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Exploring essential oil composition and mood effects

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Abstract

Despite the prevalence of aromatherapeutic practices, the molecular determinants of essential oils' mood-altering properties lack systematic investigation. This knowledge gap was addressed through an analysis of chemical composition–mood relationships across 40 botanically diverse essential oils. Gas chromatography–mass spectrometry data from peer-reviewed sources underwent Pearson correlation analysis to identify compounds most strongly associated with calming, uplifting, or stimulating effects. Binary Logistic Regression models achieved leave-one-out cross-validated accuracies of 62.5–77.5% when predicting mood categories from chemical profiles alone. Distinct molecular signatures emerged for each mood category: geraniol and citronellol dominated uplifting associations ($r = 0.414$ and 0.408; $p < 0.01$), limonene characterized uplifting effects ($r = 0.488$; $p < 0.01$), while 1,8-cineole and menthol were distinguished by their stimulant effects ($r = 0.376$ and 0.360; $p < 0.05$). Principal Component Analysis confirmed natural chemical clustering aligned with traditional mood classifications. Additionally, a supplementary physicochemical descriptor, the molar volume to polarizability ratio, demonstrated a modest discriminatory ability between calming and non-calming oils (AUC = 0.666), complementing multivariate composition-based findings. These results suggest an organization of the olfactory architecture that is different from the conventional 'lock-and-key' model, demonstrating the ability of the neuronal signaling machinery to recognize and transmit analogous, converse and null chemical codes. The results also establish semi-quantitative relationships between chemical composition and aromatherapeutic mood categories and identify promising molecular features for future mechanistic and therapeutic investigation.

Keywords

Essential Oils, Aromatherapy, Mood, Chemical composition, Predictive modeling, Logistic Regression, Gas chromatography, Polarizability, Uplifting, Stimulating, Calming

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1. Introduction

Essential oils evoke distinct psychoactive effects depending on their chemical compositions. Lavender and chamomile promote deep relaxation through their action on well-characterized anxiolytic pathways, while citrus varieties, such as sweet orange and lemon, reliably elevate mood and reduce stress (1,2). In contrast, rosemary and peppermint sharpen cognitive focus and enhance alertness through stimulating mechanisms.

These effects on mood are the result of the nature of olfactory sensation. All sensation modalities with the exception of olfaction experience the thalamus relay, resulting in a delayed and filtered sense of the stimuli (3). Olfaction, on the other hand, has a direct pathway to the limbic system, the emotional and memory center of the brain (4,5). Upon inhalation of essential oil, the volatile organic compounds bind to the olfactory receptors, where neuronal activation proceeds to olfactory bulbs and limbic sites without thalamic relay (6). As a result, olfactory inputs through aromatic sensations can alter mood rapidly without delay from cognitive systems such as visual or auditory.

Although olfactory inputs reach limbic structures rapidly, the specific emotional responses they trigger depend on how the different volatile molecules activate distinct subsets of olfactory receptors. Essential oils contain many compounds with diverse chemical structures, and each compound is capable of stimulating partially different receptor populations. These receptor-level differences generate distributed neuronal activation patterns that converge onto multiple limbic and hypothalamic sites. Consequently, a single perceptual outcome—such as relaxation or alertness—may emerge from several parallel biochemical routes rather than a single unified pathway.

This framework helps explain why botanically unrelated oils—such as lavender, chamomile, copaiba, and various resin-derived species—can all produce calming effects despite being constituted of different dominant chemical compounds. Their molecules enter the olfactory system through the same anatomical route, yet they engage distinct downstream neurochemical processes depending on their structural properties. This also means that mood categories are not governed by a single "key compound" but instead arise from families of molecules that act on partially independent networks. These mechanistic possibilities provide context for later results in this study, which show that calming, uplifting, and stimulating effects correspond to chemically heterogeneous signatures and likely involve multiple neurobiological pathways.

Prior research has associated specific compounds with specific mood changes. Linalool, lavender's primary monoterpene alcohol, for instance, induced anxiety-reducing effects (7,8). Fonseca *et al*. (9) found that acetate esters acted as a cofactor in the calming effect. Mood elevation involves limonene, a monoterpene hydrocarbon that comprises the majority of citrus oils; it triggers stress-reduction pathways while elevating mood (10). Cognitive stimulation involves another class of compounds: 1,8-cineole concentrates in

eucalyptus, rosemary, and sage to produce stimulating effects (11) while peppermint achieves similar effects through monoterpenols such as menthol and menthone (12,13).

2. Materials and Methods

Despite compelling evidence for individual compounds' mood effects, there are limited systematic analyses examining how chemical profiles influence mood changes. Previous studies have focused on single oils or isolated compounds, potentially missing important synergistic effects and the chemical patterns that characterize entire mood categories (14). To bridge this knowledge gap, chemical composition patterns across 40 essential oils were systematically analyzed, cataloging each mood effect. The objectives were to identify the chemical compounds that were the most strongly associated with each mood category and build a predictive model using logistic regression that classified oils based on their chemical profile. Lastly, chemical associations between oils and mood effects were visualized.

2.1 Dataset and essential oil selection

Based on the prevalence in aromatherapy practice, 40 natural oils representing four major aromatic families were selected: citrus, floral, woody, and minty. The citrus family consisted of lemon, sweet orange, bergamot, neroli, grapefruit, lime, mandarin, petitgrain, bitter orange, and yuzu. Commonly, these oils generally possess a high limonene content. The floral family consisted of lavender, chamomile, ylang-ylang, geranium, rose damask, jasmine, clary sage, helichrysum, palmarosa, and chamomile German, and was defined by alcohols and esters as the major constituents. The woody family consisted of sandalwood, vetiver, frankincense, atlas cedarwood, patchouli, Scots pine, cypress, myrrh, juniper berry, and copaiba balsam, characterized by sesquiterpene structural skeleton dominance. Peppermint, spearmint, eucalyptus, tea tree, rosemary, wintergreen, lemongrass, cornmint, citronella, basil sweet, characterized by menthol and cineole as major structural backbone constituents, composed the minty oil family.

