methodologies. One such field that has witnessed a paradigm shift is Essential Oil (EO) research [1, 2]. EOs, derived from plants, have long been recognized for their therapeutic properties and diverse applications [3, 4, 5]. The integration of AI into the study of EOs heralds a new era, promising deeper insights, enhanced efficiency, and accelerated discoveries [2, 6]. The conventional methods of EO analysis have often been time-consuming, resource-intensive, and limited in scope [4, 7, 8, 9]. The intricate composition of EOs, comprising a myriad of chemical compounds, poses challenges to researchers seeking to unlock their full potential. However, with the advent of AI, these challenges are met with a powerful toolset capable of deciphering complex patterns and relationships within vast datasets [10, 11].

One prominent application of AI in EO research is in the identification and classification of chemical constituents. Advanced machine learning (ML) algorithms can analyze the intricate composition of EOs, discerning subtle variations and identifying compounds that may have remained unnoticed using traditional methods [12, 13]. This expedites the analysis process and opens the door to the discovery

of novel bioactive components with potential therapeutic benefits. Furthermore, AI facilitates predictive modeling, allowing researchers to forecast the properties and activities of EOs based on their chemical profiles [7]. This predictive capability is invaluable in optimizing formulations for specific purposes, whether in aromatherapy, pharmaceuticals, or other industries. Moreover, the ability to tailor EO compositions for targeted outcomes is a testament to AI's transformative impact on the field. The integration of AI also extends to the optimization of extraction processes [14, 15]. In particular, ML algorithms can analyze historical data on extraction methods, considering factors such as temperature, pressure, and duration, to recommend optimal conditions for achieving the highest yield of bioactive compounds. This streamlines research processes while also supporting sustainable practices by minimizing resource use. As researchers embark on this exploration, it becomes evident that the combination of AI and EO research is not merely a technological evolution. Rather, it is a catalyst for groundbreaking innovations with far-reaching implications across industries and, most importantly, for human well-being.

The exploration of AI in the study of EOs represents a cutting-edge intersection between traditional herbal medicine and advanced technology. Recent research has witnessed a surge in interest in leveraging AI to deepen our understanding of the complex compositions and therapeutic applications of EOs. Notably, researchers employed ML algorithms to analyze the chemical constituents of various EOs, identifying unique compounds and elucidating their potential biological activities [12, 13, 14, 15, 16]. Correspondingly, this study laid the foundation for subsequent research by demonstrating AI's capacity to unravel the intricate molecular profiles of EOs, paving the way for targeted investigations into their therapeutic properties [14, 17]. In addition, this research delved into the predictive modeling aspects of AI in EO research. Through a comprehensive analysis of chemical data and bioactivity assays, the researchers developed ML models capable of forecasting the biological activities of EOs based on their chemical composition [18]. This predictive capability streamlines the process of identifying potential therapeutic agents and accelerates the drug discovery pipeline. Overall, the study exemplifies how AI can contribute to a more efficient, targeted approach to harnessing the therapeutic potential of EOs [19]. In a similar vein, another study focused on optimizing EO extraction processes using AI [8, 20]. By integrating historical data on extraction methods and outcomes, the researchers developed an AI-driven model that recommended optimal conditions for extracting the maximum amount of bioactive compounds from plant materials [4]. This contributes to sustainable resource use while also highlighting how AI can revolutionize traditional practices, making them more efficient and environmentally friendly.

To address the challenges of EO adulteration, several research teams proposed an innovative solution: applying AI for authenticity verification. By analyzing a large dataset of authentic and adulterated EOs, the researchers developed an ML model capable of detecting subtle deviations in chemical profiles indicative of potential adulteration [21, 22]. Importantly, this study is pivotal in ensuring the integrity of EO products on the market and in demonstrating the practical applications of AI in quality control and consumer protection. A separate study in [3, 23, 24] contributed to the field by exploring the synergistic effects of combining EOs based on AI recommendations. Using ML algorithms, the researchers identified complementary chemical profiles among different EOs, guiding the formulation of blends with enhanced therapeutic properties. As a result, this approach opens new avenues for personalized aromatherapy and tailored formulations in various industries. The existing work on AI in EO research reflects a dynamic, rapidly evolving field. From unravelling molecular complexities to optimizing extraction processes, predicting bioactivities, ensuring authenticity, and formulating synergistic blends, AI has demonstrated its transformative potential [2, 13, 24, 25, 26], As we move forward, the integration of AI will continue to drive innovation in EO research, offering novel insights and solutions with far-reaching implications for healthcare, industry, and beyond.

