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[Agriculture] Manuscript ID: agriculture-1072820 - Submission Received

1 message

Editorial Office <agriculture@mdpi.com> Mon, Dec 28, 2020 at 1:24 PM
Reply-To: agriculture@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>

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Thank you very much for uploading the following manuscript to the MDPI submission system. One of our editors will be in touch with you soon.

Journal name: Agriculture
Manuscript ID: agriculture-1072820
Type of manuscript: Article
Title: Classification of Lampung Robusta Specialty Coffee According to Different Cherry Processing Methods Using UV Spectroscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia
Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
Submitted to section: Agricultural Technology,
https://www.mdpi.com/journal/agriculture/sections/Agricultural_technology

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[Agriculture] Manuscript ID: agriculture-1072820 - Article Processing Charge Confirmation

Agriculture Editorial Office <agriculture@mdpi.com> Tue, Dec 29, 2020 at 1:24 PM
Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

Thank you very much for submitting your manuscript to Agriculture:

Journal name: Agriculture
Manuscript ID: agriculture-1072820
Type of manuscript: Article
Title: Classification of Lampung Robusta Specialty Coffee According to Different Cherry Processing Methods Using UV Spectroscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia
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E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
Submitted to section: Agricultural Technology,
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[Agriculture] Manuscript ID: agriculture-1072820 - Assistant Editor Assigned

Stephanie He <stephanie.he@mdpi.com> Tue, Dec 29, 2020 at 1:26 PM
Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Stephanie He <stephanie.he@mdpi.com>, Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

Your manuscript has been assigned to Stephanie He for further processing who will act as a point of contact for any questions related to your paper.

Journal: Agriculture
Manuscript ID: agriculture-1072820
Title: Classification of Lampung Robusta Specialty Coffee According to Different Cherry Processing Methods Using UV Spectroscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia

Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id

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[Agriculture] Manuscript ID: agriculture-1072820 - Major Revisions - Due Date 22 January 2021

Agriculture Editorial Office <agriculture@mdpi.com> Wed, Jan 13, 2021 at 9:29 AM
Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

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E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
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[Agriculture] Manuscript ID: agriculture-1072820 - Manuscript Resubmitted

Submission System <submission@mdpi.com> Mon, Jan 18, 2021 at 12:20 PM
Reply-To: Stephanie He <stephanie.he@mdpi.com>, Agriculture Editorial Office <agriculture@mdpi.com>
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>

Dear Dr. Suhandy,

Thank you very much for resubmitting the modified version of the following manuscript:

Manuscript ID: agriculture-1072820
Type of manuscript: Article
Title: Classification of Lampung Robusta Specialty Coffee According to Different Cherry Processing Methods Using UV Spectroscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia
Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
Submitted to section: Agricultural Technology,
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A member of the editorial office will be in touch with you soon regarding progress of the manuscript.

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Agriculture Editorial Office <agriculture@mdpi.com> Mon, Jan 18, 2021 at 12:54 PM
Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

Thank you very much for providing the revised version of your paper:

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Received: 28 December 2020
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[Agriculture] Manuscript ID: agriculture-1072820 - Minor Revisions - Due Date 23 January 2021

Agriculture Editorial Office <agriculture@mdpi.com> Thu, Jan 21, 2021 at 8:05 AM
Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

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E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
Submitted to section: Agricultural Technology,
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Email: stephanie.he@mdpi.com
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To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>

Dear Dr. Suhandy,

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Manuscript ID: agriculture-1072820
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Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
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Reply-To: stephanie.he@mdpi.com
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

Thank you very much for providing the revised version of your paper:

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Received: 28 December 2020
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Assistant Editor

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[Agriculture] Manuscript ID: agriculture-1072820 - Accepted for Publication

Agriculture Editorial Office <agriculture@mdpi.com> Tue, Jan 26, 2021 at 2:38 PM
Reply-To: Agriculture Editorial Office <agriculture@mdpi.com>
To: Diding Suhandy <diding.sughandy@fp.unila.ac.id>
Cc: Meinilwita Yulia <meinilwitayulia@polinela.ac.id>, Agriculture Editorial Office <agriculture@mdpi.com>

Dear Dr. Suhandy,

We are pleased to inform you that the following paper has been officially accepted for publication:

