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Compound Distribution Analysis of *Aquilaria Beccariana* Essential Oil Using Coupled GC-MS/GC-FID Instrumentation

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ABSTRACT

This study investigates the compound signal characteristics of *Aquilaria beccariana* essential oil using data acquired from a coupled Gas Chromatography–Mass Spectrometry (GC-MS) and Gas Chromatography–Flame Ionization Detector (GC-FID) system. The coupled configuration enables simultaneous identification and quantification of chemical constituents, thereby improving signal reliability and analytical precision. A total of 18 compounds were identified and grouped into four chemical classes, namely carboxylic acids, sesquiterpenes, sesquiterpenoids and other compound. To examine compound behaviour within the species, peak area (%) values were analyzed using jitter scatter plots and bar graphs. The sesquiterpene group showed the highest compound density and moderate intensity, with *allo*-aromadendrene and beta-patchoulene identified as prominent contributors. Benzyl benzoate, a non-sesquiterpenoid compound, recorded the highest peak area (10.61%), dominating the overall profile. These findings provide a detailed view of compound distribution in *A. beccariana*, offering insight into signal patterns that support future species authentication and chemical fingerprinting based on GC instrumentation data.

Keywords: *Aquilaria beccariana*, GC-MS/GC-FID, Peak Area Distribution, Compound Signal Analysis, Essential Oil Profiling

1. Introduction

Aquilaria beccariana is a native agarwood-producing species known for its fragrant, resinous heartwood, which yields a high-value essential oil used in perfumery, incense and traditional medicine [1–5]. Compared to *A. banaensis*, *A. beccariana* exhibits a broader geographic distribution and has been reported in Eastern Malaysia, Brunei and Indonesia [6]. The quality, grading and classification of agarwood oil are strongly influenced by its chemical composition, particularly the relative abundance of sesquiterpenes, chromones and other volatile organic compounds [1–3]. These compounds play a central role in defining the oil's aroma profile while also contributing to its therapeutic and pharmacological potential.

However, the compound profile of agarwood oil is highly dynamic due to influencing factors such as genetic diversity, harvesting methods, tree age, induction techniques and geographical origin [7]. Even within the same species, this variability can significantly impact quality and pose challenges in standardizing grading and authentication. Therefore, researchers and producers necessitate analytical methods capable of capturing true compound distribution and signal intensity in a consistent, reproducible manner [8], [9].

To ensure product traceability, authentication and regulatory compliance, it is essential to establish a robust and reproducible chemical profile for each agarwood species, including *A. beccariana*. Understanding which compounds dominate, how they are distributed across classes (such as sesquiterpenes or carboxylic acids), and how consistently they are detected across samples is critical not only for scientific classification but also for industrial quality control. Conventional sensory-based classification, which relies on subjective evaluation by experienced graders, is insufficient due to limitations in objectivity, reproducibility and scalability [10]. This limitation highlights the urgent need for data-driven and instrument-based analytical techniques that can provide objective, quantitative insights into compound intensity and chemical behaviour [11–14].

In recent years, chromatographic techniques have become the standard approach for essential oil profiling, especially Gas Chromatography–Mass Spectrometry (GC-MS) and Gas Chromatography–Flame Ionization Detector (GC-FID) [15–17]. These techniques offer complementary outputs where GC-MS is used for compound identification and GC-FID is used for quantification based on peak area analysis. By coupling both detectors within a single run, researchers are able to obtain more consistent and reliable data for chemical profiling [3], [16–18].

This study aims to report the compound distribution of *A. beccariana* essential oil using data acquired through a coupled GC-MS and GC-FID system. By focusing on signal analysis based on peak area (%) values, this approach allows for reliable assessment of compound intensity and variability within the species [16–18]. The findings are expected to contribute to chemical characterization, and support future applications in standardization, fingerprinting and authentication of agarwood oils [12].

