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Regression Modelling with Coupled GC–MS/GC–FID for Robust Classification of *Aquilaria* Species

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ABSTRACT

The *Aquilaria* genus is renowned for producing agarwood, a highly valuable resinous heartwood with diverse applications in perfumery, traditional medicine, and cultural practices. Accurate species identification is critical for quality control, consumer trust, and conservation, yet traditional methods are often unreliable due to chemical similarities among species. This study aimed to develop a regression-based classification model for four *Aquilaria* species (*A. beccariana*, *A. malaccensis*, *A. crassna*, and *A. subintegra*) using the chemical composition of their essential oils. Essential oils were extracted via hydrodistillation and analyzed using Gas Chromatography–Mass Spectrometry (GC–MS) coupled with Gas Chromatography–Flame Ionization Detection (GC–FID). Stepwise multiple regression identified three chemical compounds as the most significant contributors to species differentiation. The final model achieved a high predictive accuracy ($R^2 = 0.990$; adjusted $R^2 = 0.989$), with clear visual separation of species observed in three-dimensional scatter plots. These findings demonstrate that a targeted multivariate approach using a small set of chemical markers provides a robust, interpretable, and scalable method for *Aquilaria* species classification, offering valuable applications for authentication, quality control, and conservation in the agarwood industry.

Keywords: *Aquilaria* species classification, essential oil profiling, stepwise multiple regression, chemical compounds, agarwood authentication.

1. Introduction

The *Aquilaria* genus is renowned for producing agarwood, a resinous heartwood that holds significant cultural, economic, and ecological value. Agarwood is prized for its distinctive fragrance and is widely used in healthcare, religious ceremonies, and the fragrance industry [1], [2]. It is among the most valuable natural raw materials, with prices reaching up to tens of thousands of dollars per kilogram depending on quality and origin [3], [4]. This high value is attributed to the complex chemical composition of agarwood, which varies among species and environmental conditions [5], [6]. As global demand for agarwood increases, accurate identification of *Aquilaria* species becomes critical to ensure product authenticity, maintain quality control, and support conservation efforts [7].

However, distinguishing *Aquilaria* species based on chemical profiles remains challenging. Many species exhibit similar essential oil compositions, and these profiles can vary due to factors such as geographical location, climate, and tree age [2], [6]. Traditional identification methods, including visual inspection and sensory evaluation, are often insufficiently reliable. Consequently, the agarwood market faces risks of adulteration, mislabelling, and fraud, which negatively impact both producers and consumers [1], [5], [7].

This study aims to develop a robust regression-based model to classify four *Aquilaria* species: *A. beccariana*, *A. malaccensis*, *A. crassna*, and *A. subintegra*. The classification model utilizes the chemical composition of essential oils analyzed via Gas Chromatography–Mass Spectrometry (GC–MS) coupled with Gas Chromatography–Flame Ionization Detection (GC–FID). By applying stepwise regression and three-dimensional scatter plot visualization, this study aims to enhance classification accuracy and provide a scalable tool for quality control in the agarwood industry.

2. Related Works

Chemical profiling of *Aquilaria* essential oils using GC–MS has been extensively employed to characterize the complex mixtures of sesquiterpenes and chromones that contribute to agarwood's distinctive aroma [8], [9], [10]. Despite this, significant overlap in chemical profiles among species complicates direct species identification [1].

Multivariate statistical techniques such as Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) have been used to reduce data dimensionality and group samples based on chemical similarity [11], [12]. While these methods have provided some success, they often fail to capture subtle chemical interactions essential for accurate species discrimination. More recently, machine learning algorithms, including Support Vector Machines (SVM) has demonstrated improved classification performance [11], [13]. However, these approaches typically require large datasets and considerable computational resources, limiting their routine applicability in many agarwood-producing contexts [13], [14].

Stepwise regression modelling offers an interpretable and efficient alternative by identifying significant discriminant compounds and reducing model complexity [15], [16]. When combined with advanced visualization techniques such as three-dimensional scatter plots, this approach facilitates intuitive understanding of species separation within complex chemical datasets. Building upon these methodologies, the present study develops a stepwise regression model to classify four *Aquilaria* species based on essential oil composition. This approach aligns with current advancements in instrumentation data analysis and visualization, aiming to provide a practical and reliable tool for species identification and quality assurance in the agarwood industry.