2.2 Mood categorization

Practice-based and psychophysiological definitions, obtained from aromatherapy texts and peer-reviewed literature were adopted. *Calming* was defined as reductions in physiological arousal involving heart rate and/or blood pressure, decreases in state anxiety, or shifts toward parasympathetic activity following inhalation. *Uplifting* was defined as increased positive affect and/or reduced subjective stress without primary emphasis on vigilance. *Stimulating* was defined as increased alertness, attention, or psychomotor speed, such as EEG beta activity and vigilance tasks. These operational definitions followed (15,16) and were consistent with psychophysiological summaries (4). A complete oil-to-label mapping with citations is provided in Supplementary Table S1 (supplementary files).

2.3 Statistical analysis

Since this study was exploratory in nature, statistical analyses was performed; not necessarily with the intention of providing confirmatory evidence but with the intent of sorting, comparison and finding patterns and general discrimination. All statistical analyses were performed using Python 3.9 with the

following libraries: pandas (v1.4.0) for data manipulation, scikit-learn (v1.0.2) for machine learning, scipy (v1.7.3) for statistical tests, matplotlib (v3.5.1), and seaborn (v0.11.2) for visualization.

2.3.1 *Pearson's correlation*

Pearson's correlation was calculated to relatively quantify the correlation of individual chemical compounds with a particular mood effect. First, the natural oils of each mood category were coded by a binary variable (e.g., 1 for "Calming" and 0 for all others). The concentration of each constituent was treated as a continuous variable to represent its prevalence. Statistical significance of each correlation was generated using a t-test, and the five highest positively correlated compounds for each mood category were selected. An r value close to +1 implied that oils with higher levels of that compound were relatively likely to cause the target mood; an r near -1 indicated that the compound was typically absent from that category; an r value near 0 suggested no relationship between the compound and the target mood category. To construct supplementary Figure S3, compounds with ≥0.5% w/w abundance in the plant species were retained, compounds were ordered by median abundance, and minimal horizontal jitter was applied with a fixed random seed to avoid overlay.

2.3.2 *Logistic Regression modeling*

To capture multivariate relationships within the full chemical profile, Logistic Regression was employed. Three one-vs-rest models were trained to distinguish each mood category from the rest. In each model, the percentages of all chemical constituents were the predictor variables, and the outcome was whether the oil belonged to the target mood category. The standardized regression coefficients (β) were obtained from each of the final models. Given the limited sample size (n = 40), the model was evaluated by leave-one-out cross-validation.

Model performance was evaluated using standard metrics of Accuracy, Recall, Precision, F1-score and Area Under the Curve – Receptor Operating Curve (AUC-ROC). Prior to modeling, each compound column was z-scored. When multiple compounds co- occurred exclusively within the same oils, their standardized predictors became perfectly or near-perfectly collinear. In these cases, the one-vs-rest logistic regression solution was not unique, and scikit-learn returned identical β coefficients across such features. Even so, all compounds were retained to facilitate and analyze chemical interpretation and, where relevant, equivalence classes were reported in supplementary Table S2.

2.3.3 *Principal Component Analysis (PCA)*

PCA was performed to identify the broader trends within the high-dimensional dataset. The scree plot was examined to identify the appropriate number of components to retain from the PCA analysis (supplementary Figure S1). The plot showed a distinct "elbow" subsequent to the second component, which suggested that PC1 and PC2 explained the greatest amount of the total variation, and the resultant reduced dimensionality of the two-dimensional plot preserved sufficient information for subsequent analyses.

2.3.4 *Hierarchical clustering*

To probe the structural similarities between the natural oils, Hierarchical clustering was employed. The Ward's linkage method with Euclidean distance was used to generate the dendrogram and the heatmap respectively.

2.3.5 *Physicochemical descriptors*

Polarizability (Å³) and molar volume (mL/mol) per compound were compiled from curated literature sources (supplementary Table S5). Subsequently, the ratio of Molar Volume to Polarizability in units of [mL/[mol x Å³]] was computed. Since polarizability is directly proportional to molar volume (molar mass) for organic molecules, it was thought that either a different ratio would define different odor sensing or the rate of change of this ratio would differ among different odor-producing molecules. Group separation was then calculated (calming vs. uplifting and stimulating) using Welch's t-test and ROC/AUC. An optimal cutoff was selected by maximizing Youden's J. Source details and cross- checks are recorded in supplementary Table S5.

2.3.6 *Data and code availability*

All analysis code is provided as a Jupyter notebook (Supplementary Data SD6: analysis_pipeline.ipynb). The full composition tables S1b_Composition_LONG.csv and S1b_Composition_WIDE_GE0p5.csv are supplied as csv files. Supplementary Table S5 lists physicochemical descriptors with sources.

2.3.7 *Simultaneous differential effects*

Table S2 was re-arranged so that each compound's r and p for its calming effect [c], uplifting effect [u] and stimulating effect [s] appeared on the same row. The r values for each row were algebraically processed into the expressions [c-u], [c-s] and [u-s]. The first category of compounds [identified as c↔u↔s] were defined as those for which the magnitudes of these expression were similar and the magnitude of no one expression was less than 20% of the others. The objective was to identify those compounds which demonstrated significantly different effects across the calming, uplifting and stimulating categories; regardless of which category they were positively, negatively or not correlated with. The second category of compounds [identified as c↔us] were defined as those for which the magnitudes of the [c-u] and [c-s] expression were similar, as well as significantly different (>80%) from the [u-s] expression. The objective was to identify those compounds which demonstrated a significantly different effect for the calming category when compared against both the uplifting and stimulating categories. The third category of compounds [identified as cs↔u] were defined as those for which the magnitudes of the [c-u] and [u-s] expression were similar, as well as significantly different (>80%) from the [c-s] expression. The objective was to identify those compounds which demonstrated a significantly different effect for the uplifting category when compared against both the calming and stimulating categories.

2.4 Physicochemical descriptors

To evaluate whether coarse-grained molecular features track mood-related categories, two standardized physicochemical properties for each modeled compound: molecular polarizability (Å³**)** and molar volume (mL/mol)

were extracted. These values were obtained from publicly accessible databases and peer-reviewed literature sources (Supplementary Table S5). From these properties, a molar volume to polarizability ratio [cm^3/[mol. $Å^3$]] was calculated, chosen based on prior work linking molecular electronic/steric features to odor perceptual space (17-19).

