

Peer Review

Review of: "Infrared Spectroscopy (FT-NIR) and t-Distributed Stochastic Neighbor Embedding (t-SNE) as an Analytical Methodology for Rapid Identification of Tea Adulteration"

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General comments:

The paper covers the FT-NIR spectral analysis of a range of tea components. The paper would benefit from a clearer explanation of the methods used to prepare the samples. The statistical analysis of the samples could also be better explained, and the rationale and benefit of the use of deconvolution made clear. Validation of the results is essential to prove the authors' claims that this approach could work in practice.

Specific comments:

Section 2.1: Suggest adding more detail regarding sample preparation. E.g., how they were dehydrated, how they were blended/made homogenous prior to sieving, and whether the triplicate measurements were averaged.

Section 3.1: Mention figure 1 (d) in the text as well as in the figure caption.

Sections 3.2.1/2/3: Need to show the normalised spectra before deconvolution is introduced. I'm not sure deconvolution is needed here; the bands attributed to the respective chemical compounds are probably apparent without that being needed.

It is not clear how the R²R figures are derived; this needs explanation in the methods section.

Section 3.3: Need to clarify what data was used in the PCA and t-SNE experiments and explain how the ellipses for each plot were calculated. Some form of validation with new (possibly deliberately adulterated) samples is needed; currently, all figure 5 shows is that these samples form clusters. Need to provide details of the method used to give the figure 6 plot.

Declarations

Potential competing interests: No potential competing interests to declare.