3. Methodology

This study classifies four *Aquilaria* species using essential oil chemical profiles obtained via GC–MS coupled with GC–FID. Six major compounds were quantified, and stepwise multiple regression identified the most significant variables for species differentiation. The workflow is shown in Figure 1 below.

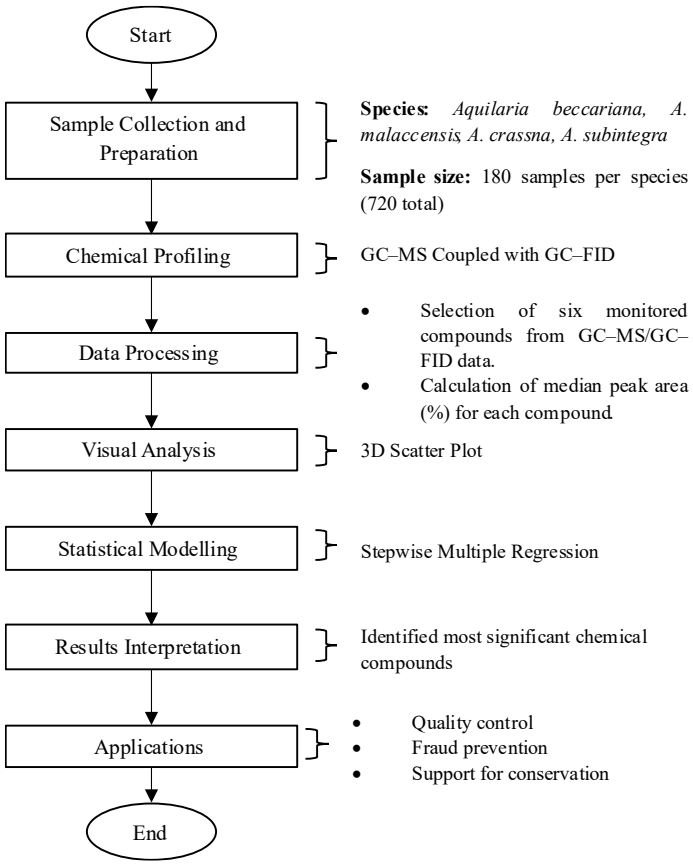

Figure 1. Workflow for Regression-Based Classification of *Aquilaria* Species Using Essential Oil Profiles

3.1 Research Design and Data Collection

This study was designed to classify four *Aquilaria* species *A. beccariana*, *A. malaccensis*, *A. crassna*, and *A. subintegra* based on their essential oil chemical profiles. The primary objective was to develop a regression-based model capable of distinguishing these species according to the chemical composition of their essential oils. Research activities were conducted at the BioAromatic Research Centre of Excellence (BARCE), Universiti Malaysia Pahang Al-Sultan Abdullah (UMPSA), where all agarwood samples were processed and analysed.

A total of 720 essential oil samples were collected, with 180 samples per species. Each sample provided data for six chemical compounds, yielding a robust dataset suitable for statistical modelling. Data collection was standardized such that each species contributed 30 data points per compound, ensuring comparability across species. Statistical and visualization techniques, including regression analysis and 3D scatter plots, were applied to develop an effective classification model. This model aims to facilitate species identification, contributing to the standardization and traceability of agarwood products and offering reliable tools for quality control to mitigate fraud and mislabelling in the agarwood market.

3.2 Essential Oil Extraction and Analysis

Essential oils were extracted from *A. beccariana*, *A. malaccensis*, *A. crassna*, and *A. subintegra* using a standardized hydro-distillation method. The hydro-distillation process lasted three to five days, after which the oils were diluted with analytical-grade dichloromethane (DCM) to improve solubility for chemical analysis. Chemical profiling was conducted using Gas Chromatography–Mass Spectrometry (GC–MS) coupled with Gas Chromatography–Flame Ionization Detection (GC–FID), combining qualitative and quantitative analytical capabilities in a complementary manner [1], [17].

