

Applications of artificial intelligence in analyzing *Aquilaria* essential oils: a review of current machine learning techniques

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ABSTRACT

This study explores the application of machine learning (ML) techniques in the classification of agarwood oil, focusing on the use of various algorithms such as k-nearest neighbors (KNN), support vector machines (SVM), random forest (RF), and artificial neural networks (ANN). Since 2013, ML has played a pivotal role in analyzing agarwood oil, particularly by leveraging data from a variety of chemical compounds found in the *Aquilaria* genus. Through a systematic review and bibliometric analysis using the SCOPUS database, this study compiles and highlights recent works that have successfully employed ML techniques for the quality assessment of agarwood oil. These studies utilize chemical data, such as gas chromatography-mass spectrometry (GC-MS) and nuclear magnetic resonance (NMR), for the classification and detection of different oil grades. The review reveals a broad range of ML applications, demonstrating their growing importance in the field of essential oil analysis. By systematically presenting the findings from recent research, this work emphasizes the potential for further exploration of ML in the standardization and improvement of agarwood oil classification techniques.

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1. INTRODUCTION

Aquilaria essential oils, extracted from trees in the *Aquilaria* genus, are highly valued for their aromatic profiles and medicinal properties, particularly in industries such as perfumery and traditional medicine [1]–[6]. However, analyzing the chemical complexity of these oils, especially their sesquiterpene content, has presented significant challenges. Traditional methods, such as human sensory evaluations, are subjective and inconsistent, making them unreliable for precise analysis [7]–[10].

In recent years, the application of artificial intelligence (AI), particularly machine learning (ML), has emerged as a promising solution to these challenges. Researchers have increasingly turned to AI-driven techniques to enhance the analysis of *Aquilaria* essential oils by identifying complex chemical patterns and processing large datasets with higher accuracy and efficiency [7], [11], [12]. ML algorithms such as artificial neural networks (ANN), random forest (RF), support vector machines (SVM), and k-nearest neighbors (KNN) have demonstrated the potential to automate and improve the accuracy of chemical compound identification from gas chromatography (GC) data [13]. These methods excel in analyzing high-dimensional

data, identifying subtle patterns and classifying compounds based on their spectral features, offering a significant advantage over traditional methods [14]–[16].

The primary focus of this review is to evaluate the functionality and performance of ANN, RF, SVM, and KNN in the analysis of *Aquilaria* essential oils. By assessing the performance criteria such as accuracy, sensitivity, specificity, and computational efficiency, this review will provide insights into which ML techniques are most suitable for processing GC data. Moreover, the paper covers research conducted from 2014–2023, providing a comprehensive overview of how these ML techniques have been applied in essential oil analysis. This review also addresses the challenges and future potential of applying AI to enhance the field of essential oil chemistry [15], [17]–[19].

2. METHOD

ML analysis of *Aquilaria* essential oils relies on GC-derived chemical profiles requiring high-quality data and effective feature extraction [10], [20]–[26]. Classical classifiers (ANN, RF, SVM, and KNN) are widely validated for essential oil analysis [20], [27]. Accordingly, a systematic literature review of Scopus-indexed studies (2013–2024) was conducted using bibliometric and content analyses.

2.1. Literature search and screening strategy

This review followed the preferred reporting items for systematic reviews and meta-analyses (PRISMA) reporting guidelines to ensure transparency and reproducibility of the literature screening process [28], [29]. Literature retrieval was conducted using the Scopus database, chosen for its comprehensive coverage of peer-reviewed journals in engineering, chemistry and applied sciences. The search employed combinations of the keywords “essential oil”, “agarwood oil”, “machine learning”, “artificial neural networks”, “random forest”, “support vector machine”, “k-nearest neighbors”, and “chemical compound classification”, applied to titles, abstracts and keywords for publications from 2013–2024. Title and abstract screening excluded studies not related to essential oils or ML-based analysis, while full-text assessment further removed articles lacking quantitative performance evaluation or sufficient chemical analytical data. The final set of eligible studies was subjected to qualitative content analysis, as summarized in Figure 1.