2. Coupled GC-MS/GC-FID Instrumentation

GC-MS and GC-FID are two of the most widely used instrumental techniques for chemical analysis in essential oil studies [3], [16–18]. GC-MS enables compound identification through the separation of volatile components followed by detection based on their mass-to-charge (m/z) ratios and fragmentation patterns. The resulting mass spectra are matched against reference spectral libraries such as the NIST (National Institute of Standards and Technology) database to confirm compound identity with high specificity [15]. This makes GC-MS particularly valuable for profiling complex natural products, such as essential oils, which contain numerous structurally similar constituents.

In contrast, GC-FID is used primarily for the quantification of organic compounds. As compounds elute from the GC column, they pass through a hydrogen–air flame in the FID detector, where they are ionized and burned, producing an electrical signal proportional to the number of carbon atoms in the molecule [18]. This signal is translated into peak area (%), which reflects the relative abundance of the compound in the sample. GC-FID offers excellent sensitivity for hydrocarbons and other volatile organics, and it is well-known for its repeatability and wide linear dynamic range. These advantages make it particularly suitable for quantitative analysis, even when sample concentrations vary significantly.

When these two techniques are coupled, especially when both GC-MS and GC-FID detectors are connected to the same gas chromatograph via a post-column splitter, the analytical setup benefits from the strengths of both systems. The GC column performs the same separation, but the effluent is split and simultaneously delivered to both detectors. This configuration allows for real-time compound identification and quantification within a single run, enhancing data integrity and reducing the need for repeat analyses [11], [19–21]. It also increases detection reliability by ensuring that both identity and intensity are captured for every analyte. In samples such as essential oils, where many compounds co-elute or have similar retention times, this dual-detection system helps minimize ambiguity, particularly for minor or trace-level compounds that may be overlooked or misidentified in a single-detector system [16].

In this study, the coupled GC-MS/GC-FID system was applied to the chemical profiling of *A. beccariana* essential oil, a species known for its commercial and medicinal value. A total of 18 compounds were detected, and each was assigned to one of four chemical classes, namely carboxylic acids, sesquiterpenes, sesquiterpenoids and other compounds [22]. The GC-MS detector was used to confirm compound identities based on spectral matching, while the GC-FID detector provided peak area (%) data representing relative compound concentration.

The acquired peak area data served as the core input for downstream signal-based analysis. Each compound's intensity was assessed not only individually, but also in relation to other compounds within the same group, enabling intra-group and inter-group comparisons. These values were subsequently visualized using jitter scatter plots and bar graphs, providing a clear overview of signal distribution patterns and compound dominance across the species. This graphical approach allowed researchers to assess signal consistency and variability, helping identify candidate compounds that could serve as species-specific chemical markers.

By integrating both qualitative and quantitative analysis in a single framework, the use of GC-MS/GC-FID significantly improved the robustness and depth of the chemical profiling process. This methodology provided reliable insights into compound behaviour and composition, forming a strong foundation for species characterization, standardization and potential authentication of *A. beccariana* oil in future studies.

3. Methodology

This methodology outlines the analytical approach taken to examine the chemical composition of *A. beccariana* essential oil using a GC-based dual detection system. The study was conducted to evaluate signal intensity and compound distribution using peak area (%) data derived from a structured instrumental workflow. The analytical process was specifically designed to capture reliable compound-level information from a single experimental run.

A total of 18 volatile compounds were detected and systematically organised into four distinct chemical classes, namely carboxylic acids, sesquiterpenes, sesquiterpenoids, and other compound types [22]. Each compound was assigned

a label according to its spectral identity, and its corresponding peak area was used as a quantitative measure for comparing signal behaviour. The classification framework facilitated a clearer interpretation of chemical trends within the species.

Data tabulation and categorization were followed by graphical interpretation to examine distribution patterns across compounds. Visualization techniques such as jitter plots and bar graphs were employed to explore the variability, intensity and potential dominance of specific compounds. This step enabled a signal-based evaluation of the oil's chemical structure from a species specific perspective.