To assess whether this descriptor differed across mood categories, calming versus uplifting /stimulating oils were compared using Welch's t-test, and the discriminatory ability of this single feature was evaluated using ROC/AUC analysis. Optimal cutoffs were determined by maximizing Youden's J statistic, and sensitivity/specificity values were computed accordingly. This analysis served as an auxiliary, low-dimensional baseline to complement the multivariate composition-based predictive models.

2.5 Sensitivity to label definition

To assess the robustness of mood classification results to alternative labeling strategies, the entire modeling pipeline was re-run using a literature-first label set, in which each essential oil was assigned mood categories according to prior aromatherapy reports rather than the majority-vote or dominant-label scheme used in the main analysis.

The full workflow, including Pearson correlations, logistic regression modeling, cross-validation, ROC/AUC computation, and feature ranking, was re-run under this literature relabeled framework. Model performance metrics, rank order of top positive and negative predictors, and coefficient stability were then compared to the main-label results. Minor variations in coefficients were evaluated using identical standardization protocols, and sensitivity/specificity values were recalculated for consistency across analyses.

This sensitivity analysis examined whether the findings depended primarily on the specific labeling definition or remained stable under a plausible alternative annotation method.

3. Results

3.1 Pearson's correlation

Compound correlations with mood categories

Pearson correlation analysis found distinct chemical signatures for each mood classification, with results summarized in Table 1.

Calming oils demonstrated a strong correlation with a distinct set of woody–floral constituents rather than citrus–floral alcohols. As listed in Table 1, the top calming-associated compounds were β-caryophyllene ($r = 0.258$), linalyl acetate ($r = 0.235$), α-terpineol ($r = 0.191$), and two angelate esters (methallyl angelate and isoamyl angelate, $r = 0.177$ each). Although the magnitudes were modest, this pattern reflected the chemical diversity of relaxation-oriented oils: β-caryophyllene is abundant in woody oils such as sandalwood and copaiba; linalyl acetate defines lavender chemotypes; and α-terpineol is a frequent component of floral–woody calming profiles.

Table 1. Top five chemical compounds positively correlated with each mood effect category

Mood Effect	Compound	r	p
Calming	β-Caryophyllene	0.258	0.108
	Linalyl Acetate	0.235	0.144
	α-Terpineol	0.191	0.239
	Methallyl angelate	0.177	0.274
	Isoamyl angelate	0.177	0.274
Uplifting	Limonene	0.488	0.001
	Geraniol	0.414	0.008
	Citronellol	0.408	0.009
	β-Pinene	0.274	0.088
	Citronellal	0.260	0.105
Stimulating	1,8-Cineole	0.376	0.017
	Menthol	0.360	0.022
	Menthone	0.340	0.032
	Estragole	0.260	0.105
	Neral	0.260	0.105

Note. The table shows the results of a point-biserial correlation analysis between the percentage of each compound and the binary classification of mood categories (n=40). The value r represents the Pearson correlation coefficient. The value p represents the significance -value for the correlation; values < 0.05 are typically considered statistically significant.

Importantly, geraniol and citronellol—while strongly uplifting—did not appear among the top calming correlates, which may indicate that positive affect elevation (uplifting) and physiological relaxation (calming) arise from chemically distinct signatures. Linalool demonstrated a moderate correlation with calming effects (r=0.330) and thus did not make the top five list. Altogether, these results suggested that calming effects originated from combinations of sesquiterpenes and esters rather than from citrus-floral monoterpene alcohols.

Uplifting effects demonstrated the strongest linkage to citrus oils. Limonene showed the strongest correlation (r = 0.488, p = 0.001), which corresponds to its high prevalence across citrus oils within the dataset. Geraniol and citronellol ranked among the top uplifting r-values, suggesting they contributed to both calming and uplifting moods, depending on the chemical composition and/or concentration. β-Pinene, a component that consistently presented in the citrus oil groups alongside limonene, also showed modest correlation, approaching significance (r = 0.274, p = 0.088).

Stimulating classifications correlated most strongly with minty aromatics. 1,8-cineole was the primary stimulating correlate (r = 0.376, p = 0.017), which corresponded with its reported stimulating effect from the literature. Menthol followed closely as another strong marker for this category (r = 0.360, p = 0.022). Both constituents generate the sharp, clearing scents,

which align with eucalyptus, peppermint, and rosemary oils. Menthone, with its structural similarity, also showed a significant association ($r = 0.340$, $p = 0.032$).

For transparency, Supplementary Figure S3 visualizes all data points (compound-by-oil % by weight, ≥0.5%) stratified by mood label.

3.2 Predictive modeling

Binary Logistic Regression models demonstrated variable predictive capacity across mood categories (Table 2). Uplifting classifications showed the strongest performance, with 77.5% accuracy and an AUC-ROC of 0.824. Stimulating oils showed comparable accuracy (77.5%) with lower discriminative power (AUC-ROC = 0.655), while calming categories proved most challenging to predict (62.5% accuracy; AUC-ROC = 0.702).

Table 2. Logistic Regression model performance using Leave-one-out-cross-validation (LOOCV)

Model	Accuracy	Precision	Recall	F1-Score	AUC-ROC
Calming vs. Rest	62.5%	0.58	0.70	0.63	0.702
Uplifting vs. Rest	77.5%	0.75	0.82	0.78	0.824
Stimulating vs. Rest	77.5%	0.71	0.83	0.77	0.655

Performance metrics were calculated using LOOCV for each of the three binary classifiers. Per established metrics, Accuracy represents the proportion of correct predictions, Precision measures the accuracy of positive predictions. Recall measures the model's ability to identify all relevant instances. F1-Score is the harmonic mean of precision and recall. AUC-ROC represents the model's ability to distinguish between classes.

