Peer-Review

Kim, Aiden. 2026. “Exploring Essential Oil Composition and Mood Effects.” *Journal of High School Science* 10 (1): 14–36. https://doi.org/10.64336/001c.155127

Good work. This can be taken further though which will add even more value to your manuscript (see comments below and attached references and spreadsheet).
1.Please present formal definitions of calming, uplifting and stimulating. If it is in one of your references, please mention that the definition can be obtained from reference X.
2.Your figure 2 shows only 19 oils, though you mention that you obtained data from 40. Where are the rest? Please discuss in the manuscript.
3.Please include a supplementary file with data that includes exactly which manuscript/literature/publication, each compound’s data was obtained from (such as olfactory (mood) effect, concentration, chemical composition patterns. This is important as it helps readers replicate your work. If this is in a repository such as Github, please provide a link in the manuscript.
4.Present actual graphs showing datapoints with effect for calming, uplifting and stimulating compounds. Present all datapoints for each category (for the 3 categories) in the graphs (not just the top five as you have done in the table).
5.I want you to take this concept further. See reference 3. I used your figure 2 and found the polarizability (corresponding to electronicity) and molar volume (corresponding to stereocity) of 5 compounds showing a calming effect and 5 compounds showing uplifting and/or stimulating effects. See spreadsheet attached. It seems like there is a categorization cut off betwen these two categories based on the ratio of molar volume to polarizability; i.e. the greater this ratio, the compound is more likely to be uplifting and/or stimulating and the lesser this ratio, the more likely the compound is to be calming. I obtained the polarizability and molar volumes from the internet. It seems to me that your work does confirm an association between electronicity, stereocity and mood. Please present this data in the manuscript after you expand it to all your tested compounds.. This will add more value to your manuscript. Also cite references a through c below in the manuscript.
References:
a. Debnath T, Nakamoto T (2020) Predicting human odor perception represented by continuous values from mass spectra of essential oils resembling chemical mixtures. PLoS ONE 15(6): e0234688. https://doi.org/10.1371/journal.pone.0234688
b. https://iopscience.iop.org/article/10.1149/1945-7111/ac33e0/pdf
c. https://img.perfumerflavorist.com/files/base/allured/all/document/2016/02/pf.PF_28_01_036_09.pdf
_____Sheet1Polarizability

molar

	Label	ratio of molar volume (Angstroms cube)	molar volume(mL/mole)	ratio of molar volume to polarizability
delta-3-carene	calming	17.33	158.4	9.14
Alpha-terpineol	calming	19.07	165.9	8.7
Gamma-terpinene	calming	17.8	160.27	9
alpha pinene	calming	17.22	120.3	7
Lavandulol	calming	19.23	175.7	9.14
beta pinene	uplifting/stimulating	17.14	156	9.1
terpinen-4-ol	uplifting/stimulating	18.7	174.4	9.3

sabinene	uplifting/stimulating	17.24	161.81	9.3
limonene	uplifting/stimulating	18	170	9.44
1,8-cineole	uplifting/stimulating	18.18	174.4	9.59

calming (avg, std)	8.572, 0.813	
uplifting/stimulating	9.346, 0.163	
n		5
P-value		0.07

reference https://img.perfumerflavorist.com/files/base/allured/all/document/2016/02/pf.PF_28_01_036_09.pdf

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Open response questions

Comments to author

Good work. This can be taken further though which will add even more value to your manuscript (see comments below and attached references and spreadsheet).

1. Please present formal definitions of calming, uplifting and stimulating. If it is in one of your references, please mention that the definition can be obtained from reference X.

I now present operational definitions in Section 6.2 (Mood Categorization) and cite the sources. Briefly, calming refers to reductions in arousal/tension (e.g., parasympathetic-leaning responses), uplifting to positive valence with mild arousal, and stimulating to increased alertness/arousal. Definitions synthesize practice texts and psychophysiological literature (e.g., Battaglia, 2018; Tisserand & Young, 2014; Sowndhararajan & Kim, 2016), and I explicitly note where readers can find them in the cited references.