Manuscript ID: agriculture-1072820
Type of manuscript: Article
Title: Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spec-troscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia
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Type of manuscript: Article
Title: Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spec-troscopy and Chemometrics
Authors: Diding Suhandy *, Meinilwita Yulia
Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
Submitted to section: Agricultural Technology,
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Type of manuscript: Article
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Authors: Diding Suhandy *, Meinilwita Yulia
Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
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Type of manuscript: Article
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Authors: Diding Suhandy *, Meinilwita Yulia
Received: 28 December 2020
E-mails: diding.sughandy@fp.unila.ac.id, meinilwitayulia@polinela.ac.id
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Dear Authors,

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Abstract: https://www.mdpi.com/2077-0472/11/2/109
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Classification of Lampung Robusta Specialty Coffee According to Different Cherry Processing Methods Using UV Spectroscopy and Chemometrics

Classification based on spectroscopic data offers many possibilities. UV range data is less commonly used, which is definitely a novelty.

My content comments:

- Needless to say, it was measured in transmittance mode. Absorbance is measured with a UV spectrophotometer, so no other phenomenon can be detected
- Lines 58-64: shows with literature references how the processing method affects other properties (glucose and fructose concentration, amino acid, etc.) Here it is worth explaining this better and e.g. table to present comparative data. It is not known whether these data are given for dry matter or fresh product. Thus, the terms "higher" or "lower" concentration cannot be interpreted.
- Chapter 2.2: Sample preparation for coffee is not clear to me: “Stirred with hot distilled water at 98°C for 10 minutes”. How was it ensured that the water temperature was 98°C throughout? Why was the technique of making espresso coffee not used: extraction with high pressure, water vapor? The dissolution of valuable components is thus more efficient.
- Chapter 2.3.: the near UV range does start at 190 nm, but we don't really use it below 200 nm anymore - as you can see in the spectra, the signal-to-noise ratio is bad.

The equation is unnecessary it is evident.

- Chapter 2.4.: The difference between the methods must be presented in at least one sentence. If the accuracy is given as a percentage, then Equation 2 is incorrect, it must be multiplied by 100.
- Chapter 3.1. these are different data processing operations. It is not mentioned later which pre-treatment method and where it was used.
- Chapter 3.2. For PCA, PC1 and PC2 explain only 82% of the variance. This is not enough, it is too low. In this case, the value of PC3 must also be taken into account.

What percentage was the accuracy of the classification using PCA?

- Chapter 3.3. The accuracy of the calibration is not usually reported because, in fact, the accuracy of the validation is crucial. This is also confusing because for the PCA-LDA model, the accuracy is once 93.33% and then 91.7% in the table.

What is the difference between the LDA and the PCA-LDA model?

During LDA, the data are previously subjected to PCA data reduction in all cases. I do not understand. This also shows that 2.4. Chapter 2 lacks a description and explanation of the methods.

In the end, for the classification models, were only the absorbance values of the designated wavelengths used?

It would have been worth considering the entire spectral data set, precisely because of the overlaps.

- Chapter 4 The Conclusion chapter is very short.

My formal comments:

Lines 38 and 39: the name of the coffee plant must be written in italics

Line 99: Lampung Robusta – italics

The manuscript is interesting, but I recommend it only after a very thorough revision.

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Manuscript ID: agriculture-1072820

Type: Article

Number of Pages: 9

Title: Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spectroscopy and Chemometrics

Authors: Diding Suhandy * , Meinilwita Yulia

Abstract: The postharvest processing factors including cherry processing methods highly influence the final quality of coffee beverages, especially in the composition of several coffee metabolites such as glucose, fructose, the amino acid (glutamic acid), and chlorogenic acids (CGA) as well as trigonelline contents. In this research, UV spectroscopy combining with chemometrics was used to classify a ground roasted Lampung robusta specialty coffee according to different cherry processing methods. Total 360 samples of Lampung robusta specialty coffee with 1 gram of weight for each sample from three different cherry processing methods were prepared as samples: 100 samples of pure dry coffee (DRY), 100 samples of pure semi-dry coffee (SMD), 100 samples of pure wet coffee (WET) and 60 samples of adulterated coffee (ADT) (SMD coffee was adulterated with DRY and WET coffee). All samples were extracted using a standard protocol as explained by previous works. A low-cost benchtop UV-visible spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, the USA) was utilized to obtain UV spectral data in the interval of 190-400 nm using transmittance mode. Using the first two principal components (PCs) with a total of 82% of explained variance, there was good separation between samples. The samples were clustered into four possible groups according to different cherry processing methods: dry, semi-dry, wet, and adulterated. Four supervised classification methods, partial least squares-discriminant analysis (PLS-DA), principal component analysis-linear discriminant analysis (PCA-LDA), linear discriminant analysis (LDA), support vector machine classification (SVMC), were selected to classify the Lampung robusta specialty coffee according to differences in cherry processing methods. PCA-LDA is the best classification method with 91.7% classification accuracy in prediction. PLS-DA, LDA and SVMC give accuracy of 56.7%, 80.0% and 85.0%, respectively. The present research suggested that UV spectroscopy combining with chemometrics will be highly useful in Lampung robusta specialty coffee authentication.