While AI and ML techniques have been increasingly adopted in EO research for identification, classification, and bioactivity prediction, the reliability of these approaches depends strongly on appropriate validation. Most reported studies validate AI outputs through comparison with established analytical techniques such as gas chromatography-mass spectrometry (GC-MS), gas chromatography-flame ionization detection (GC-FID), and nuclear magnetic resonance (NMR). This includes statistical performance evaluation using cross-validation and standard accuracy metrics. In several cases, AI and ML predictions are further supported by experimental or laboratory-based confirmation, particularly in antimicrobial and authentication studies. In essence, AI methods in EO research are generally applied as complementary tools rather than standalone replacements, enhancing analytical efficiency while maintaining scientific rigor through established validation practices.

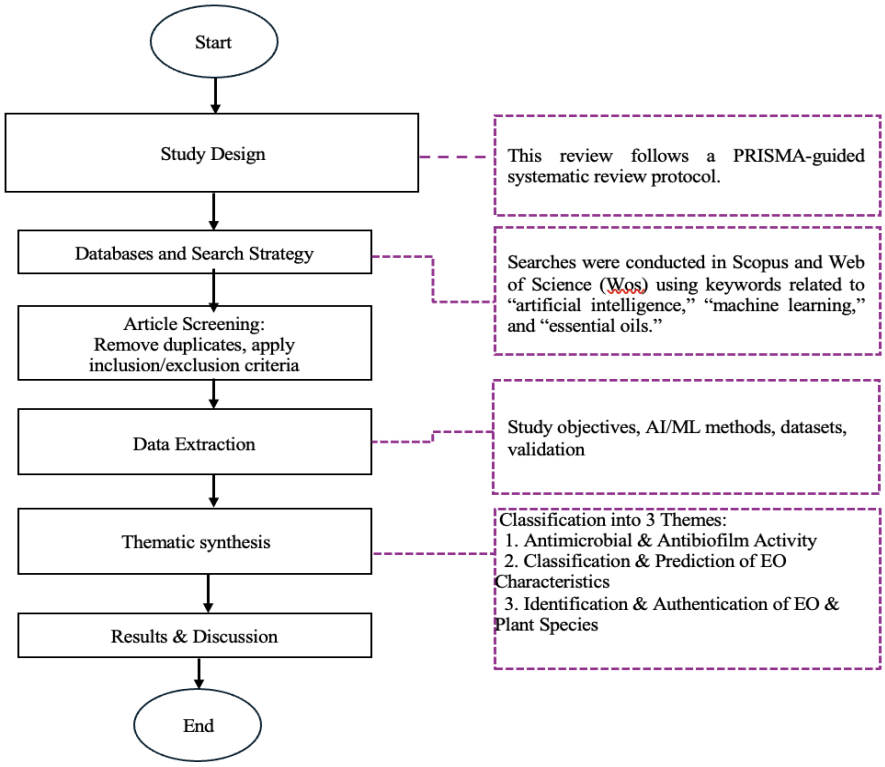


Figure 1. General Methodology

Methodology

The methodology employed in this study adheres to the Preferred Reporting Items for Systematic Reviews and Meta-Analysis (PRISMA) framework, incorporating synthesis and quality appraisal. The PRISMA framework encompasses four key processes: identification, screening, eligibility, and inclusion [27]. Originating as a global initiative, PRISMA addresses concerns such as the lack of transparent and well-documented review methods in published articles [27]. Following PRISMA's guidelines, the subsequent phase involves synthesis analysis, focusing on achieving the goals of the Systematic Literature Review (SLR) and organizing variables of interest based on the overall characteristics of the included articles [28]. Furthermore, in the context of quality appraisal, consideration is given to whether the scale utilized to assess the quality of individual studies is suitable for the specific designs under consideration [28], [29]. The general methodology is displayed in **Figure 1**.

Identification

This investigation focused on scrutinizing articles from two databases, Institute for Scientific Information (ISI) Web of Science (WoS) and Scopus, to ensure a comprehensive collection of relevant literature. The initial query yielded 209 articles, of which 115 were sourced from Scopus and 94 from WoS, as illustrated in **Figure 1**. The search string method detailed in **Table 1** was employed to retrieve these articles. Noteworthy keywords such as "essential oil," "artificial intelligence," and "machine learning" were pivotal in capturing the scope of the study.