2. Your figure 2 shows only 19 oils, though you mention that you obtained data from 40. Where are the rest? Please discuss in the manuscript.

The original Figure 2 is a coefficient plot from one-vs-rest logistic models and displays compounds (top 5 positive and top 5 negative predictors per class) and does not display full data. All models were trained and evaluated on the full set of n=40 oils (LOOCV). To prevent confusion, I (i) clarified the caption and axis labels, and (ii) explicitly direct readers to figures that include all 40 oils (PCA and clustering in Figures 3–4; full per-compound datapoints in Supplementary Figure S3).

3. Please include a supplementary file with data that includes exactly which manuscript/literature/publication, each compound's data was obtained from (such as olfactory (mood) effect, concentration, chemical composition patterns. This is important as it helps readers replicate your work. If this is in a repository such as Github, please provide a link in the manuscript.

I added provide full code and data:

a. Supplementary Table S1a. Oil-to-label mapping with literature citations (title, journal, DOI/URL) and GC–MS source for each oil.

b. Supplementary Data

a. S1a_GC_MS. oil-to-label mapping with full literature citations (title, journal, DOI/URL) and GC–MS source per oil.

b. S1b_Composition_LONG. Oil, Compound, % by weight, Mood_Association, ≥0.5%
flag.

c. S3_Composition_WIDE. Oil × Compound matrix with Mood_Association.

d. S4_Logistic_Coefficients_ALL. and S2_full_logistic_coefficients.xlsx.

e. S5_Descriptors_STANDARDIZED. per-compound Polarizability_A3, MolarVolume_mL_per_mol, MV_over_alpha, Mood_Association, Descriptor_Source, Notes (proxy/temperature handling).

f. SD6_analysis_pipeline.ipynb. end-to-end notebook reproducing all tables/figures from raw inputs.

4. Present actual graphs showing datapoints with effect for calming, uplifting and stimulating compounds. Present all datapoints for each category (for the 3 categories) in the graphs (not just the top five as you have done in the table).

I added Supplementary Figure S3:

g. S3a beeswarm-style scatter of all compound–oil observations ≥0.5% stratified by mood

h. S3b mood-wise medians and IQRs per compound

These figures complement Table 1 (top correlations) by displaying the complete distributions.

5. I want you to take this concept further. See reference 3. I used your figure 2 and found the polarizability (corresponding to electronicity) and molar volume (corresponding to stereocity) of 5 compounds showing a calming effect and 5 compounds showing uplifting and/or stimulating effects. See spreadsheet attached. It seems like there is a categorization cut off betwen these two categories based on the ratio of molar volume to polarizability; i.e. the greater this ratio, the compound is more likely to be uplifting and/or stimulating and the lesser this ratio, the more likely the compound is to be calming. I obtained the polarizability and molar volumes from the internet. It seems to me that your work does confirm an association between electronicity, stereocity and mood. Please present this data in the manuscript after you expand it to all your tested compounds.. This will add more value to your manuscript. Also cite references a through c below in the manuscript.

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a. Debnath T, Nakamoto T (2020) Predicting human odor perception represented by continuous values from mass spectra of essential oils resembling chemical mixtures. PLoS ONE 15(6): e0234688. https://doi.org/10.1371/journal.pone.0234688

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c. https://img.perfumerflavorist.com/files/base/allured/all/document/2016/02/pf.PF_28_01_036_09.pdf

I implemented the suggested descriptor analysis across my compound list:

a. Compiled molar volume (mL/mol) and polarizability (Å³) per compound (Supplementary Table S5 with sources).

b. Evaluated MV/α ratio as a single descriptor. Pooling Uplifting+Stimulating vs. Calming, the ratio showed group separation (Welch's t-test $t = 1.71$, $p = 0.092$) and AUC = 0.666 with an optimal cutoff of approximately 8.76 (sensitivity 0.667, specificity 0.681) on our dataset.

c. Added an ROC plot (Supplementary Figure S4) and the exact table used.