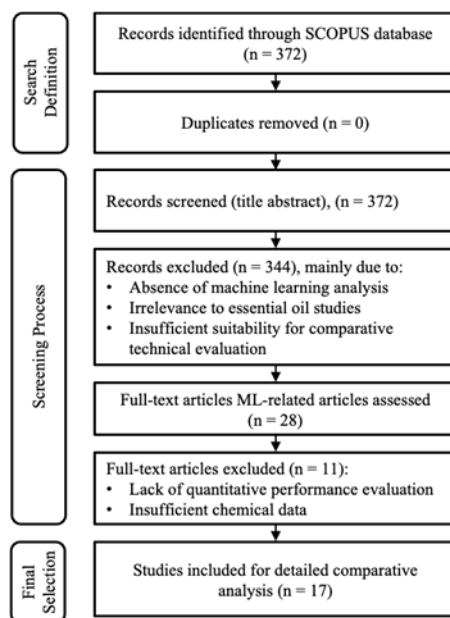


Figure 1. PRISMA-style flow diagram of the literature search, screening and selection process

2.2. *Aquilaria* species overview

The study focuses on four common species of *Aquilaria* found in Malaysia, which include *A. malaccensis*, *A. hirta*, *A. beccariana*, and *A. rostrata*. These species are known for their economic value due to the high demand for agarwood, a fragrant resin used in traditional medicine, perfumes and religious rituals. Table 1 summarizes the key characteristics, commercial value and conservation status of these species.

All of these species are listed under Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES) Appendix II, which regulates their trade to ensure sustainability, while their International Union for Conservation of Nature (IUCN) statuses range from vulnerable to near threatened, reflecting concerns over habitat loss and overharvesting [30], [31].

Table 1. Characteristics and applications of common *Aquilaria* species found in Malaysia [3], [32], [33]

<i>Aquilaria</i> species	Habitat	Leaf characteristics	Key compounds in essential oils	Commercial value (agarwood)	Conservation status (CITES/IUCN)
<i>Aquilaria malaccensis</i>	Lowland tropical forests	Large, elliptic-oblong leaves with smooth surface	Agarol, sesquiterpenes	High, due to high-grade resin	CITES Appendix II, IUCN: vulnerable
<i>Aquilaria hirta</i>	Hill slopes and highland areas	Small, velvety, pubescent leaves on abaxial surface	aromadendrene, guaiene	Moderate	CITES Appendix II, IUCN: near threatened
<i>Aquilaria beccariana</i>	Swampy lowland areas	Broad leaves with smooth upper surface	A-guaiene, β -eudesmol	High, valued for fragrance use	CITES Appendix II, IUCN: vulnerable
<i>Aquilaria rostrata</i>	Coastal tropical forests	Narrow, lanceolate leaves with distinct veins	Eudesmol, agarol	Moderate	CITES Appendix II, IUCN: near threatened

*Note: conservation status is the threat level faced by the species, according to the IUCN Red List [30] or Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES) [31].

2.3. Investigating advanced machine learning techniques

This study reviewed four widely used ML algorithms, ANN, RF, SVM, and KNN, for essential oil classification based on chemical composition, reflecting their dominance in agarwood-related research. SVM with radial basis function (RBF) kernels is frequently applied due to its robustness on small and complex gas chromatography-mass spectrometry (GC-MS) datasets [15], [34], [35], while RF provides reliable performance through ensemble learning and feature-importance analysis [19], [21]. KNN remains an effective approach for species and quality-grade discrimination [36], [37], and ANN has shown high predictive accuracy in modelling essential-oil composition patterns [16], [38], [39]. Most studies employed preprocessing steps such as normalization, noise reduction, feature selection and principal component analysis (PCA) to improve data quality [16], [26], with model parameters optimized using cross-validation and grid search. Performance was evaluated using standard metrics including accuracy, precision, recall, specificity, and F1-score [13], [40]. Table 2 presents a comparative analysis of these four ML techniques, highlighting their features, advantages, and disadvantages. Despite the potential of advanced and hybrid models, their adoption remains limited due to small and imbalanced datasets, making these classical algorithms the most practical choices in current studies.

Table 2. Comparative analysis of ML techniques for essential oil classification

Features	ANN	RF	SVM	KNN
Algorithm	ANN	Ensemble of decision trees	Hyperplane with largest margin	Classifies based on KNN
Suitable for	Complex, non-linear problems	Classification (primarily)	High-dimensional data, outlier-resistant	Simple data, classification and regression
Advantages	Captures intricate patterns, efficient with large datasets	Robust to outliers, handles complex interactions	Effective for high-dimensional data, robust to outliers	Simple to implement, versatile
Disadvantages	Black box model, hyperparameter sensitive	Computationally expensive for large datasets	Sensitive to kernel choice, computationally expensive	Sensitive to noise and outliers, high dimensionality issues

3. RESULTS AND DISCUSSION

This study conducted an in-depth analysis of ML applications for the classification of *Aquilaria* essential oils. It examined key challenges in chemical analysis, particularly the complex sesquiterpene composition of agarwood oil. The growing integration of AI and ML has significantly improved the precision, automation, and efficiency of essential oil detection and classification.