Table 1. The search string

Scopus	TITLE-ABS-KEY ("essential oil*" AND ("artificial intelligence" OR "machine learning")) AND (LIMIT-TO (DOCTYPE , "ar")) AND (LIMIT-TO (PUBSTAGE , "final")) AND (LIMIT-TO (LANGUAGE , "English")) AND (LIMIT-TO (SRCTYPE , "j")
Web of Science (WoS)	"essential oil*" AND ("artificial intelligence" OR "machine learning") (Topic) and Article (Document Types) and English (Languages)

Screening

During the screening process, a thorough examination was conducted on a diverse range of potential research materials to identify content aligning with the predefined research objectives. The criteria used during this screening phase prominently featured the application of AI and ML to select research items on EOs. The initial screening phase resulted in the exclusion of 144 publications. Subsequently, meticulous assessment was conducted on 65 papers based on distinct inclusion and exclusion criteria outlined in this study, as detailed in **Table 2**. The primary criterion for inclusion was literature, specifically research papers, as they serve as the primary source for practical recommendations. This encompassed a comprehensive array of materials, such as reviews, meta-syntheses, meta-analyses, books, book series, chapters, and conference proceedings, that were not considered in the most recent study. Moreover, the review focused exclusively on English-language publications and confined the analysis to 2008 and 2024. In total, 31 publications were excluded due to duplication criteria.

Eligibility

In the third phase, the eligibility assessment, a compilation of 113 articles was curated. This stage required a thorough review of both titles and core content across all articles to confirm their alignment with the inclusion criteria and relevance to the present research objectives. As a result, 58 reports were excluded due to factors such as straying beyond the study scope, possessing titles lacking in significance, featuring abstracts unrelated to the study's objective, and lacking full-text access corroborated by empirical evidence. Ultimately, 55 articles fulfilled the criteria and are currently accessible for review, as illustrated in **Figure 2**.

Data abstraction and analysis

In this investigation, an integrative analysis played a pivotal role as one of the assessment strategies aimed at scrutinizing and synthesizing various research designs, with a predominant emphasis on quantitative methods. Specifically, the primary goal of this meticulous examination was to identify relevant topics and subtopics. The initial phase of theme development began with data collection, which showcased the authors' in-depth analysis of 55 publications directly relevant to the study's topics. The authors systematically evaluated significant studies on AI in the EO field, thoroughly examining methodologies and research findings. Subsequently, collaborative efforts among the authors contributed to the formulation of themes grounded in the evidence presented throughout this study. A comprehensive log meticulously documents analyses, perspectives, or other insights crucial for data interpretation throughout the analytical process. Following this, a rigorous comparison of results was executed to pinpoint any inconsistencies in the theme design process. The resulting themes underwent adjustments to ensure coherence.

Following study selection, an integrative thematic synthesis approach was employed to categorize the findings of the included articles. Two reviewers independently extracted key attributes from each study, including research objectives, EO type, analytical data, AI or ML techniques applied, and primary outcomes. Initial grouping of studies was conducted based on their dominant research objectives. An inductive thematic analysis was then performed to identify recurring patterns and conceptual similarities among the extracted data. Through iterative comparison, the studies were systematically organized into three overarching themes: (1) antimicrobial and antibiofilm activity of EOs, (2) classification and prediction of EO characteristics, and (3) identification and authentication of EOs and plant species. Any discrepancies in categorization were resolved through discussion until complete agreement was achieved, ensuring transparency and methodological rigor in the synthesis process.

Table 2. The inclusion and exclusion criteria

Criterion	Inclusion	Exclusion
Language	English	Non-English
Timeline	2008 – 2024	< 2008
Literature Type	Journal (Article)	Conference, Book, Review
Publication Stage	Final	In Press

