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Lutfun Nahar <onbehalfof@manuscriptcentral.com>

Do 08.09.2022 13:34

An:Liling Triyasmono <liling.triyasmono@uni-wuerzburg.de>;

08-Sep-2022

Dear Mr. Triyasmono

Welcome to the online submission system for Phytochemical Analysis. An account has been created for you as Co-Author on a manuscript.

Your case-sensitive USER ID at https://mc.manuscriptcentral.com/pca is as follows:

USER ID:
liling.triyasmono@uni-wuerzburg.de

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After completing the set-up of your account you will be able to log-in and track the progress of your submission, through the peer-review process, to the point of final decision.

Thank you for your participation.

Yours sincerely

Phytochemical Analysis Editorial Office

(this is an automated email)

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WG: PCA-22-0406 - Decision

Liling Triyasmono

Di 18.10.2022 09:56

Gesendete Elemente

An:Ludwig Höllein <ludwig.hoellein@uni-wuerzburg.de>;

Dear Dr. Ludwig,

Here is an email link and instructions from the editor for re-submission.

Thank you for your time and assistance.

Best regards,
Liling

Von: Ulrike Holzgrabe
Gesendet: Dienstag, 11. Oktober 2022 08:51
An: Liling Triyasmono
Betreff: WG: PCA-22-0406 - Decision

Hi Liling,

this looks very good. Would you please prepare the revision and rebuttal letter.

Ulrike

-----Ursprüngliche Nachricht-----
Von: Anupam Talukdar <onbehalfof@manuscriptcentral.com>
Gesendet: Dienstag, 11. Oktober 2022 06:24
An: Ulrike Holzgrabe <ulrike.holzgrabe@uni-wuerzburg.de>
Betreff: PCA-22-0406 - Decision

Dear Prof. Holzgrabe

I have now received the referees reports about your manuscript - see attached.

You will see that the referees conclude that your paper is basically acceptable but requires some minor revision with respect to a few points before it can be published in Phytochemical Analysis (PCA).

Might I invite you to revise your manuscript by attending carefully to the points raised by the referees in their reports?
When you submit your revised paper, please could you also enclose a covering letter in which you indicate the actions (or otherwise)

that you have taken with respect to each of the points raised by the referees?

Wiley Editing Services Available to All Authors Should you be interested, Wiley Editing Services offers expert help with manuscript, language, and format editing, along with other article preparation services. You can learn more about this service option at www.wileyauthors.com/eeo/preparation. You can also check out Wiley's collection of free article preparation resources for general guidance about writing and preparing your manuscript at www.wileyauthors.com/eeo/prepresources.

PCA house-rules allow FOUR weeks for the minor revision of submitted manuscripts. I look forward to hearing from you in due course.

Yours sincerely,

Dr. Anupam Talukdar

PS: reviewers comments
Reviewer: 1

Comments to the Author - note these may be passed on unedited.
The project is interesting, and the manuscript is well-written. However, there are several critical issues. First of all, you cannot talk about classification/recognition. PCA is not used to classify as the authors stated at line 82. PCA is an unsupervised method to visualize similarities and differences among samples. On the contrary, PLS-R is a supervised regression method used to predict values (such as concentrations, and unsaturation levels) in unknown samples.
Generally, PCA is performed prior to supervised methods to assess their applicability to the dataset. Classification models can be achieved through PLS-DA or LDA or other supervised machine learning techniques. For this reason, this project cannot be accepted as it is for publication. Classification methods have to be added. Additionally, the number of samples is not enough for classification. At least, you have to increase the number of binary mixtures.
Moreover, the comparison of the achieved results with other methods in the literature is completely missing. The recognition of vegetable oils has been attempted by several authors with NMR and FTIR. The advantages of your method should be highlighted. Here are some examples of similar articles that should be discussed:
https://doi.org/10.1021/acs.jafc.1c02279 : the recognition was achieved using 13C-NMR without the employment of chemometrics.
https://doi.org/10.1007/s11746-002-0472-z : 13C-NMR
https://doi.org/10.1016/j.foodcont.2014.04.046 : NMR and descriptive PCA
https://doi.org/10.1016/j.foodcont.2011.08.013: ATR-FTIR and chemometrics

In the figures' captions, it might be useful to insert the abbreviation to help the reader.
In figures 5 and 6 insert the meaning of colored circles.
- Material of ATR cell?
- Why did not you mean-centered spectral data after baseline correction/first derivative? This pretreatment is strongly recommended.
- Savitzky-Golay which derivative? Provide more details.
- Lines 144 and 148: PCA is not a supervised classification method!!!
- Line 203 there is a repetition of the verb "show".
- In PLS, the number of samples used for the training set (70%) should be higher than that of the test set (30%). You used 19

samples for building the models and 21 for the prediction.

Reviewer: 2

Comments to the Author - note these may be passed on unedited.
The overall paper is well written.
Considering readers in the Western nations are less family with this fruit a photograph and some mention of the taste of this fruit/oil may interest.

More importantly the axes of all the figures are rather small and hard to read. They should be reproduced somewhat larger than those submitted to permit interested readers to understand them more readily.

Finally, using 4cm-1 as a sampling interval was used to ensure binning should be explained as has been for the NMR spectrum.