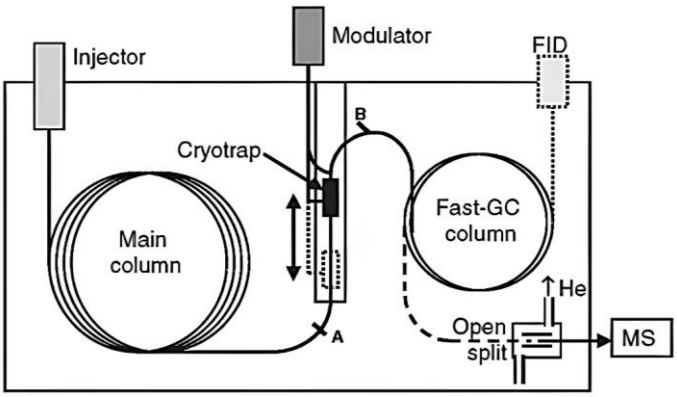

Figure 2. GC×GC System with Dual Detection: MS and FID[17]

Table 1. Concentration of chemical compounds across *Aquilaria* species (%)

Code	Chemical Compounds	Molecular formula	Ident. Mode	Peak Area (%)			
				AB	AM	AC	AS
A	β-selinene	$C_{15}H_{24}$	FID, MS	0.66	0.56	0.11	0.37
B	dihyro-β-agarofuran	$C_{15}H_{26}O$	FID, MS	1.25	0.55	0.48	0.44
C	δ-guaiene	$C_{15}H_{24}$	FID, MS	0.74	2.02	0.21	0.35
D	10-epi-γ-eudesmol	$C_{15}H_{26}0$	FID, MS	0.34	6.73	2.54	2.16
E	γ-eudesmol	$C_{15}H_{26}0$	FID, MS	0.26	2.17	0.95	1.85
F	Pentadecanoic acid	$C_{15}H_{3O}O_2$	FID, MS	0.15	0.15	0.14	0.46

GC–MS provides detailed qualitative identification by separating volatile compounds chromatographically and then detecting them using mass spectrometry [18], [19]. Each compound's unique mass spectral pattern enables precise identification through comparison with spectral libraries and reference standards. This method is essential for characterizing the complex chemical composition of agarwood essential oils. GC–FID offers sensitive and reliable quantification of the compounds identified by GC–MS. Following chromatographic separation, the flame ionization detector measures the ions produced by burning the compounds in a hydrogen-air flame, generating signals proportional to compound concentration. This technique allows accurate determination of the relative abundance of each component within the essential oils [20].

The coupling of GC–MS and GC–FID leverages the strengths of both methods: GC–MS's ability to identify compounds and GC–FID's capacity to provide precise quantitative data [8], [21]. This integrated approach ensures

comprehensive chemical analysis, crucial for robust species classification based on essential oil profiles. Analyses were performed using an Agilent 7890B GC System with a 5977A Mass Spectrometer and a DB-1ms column (30 m × 250 µm × 0.25 µm), as detailed in Figure 2. The column temperature was programmed from 80°C to 250°C at 3°C/min, with helium as the carrier gas at 1.0 mL/min. The GC–FID detector operated at 250°C to optimize sensitivity [1], [22]. Each sample was analysed in triplicate to ensure reproducibility. Six key chemical compounds (β-selinene, dihydro-β-agarofuran, δ-guaiene, 10-epi-γ-eudesmol, γ-eudesmol, and pentadecanoic acid) were consistently detected across all species and selected for further analysis, as summarized in Table I. In Table 1, AB, AM, AC, and AS denote *Aquilaria beccariana*, *Aquilaria malaccensis*, *Aquilaria crassna*, and *Aquilaria subintegra*, respectively. The resulting dataset formed the basis for subsequent statistical modelling and species classification.

3.3 Statistical Methods and Data Analysis

Stepwise regression is a systematic and iterative statistical technique used to identify the most significant predictor variables from a larger set of potential candidates. It combines both forward selection, which adds variables to the model one at a time based on their statistical significance, and backward elimination, which removes variables that do not contribute meaningfully to the model [15]. This dual approach enables the construction of a parsimonious regression model by retaining only those chemical compounds that provide substantial explanatory power for species classification. Stepwise regression is particularly useful when dealing with multiple, potentially correlated variables, as it reduces the risk of overfitting and enhances model interpretability [15], [16]. In this study, stepwise regression was selected to refine the dataset of chemical compounds and to develop a robust model capable of accurately distinguishing among the four *Aquilaria* species [14], [15].