Figure 1 illustrates the complete experimental workflow, encompassing key stages such as sample preparation, detector output acquisition, compound classification and signal analysis. The structured process ensures that each stage, from compound detection to behaviour interpretation, contributes to a consistent and reproducible methodology for profiling essential oil from a *A. beccariana* species.

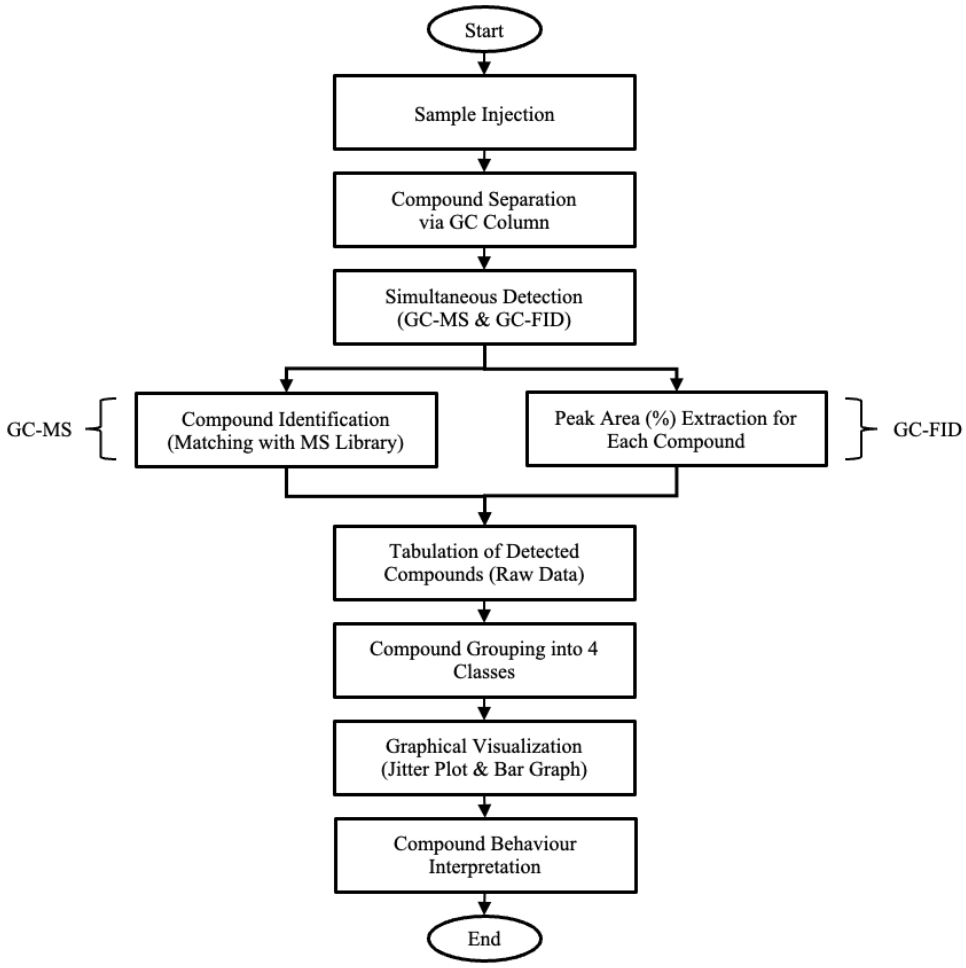

Figure 1. Workflow of compound acquisition and analysis in *A. beccariana* using GC-MS/GC-FID

The process begins with injecting the oil sample into the gas chromatograph, where volatile constituents are separated within the GC column based on their physicochemical properties, primarily boiling points and polarity. As each compound elutes from the column at its specific retention time, it is directed simultaneously to both GC-MS and GC-FID detectors via a post-column splitter.

The GC-MS detector identifies compounds by comparing their fragmentation patterns against a spectral database, ensuring precise structural recognition. Simultaneously, the GC-FID detector generates quantitative data in the form of peak area (%) for each compound, reflecting its relative abundance within the oil matrix. The dual output, qualitative from GC-MS and quantitative from GC-FID, ensures comprehensive compound-level profiling in a single analysis.