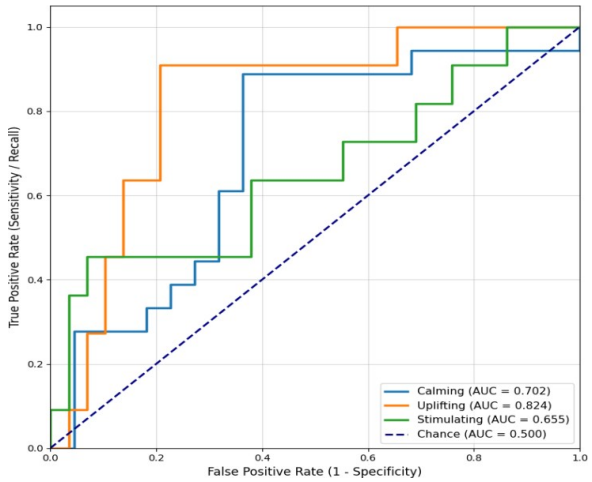

Figure 1. ROC curves for three binary classifiers

Discriminative ability varied considerably among mood categories, as illustrated by the ROC curves in Figure 1. The uplifting model's curve demonstrated a modest separation from random classification, with an AUC of 0.824. In contrast, the calming model reached only moderate discrimination levels, reflecting the chemical complexity of relaxation-inducing mood changes.

ROC curves for the one-vs-rest logistic regression models were shown. These curves demonstrate the classification performance for each mood category. The diagonal dashed line represents the performance of a random classifier (AUC = 0.5).

As an auxiliary single-feature baseline, the molar volume to polarizability ratio modestly distinguished calming oils from uplifting/stimulating oils (Welch's t-test: t = 1.71, p = 0.092). When treated as a classifier, this descriptor achieved AUC = 0.666, with an optimal cutoff of 8.76 yielding a sensitivity of 0.667 and a specificity of 0.681. Although coarse, this result suggests that a broad steric/electronic balance captured by this ratio tracks mood category at a low resolution and complements multivariate models. It may be that a ratio of broader stearic (molar surface area, molecular shape (linear, branched), Taft parameter to measure spatial hindrance, conformational energy and connectivity) and electronic (electron density, orbital energies (HOMO/LUMO), electronegativity, Electron-Ion Interaction Potential (EIIP) and Van der Waals surface) descriptors may be more successful in discriminating these mood categories. Research into other descriptors and mechanisms (20-28) is ongoing.

Repeating the entire workflow with literature-first labels produced performance patterns that closely matched the primary analysis. The Uplifting model remained the best-performing classifier, with accuracy and AUC values differing only slightly from the main-label results (AUC ≈ 0.824 in the primary set). The Stimulating model demonstrated similar robustness, with performance remaining within a narrow range relative to the original model (AUC ≈ 0.655). The Calming model likewise exhibited minimal change (AUC ≈ 0.702), consistent with its broader chemical diversity.

Importantly, the top-ranked positive and negative predictors (e.g., limonene, β-pinene, 1,8-cineole) retained their positions across labeling schemes, with only minor coefficient shifts (Supplementary Table S6). These results indicate that the primary conclusions did not depend strongly on the specific labeling rule applied and are robust to reasonable relabeling.

3.3 Key chemical compounds

The prediction model revealed chemical compounds for each mood category. Standardized Logistic-Regression coefficients identified the most influential compounds when all constituents were modeled together. Figure 2 displays, for readability, the top five positive and top five negative compounds per class; the full coefficient vectors for all compounds are provided in Supplementary Table S4.

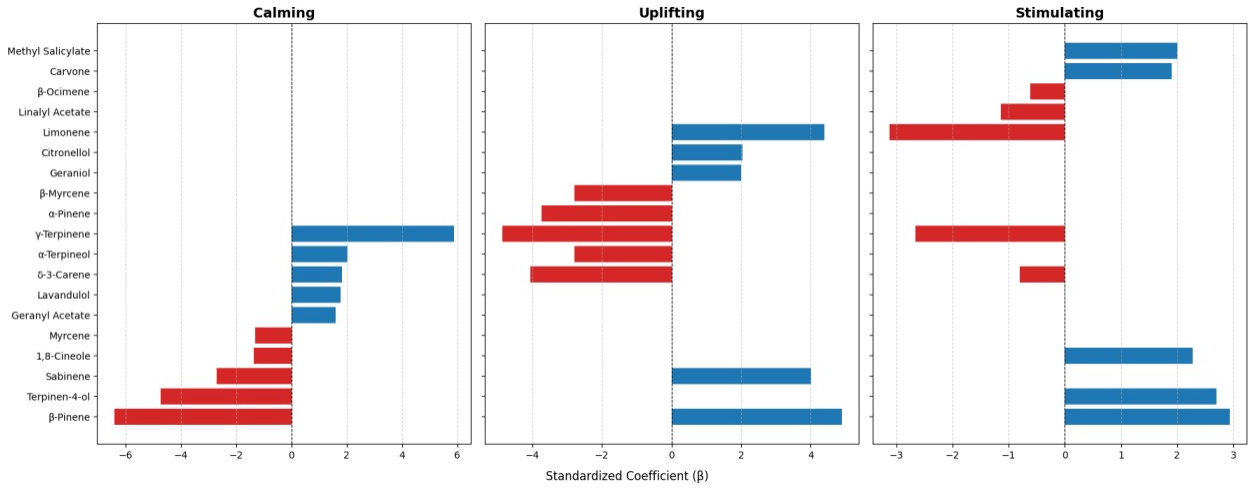

Figure 2. Key chemical compounds from Logistic Regression models. Standardized logistic- regression coefficients (β) for compounds in one-vs-rest models. For visual clarity, the top five positive and top five negative compounds are shown per mood class (i.e., 30 bars total). All models were trained and evaluated on n=40 oils (LOOCV). The full coefficient vectors for all compounds are provided in Supplementary Table S4.

Standardized Logistic Regression coefficients (β) for one-vs-rest mood classification models. Blue bars represent the five strongest positively associated compounds for each category, while red bars indicate the five strongest negatively associated compounds. Bar length corresponds to coefficient magnitude; a rightward extension indicates positive association, and a leftward extension indicates negative association.