The statistical analysis was performed using SPSS (v.26). Stepwise regression served as the primary method to identify the chemical compounds that significantly differentiate the species. Through iterative evaluation, the model retained only those compounds with strong statistical relevance, resulting in a refined set of predictors for species classification. The final regression equation can be expressed in the following general form in Equation (1):

$$Species = \beta_0 + \beta_1(C) + \beta_2(D) + \beta_3(E) \quad (1)$$

Where compounds C, D, and E represent the peak areas of δ-guaiene, 10-epi-γ-eudesmol, and γ-eudesmol, respectively. The parameters β_1, β_2, and β_3 are the regression coefficients that quantify the strength and direction of the relationship between each compound's concentration and the predicted species classification. A higher β value indicates a greater influence of that compound on differentiating species. β_0 is the intercept term, representing the baseline value of the model when all compound concentrations are zero. Three-dimensional scatter plots were subsequently generated to visualize the relationships among the most discriminative chemical compounds and their contribution to species separation. Each axis represented one of the selected compounds, enabling clear visualization of species clusters in multidimensional chemical space.

The final regression model's performance was assessed using the coefficient of determination (R^2), which quantifies the proportion of variance in species classification explained by the selected compounds. A high R^2 value indicates that the model effectively captures the variability necessary for accurate species differentiation. This metric provided an objective measure of the model's predictive accuracy and robustness. The integration of stepwise regression and 3D visualization facilitated a comprehensive analysis, supporting both model refinement and a deeper understanding of the chemical interactions underlying species classification.

4. Results and Discussion

The chemical analysis focused on six compounds consistently detected across the four *Aquilaria* species: β-selinene (A), dihydro-β-agarofuran (B), δ-guaiene (C), 10-epi-γ-eudesmol (D), γ-eudesmol (E), and pentadecanoic acid (F). These compounds were quantified based on their relative peak area percentages obtained from GC-MS and GC-FID analyses. Figure 3 illustrates the median peak area percentages for each compound across all samples.

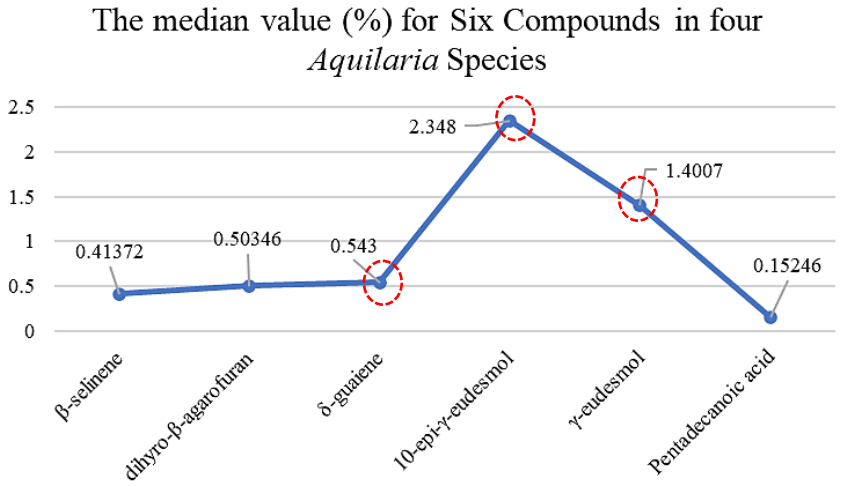

Figure 3. Median Peak Area (%) Values of Chemical Compounds in *Aquilaria* Species

Among the six compounds, 10-epi-γ-eudesmol (D) displayed the highest median peak area at 2.348%, indicating its prominence in the essential oil profiles of the *Aquilaria* species studied. The compound γ-eudesmol (E) also showed a substantial median peak area of 1.4007%, suggesting its significant presence across species. δ-guaiene (C), with a median of 0.543%, exhibited moderate abundance and contributed notable variability in concentration between species.

Conversely, β-selinene (A) and pentadecanoic acid (F) had consistently low median peak areas and showed minimal variability across species, suggesting a limited role in distinguishing among them. Dihydro-β-agarofuran (B) exhibited a low median peak area (0.50346%) and narrow interquartile range, further indicating its limited discriminatory capacity. The higher variability and median values observed in δ-guaiene (C), 10-epi-γ-eudesmol (D), and γ-eudesmol (E) suggest that these compounds are the most informative for differentiating the *Aquilaria* species. Their distributions across species highlight potential chemical signatures unique to each species' essential oil profile.