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Comments and Suggestions for Authors

Classification based on spectroscopic data offers many possibilities. UV range data is less commonly used, which is definitely a novelty.

The manuscript is interesting, but I recommend it only after a very thorough revision.

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Number of Pages: 9

Title: Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spectroscopy and Chemometrics

Authors: Diding Suhandy * , Meinilwita Yulia

Abstract: The postharvest processing factors including cherry processing methods highly influence the final quality of coffee beverages, especially in the composition of several coffee metabolites such as glucose, fructose, the amino acid (glutamic acid), and chlorogenic acids (CGA) as well as trigonelline contents. In this research, UV spectroscopy combining with chemometrics was used to classify a ground roasted Lampung robusta specialty coffee according to different cherry processing methods. Total 360 samples of Lampung robusta specialty coffee with 1 gram of weight for each sample from three different cherry processing methods were prepared as samples: 100 samples of pure dry coffee (DRY), 100 samples of pure semi-dry coffee (SMD), 100 samples of pure wet coffee (WET) and 60 samples of adulterated coffee (ADT) (SMD coffee was adulterated with DRY and WET coffee). All samples were extracted using a standard protocol as explained by previous works. A low-cost benchtop UV-visible spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, the USA) was utilized to obtain UV spectral data in the interval of 190-400 nm using transmittance mode. Using the first two principal components (PCs) with a total of 82% of explained variance, there was good separation between samples. The samples were clustered into four possible groups according to different cherry processing methods: dry, semi-dry, wet, and adulterated. Four supervised classification methods, partial least squares-discriminant analysis (PLS-DA), principal component analysis-linear discriminant analysis (PCA-LDA), linear discriminant analysis (LDA), support vector machine classification (SVMC), were selected to classify the Lampung robusta specialty coffee according to differences in cherry processing methods. PCA-LDA is the best classification method with 91.7% classification accuracy in prediction. PLS-DA, LDA and SVMC give accuracy of 56.7%, 80.0% and 85.0%, respectively. The present research suggested that UV spectroscopy combining with chemometrics will be highly useful in Lampung robusta specialty coffee authentication.

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Are the results clearly presented?	( )	( )	( )	( )
Are the conclusions supported by the results?	( )	( )	( )	( )

Comments and Suggestions for Authors

The authors used UV and chemometrics to classify coffees obtained by different process. Despite being an incremental progress, it is an interesting tool for the quality assessment of products, having interest to the audience. However, I believe there are aspects in the paper that need to be clarified to make it robust.

1) I believe the ranges of the values, such as grain size and sample weight should be informed, instead of the average value only.

2) Authors should address better the differences between Fig. 1 and Fig. 2, where some peaks seems to be appeared. Is it an artifact of the pre-treatment?

3) In Fig. 5, the training and validation points for dry and adulterated are mixed, not supporting the claim that the samples were correctly classified.

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Manuscript ID	agriculture-1072820
Type	Article
Number of Pages	9
Title	Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spectroscopy and Chemometrics
Authors	Diding Suhandy * , Meinilwita Yulia

Abstract The postharvest processing factors including cherry processing methods highly influence the final quality of coffee beverages, especially in the composition of several coffee metabolites such as glucose, fructose, the amino acid (glutamic acid), and chlorogenic acids (CGA) as well as trigonelline contents. In this research, UV spectroscopy combining with chemometrics was used to classify a ground roasted Lampung robusta specialty coffee according to different cherry processing methods. Total 360 samples of Lampung robusta specialty coffee with 1 gram of weight for each sample from three different cherry processing methods were prepared as samples: 100 samples of pure dry coffee (DRY), 100 samples of pure semi-dry coffee (SMD), 100 samples of pure wet coffee (WET) and 60 samples of adulterated coffee (ADT) (SMD coffee was adulterated with DRY and WET coffee). All samples were extracted using a standard protocol as explained by previous works. A low-cost benchtop UV-visible spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, the USA) was utilized to obtain UV spectral data in the interval of 190-400 nm using transmittance mode. Using the first two principal components (PCs) with a total of 82% of explained variance, there was good separation between samples. The samples were clustered into four possible groups according to different cherry processing methods: dry, semi-dry, wet, and adulterated. Four supervised classification methods, partial least squares-discriminant analysis (PLS-DA), principal component analysis-linear discriminant analysis (PCA-LDA), linear discriminant analysis (LDA), support vector machine classification (SVMC), were selected to classify the Lampung robusta specialty coffee according to differences in cherry processing methods. PCA-LDA is the best classification method with 91.7% classification accuracy in prediction. PLS-DA, LDA and SVMC give accuracy of 56.7%, 80.0% and 85.0%, respectively. The present research suggested that UV spectroscopy combining with chemometrics will be highly useful in Lampung robusta specialty coffee authentication.