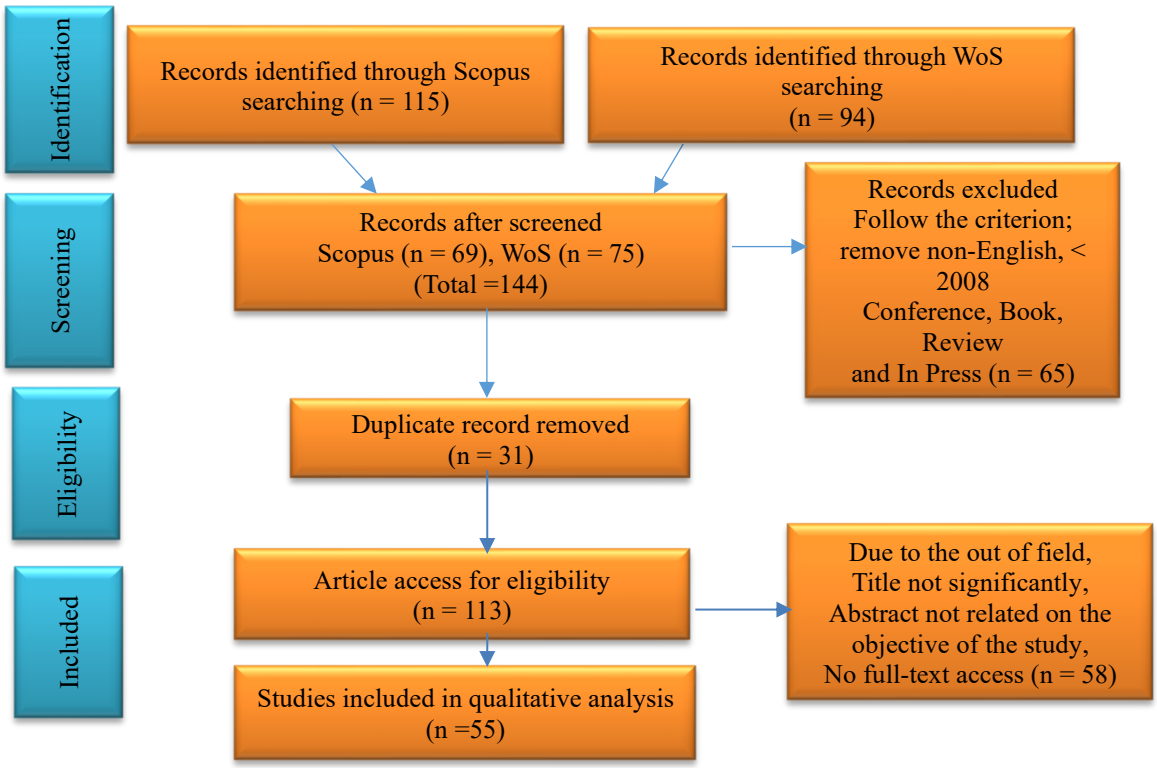


Figure 2. PRISMA framework

Results and Discussion

This research unveils significant insights into the application of AI in EO research across three distinct themes. Firstly, the investigation examined the antimicrobial and antibiofilm activity of EOs, providing compelling evidence of their efficacy against various microbial strains. Secondly, employing AI techniques facilitated the classification and prediction of EO characteristics, demonstrating remarkable accuracy in delineating their chemical composition and properties. Lastly, the analysis emphasized the pivotal role of AI in identifying and authenticating plant species used in EO production, thereby ensuring the integrity and quality of the final products. Collectively, these findings underscore the transformative potential of AI to advance EO research and its multifaceted applications across the pharmaceutical, cosmetic, and agricultural industries.

Theme 1: Antimicrobial and antibiofilm activity of essential oils

The investigation into the antimicrobial and antibiofilm properties of EOs has garnered considerable attention in recent years. In this context, this SLR synthesizes findings from selected journal articles to provide comprehensive insights into the application of AI in EO studies, particularly concerning antimicrobial and antibiofilm activities. Antimicrobial and antibiofilm properties of EOs have attracted attention for their potential to combat infections, particularly those associated with Cystic Fibrosis (CF) [30, 31]. Accordingly, EOs have emerged as potential candidates for preventing and treating biofilm-associated infections caused by pathogens such as *Staphylococcus aureus*, *Staphylococcus epidermidis,* and *Pseudomonas aeruginosa*. Recent investigations have explored the efficacy of EOs in modulating biofilm production, with ML algorithms aiding in predicting the antibiofilm activity of individual chemical components within EOs [31]. Another significant aspect of AI in EO research lies in the Quantitative Structure-Retention Relationship (QSRR) modeling of EO components [31]. Notably, this approach enables the prediction of EO component Retention Indices (RIs) using linear and nonlinear chemometric methods, including Multiple Linear Regression (MLR), Partial Least Squares (PLS), Polynomial PLS (Poly-PLS), and Support Vector Machines (SVMs). A study comparing different chemometric methods discovered that SVM outperformed MLR, PLS, and Poly-PLS in QSRR modeling. The reliability of SVM was evidenced by low relative Standard Error (SE%) and high square correlation coefficients, affirming its

utility as a robust modeling tool for QSRR studies [31].

One study examined the efficacy of *ethylene-vinyl alcohol copolymer* (EVOH) films containing pure components of EOs: *cinnamaldehyde* (cinho), *citral* (cit), *isoeugenol* (ieg), or *linalool* (lin), against *Fusarium sporotrichioides* growth and production of T-2 and HT-2 toxins under varying temperature and water activity conditions [32]. Overall, the results indicated that the films' effectiveness in controlling fungal Growth Rate (GR) and toxin production varied depending on the type of EO component. ML methods, including XGBoost and Random Forest (RF), demonstrated superior performance in predicting *F. sporotrichioides* GR and toxin production compared to SVM and neural network algorithms. Taken together, this comparative analysis underscores the potential of ML techniques in optimizing the efficacy of EO-based formulations for combating fungal infections. Another study focused on the classification of bitter orange EOs according to fruit ripening stage using untargeted chemical profiling and ML [33]. As documented, bitter orange EOs exhibit variations in quality and composition based on the ripening stage of the citrus fruit. By leveraging headspace gas chromatography-mass spectrometry (HS-GC-MS) and artificial neural networks (ANN), the study proposed an objective approach to assess the ripening stage of bitter orange EOs. Key volatile compounds identified by HS-GC-MS analysis demonstrated predictive power in accurately classifying EOs by ripening stage. Consequently, this innovative strategy provides a reliable method for quality control of bitter orange EOs, enabling their use across various industries.