To visualize species differentiation, a 3D scatter plot was constructed using the peak area percentages of δ-guaiene (C), 10-epi-γ-eudesmol (D), and γ-eudesmol (E) (Figure 4). The plot reveals distinct clusters corresponding to each species, demonstrating clear separation in multidimensional chemical space. Specifically, *Aquilaria beccariana* samples clustered towards the lower ends of all three compound axes, reflecting comparatively low concentrations. In contrast, *Aquilaria malaccensis* exhibited elevated values along the 10-epi-γ-eudesmol (D) and γ-eudesmol (E) axes, forming a clearly distinct cluster. *Aquilaria crassna* and *Aquilaria subintegra* showed moderate levels of δ-guaiene and overlapping γ-eudesmol values but remained distinguishable due to subtle shifts along the 10-epi-γ-eudesmol axis. This clear spatial differentiation confirms that the combined variation in these compounds effectively captures interspecies chemical differences, supporting their utility as classification markers.

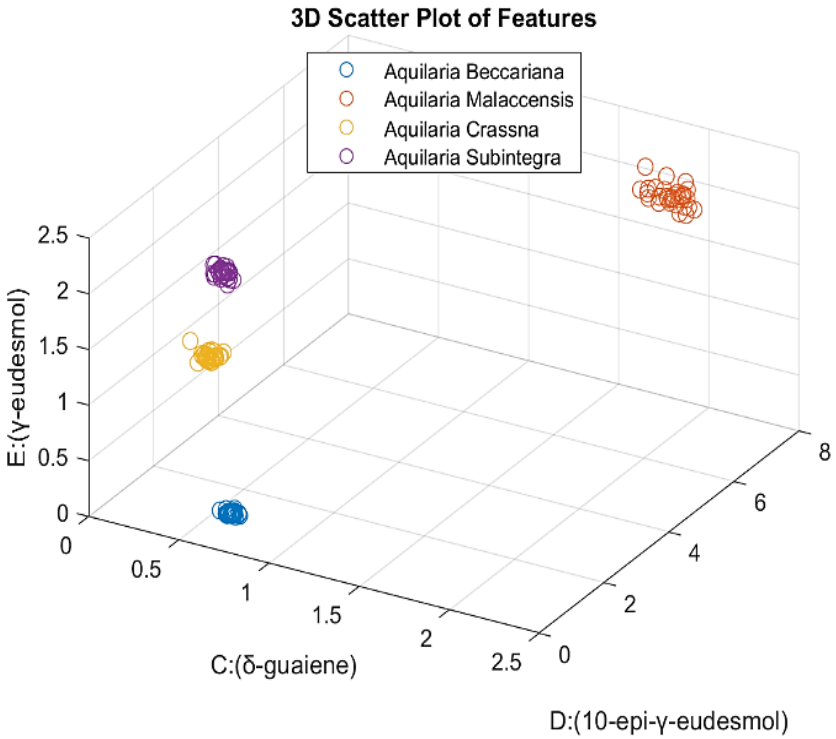

Figure 4. Median 3D Scatter Plot of *Aquilaria* Species Clustering by Significant Chemical Compounds

Following the identification of most significant compounds, a stepwise multiple regression analysis was performed to statistically model the relationship between chemical composition and *Aquilaria* species classification. The regression approach aimed to determine which compounds significantly contributed to species differentiation while optimizing model simplicity and predictive performance [15].

In Table 2, the note "Dependent Variable: Species" indicates that the categorical outcome being predicted in the regression model is the *Aquilaria* species identity. Each essential oil sample was assigned to one of four species (*A. beccariana*, *A. malaccensis*, *A. crassna*, or *A. subintegra*) and this variable was numerically encoded to enable statistical analysis. Thus, the regression model predicts species classification based on the quantitative inputs (peak areas of chemical compounds), allowing species differentiation according to essential oil composition.

The analysis considered all six monitored compounds (A–F) as independent variables and employed the stepwise multiple regression method, which combines forward selection and backward elimination. This means that variables were added to or removed from the model sequentially based on their statistical significance (entry criterion: $p \leq 0.05$; removal criterion: $p \geq 0.10$).