Calming model coefficients revealed several unexpected patterns alongside traditionally representative compounds. γ-Terpinene emerged with the highest positive coefficient (β = 5.89), an unexpected finding given its typical occurrence in citrus rather than relaxation-focused oils. Traditional calming indicators like linalool contributed more modestly (β = 1.09), while β- pinene demonstrated the most pronounced opposition to calming classification (β = -6.42), followed by terpinen-4-ol (β = -4.75). Although 1,8-cineole predictably opposed calming effects (β = -1.37), its influence proved weaker.

Uplifting classifications corresponded to the anticipated chemical patterns. β-Pinene (β = 4.90, *SE* = 1.82) and limonene (β = 4.40, *SE* = 1.65) dominated positive predictions, consistent with the citrus associations. Notably, γ-terpinene acted as a strong negatively associated compound (β = -4.87, *SE* = 1.93).

Stimulating oil predictions followed more expected patterns. β-pinene emerged as the strongest positive predictor of this mood effect (β = 2.93, *SE* = 1.21). It was followed by terpinen-4-ol (β = 2.69, *SE* = 1.15), 1,8-cineole (β = 2.27, *SE* = 0.98), and menthol (β = 1.22, *SE* = 0.56). Limonene's strong negative coefficient (β = -3.12, *SE* = 1.24) could be taken to be indicative of purely citrus profiles being

negatively associated with stimulating classifications.

3.4 PCA and clustering

Forty essential oils were projected onto the two principal components. Each colored point corresponded to its category. Arrows indicate the direction and magnitude of influence for the most important chemical compounds.

Principal Component Analysis demonstrated modest mood category separation within multivariate chemical space (Figure 3). Combined variance explanation reached 39.6% across the first two components (PC1: 30.9%, PC2: 8.7%), with complete loading matrices provided in Supplementary Table S4. The primary axis (PC1) classified uplifting oil as being distinct from the remaining categories. Limonene's dominant positive loading (0.98) drove this separation, resulting in segregating citrus-abundant uplifting oils toward high positive values.

Secondary differentiation (PC2) distinguished stimulating from calming profiles across the remaining chemical space. This axis featured strong positive contributions from α-pinene (0.63) and a moderate contribution from 1,8-cineole (0.34), contrasted against negative loadings from linalool (-0.52) and linalyl acetate (-0.42). Consequently, stimulating oils clustered in the upper plot region (positive PC2), while calming oils predominantly occupied lower areas (negative PC2).

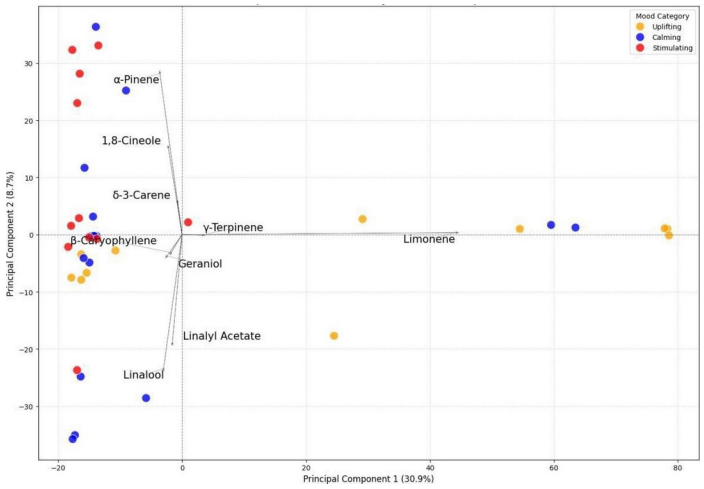

Figure 3. PCA biplot of essential oils colored by mood category

Hierarchical clustering analysis using Ward's linkage method (Figure 4) showed similar patterns, with three large clusters closely aligned to mood categories with 75% agreement. The subclusters within each major grouping signify functional subdivisions, such as floral calming clusters (rose, geranium) and wood calming clusters (sandalwood, cedarwood).