After data acquisition, the results from both detectors are compiled into a unified table consisting of compound names, structural types and corresponding peak areas. This tabulated output serves as the primary dataset for further analysis [22]. Each compound is subsequently assigned to one of four predefined chemical groups: Group 1 (carboxylic acids), Group 2 (sesquiterpenes), Group 3 (sesquiterpenoids) and Group 4 (other compound). This classification enhances clarity in interpretation and supports group-wise visualization.

To evaluate compound distribution and intensity patterns, two visualization techniques were employed: jitter scatter plots and grouped bar graphs. These graphical outputs allow for easy comparison between compounds within and across groups, highlighting signal behaviour trends and dominant peaks. Based on these results, a signal-driven interpretation

was performed to identify key compounds that exhibit high intensity or recurring detection, potentially serving as markers for species-specific profiling.

The final dataset, including compound names, peak area values and assigned chemical groups, is presented in Table 1. This structured approach from injection to classification and visual interpretation provides a repeatable and objective method for analysing essential oil composition using GC-MS/GC-FID instrumentation.

Table 1. List of chemical compounds dataset and peak area (%) for each *Aquilaria* oil species [22]

Group	Peak Area (%)	Compounds	Type of Compounds
1	0.14	*n*-decanoic acid	Carboxylic acid
1	0.15	pentadecanoic acid	Carboxylic acid
2	1.53	β-patchoulene	Sesquiterpene
2	0.11	β-elemene	Sesquiterpene
2	1.14	cyperene	Sesquiterpene
2	0.10	β-gurjunene	Sesquiterpene
2	0.73	α-guaiene	Sesquiterpene
2	1.98	*allo*-aromadendrene	Sesquiterpene
2	0.66	β-selinene	Sesquiterpene
2	0.31	valencene	Sesquiterpene
2	0.74	δ-guaiene	Sesquiterpene
2	0.55	δ-cadinene	Sesquiterpene
3	1.25	dihyro-β-agarofuran	Sesquiterpenoid
3	0.34	10-epi-γ-eudesmol	Sesquiterpenoid
3	0.26	γ-eudesmol	Sesquiterpenoid
3	0.16	cyperotundone	Sesquiterpenoid
3	0.00	dehydrofukinone	Sesquiterpenoid
4	10.61	benzyl benzoate	Other Compound

4. Results and Discussion

This section presents the compound behaviour of *Aquilaria beccariana* essential oil based on quantitative data obtained from GC-MS coupled with GC-FID analysis. A total of 18 compounds were successfully detected and grouped into four chemical classes [22]: Group 1 (Carboxylic acids), Group 2 (Sesquiterpenes), Group 3 (Sesquiterpenoids, and Group 4 (Other compound). The classification was performed to facilitate structural interpretation and comparative signal analysis. Each compound was quantified using its corresponding peak area (%) from GC-FID output, which reflects its relative abundance in the essential oil. Figure 2 displays the jitter scatter plot visualizing the distribution of compound peak areas across the four groups.