Moreover, ML analyses were employed to investigate the relationship between the chemical composition of EOs and in vitro antibiofilm activities against *Staphylococcus* species [4]. *Staphylococci*, including *S. aureus* and *S. epidermidis,* are among the most prevalent causes of biofilm-associated infections. The study evaluated the antibiofilm capabilities of 89 EOs against different strains of *S. aureus* and *S. epidermidis*. ML algorithms were utilized to analyze the chemical compositions of EOs and their associated anti-biofilm potencies. Robust ML models enabled the identification of chemical components that modulate biofilm production, inhibition, or stimulation in each strain. This comprehensive analysis sheds light on the potential of EOs as non-biocidal agents for combating biofilm-associated infections caused by *Staphylococcus* species.

The study by Lebanov et al. [18] used ML classification models trained on experimental data to predict the bioactivity of EOs against HSV-1 infection. Using in vitro assays and gas chromatography/mass spectrometry, the authors identify EOs with potent antiviral activity and low toxicity, highlighting the potential of ML to predict the efficacy of complex mixtures such as EOs. In a similar vein, research by [10] investigated the inhibitory activity of EOs against *Plasmodium* in early mosquito stages, which are crucial for malaria transmission. By combining in vitro assays with ML analysis, the study identifies EOs and their components as potential inhibitors of malaria parasites, demonstrating the innovative use of AI in malaria control strategies. Moreover, Brown et al. [16] explored the antimicrobial activity of EOs against bacterial isolates from CF patients. Using unsupervised ML, the authors identified EOs capable of inhibiting bacterial growth, regardless of antibiotic resistance profiles. This highlights the potential of EOs as alternative antimicrobial agents in combating antibiotic-resistant infections.

One study employed ANNs to predict the antimicrobial activity of 49 EOs against common pathogens, including *S. aureus* and *Escherichia coli*, achieving a prediction accuracy of over 70% within a 10 mm error range [34]. Similarly, a hybrid analytical approach combining hypothesis-based and data-driven methods was proposed to identify antiviral substances in medicinal plant extracts. This method effectively segmented chromatographic data and identified volatile compounds responsible for antiviral effects, such as *beta-cis-caryophyllene* and *linalool* [35]. Furthermore, interpretable ML techniques were applied to *heterogeneous* antibody-virus datasets, enabling the prediction of antibody inhibition against diverse influenza virus variants. This approach facilitates pandemic preparedness and enhances understanding of serum potency and breadth in vaccination and infection studies [36]. ML algorithms were employed to screen potential compounds against MCF7 human breast cancer cells, and Ocimum basilicum EOs were identified as promising candidates. Molecular docking analysis revealed the anticancer mechanisms of selected EO components, offering insights for novel breast cancer treatments [23, 37, 38, 39, 40, 41]. Essentially, these findings underscore the pivotal role of AI in elucidating the therapeutic potential of EOs and guiding future research in antimicrobial and anticancer drug discovery.

Theme 2: Classification and prediction of essential oil characteristics

In recent years, AI techniques have emerged as powerful tools for analyzing complex chemical compositions and predicting the properties of EOs, as

summarized in **Table 3**. In this section, the investigation delves into how AI methodologies have been applied to classify and predict EO characteristics, shedding light on the advancements and potential implications in this field. Through a systematic analysis of the literature, compelling insights into the accuracy and efficacy of AI-driven approaches in delineating the chemical makeup and properties of EOs are presented, offering valuable guidance for future research and practical applications.