3.1. Yearly distribution of ML algorithms in agarwood oil (2014-2024)

The temporal distribution of studies published between 2013 and 2024, as shown in Figure 2, illustrates the evolution of ML algorithm usage for agarwood oil classification. ANN was the sole algorithm applied in 2013, marking the initial adoption of ML in this field [41], followed by ANN and KNN in 2014.

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By 2017, SVM, RF, and KNN were introduced, reflecting increasing interest in multi-algorithm evaluation to better handle complex GC-MS data. RF gained prominence between 2018 and 2019, with multiple studies reported, while ANN and KNN were temporarily absent. In 2021, RF, SVM, and ANN were concurrently explored, indicating renewed multi-model comparison. Subsequently, KNN, SVM, and ANN became more prominent in 2022 and 2024, whereas RF was no longer applied in 2024. Overall, ANN dominated early studies, RF prevailed in mid-years, and KNN and SVM gained prominence in recent research, reflecting continual methodological refinement.

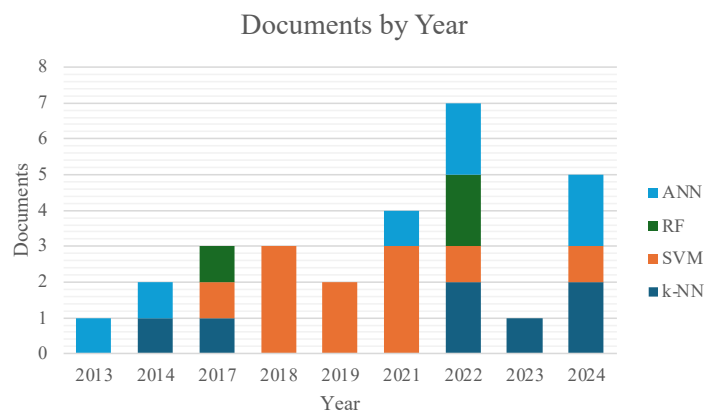


Figure 2. Number of studies applying ANN, RF, SVM, and KNN algorithms for agarwood oil classification

3.2. ML algorithm distribution in agarwood oil studies

Figure 3 illustrates the distribution of ML algorithms used in agarwood oil classification across the reviewed studies. SVM was the most frequently applied method (39%), reflecting its robustness in handling non-linear, high-dimensional chemical data with strong accuracy, and generalization. Both KNN and ANN were each used in seven studies (25%), demonstrating complementary strengths: KNN performed well on smaller, well-separated datasets, while ANN achieved strong predictive performance, particularly when trained with synthetic data. RF appeared in three studies (11%), providing reliable multi-dimensional analysis and useful feature-importance evaluation, confirming its continued relevance in agarwood oil research.

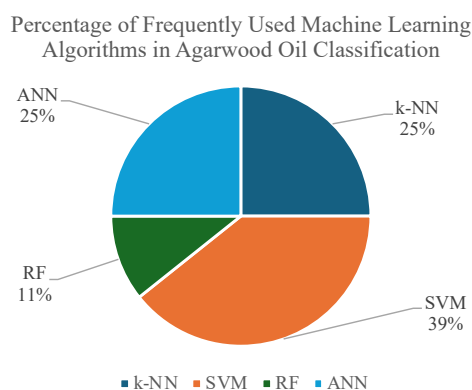


Figure 3. Distribution of ML algorithms applied in agarwood oil classification studies

3.3. Summary of ML applications in essential oil classification

Table 3 summarizes successful ML applications in agarwood and essential oil classification. ANN, RF, SVM, and KNN are most frequently reported due to their ability to model complex, non-linear GC-based chemical data [15], [19], [21]. Collectively, these approaches support accurate, reproducible, and objective quality evaluation across *Aquilaria* species [34], [37], [42], [43].