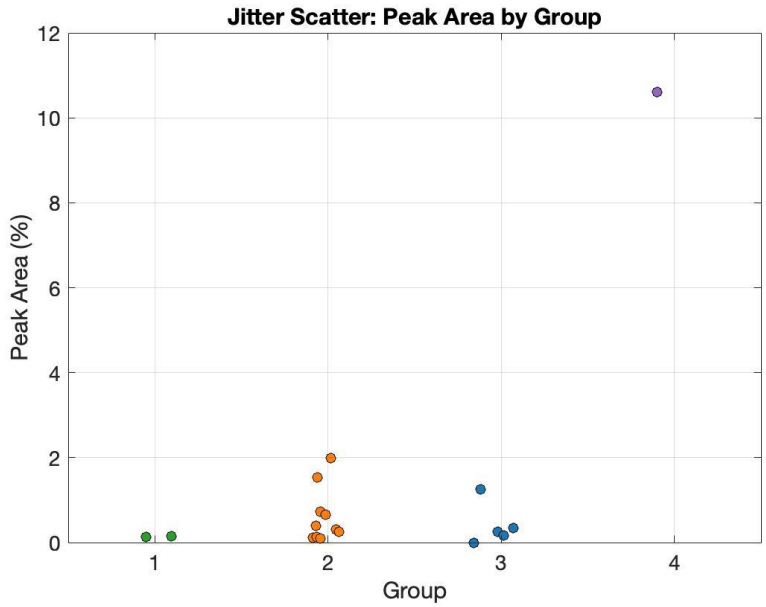

Figure 2. Jitter scatter plot of compound peak area (%) grouped by chemical class in *Aquilaria beccariana* essential oil. Group 1: Carboxylic acid (green), Group 2: Sesquiterpene (orange), Group 3: Sesquiterpenoid (blue), Group 4: Other compound (purple)

From Figure 2, it is evident that Group 2 dominates the compound profile in terms of both variety and signal spread. This group includes a range of compounds such as β-patchoulene (1.53%), allo-aromadendrene (1.98%), α-guaiene (0.73%) and β-selinene (0.66%), which contribute moderately to the overall oil intensity. Notably, allo-aromadendrene showed the highest peak area within Group 2, indicating its significant role in defining the chemical fingerprint of *A. beccariana*. Other sesquiterpenes like β-gurjunene (0.10%) and β-elemene (0.11%) appeared in lower concentrations, suggesting secondary contributions.

In contrast, Group 1 consists of only two compounds, *n*-decanoic acid and pentadecanoic acid, with peak areas of 0.14% and 0.15% respectively. Their low intensity indicates limited influence in the aroma and pharmacological properties of the oil, though they may still contribute to minor functional roles. This group showed the least variation and concentration, consistent with previous findings that carboxylic acids are often present in trace amounts in agarwood oils.

Group 3, though smaller in number, includes structurally oxygenated sesquiterpenes such as dihydro-β-agarofuran (1.25%) and 10-epi-γ-eudesmol (0.34%). These compounds displayed moderate intensity and are of particular interest due to their potential pharmacological activity and fragrance value. Their presence complements the more dominant sesquiterpene signals and adds depth to the oil profile.

Group 4 is represented solely by benzyl benzoate, which demonstrated a strikingly high peak area of 10.61%, far exceeding all other compounds. This clear outlier in both intensity and grouping signifies its substantial contribution to the oil's chemical character and may serve as a potential marker compound for *A. beccariana*. Its separation from the rest is visually emphasised in the scatter plot, reinforcing its dominant role.

To further quantify and compare compound intensities, Figure 3 displays a bar graph representing the peak area (%) values for each of the 18 compounds detected in *A. beccariana* essential oil. This graphical format allows direct visual assessment of individual compound concentration across all groups. By displaying exact peak area values, the bar graph highlights key contributors to the oil's chemical composition beyond general group trends.