Table 2. Regression Variable Selection

Variables Entered/Removed[a]			
Model	**Variables Entered**	**Variables Removed**	**Method**
1	Compound_E	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
2	Compound_C	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
3	Compound_D	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).

a. Dependent Variable: Species

Table 2 summarizes the variable selection process. Each row represents a step in which a new compound was added to the model. The column "Method" indicates that the same stepwise selection procedure was applied at every stage. The entry "Variables Removed = None" signifies that no previously entered variable was excluded during that step because all retained variables continued to meet the significance threshold.

In this process, Compound E (γ-eudesmol) was entered first, followed by Compound C (δ-guaiene) and Compound D (10-epi-γ-eudesmol). Compounds A (β-selinene), B (dihydro-β-agarofuran), and F (pentadecanoic acid) were not included in the final model because their contributions were statistically insignificant ($p > 0.05$). This stepwise inclusion

pattern demonstrates that the three retained compounds provided the most significant explanatory power for species differentiation.

Table 3. Model Summary

Model Summary[d]	
R	**R^2**
0.516[a]	0.267
0.994[b]	0.988
0.995[c]	0.990

a. Predictors: (Constant), Compound_E
b. Predictors: (Constant), Compound_E, Compound_C
c. Predictors: (Constant), Compound_E, Compound_C, Compound_D
d. Dependent Variable: Species

In Table 3, the term *Model Summary*^{d} refers to the statistical output produced by the SPSS stepwise multiple regression analysis, which presents the overall performance of each model iteration. The superscript *d* corresponds to the footnote indicating that the dependent variable in all regression models is *Species*. Each row (Models 1 to 3) represents a sequential stage of the stepwise regression process in which additional predictors were entered based on statistical significance criteria ($p \leq 0.05$ for entry and $p \geq 0.10$ for removal).

The column "Predictors" lists the independent variables (chemical compounds) retained in each stage of model development. Specifically, Model 1 included Compound E (γ-eudesmol), Model 2 added Compound C (δ-guaiene), and Model 3 further incorporated Compound D (10-epi-γ-eudesmol) to produce the final model. The coefficients R, R^2, and Adjusted R^2 represent the correlation strength and the proportion of variance in species classification explained by each successive model. The steady increase in R^2 from 0.267 in Model 1 to 0.990 in Model 3 indicates progressive enhancement in model fit as additional significant predictors were introduced. This pattern confirms that the combined influence of γ-eudesmol, δ-guaiene, and 10-epi-γ-eudesmol provides the most statistically robust framework for distinguishing *Aquilaria* species.

The results presented in Table 3 indicate that the final regression model achieved a high degree of predictive accuracy, with a correlation coefficient (R) of 0.995 and a coefficient of determination (R^2) of 0.990. This demonstrates that 99% of the variance in species classification is explained by the three selected compounds, reflecting the strong explanatory power and robustness of the model. Diagnostic assessments confirmed that the residuals were normally distributed and homoscedastic, validating the model's statistical assumptions and reliability.

These findings suggest that a regression model based on a limited set of significant chemical predictors can effectively classify *Aquilaria* species with high precision. From a practical standpoint, focusing on γ-eudesmol, δ-guaiene, and 10-epi-γ-eudesmol as primary discriminatory markers simplifies analytical procedures and enhances efficiency in species authentication. This targeted approach offers substantial value for agarwood quality control, authentication, and fraud prevention within the commercial supply chain.

Despite the strong performance of the regression model, certain limitations must be acknowledged. Although the high R^2 values indicate an excellent fit within the present dataset, the model's generalizability requires further validation using larger and more diverse sample populations. Environmental and biological factors, such as geographic variation, tree age, soil composition, and extraction methods, may influence the chemical composition of essential oils and consequently affect classification accuracy.

Future research should therefore focus on expanding the dataset to include additional *Aquilaria* species and broader geographic regions to ensure greater representativeness. Integrating chemical profiling with advanced analytical approaches, such as machine learning algorithms or genetic-based identification techniques, could further enhance classification robustness and adaptability. Such developments would strengthen the scientific foundation for agarwood authentication, support sustainable resource management, and improve traceability throughout the agarwood value chain.