Table 3. Summary of successful studies leveraging ML for agarwood oil and other essential oil classification

Article	Algorithms	Functionality	Performance criteria results/findings
[38], [44]	ANN	To classify the grade of agarwood oil based on its chemical composition.	<p>i) Original GC-MS data (n=16):</p> <ul style="list-style-type: none"> - Accuracy: 75% - Sensitivity: 0% - Specificity: 100% <p>ii) Original GC-MS with synthetic data (n=90):</p> <ul style="list-style-type: none"> - Accuracy: 100% - Sensitivity: 100% - Specificity: 100% <p>Synthetic data effectively mitigated small-sample limitations in ANN-based agarwood oil classification.</p>
[39], [45], [46]	ANN with LM algorithm	An ANN-Levenberg Marquardt (LM) model was developed to grade agarwood oil quality using 11 chemical inputs across four quality levels, trained on 660 samples.	<ul style="list-style-type: none"> - Accuracy: 100% - Sensitivity: 100% - Specificity: 100% - Precision: 100% <p>The model demonstrated excellent classification performance with rapid convergence.</p>
[43], [47]	PLS-DA and RF	To classify the <i>gaharu</i> (agarwood) samples into one of three grades (high, intermediate, or low) based on their chemical constituents.	The ¹ H-NMR-based metabolomics approach demonstrated good grading performance (72.92% agreement; $\kappa=0.69$), supporting its effectiveness for <i>gaharu</i> quality assessment based on chemical composition.
[19], [21], [48]	RF	To discriminate between the formation modes of natural agarwood using the GC-MS raw data of artificial agarwood as the training sets. Agarwood samples formed by four different methods: <ul style="list-style-type: none"> - Physical injury - Chemical stimulation - Fungal infection - Comprehensive stimulation 	<p>i) Highest accuracy: 81.7%</p> <p>ii) Kappa value: 75.2%</p> <p>iii) Cross-validation: 45.5%</p> <p>iv) R boundary: 0.9</p> <p>Natural agarwood samples:</p> <ul style="list-style-type: none"> - Physical injury: 17.1% - Chemical stimulation: 22.9% - Fungal infection: 2.9% - Comprehensive stimulation: 57.1% <p>The GC-MS derived apparent abundance (R) was closely associated with agarwood quality and can serve as a quality index.</p>
[15], [49]	SVM	Evaluated the agarwood oil quality to high and low using RBF and multilayer perceptron (MLP).	<p>RBF: i) accuracy: 94.7368%, ii) sensitivity: 100.00%, iii) specificity: 93.3333%, and iv) precision: 80.00%.</p> <p>MLP: i) accuracy: 89.4737%, i) sensitivity: 100.00%, iii) specificity: 86.6667%, iv) precision: 66.6667%.</p> <p>RBF tuned kernel parameter is better compared to MLP.</p>
[34], [42]	SVM	Implemented the RBF tuned parameter in SVM for agarwood oil quality classification.	<p>RBF: i) accuracy: 94.7368%, ii) sensitivity: 100.00%, iii) specificity: 93.3333%, iv) precision: 80.00%.</p> <p>The RBF-tuned SVM model met all classification performance criteria for agarwood oil quality.</p>
[14], [50]	BSVM	Assess statistical learning model Boolean support vector machines (BSVM) to the problem of agarwood oil quality categorization.	Performance measures for BSVM: i) accuracy: 89.4737%, i) sensitivity: 100.00%, iii) specificity: 86.6667%, iv) precision: 66.6667%. Boolean learning functions showed limited tolerance in maximizing hypermargin for agarwood oil classification.
[51], [52]	KNN	KNN was applied to classify agarwood oil quality based on chemical compounds.	Min-max scaling (0-1) was applied, and the KNN model (k=1-8) achieved 100% classification accuracy for agarwood oil quality.
[36], [53]	KNN	To classify Cymbopogon oil species (citronella and lemongrass) using a KNN model.	<p>Accuracy (k=1 until k=5):</p> <ul style="list-style-type: none"> - Training test: range between 88% to 100% - Testing test: range between 66% to 100% <p>KNN (k=1, 2) achieved 100% accuracy for classifying citronella and lemongrass oils.</p>
[54], [55]	KNN	To classify agarwood oil samples based on their origin (lab, local manufacturer, market) using a KNN model.	<p>Accuracy (k=1 and k=2):</p> <ul style="list-style-type: none"> - Training test: 98.63% - Testing test: 100% <p>KNN effectively classified agarwood oil samples into three sources.</p>
[37]	KNN	To developed a new method for classifying agarwood oil quality using chemical composition analysis and a KNN model.	<ul style="list-style-type: none"> - Accuracy: 100% - Sensitivity: 100% - Specificity: 100% - Precision: 100% <p>The KNN model successfully classified all samples correctly based on their quality grade.</p>

Figure 4 compares the performance of four ML algorithms using mean±standard deviation (SD) accuracy and F1-score distributions. Figure 4(a) shows the mean±SD accuracy across studies, where ANN and KNN achieved the highest mean accuracies (87.5%±17.7 and 99.3%±1.1, respectively), while RF exhibited greater variability, indicating sensitivity to dataset composition. Figure 4(b) presents the