Table 3. Classification and Prediction of EO Characteristics using AI

Ref	Objectives	Problem Statement	Methodologies	Findings	Advantages/ Shortcomings
[42]	Identification of components in EOs	To present a computer-aided method for identifying known and new chemical constituents in EOs using C-13 NMR data.	Computer-aided method	Developed a novel program for analyzing C-13 NMR data to identify components in EOs.	Future research could validate the accuracy and applicability of the developed program in a broader range of EOs.
[43]	Classification and selection of fish gelatin packaging film	To classify and select biodegradable packaging produced from fish gelatine incorporated with palm oil and EOs.	K-nearest neighbor algorithm (kNN)	Demonstrated the efficiency of the kNN algorithm in classifying and selecting biodegradable packaging incorporating palm oil and EOs.	Further studies could explore optimization techniques for enhancing the efficiency and applicability of the classification algorithm.
[15]	Classification and bioactivity prediction of EO-producing plants	To develop a deep learning model for classifying and predicting the bioactivities of EO-producing plants from Egypt.	Convolutional Neural Networks (CNN), Multiclass Neural Network (MNN)	Established a CNN model with high accuracy in classifying and predicting the bioactivities of EO-producing plants.	Future research may focus on extending the application of deep learning models to classify and predict bioactivities of EOs from other regions.
[44]	Identification of drying temperatures of *Amomum tsao-ko*	To identify drying temperatures of *Amomum tsao-ko* using FT-NIR spectroscopy and ML techniques.	PCA, PLS-DA, SVM, ResNet	Demonstrated the feasibility of FT-NIR spectroscopy coupled with ML for identifying drying temperatures of *Amomum tsao-ko*.	Further validation studies could assess the reliability and accuracy of the developed models under varying experimental conditions.
[45]	Estimation of clove bud yield using remote sensing data and methodologies	Limited availability of data on local clove production	Circular Hough Transform (CHT) for automated detection of individual clove trees, RF classifier for tree species classification	97.9% detection of reference clove trees using CHT, 70.7% producer accuracy, and 59.2% user accuracy for clove tree classification, 77.9% overall accuracy for classifying clove production systems	Future research could focus on refining classification algorithms to improve accuracy and on exploring additional features to improve predictive performance.
[46]	Identification of potential natural antibiotic plants from Jamu formulas using ML	Addressing antibiotic resistance by discovering potential herbal plants with antibacterial properties	RF classifier	Identified 14 plants as potential natural antibiotic candidates with high accuracy	Future research could validate the efficacy of identified plants in clinical trials and investigate their mechanisms of action.
[47]	Assessment of EOs biofilm modulation activity against *P. aeruginosa* isolates from CF patients	Investigating the potential of EOs in controlling biofilm formation by *P. aeruginosa*	ML for the classification of antibiofilm action of chemical components	Identified commercial EOs capable of modulating biofilm production by *P. aeruginosa* strains	Future research could explore the clinical applications of identified EOs in managing biofilm-related infections

[48]	Assess the antioxidant activity of EOs and establish quantitative composition-activity relationships using ML.	Understanding the antioxidant properties of EOs and their constituents is important but insufficiently explored.	ML classification algorithms	Active EOs demonstrated potent antioxidant properties, with ML models highlighting key chemical compounds.	ML models offer insights into the antioxidant properties of EOs, facilitating the identification of potent antioxidants. Further research could explore complex antioxidant mechanisms and validate findings in vivo.
[49]	Design an Artificial Intelligence of Things (AIoT)-based plant pot for growing mint in offices to maximize extract production.	Despite advancements, growing plants indoors remains challenging.	Case-Based Reasoning (CBR), sensors	Identified optimal conditions for mint growth in offices.	Potential for enhancing indoor plant growth; need for real-world testing.
[19]	Develop ML models for predicting GC RIs to aid compound identification	Limited data hinders compound identification in gas chromatography.	Neural networks, gradient boosting	Accurately predict compound RIs, outperforming previous methods.	Valuable tool for compound identification; explore broader applications.
[50]	Optimize ultrasound-assisted extraction of polyphenolic compounds from plants using AI and optimization techniques.	Improving extraction efficiency and environmental impact is crucial.	ANN, multi-objective optimization	Identified optimal extraction conditions for maximizing *polyphenol* extraction.	Contribute to sustainable production practices; explore scalability.
[51]	Evaluate ML models for predicting the nutritional status of oil palm leaves using proximal multispectral images.	Traditional methods for assessing plant health are time-consuming.	RF, support vector regression, neural network	Models show promise for accurately predicting leaf nutrition.	Potential for precision agriculture; investigate applicability to other plants.

To contextualize Theme 2, the AI approaches used for classification and prediction of EO characteristics were compared across the included studies (Table 3). For example, SVM models applied to GC-MS datasets frequently reported classification accuracies above 90%, highlighting their effectiveness in distinguishing closely related EOs. In contrast, ANNs were used in some studies to predict chemical concentrations. They demonstrated robust performance for complex multicomponent EOs. Other studies employed RF and K-Nearest Neighbor (KNN) algorithms, with varying success depending on dataset size and preprocessing techniques such as principal component analysis (PCA) or feature selection. Cross-validation strategies and external validation sets were also noted to influence reported performance metrics such as accuracy, root mean square error (RMSE), and R^2. By comparing these methodological choices and outcomes, it is evident that algorithm selection, data quality, and validation approaches significantly affect the predictive capabilities of AI/ML models, guiding future research and practical applications in EO characterization.

Theme 3: Identification and authentication of plant species

Traditional methods for verifying plant species can be time-consuming and often rely on subjective assessments. Nevertheless, recent advancements in AI, as outlined in **Table 4**, offer promising solutions to this challenge. In this section, the exploration focuses on the application of AI methodologies in the identification and authentication of plant species used in EO production. By analyzing the literature and synthesizing key findings, the discussion uncovers the transformative potential of AI to streamline and improve the accuracy of plant species authentication, thereby safeguarding the quality and reliability of EO products.