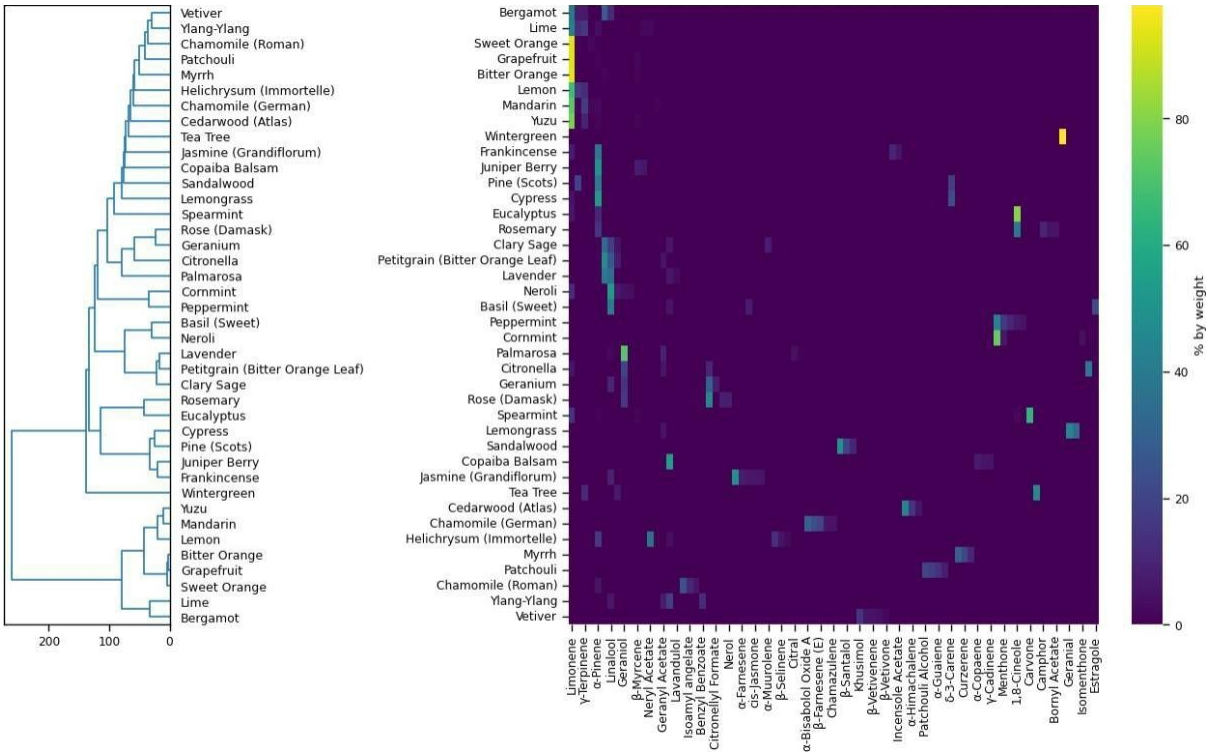

Figure 4. Hierarchical clustering and heatmap of essential oil chemical composition

The hierarchical clustering analysis on 40 essential oils based on their chemical profiles is shown in Figure 4. The dendrogram on the left demonstrates the notable clusters within the oils. The heatmap on the right visualizes the relative percentage (% by weight) of each chemical compound for every oil. Brighter colors indicate higher concentrations.

Table 3. Category differentiation among essential oils

Category	Compounds
c↔u↔s	β-pinene, **1,8-cineole**, β-myrcene, **Sabinene**, Menthol, Menthone, L-Bornyl acetate, Camphor, Verbenone, Benzyl acetate, Methyl acetate, Isomenthone, Estragole, Methyl salicylate, Menthofuran, Carvone, **Terpinen-4-ol**, γ-Terpinene, Geranyl acetate, **α-Terpineol**, γ-Cadinene, patchovlol, Linalyl acetate, Linalool, β-Caryophyllene, Citronellol
c↔us	β-Farnesene, Incensole acetate, β-Ocimene, δ-Cadinene, β-Selinene, β-Vetivene, Curzerene, γ-Curcumene, Chamuzulene, Isobutyl angelate, α-Guaiene, Seychellene, Methallyl angelate, Citronellyl angelate, Eugenol, Benzyl acetate, epi-β-Santalol, Benzyl benzoate, Italidione II, Khusimol, Lavandulol, α and β Vetivone, Lindestrene, α-Thujene, Isovalencenol, α-muurolene, Neral, α-Copaene, Nonadecane, α-Bisabolol, α and β-Himachalene, p-Cymene
cs↔u	δ-3-Carene, γ-Terpinene, Geraniol, Farnesol, α-Farnesene, Cis-Jasmone, Citronellal, Indole, Limonene

The compounds in bold exhibit similar differentiation shown in Figure 2. Data from supplementary Table S6 was used to construct the category differentiation worksheet, from which these compounds emerged.

Table 3 presents a different interpretation of the results wherein a specific molecule is not only associated with a specific (on-off) effect for a given category; but is instead, *simultaneously* associated with three coding correlative states of associative (+1), dis-associative (-1) or none (0) for all of the categories (calming, uplifting and stimulating). This observation necessitates a nuanced olfactory architecture frame-shift that is discussed below.

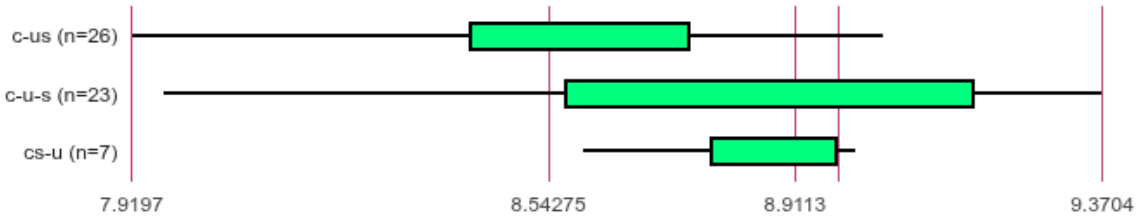

Figure 5. Molar volume to polarizability ratio [cm^3/[mol. $Å^3$]]. Box and whisker plots of single molecules that simultaneously produce (whether associative, dissociative or none) sensations of calming, uplifting and stimulating (c-u-s), those (single molecules) that simultaneously produce a calming effect without producing uplifting or stimulating effects (c-us) and those single molecules that simultaneously produce a calming and stimulating effect without producing an uplifting effect (cs-u). Data from supplementary Table S6 was used to construct the category differentiation worksheet. The resulting emerging compounds (Table 3) were cross referenced against descriptors.csv sheet, from which Figure 5 was derived. The accompanying Table 5A1 is appears in Appendix 1.

4. Discussion

4.1 The chemical basis for mood effects

The results confirmed traditional aromatherapy patterns while revealing important complexities in the chemical basis of mood effects. Pearson correlation analyses generally aligned with expected associations, whereas the multivariate models captured variance that single-compound correlations could not, reflecting the combined influence of multiple constituents without explicitly modeling interactions.

The correlation patterns for calming oils revealed a chemically heterogeneous group driven predominantly by woody sesquiterpenes and floral esters, rather than the citrus–floral monoterpene alcohols characteristic of uplifting profiles. β-Caryophyllene, the strongest calming correlate in the dataset, aligns with extensive literature demonstrating anxiolytic and anti-inflammatory effects through CB2 receptor–mediated pathways. Linalyl acetate, a defining ester in lavender, also aligned well with calming profiles and is consistent with reports that its hydrolysis product (linalool) contributes to reduced physiological arousal.

The presence of α-terpineol and two angelate esters further supports a multi-pathway model of calming effects. These compounds originate from botanically diverse families—lavender, chamomile, copaiba, and resinous oils—suggesting that relaxation responses arise from multiple, partially independent neurochemical pathways. This diversity also helps explain why the Logistic Regression model produced the lowest classification accuracy for calming oils:

the group spans multiple botanical lineages and structural classes, creating substantial chemical variability.

In contrast, geraniol and citronellol showed their strongest correlations with uplifting—not calming—effects. This may indicate that positive affect elevation and physiological relaxation rely on different chemical signatures. Collectively, these findings refine earlier assumptions and demonstrate that calming effects are more reliably associated with sesquiterpenes and esters than with citrus–floral monoterpene alcohols.