These results support the hypothesis that a steric/electronic balance tracks mood at a coarse level and complement my multivariate composition models. I have cited the three suggested references (a–c).

SD6_analysis_pipeline.ipynb

Github Link: https://github.com/aiden276115/Supplementary-Data-SD6--analysis_pipeline.git

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Thank you for addressing my comments. The paper is significantly improved but some inconsistencies, formatting and organization issues remain. In addition, please include a "limitations" section if not already done so and include content in point 3 in this limitations section.

1.Formatting: Section numbering and table text are occasionally irregular, placeholders remain (e.g., '[..]' in §4.6), and chemical names are sometimes inconsistently formatted. Please check the manuscript thoroughly for placeholders or missing values.

2.Factual errors: Internal contradictions (e.g., geraniol/citronellol asserted as top calming correlates vs their appearance under uplifting in Table 1) and coefficient sign inconsistencies (negative predictors reported with positive β) are present; the claim that olfaction uniquely bypasses thalamic relay is an oversimplification. Please check the manuscript thoroughly for factual errors.
3.Include these following inadequacies under the "Limitations section" [1] Only LOOCV is reported; no bootstrap CIs, permutation testing, or external validation; §4.6 label-sensitivity analysis is incomplete; batch/source variability of GC–MS data is not modeled. [2] no multiple testing correction (Benjamini–Hochberg) across many correlations, no regularization for high p/n with collinearity, no CIs for metrics or coefficients, potential class imbalance not addressed, and assumptions (normality for Pearson, linear log-odds) not tested. [3] No adjustments for confounders such as extraction method, cultivar/chemotype, geographic origin, or publication heterogeneity; no batch effects modeling or meta-analytic weighting. [4] Collinearity is acknowledged, but no mitigation (e.g., ridge/elastic net, VIF screening, feature grouping) is applied; coefficients may be unstable and uninterpretable. [5] No explicit modeling was performed for synergy/antagonism and label uncertainty (e.g., probabilistic labels, interaction terms).
4.Tone down all claims that over-reach (without supporting evidence) such as "…establish quantitative chemical foundations….." given small n, collinearity, and modest AUCs.
5.Include physico-chemical descriptors briefly in abstract and conclusion. Rearrange your manuscript sections to a format that is accepted by this Journal (Introduction, Materials and Methods, Results, Discussion, Limitations, Perspectives, Conclusion).

Response to Reviewer
Below, I provide each reviewer comment verbatim, followed by a detailed description of how and where the manuscript was revised to address that specific point. All changes refer to the updated manuscript entitled "Exploring Essential Oil Composition and Mood Effects (Revised)".

1. Formatting Issues
Reviewer Comment:
"Formatting: Section numbering and table text are occasionally irregular, placeholders remain (e.g., '[..]' in §4.6), and chemical names are sometimes inconsistently formatted. Please check the manuscript thoroughly for placeholders or missing values."
Response:
To address this comment, the manuscript underwent a full formatting audit from start to finish:

- **Section numbering:**

All section and subsection numbers were standardized to match the journal's required structure. Nested subsections were checked for logical order and consistency.

- **Placeholder removal:**

All remaining placeholders such as "[…]", "TBD", or incomplete sentences in the previous version —especially in the sensitivity analysis subsection—were fully removed or replaced with finalized analysis text.

- **Chemical name consistency:**

Chemical names were standardized following IUPAC and common aromatic chemistry conventions, including consistent use of Greek letters (α-pinene, β-caryophyllene) and correct hyphenation/spelling (e.g., 1,8-cineole rather than 1.8 cineole).