Table 4. Identification and authentication of plant species

Ref.	Objectives	Problem Statement	Methodologies	Findings	Advantages/ Shortcomings
[52]	To discriminate the age of *Valeriana jatamansi* using hyperspectral remote sensing and ML techniques	Identifying the age of *V. jatamansi* using traditional methods is time-consuming and labor-intensive	PCA, ML Classifiers (ANN, SVM, RF, BDT, DT, KNN)	Classifier accuracies improved after PCA feature selection. ANN resulted in 100% overall accuracy. Specific wavelength regions were identified for discriminating age groups. The developed model provided rapid on-site identification of plant age.	Future research can explore the application of this technology to other valuable plants for optimizing harvesting.
[49]	Designing an AIoT-based indoor planting model for *Mentha spicata*	Lack of efficient methods for monitoring and controlling indoor plant growth	AIoT, CBR Inference Engine	AIoT-based plant pot design enables precise monitoring and control of *M. spicata* growth. Specific illumination and moisture conditions optimized mint extract production.	Future research could focus on the scalability and adaptability of the proposed AIoT model to different plant species and environments.
[53]	To differentiate between morphologically similar species in the genus Cinnamomum using a deep CNN	Difficulty in visually distinguishing between morphologically similar Cinnamomum species	Deep CNN, Image Processing	Developed CNN classifiers achieved high accuracy in species differentiation. Outperformed traditional classifiers.	Further research could explore the application of CNNs for species identification in other plant genera with similar morphological challenges.
[54]	Investigating the effect of rosemary odor on mental workload using EEG and AI	Understanding the impact of rosemary odor on mental workload	EEG Signal Processing, Decision Tree Feature Importance Method, Classification and Regression Tree Algorithm	Rosemary odor reduced mental workload during cognitive tasks. EEG signals were used to classify mental workload with high accuracy.	Future studies could investigate the potential therapeutic applications of rosemary odor in reducing mental stress in various settings.
[55]	Forecasting Lyme disease risk using web search data	Delayed estimation of Lyme disease spread using traditional surveillance methods	Machine-Learned Classifier of Web Search Sessions	Web search data enabled real-time monitoring and estimation of Lyme disease incidence. High correlation with official case count data.	Potential for real-time disease surveillance and timely interventions. Further research could explore extending this method to monitor

					other vector-borne diseases.
[56]	To identify the authenticity, botanical sources, and geographical origins of Atractylodis Rhizomai (AR) decoction pieces	Difficulty in authenticating AR decoction pieces due to counterfeit products	Near-Infrared Spectroscopy (NIRS), ML (Extreme Learning Machine (ELM), Back Propagation Neural Network, Support Vector Classification)	NIRS combined with ML effectively identified the authenticity, botanical sources, and geographical origins of AR. ELM performed best in authenticity identification.	Future research could explore the scalability and adaptability of the proposed method to authenticate other herbal products with similar authentication challenges.
[57]	To distinguish between aromatic fragrances with different concentrations using electronic nose technology and an SVM	Difficulty in distinguishing between aroma samples with multiple concentrations using electronic nose technology	Electronic Nose, SVM	SVM technology is effectively distinguished between four fragrance samples with three concentrations using electronic nose data. Feature reduction enhanced the electronic nose's resolving power.	Further research could investigate the application of SVMs for distinguishing aroma samples in real-world scenarios with varying concentrations and environmental conditions.
[58]	To explore the polypharmacological mechanism of Traditional Chinese Medicine (TCM) using unsupervised ML	Challenges in investigating the polypharmacological mechanism of TCM with multiple components	Unsupervised ML, Hierarchical Clustering, Cellular Functional Similarity	Unsupervised learning strategy effectively explored the polypharmacological mechanism of TCM using hierarchical clustering based on cellular functional similarity. Identified potential active compounds and mechanisms of action.	Future research could validate the findings of the unsupervised learning strategy through experimental studies and clinical trials. Additionally, integrating quantitative omics data could provide further insights into the therapeutic mechanisms of TCM.
[59]	To predict Adverse Drug Reactions (ADRs) of combined medication using ML from heterogeneous pharmacologic databases	Difficulty in early and accurate prediction of potential ADRs for combined medications	ML, Network Analysis, PCA	The proposed method (HCNS-ADR) effectively predicted ADARs for combined medications by building highly credible negative samples. Significant performance improvements compared to baseline approaches.	Future research could focus on the scalability and generalizability of the proposed method for predicting ADRs across a broader range of medications and patient populations.
[60]	To evaluate the capability of electronic nose technology coupled with chemometrics tools for spearmint grading	Difficulty in fast, real-time, and non-destructive spearmint grading	Electronic Nose, Chemometrics (PCA, PLS-DA, Fuzzy Clustering), ANN	An electronic nose coupled with chemometrics tools accurately graded spearmint based on volatile organic compounds, with high prediction accuracy and sensitivity.	Future research could focus on validating the developed system with larger datasets and under different environmental conditions to enhance its robustness and reliability in real-world applications.
[61]	To correlate the toxicity of major constituents of EOs	Difficulty in correlating the toxicity of EO	Gas Chromatography, In Silico Analyses,	In silico analyses identified key chemical constituents associated with the toxicity	Future research could validate the in-silico findings through