Limonene's strong correlation with uplifting effects ($r = 0.488$; $p < 0.001$) further supports the role of citrus volatiles in positive mood modulation, consistent with prior reports of monoaminergic activity (29). Oxygenated monoterpenes such as 1,8-cineole and menthol displayed the expected stimulating associations ($r = 0.376$; $p < 0.05$). These findings are consistent with work showing that these compounds modulate physiological arousal through TRPM8 channel activation and cholinesterase inhibition (12,30).

The multivariate analysis found complexities beyond correlation-based trends. It highlighted the contradictory role of γ-terpinene: although typically characteristic of citrus oils, the logistic regression model identified it as the strongest positive coefficient for the calming category ($\beta = 5.89$) and a strong negative coefficient for the uplifting category ($\beta = -4.87$). These observations align with studies reporting anxiolytic effects of isolated γ-terpinene, potentially involving modulation of the GABAergic system (31). Furthermore, γ-terpinene-rich oils exhibit neuroprotective properties that may contribute indirectly to stress-reduction pathways (32); however, direct evidence linking such neuroprotection to acute calming effects remains limited, and this relationship should be regarded as tentative rather than causal. Importantly, these coefficients must also be interpreted with caution, as γ-terpinene co-occurs with several citrus-related monoterpenes, and the high collinearity in $p \lll n$ conditions may inflate or destabilize Logistic Regression estimates.

Predictive model performance reflected the underlying chemical structure of each mood category. Uplifting oils achieved the highest classification accuracy (77.5%; AUC = 0.824), consistent with their chemical homogeneity dominated by limonene, β-pinene, and γ-terpinene, which form a cohesive citrus-derived motif. Stimulating oils likewise produced reliable classification driven by oxygenated monoterpenes closely associated with cognitive activation. In contrast, calming oils demonstrated modest model performance (62.5%; AUC = 0.702), reflecting their far greater chemical heterogeneity. The calming oil dataset spans plant-derived oils (lavender, rose, geranium), wood oils (sandalwood, cedarwood), and resin oils (frankincense), each with distinct biosynthetic pathways. This structural diversity suggests that calming effects may arise from several independent neurochemical mechanisms rather than a single dominant chemical axis.

Principal component visualization further clarified the chemical architecture underlying the mood categories. PC1 differentiated citrus-

dominant oils through limonene-driven loadings, whereas PC2 captured a stimulating–calming continuum defined by opposing contributions from oxygenated monoterpenes and ester/terpene profiles. Together, these dimensions illustrate how chemically coherent uplifting and stimulating groups diverge from the more dispersed calming cluster. This spatial arrangement is consistent with the idea that botanically diverse species may yield similar perceptual outcomes; however, PCA-based proximity alone does not establish evolutionary convergence, and such interpretations should remain cautious.

4.2 Implications for olfactory architecture

The results of this study set up some interesting observations; which cannot be completely explained with the conventional lock-and-key, receptor-ligand interaction model. The implications for olfactory architecture can be speculated, once it is assumed that the negative correlation of a chemical compound with any given effect is not the same as that molecule not *having* an effect – that definition would be demonstrated by the compound having no (zero) correlation. For example, β- pinene and terpinen-4-ol demonstrating the most pronounced opposition to calming classification (β = -6.42 and -4.75 respectively) is not the same as the *mere absence* of the calming effect; these compounds may be positively associated with uplifting-congruent (or uplifting-mimetic) or stimulating-congruent (or stimulating-mimetic) effects. A mechanistic interpretation would imply that there are either [1] specific spatially separated receptor pockets per receptor (33) (since current research is suggestive of one specific type of receptor (among the ~400 receptors known thus far) per neuron (distributed among a total of an order-of-magnitude of 10^6 neurons)) (34), or [2] one receptor (either associative or dis-associative) per receptor type that accommodates every molecule (within enthalpy constraints) and codes a signal (1, -1 or 0) depending on its (the receptor's shape – and/or free energy change? - when docked with the ligand) (35,36) or [3] a 'shape-shifting' receptor (37). Observations from this study fit a first-approximation model where the receptor (when docked with the appropriate molecule) codes for either an associative, a dis-associative, or no effect; corresponding to a Pearson's correlation of 1, -1 or 0 respectively. This interpretation explains why a single molecule can *simultaneously* be associated with a positive, negative or no correlation with a palpable effect (calming, uplifting and/or stimulating); corresponding with nine sub-receptor or receptor coding states of c^+, c^-, c^0, u^+, u^-, u^0, s^+, s^- and s^0. This is different from the conventional 'lock-and-key' weltanschauung, and demonstrates the ability of the neuronal signaling machinery to recognize and transmit analogous, converse and null chemical codes.

The considerable overlap between the box plots in Figure 5 implies an overlap between different olfactory receptors for similar molecules, or for the same receptor to behave differently upon engagement with different molecules and/or the capability of one molecule to differentially activate (in terms of olfactory sensation) similar (ensemble of) receptors.

4.3 Summary

Overall, these findings suggest that mood-

modulating effects in essential oils may originate [1] not from singular marker compounds but from ensembles of constituents operating across distinct chemical and neurobiological pathways and/or [2] from singular marker compounds engaging with ensembles of different accommodative receptor types – each type in turn coding for the different docked states of positive correlation, negative correlation or no correlation. Uplifting and stimulating categories reflect chemically cohesive motifs, whereas calming effects emerge from a broader and more heterogeneous mixture of molecules. These patterns provide a quantitative foundation for traditional mood classifications while highlighting the need for more mechanistically grounded and multidimensional models of aroma–emotion relationships and olfactory architecture.

5. Limitations

5.1 Statistical limitations

This study – by its very nature to classify molecular ensembles into mood categories - has several statistical constraints. The predictive models rely solely on leave-one-out cross-validation, with no bootstrap confidence intervals, permutation tests, or external validation, limiting assessment of model uncertainty and stability. Correlation analyses lack multiple-testing correction, and both correlations and regression outputs are reported without confidence intervals, reducing interpretability. Additionally, mild class imbalance and the unverified assumptions of Pearson correlation (e.g., normality) indicate that all statistical findings should be considered exploratory.