5. Conclusions

This study developed and validated a regression-based model with high predictive accuracy for the classification of four *Aquilaria* species using their essential oil chemical profiles. The identification of γ-eudesmol, δ-guaiene, and 10-epi-γ-eudesmol as the most significant chemical markers demonstrates their effectiveness as reliable indicators for interspecies differentiation. The model's strong statistical performance ($R^2 = 0.990$) confirms that a multivariate regression approach provides superior precision compared with single-compound analyses, offering a scientifically robust framework for agarwood authentication. The findings have important implications for the agarwood industry. By utilizing a focused set of the most significant chemical predictors, this approach facilitates efficient and reproducible species identification, strengthens quality assurance practices, and supports regulatory efforts to prevent mislabelling and adulteration. Moreover, the model contributes to sustainable resource management by enabling

traceable and verifiable species classification, which is critical for conservation initiatives involving *Aquilaria* species. Although this study was limited to four species and samples obtained under controlled conditions, the established methodology can be adapted to broader datasets encompassing additional species, geographic origins, and environmental variables. Future research should focus on integrating this chemical profiling approach with advanced analytical frameworks, such as machine learning algorithms and genetic-based identification tools, to enhance classification accuracy, scalability, and global applicability. Overall, this work presents a practical, interpretable, and scientifically grounded solution for addressing the ongoing challenges of agarwood species authentication, quality assurance, and conservation management within the global agarwood trade.

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References

[1] N. A. Syafiqah Noramli, N. A. S. Ahmad Sabri, M. I. Roslan, N. Ismail, Z. M. Yusoff, and M. N. Taib, "Unraveling the relationships among essential oil compounds in Aquilaria species using GC-MS and GC-FID techniques," *Indonesian Journal of Electrical Engineering and Computer Science*, vol. 39, no. 1, p. 167, Jul. 2025, doi: 10.11591/ijeecs.v39.i1.pp167-177.

[2] P. Shivanand, N. F. Arbie, S. Krishnamoorthy, and N. Ahmad, "Agarwood—The Fragrant Molecules of a Wounded Tree," *Molecules*, vol. 27, no. 11, p. 3386, May 2022, doi: 10.3390/molecules27113386.

[3] S. M. H. Mohd Huzir, S. N. Tajuddin, Z. Mohd Yusoff, N. Ismail, A. A. Almisreb, and M. N. Taib, "Agarwood oil quality identification using artificial neural network modelling for five grades," *International Journal of Electrical and Computer Engineering (IJECE)*, vol. 14, no. 2, p. 2254, Apr. 2024, doi: 10.11591/ijece.v14i2.pp2254-2261.

[4] M. Huang, S. Ma, M. Qiao, Y. Fu, and Y. Li, "Quality Similarity between Induced Agarwood by Fungus and Wild Agarwood," *J Agric Food Chem*, vol. 71, no. 42, pp. 15620–15631, Oct. 2023, doi: 10.1021/acs.jafc.3c04322.

[5] P. Zhang, X. Li, Z. Cui, and D. Xu, "Morphological, physiological, biochemical and molecular analyses reveal wounding-induced agarwood formation mechanism in two types of Aquilaria sinensis (Lour.) Spreng," *Ind Crops Prod*, vol. 178, p. 114603, Apr. 2022, doi: 10.1016/j.indcrop.2022.114603.

[6] X. Wang, S. W. Chan, N. Singaram, M.-L. Teoh, S. H. Mah, and C. Y. Looi, "Essential oil from Aquilaria spp. (agarwood): a comprehensive review on the impact of extraction methods on yield, chemical composition, and biological activities," *Journal of Essential Oil Research*, vol. 37, no. 1, pp. 110–144, Jan. 2025, doi: 10.1080/10412905.2024.2447706.

[7] Z.-Q. Xie, J.-Y. Xu, M. Rafiq, and C.-S. Cheng, "An analysis of Agarwood trade patterns, historical perspectives, and species identification challenges: repercussions for importing nations," *TMR Modern Herbal Medicine*, vol. 7, no. 1, p. 1, 2024, doi: 10.53388/MHM2024001.

[8] N. A. S. Noramli, N. A. S. A. Sabri, M. I. Roslan, N. Ismail, Z. M. Yusoff, and M. N. Taib, "Analytical Characterization of Aquilaria Species Essential Oils Using Advanced Chromatographic Techniques Based on GC-MS and GC-FID," in *2025 21st IEEE International Colloquium on Signal Processing & Its Applications (CSPA)*, IEEE, Feb. 2025, pp. 10–15. doi: 10.1109/CSPA64953.2025.10933407.