	from two *Ipomoea* species using in silico analyses	constituents with molecular mechanisms using traditional experimental methods	ML-based Algorithm	of EOs from *Ipomoea* species. Chemical composition and toxicity were correlated using ML-based algorithms.	experimental studies and clinical trials to enhance understanding of the toxicity mechanisms of EO constituents.
[62]	To evaluate the use of bioactive EVOH films containing pure components of Eos and ML methods in controlling fungal growth and mycotoxin production	Challenges in controlling fungal growth and mycotoxin production using traditional antifungal chemicals	Bioactive EVOH Films, ML (Neural Networks, RF, Extreme Gradient Boosted Trees), MLR	Bioactive EVOH films containing EOCs effectively controlled fungal growth and mycotoxin production. ML models accurately predicted fungal growth and mycotoxin production under different environmental conditions.	Future research could explore the scalability and adaptability of bioactive EVOH films containing EOCs in real-world food packaging applications to mitigate the risks posed by toxigenic fungi and mycotoxins.
[7]	To classify agarwood EO grades using ML techniques	Difficulty in grading EOs using traditional human sensory evaluation methods	ML (SVM)	SVM achieved high accuracy in classifying agarwood EO grades. SVM using the versus all (OVA) approach showed promising results for future classification studies.	Future research could further explore integrating multiple ML algorithms and feature engineering techniques to improve classification accuracy for EO grades.
[63]	To propose a green approach for the multivariate consecutive extraction of EOs and total flavonoids from daidaihua	Difficulty in optimizing extraction processes for EOs and flavonoids from daidaihua using traditional methods	Steam Distillation, Alkali Extraction, Acid Precipitation, ANN, Genetic Algorithm	The proposed green extraction approach effectively optimized process parameters for the extraction of EOs and flavonoids from daidaihua. The extraction yields were significantly improved, and the mass transfer mechanism was elucidated.	Future research could explore the scalability and adaptability of the proposed extraction approach for other plant materials and optimize it for large-scale industrial applications.

For plant species identification and authentication, AI techniques were applied to analytical data obtained from EOs or plant extracts. Standard datasets included GC-MS chemical fingerprints, Fourier Transform Infrared Spectroscopy (FTIR), and NMR spectra, and multispectral or chromatographic profiles. Classification algorithms such as SVMs, RF, and PCA-based methods were frequently used to distinguish closely related plant species and detect adulteration. Validation strategies, including cross-validation, external test sets, and performance metrics such as accuracy and R^2, were reported to assess model reliability.

Conclusion

Overall, the use of AI in EO studies has revolutionized the field by providing valuable insights into their antimicrobial, antibiofilm, anticancer, identification, and prediction properties. By harnessing ML algorithms, researchers can predict the activities of EOs and their components, enabling the optimization of their efficacy in combating infections and diseases. Notably, one of the key advantages of AI techniques in EO research is the ability to classify and assess the quality of different oils. By analyzing vast amounts of data, AI algorithms can accurately categorize EOs based on their chemical composition and therapeutic properties. This streamlines the identification and selection of the most suitable oils for specific applications while also ensuring consistent, reliable use.

AI is proving to be a valuable tool in predicting the bioactivity of EOs. By analyzing the chemical composition and structure of oils, ML algorithms can accurately predict their potential effects on the human

body. As a result, this allows researchers to identify oils with specific bioactive properties, such as anti-inflammatory or antioxidant effects, and tailor their use accordingly. The potential of AI in enhancing our understanding and application of EOs in healthcare is vast. By combining AI with traditional research methods, scientists can uncover new insights into the therapeutic properties of EOs and develop more effective treatments for various health conditions. Consequently, this benefits patients by providing alternative and potentially more natural treatment options while also opening new avenues for drug discovery and development. In conclusion, the integration of AI into EO studies has revolutionized the field by enabling researchers to explore the properties of EO data better. ML algorithms aid in predicting the activities of EOs and their components, optimizing their efficacy in combating infections and diseases. Additionally, AI techniques are used to classify EOs, assess their quality, and predict their bioactivity, underscoring the immense potential of AI to enhance our understanding and applications of EOs in healthcare.

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