5.2 Modeling and data structure limitations

The modeling framework uses only linear logistic regression, which cannot capture non-linear patterns, interactions, or synergistic effects common in essential-oil mixtures. The high-dimensional $p \lll n$ structure is not addressed with standard regularization techniques (ridge, lasso, elastic net), increasing the risk of unstable or inflated coefficients. Furthermore, input GC–MS abundance values are treated as noise-free, without accounting for known batch-to-batch or instrument variability.

5.3 Confounding and heterogeneity limitations

Several potential confounders, such as extraction method, cultivar/chemotype, geographic origin, harvest conditions, and source-level heterogeneity, were not (and could not) be taken into consideration. Since oils within the same mood category can originate from chemically diverse species, these unaccounted factors may have increased within-category variance and obscured true associations. Similarly, GC–MS batch effects were not incorporated, limiting cross-source comparability. Additionally, essential oil compound isomers frequently present with different odors; and hence, potentially can exert different mood-effects (38). Isomerization was not explicitly modeled or considered in this study.

5.4 Collinearity

Strong collinearity among monoterpenes and sesquiterpenes remains unaddressed. No VIF filtering, PCA grouping, cluster aggregation, or regularized models were used, making logistic regression coefficients potentially unstable or difficult to interpret. Future analyses should

explicitly mitigate collinearity to obtain more reliable predictor estimates.

5.5 Generalizability

Generalizability is limited by the small dataset and by collapsing complex affective experiences into three broad categories. Label assignments drawn from heterogeneous literature sources may reflect publication bias or inconsistent methodological standards. Accordingly, these findings should be viewed as preliminary and require confirmation with larger, standardized, and experimentally controlled datasets.

6. Perspective

This research demonstrates how quantitative composition-based methods can be used to analyze mood responses but requires better data collection and modeling systems for accurate results. The research requires additional standardized GC–MS data from controlled cultivation and extraction procedures to minimize batch inconsistencies and separate effects from chemotype and geographic source and extraction techniques. The observed diversity in calming oils would become clearer through datasets that show whether different mechanisms exist or if the results stem from measurement errors between sources.

Future modeling research should use non-linear algorithms with interaction detection capabilities including random forests and boosting and kernel methods and manifold learning to discover complex patterns that linear models cannot detect. The use of probabilistic and multidimensional labeling systems would provide better representation of mood responses which exist on a continuum and depend on specific situations. The validation of chemical motifs through human-subject data collection including odor exposure tests and mood assessments and physiological measurements and neuroimaging results will confirm their relationship to psychological and autonomic changes.

Additional research must establish direct links between molecular characteristics and how people perceive them. The use of polarizability and molecular volume as interpretable descriptors can link chemical structures to receptor interactions and emotional responses. The proposed research directions will create a framework for developing models that explain aroma-emotion relationships through experimental evidence to establish a quantitative science of aroma-emotion relationships.

7. Conclusion

This systematic study of 40 essential oils provides quantitative chemical evidence for the traditional aromatherapeutic mood categories and demonstrates both expected and unexpected patterns of structure–function relationships. Correlation analyses confirmed existing associations: limonene with uplifting effects (r = 0.488); 1,8-cineole with stimulation (r = 0.376); and woody sesquiterpenes and floral esters, such as β-caryophyllene, linalyl acetate, and α-terpineol, with calming properties.

Multivariate modeling revealed additional patterns not apparent from correlations alone. γ-Terpinene, commonly found in citrus oils, unexpectedly emerged as a strong positive

coefficient for calming and a negative coefficient for uplifting, although these findings should be interpreted with caution given the high collinearity typical of essential-oil mixtures. The varying model accuracy across mood categories (62.5–77.5%) reflects the underlying chemical diversity: uplifting citrus oils, with relatively homogeneous chemical profiles, showed the most reliable performance.

PCA results indicated that mood types partially align with chemical dimensions. Limonene strongly defined the primary axis representing citrus compositions, while oxygenated monoterpenes distinguished stimulating from calming oils along the secondary axis. Calming oils, however, displayed greater dispersion, consistent with their heterogeneous chemical origins.

In addition to composition-based analyses, a coarse physicochemical descriptor—the polarizability-to-volume ratio—showed modest ability to distinguish calming from non-calming oils (AUC = 0.666). Although limited, this suggests that broad electronic and steric properties may contribute to mood-related perceptual differences and can complement multivariate chemical modeling. The study found that a similar compound may exhibit simultaneous positive, negative or no correlation with any given category of mood, suggestive of an organization of the olfactory architecture that is different from the conventional 'lock-and-key' model. Hence, the ability of the neuronal signaling machinery to recognize and transmit analogous, converse and null chemical codes cannot be discounted.

These findings advance the semi-quantitative understanding of aromatherapeutic mood effects by identifying chemical correlates associated with calming, uplifting, and stimulating classifications. For future research, larger and more standardized datasets combined with non-linear or interaction-sensitive modeling approaches may better capture the synergistic properties of whole-oil mixtures. The revealed chemical–mood relationships further suggest that multiple neurochemical pathways—such as GABAergic, monoaminergic, and cholinergic mechanisms documented in prior literature—may contribute, although direct mechanistic confirmation will require targeted physiological studies.

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Appendix 1

Table 5A1. Companion to Figure 5

Groups	cs-u	c-u-s	c-us
Sample size (n)	7	23	26
Minimum	8.59285	7.9656	7.9197
Q1	8.783345	8.563649	8.4223
Median	8.9772	8.9113	8.54275
Q3	8.97735	9.18005	8.757
Maximum	9.0018	9.3704	9.043
Mean ($\bar{x}$)	8.870463	8.854687	8.52268
Skewness	-1.074695	-0.701062	-0.44011
Excess kurtosis	-0.0451929	-0.392575	-0.580067
Outliers	9.3702, 7.0914,		9.6883, 9.4795, 7.712, 9.3705, 9.5562