Reviewer: 3

Comments to the Author - note these may be passed on unedited.
This is an interesting, comprehensive and well conducted study. The proposed method for determination of red fruit oil quality is chemometrically supported 1H NMR and FTIR spectra analysis that contributed to the classification of red fruit oil depending on its content of the unsaturation and FFA values.
I strongly recommend this paper to be published since this technique, compared to other techniques frequently used, is fast, economical (as authors recognized) but also nondestructive.
The chemometric methods (PCA and PLSR) are properly used and discussed, so I have no addition suggestions that can improve the quality of the paper. However, it is commendable that the authors used chemometric methods that have been around for more than a century, but their full potential has not yet been exploited. Their application leads to valid and accurate conclusions in a simple and much faster way, which is also demonstrated in this paper.
I have only two technical suggestion:

Page 5, line 1, the verb informations should be corrected to information, information has no plural form.
Page 10, line 9, neighbourhood is not spelled properly, please correct.

PS: How to submit your revised manuscript:

Log into https://mc.manuscriptcentral.com/pca and enter your Author Center, where you will find your manuscript title listed under "Manuscripts with Decisions". Click on "create revision"

You will be required to respond to the comments made by the referee(s) in the space provided. You can use this space to document any changes you make to the original manuscript.

[E-Mail reference DL-SW-9]

AW: PCA-22-0406.R2 - Decision

Liling Triyasmono

Mo 21.11.2022 08:27

Gesendete Elemente

An:Ulrike Holzgrabe <ulrike.holzgrabe@uni-wuerzburg.de>;

Dear Prof. Ulrike,

Thank you for all your time, support, direction, correction, and guidance, Professor.
Finally, our manuscript has been accepted.
Without your tremendous support, the article would not have been accepted there.
I am delighted to receive this news.

Thank you again for everything, Professor.
Best regards,
Liling

Von: Ulrike Holzgrabe
Gesendet: Montag, 21. November 2022 07:10:31
An: Liling Triyasmono
Betreff: Fwd: PCA-22-0406.R2 - Decision

Congratulations!
Ulrike

Anfang der weitergeleiteten Nachricht:

> Von: Anupam Talukdar <onbehalfof@manuscriptcentral.com>
> Datum: 21. November 2022 um 06:14:51 MEZ
> An: Ulrike Holzgrabe <ulrike.holzgrabe@uni-wuerzburg.de>
> Betreff: PCA-22-0406.R2 - Decision
> Antwort an: anupam@bioinfoaus.ac.in
>
> Dear Prof. Holzgrabe
>
> I am pleased to be able to inform you that the paper you submitted to Phytochemical Analysis (PCA), as indicated above, has been recommended for acceptance by the referees in its original version.
>
> Your manuscript will be edited according to PCA format and house-style, and transmitted to the publishers (Wiley & Sons, Chichester, UK) for copy-editing and proofing. The proofs will be sent to you (as pdf files) directly by the printers according to their work schedule.
>
> Should any problems occur during the processing of your paper, I will contact you by e-mail - so please do keep me updated of any change in your e-mail address.
>
> Thank you for your support of Phytochemical Analysis: we look forward to receiving your next submission.

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With best regards,

Dr. Anupam Talukdar

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*Wiley's Author Services: https://authorservices.wiley.com/home.html

[E-Mail reference DL-RW-11]

Your article has been accepted! Here's what comes next

cs-author@wiley.com

Fr 25.11.2022 09:01

An:Liling Triyasmono <liling.triyasmono@uni-wuerzburg.de>;

Dear Liling Triyasmono,

Article ID: PCA3196
Article Title: Chemometric analysis applied to 1H NMR and FTIR data for a quality parameter distinction of Red Fruit (Pandanus conoideus, Lam.) Oil products
Journal Title: Phytochemical Analysis

Congratulations your article has been accepted in Phytochemical Analysis! To register with Author Services, simply click here or paste this link into your browser.

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Before You Submit

Manuscripts I Have Co-Authored

STATUS	ID	TITLE	CREATED	SUBMITTED
Accepted (21-Nov-2022)	PCA-22-0406.R2	Chemometric analysis applied to ^{1}H NMR and FTIR data for a quality parameter distinction of Red Fruit (Pandanus conoideus, Lam.) Oil products View Submission Submitting Author: Holzgrabe, Ulrike	08-Nov-2022	08-Nov-2022
Minor Revision (06-Nov-2022)	PCA-22-0406.R1	Chemometric analysis applied to 1H NMR and FTIR data for a quality parameter distinction of Red	21-Oct-2022	21-Oct-2022

1

STATUS	ID	TITLE	CREATED	SUBMITTED
a revision has been submitted		Fruit (Pandanus conoideus, Lam.) Oil products View Submission Submitting Author: Holzgrabe, Ulrike		
Minor Revision (11-Oct-2022) a revision has been submitted	PCA-22-0406	Chemometric analysis applied to 1H NMR and FTIR data for a quality parameter distinction of Red Fruit (Pandanus conoideus, Lam.) Oil products View Submission Submitting Author: Holzgrabe, Ulrike	07-Sep-2022	08-Sep-2022