F1-score distribution, with SVM demonstrating stable and strong performance comparable to KNN, confirming their robustness across diverse essential oil datasets [47], [54]. Across the reviewed literature, ANN performed well on larger or synthetically augmented datasets [38], [39], [44], RF delivered moderate but reliable results [19], [21], [43], [47], SVM with RBF kernels showed strong accuracy and generalization on complex GC-MS data [42], [49], and KNN achieved near perfect classification on smaller, well separated datasets [37], [52], [54]. These findings indicate that algorithmic robustness improves with dataset representativeness, while classical ML approaches remain the most practical choice due to limited data availability and standardization.

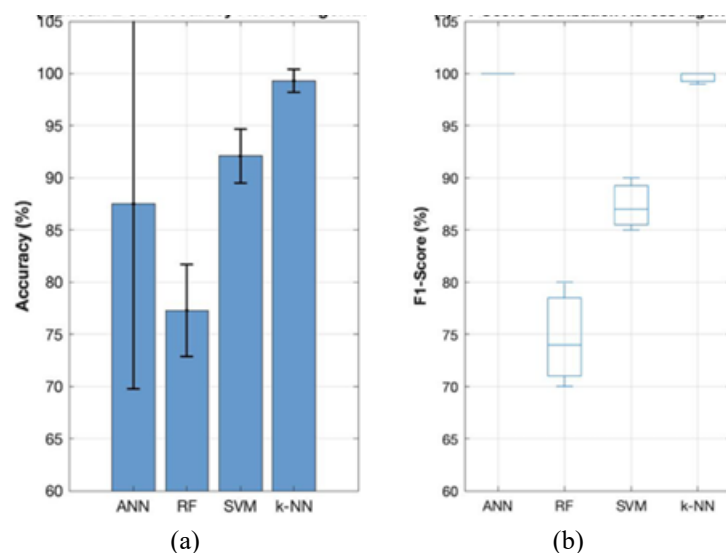


Figure 4. Comparative performance of ML algorithms for *Aquilaria* essential oil classification of (a) mean±SD accuracy and (b) F1-score distribution across algorithms

3.4. Challenges and limitations

Despite promising performance, several challenges limit the broader application of ML for agarwood essential oil classification. Most studies rely on small and imbalanced datasets, often requiring synthetic data augmentation, which may introduce bias and overfitting, reducing generalizability. The absence of standardized GC-MS data formats, acquisition parameters, compound reporting and preprocessing pipelines further complicates performance comparison, model transferability and reproducibility. Variations in feature selection, scaling and validation strategies contribute to data heterogeneity, meaning aggregated performance metrics should be interpreted cautiously. These limitations highlight the need for standardized chemical datasets, consistent analytical workflows, explicit reporting of ML configurations, larger multi-species samples and cross-laboratory validation to support reliable real-world deployment.

4. CONCLUSION

This review demonstrates the effectiveness of AI and ML techniques, particularly ANN, RF, SVM, and KNN, in advancing the classification and quality assessment of *Aquilaria* essential oils using GC-MS-derived chemical data. Model robustness and classification accuracy are strongly influenced by dataset quality, compound diversity and parameter optimization. Future research should explore transfer learning, deep convolutional neural networks and multimodal data fusion integrating GC-MS with complementary spectroscopic techniques such as Fourier transform infrared (FTIR). The establishment of open, standardized benchmark datasets would further enhance reproducibility and fair model comparison. Although limited to published studies with heterogeneous experimental settings, these constraints reflect the current state of the literature. Overall, AI-driven frameworks offer strong practical potential for automated quality control and authentication in the perfumery and agarwood industries.

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AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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Ahmad Sabri														
Nur Athirah Syafiqah	✓	✓	✓			✓		✓		✓	✓			
Noramli														
Muhammad Ikhsan	✓		✓	✓		✓				✓	✓			
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C : Conceptualization

M : Methodology

So : Software

Va : Validation

Fo : Formal analysis

I : Investigation

R : Resources

D : Data Curation

O : Writing - Original Draft

E : Writing - Review & Editing

Vi : Visualization

Su : Supervision

P : Project administration

Fu : Funding acquisition

CONFLICT OF INTEREST STATEMENT

Authors state no conflict of interest.

INFORMED CONSENT

We have obtained informed consent from all individuals included in this study.

DATA AVAILABILITY

Data availability is not applicable to this paper as no new data were created or analyzed in this study.

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