- **Table uniformity improvements:**

Tables were reformatted to ensure:

- consistent font size (11 pt),
- left alignment for numerical fields,
- uniform caption style according to journal instructions,
- correction of any leftover italicization errors.

- **Proofreading for missing values:**

A manuscript-wide pass ensured that all statistical values (p-values, correlation coefficients, AUCs, sample counts) are fully present and consistent across the text, tables, and figures.

Locations Updated:

i. Sections 2, 3, 4, 5, and 6 (global edits throughout Manuscript)
j. Table 1, Table 2 formatting fixed
k. Former §4.6 corrected and rewritten

2. Factual Errors and Inconsistencies
Reviewer Comment:
"Factual errors: Internal contradictions (e.g., geraniol/citronellol asserted as top calming correlates vs their appearance under uplifting in Table 1) and coefficient sign inconsistencies (negative predictors reported with positive β) are present; the claim that olfaction uniquely bypasses thalamic relay is an oversimplification."
Response:
This comment required multiple factual and interpretive corrections:

- **Geraniol/citronellol classification fixed:**

Earlier drafts mistakenly included these as calming compounds, but corrected literature comparison and the study's own Pearson values show they are **uplifting-associated**. All relevant narrative text now reflects this.

- **Regression coefficient sign corrections:**

Logistic regression β values were re-checked against the original model output, and all mismatched signs were corrected in both text and visualized results.

- **Neuroscience clarification:**

The claim about olfaction bypassing the thalamus was revised to reflect current neuroscientific understanding:
"Olfactory pathways partially bypass the thalamus during initial processing while still engaging multiple distributed cortical–limbic circuits."

- **Chemical category consistency check:**

Each compound's placement under calming, uplifting, or stimulating was revalidated to eliminate internal contradictions.

Locations Updated:

- Introduction (Paragraph 2)
- Results 3.1 (Calming and Uplifting paragraphs)
- Results 3.3 (Predictor Sign Corrections)
- Discussion (Sections 4.1–4.2)

3. Required *Limitations* Section Content
Reviewer Comment:
"Include these following inadequacies under the Limitations section:
[1] Only LOOCV is reported; no bootstrap CIs, permutation testing, or external validation; §4.6 label-sensitivity analysis is incomplete; batch/source variability not modeled.
[2] No multiple testing correction; no regularization for high p/n; no CIs reported; class imbalance not addressed; assumptions not tested.
[3] No adjustments for confounders (extraction method, cultivar, geographic origin, publication heterogeneity); no batch effects modeling.
[4] Collinearity not mitigated; coefficients may be unstable.
[5] No explicit modeling of synergy/antagonism or label uncertainty."
Response:
A completely rewritten and expanded Section 5 (Limitations) now directly addresses each point in structured subsections:

5.1 Statistical Limitations

- lack of bootstrap confidence intervals,
- absence of permutation tests,
- reliance solely on LOOCV as internal validation.

5.2 Modeling/Data Structure Limitations

- no regularization despite high p/n,
- no BH/FDR multiple testing correction,
- class imbalance concerns.

5.3 Confounding & Heterogeneity

- unadjusted variation in extraction methods, cultivars, origins, and publication heterogeneity.

5.4 Collinearity Constraints

- highly correlated molecules likely caused instability in regression coefficients.

5.5 Unmodeled Interactions & Label Uncertainty

- no modeling of synergistic/antagonistic effects,
- no sensitivity analyses regarding ambiguous mood labels.

Each subsection explicitly cites why the issue matters for interpretation and how it limits generalizability, as the reviewer requested.

Locations Updated:

- Entire Section 5 (Limitations), paragraphs 5.1–5.5
- New text added explicitly referencing LOOCV, lack of bootstrap CIs, no batch adjustment, no BH correction, collinearity instability, and absence of interaction modeling.

4. Tone Down Over-Reaching Claims

Reviewer Comment:

"Tone down all claims that over-reach (without supporting evidence) such as '…establish quantitative chemical foundations…' given small n, collinearity, and modest AUCs."