[9] S. Gutiérrez *et al.*, "A synthetic biology and green bioprocess approach to recreate agarwood sesquiterpenoid mixtures," *Green Chemistry*, vol. 26, no. 5, pp. 2577–2591, 2024, doi: 10.1039/D3GC03708H.

[10] X. Zhang *et al.*, "Sesquiterpenoids in Agarwood: Biosynthesis, Microbial Induction, and Pharmacological Activities," *J Agric Food Chem*, vol. 72, no. 42, pp. 23039–23052, Oct. 2024, doi: 10.1021/acs.jafc.4c06383.

[11] R. Hayati, A. A. Munawar, E. Lukitaningsih, N. Earlia, T. Karma, and R. Idroes, "Combination of PCA with LDA and SVM classifiers: A model for determining the geographical origin of coconut in the coastal plantation, Aceh Province, Indonesia," *Case Studies in Chemical and Environmental Engineering*, vol. 9, Jun. 2024, doi: 10.1016/j.cscee.2023.100552.

[12] G. Catinella, N. Badalamenti, V. Ilardi, S. Rosselli, L. De Martino, and M. Bruno, "The essential oil compositions of three teucrium taxa growing wild in sicily: Hca and pca analyses," *Molecules*, vol. 26, no. 3, Feb. 2021, doi: 10.3390/molecules26030643.

[13] M. A. Haqmi Abas, "Agarwood Oil Quality Classification using Support Vector Classifier and Grid Search Cross Validation Hyperparameter Tuning," *International Journal of Emerging Trends in Engineering Research*, vol. 8, no. 6, pp. 2551–2556, Jun. 2020, doi: 10.30534/ijeter/2020/55862020.

[14] M. Awad and R. Khanna, "Support Vector Machines for Classification," in *Efficient Learning Machines*, Apress, 2022, pp. 39–66. doi: 10.1007/978-1-4302-5990-9_3.
[15] S. M. H. M. Huzir *et al.*, "Stepwise regression of agarwood oil significant chemical compounds into four quality differentiation," *Indonesian Journal of Electrical Engineering and Computer Science*, vol. 29, no. 2, p. 735, Feb. 2023, doi: 10.11591/ijeecs.v29.i2.pp735-741.
[16] N. Zawani Mahabob, A. F. Mohd Amidon, Z. Mohd Yusoff, N. Ismail, and S. N. Tajjudin, "Comparison of ANN Performance Towards Agarwood Oil Compounds Pre-processing Based on Principal Component Analysis (PCA) and Stepwise Regression Selection Method," *Journal of Electrical & Electronic Systems Research*, vol. 19, no. OCT2021, pp. 51–55, Oct. 2021, doi: 10.24191/jeesr.v19i1.007.
[17] G. Schomburg, "Two-dimensional gas chromatography: Principles, instrumentation, methods," *J Chromatogr A*, vol. 703, no. 1–2, pp. 309–325, Jun. 1995, doi: 10.1016/0021-9673(95)00190-X.
[18] S. S.S.S.M, V. Atyam, M. Avidi, and D. Ayinala, "A Review on Gas chromatography – Mass spectroscopy: Short Communication," *Journal of Pharma Insights and Research*, vol. 2, no. 1, pp. 009–013, Feb. 2024, doi: 10.5281/zenodo.10614850.
[19] L. Mondello, C. Cordero, H. G. Janssen, R. E. Synovec, M. Zoccali, and P. Q. Tranchida, "Comprehensive two-dimensional gas chromatography–mass spectrometry," *Nature Reviews Methods Primers 2025 5:1*, vol. 5, no. 1, pp. 1–18, Feb. 2025, doi: 10.1038/s43586-024-00379-3.
[20] Ł. Dąbrowski, "Some Aspects of the Use of Carbon Dioxide as a Carrier and Makeup Gas in GC–FID Analysis," *Separations*, vol. 11, no. 12, p. 347, Dec. 2024, doi: 10.3390/SEPARATIONS11120347/S1.
[21] N. I. N. A. and S. N. T. N. M. Sarih, "Analysis of GC-FID and GC-MS Microwave-Assisted Hydrodistillation Extraction(MAHD)of Agarwood Chips," 2021.
[22] Z. M. Yusoff and N. Ismail, "Datasets of chemical compounds in three different species of aquilaria using GC-MS coupled with GC-FID analysis," *Data Brief*, vol. 53, p. 110209, Apr. 2024, doi: 10.1016/j.dib.2024.110209.