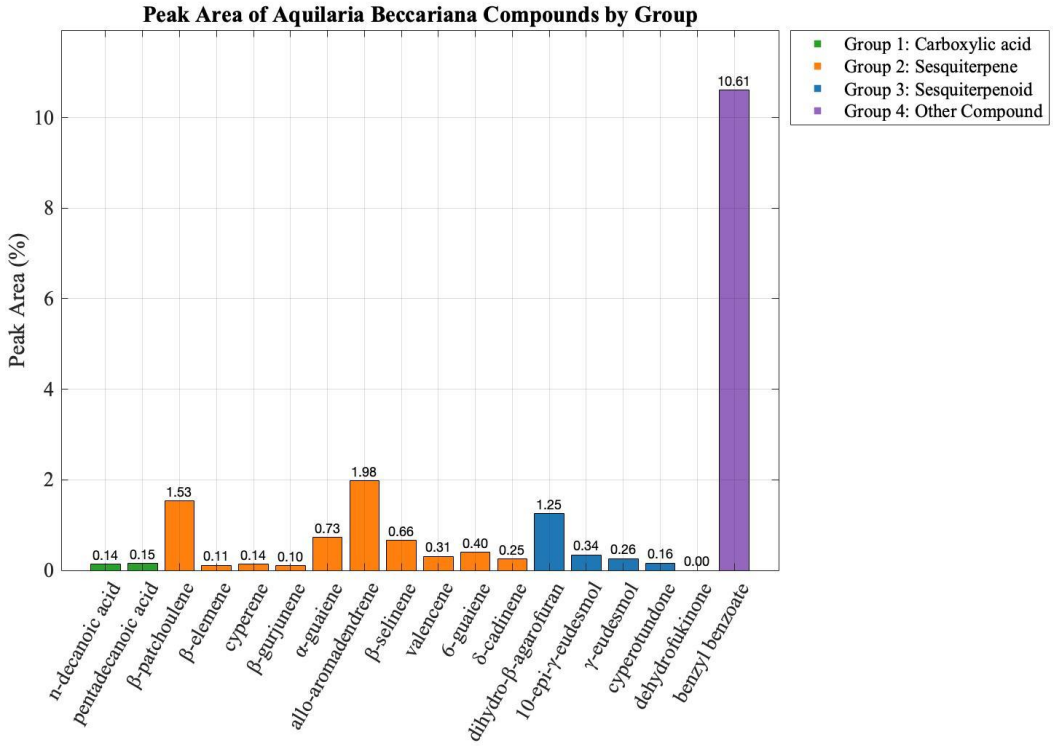

Figure 3. Bar graph showing peak area (%) of 18 compounds detected in *Aquilaria beccariana* essential oil. Compounds are colour-coded by chemical group

The compound benzyl benzoate clearly dominates the profile with a peak area of 10.61%, standing in sharp contrast to the rest and confirming its unique quantitative significance in this sample. Its distinct intensity, compared to all other compounds, underscores its potential as a primary chemical marker for the species. While the jitter plot revealed this outlier qualitatively, the bar graph quantifies the extent of its prominence.

Group 3 shows notable variation, with dihydro-β-agarofuran leading at 1.25%, followed by smaller yet consistent contributions from eudesmol-type compounds. These secondary contributors add structural diversity and may contribute to functional or aromatic properties. Although not as concentrated as sesquiterpenes, they provide supporting intensity in the compound spectrum.

In contrast, the bar graph confirms the minimal presence of Group 1 compounds, with carboxylic acids contributing less than 0.20%. Their low abundance suggests a limited role in defining the oil's dominant characteristics. Nevertheless, their detection remains valuable for holistic profiling and inter-species comparison.

The bar graph, when viewed alongside the jitter plot, enables both group-wise visualisation and compound-specific comparison, allowing for a robust understanding of compound behaviour within this *A. beccariana* sample. Together, these visual tools highlight the quantitative hierarchy of chemical components and reinforce the analytical strength of GC-based instrumentation in essential oil studies.

5. Conclusions

This study successfully characterized the chemical compound distribution of *A. beccariana* essential oil using peak area (%) data acquired from a GC-MS coupled with GC-FID instrumentation. Through the dual-detector approach, both qualitative identification and quantitative assessment of 18 compounds were achieved in a single run, enhancing the reliability and resolution of the profiling process. The compounds were grouped into four chemical classes, namely carboxylic acids, sesquiterpenes, sesquiterpenoids and other compounds for clearer interpretation of their signal behaviour and contribution to the oil's composition. The visualization via jitter plot and bar graph provided insights into the distribution pattern of compounds within the species. Benzyl benzoate was identified as the dominant compound, while sesquiterpenes and sesquiterpenoids formed the structural backbone of the oil. The integration of compound grouping with intensity analysis offers a signal-driven framework that supports future efforts in species authentication, chemical fingerprinting and standardisation of agarwood essential oils. This approach demonstrates the capability of coupled GC-MS/GC-FID systems to generate reproducible and interpretable compound-level data studies.

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