Response:

To ensure alignment with data strength:

- Removed or softened language that implied definitive causal relationships.
- Replaced strong verbs (e.g., "establish", "demonstrate definitively") with "suggest", "indicate", "exploratory findings show…".
- Conclusion rewritten to highlight preliminary nature and future research needs.

Locations Updated:

- Abstract (last sentence)
- Discussion (throughout)
- Conclusion (last three paragraphs toned down)

5. Physicochemical Descriptor Inclusion

Reviewer Comment:

"Include physico-chemical descriptors briefly in abstract and conclusion."

Response:

- Abstract now incorporates the polarizability-to-volume ratio descriptor and its exploratory relevance.
- Conclusion includes a summary acknowledging its modest discriminatory performance (AUC = 0.666) and potential for future multi-feature modeling.

Locations Updated:

- Abstract (final two sentences)
- Conclusion (paragraph 3)

6. Reorganization of Manuscript Sections

Reviewer Comment:

“Rearrange your manuscript sections to a format that is accepted by this Journal (Introduction, Materials and Methods, Results, Discussion, Limitations, Perspectives, Conclusion).”

Response:

The manuscript was structurally reorganized into the required format:

1. Introduction
2. Materials and Methods
3. Results
4. Discussion
5. Limitations
6. Perspectives
7. Conclusion

Subsection numbering was updated accordingly to maintain internal consistency.

Locations Updated:

- Global restructuring (Sections 1–7 reordered and renumbered)

Summary Statement

All the reviewer’s comments have been carefully addressed and reflected throughout the revised manuscript. I corrected the formatting issues, fixed factual inconsistencies, clarified the statistical explanations, reorganized the sections into the required structure, and adjusted the tone so that the claims are more appropriate for the data. With these changes, the updated manuscript now follows the journal’s guidelines and resolves all the problems that were previously pointed out.

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Thank you for addresing my comments. Accepted.

HOWEVER, I have made additions and changes to capture more information. Please check thoroughly. If you are in agreement with the changes, please let us know at the discussion board so that we may proceed with copyediting.

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I have reviewed the additions and changes, and I agree with them. Please proceed with copyediting.

•Shireesh Apte
Jan 6, 2026 - 10:35 am IST

Dear author,
Thank you. As we continue copyediting, I had a questtion. Why do the r and p values in Table 1 in the manuscript differ from those in Supplemenatary Table 6 ? Are they supposed to be different? And if yes, can you provide me with an example of how you derived one representative value?
Best,
Shireesh Apte

•Aiden Kim
Jan 7, 2026 - 12:14 pm IST

Dear Dr. Apte,

Thank you for the question.
Table 1 reports the top 5 point-biserial (Pearson) correlations per mood category using the literature-based labels, with uncorrected two-sided p-values. Supplementary Table S6 lists the full set of correlations from the same analysis and additionally includes Benjamini-Hochberg FDR-adjusted q values. Because S6 is rounded to three decimals, very small p-values may appear as 0.000 (i.e., $p < 0.001$). Also, the same compound appears separately under each mood category in S6, so values should be compared within the same Mood-Compound row.
Representative example (Uplifting-Limonene): we create a binary indicator y (1 = Uplifting, 0 = otherwise) across n = 40 oils, correlate limonene % (continuous) with y using the point-biserial correlation (equivalent to Pearson's r with a binary variable), and compute the two-sided p-value from the standard t-test for r. For this case, r = 0.584 and the two-sided p = 7.6 X 10^(-5), which rounds to 0.000 at three decimals (i.e., $p < 0.001$).
To keep the manuscript and supplement consistent, please feel free to report any p-values < 0.001 as < 0.001 (rather than 0.000), and update Table 1 accordingly (e.g., Uplifting-Limonene p should be < 0.001).

Thank you!

We are OK to copyedit. Thank You!