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Are the results clearly presented?	( )	( )	(x)	( )
Are the conclusions supported by the results?	( )	( )	(x)	( )

Comments and Suggestions for Authors

The manuscript *"Classification of Lampung Robusta specality coffee according to different cherry processing methods using UV spectroscopy and chemometrics"* addressed an interesting application for spectroscopy. The manuscript provides a sufficient background and introduction to the research. However, there are several areas to be addressed before this manuscript is considered for publication. Major concerns are in the lack of information provided in selecting these 4 supervised classification approaches and not enough background information behind the algorithms. The Unscrambler is a powerful software tool, but picking four approaches and stating accuracy results is not enough. I hope the following comments are helpful in progressing with the manuscript.

Subjective language used throughout, such as "good", "better", or "best" and should be reworded.

Sample division into cal, val, test is well constructed.

Should list the explained variance for the selected 10 PCs

P3, L128: is not correct. It states that "PCA is used for unsupervised classification". PCA is not a classification method, but rather a visualization tool that does not explicitly calculate classification. This should be reworded.

There is not enough information given on the four supervised classification approaches. Stating that "A detailed explanation of

classification approaches. Stating that "A detailed explanation of those methods can be found …" is not enough information to tell the reader any details of those approaches for this dataset. For example: there are many different parameters that are needed to run a SVMC such as the gamma, kernel type, cost-of-classification… Info is listed for SVMC in results and discussion, but there is no justification to why these were selected. Was a grid search performed to identify optimal SVMC parameters in Unscrambler? If so, that should be listed in materials and methods.

Should justify why a PC-LDA/LDA was chosen over QDA or Mahalanobis DA which are options that can be selected in the Unscrambler software as well, dealing with non-linearity or scaling issues. Was there a pattern in the covariance of the data structure that justified LDA or was the accuracy simply higher for that approach?

Preprocessing spectral data – SNV is appropriate, but was derivative processing necessary? If so, the authors should state classification results of the raw data to justify the use of Savitzky-Golay (SG). Baseline correction is addressed with (SG), but less invasive adjustments can also be used for baseline correction.

P6, L184: should state "…differences in cherry processing methods.", not "different"

Good job from authors in noting the PC-LDA benefit over LDA for highly correlated spectral data.

Chemometric results: What about the downside of PC-LDA / LDA? These methods may give improved accuracy by forcing classification into a group but may not be realistic. Whereas PLS-DA or SVMC do not force a sample into a classification group.

Chemometric results: What does the model fit look like for each of the four approaches? Reporting an accuracy is not enough information. How do we know that approach is the most robust? Possibly reporting the delta accuracy between training and prediction of each method would help.

Submission Date	28 December 2020
Date of this review	06 Jan 2021 15:29:45

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Journal: Agriculture (https://www.mdpi.com/journal/agriculture) (ISSN 2077-0472)

Manuscript ID: agriculture-1072820

Type: Article

Number of Pages: 9

Title: Classification of Lampung Robusta Specialty Coffee According to Differences in Cherry Processing Methods Using UV Spectroscopy and Chemometrics

Authors: Diding Suhandy * , Meinilwita Yulia

Abstract: The postharvest processing factors including cherry processing methods highly influence the final quality of coffee beverages, especially in the composition of several coffee metabolites such as glucose, fructose, the amino acid (glutamic acid), and chlorogenic acids (CGA) as well as trigonelline contents. In this research, UV spectroscopy combining with chemometrics was used to classify a ground roasted Lampung robusta specialty coffee according to different cherry processing methods. Total 360 samples of Lampung robusta specialty coffee with 1 gram of weight for each sample from three different cherry processing methods were prepared as samples: 100 samples of pure dry coffee (DRY), 100 samples of pure semi-dry coffee (SMD), 100 samples of pure wet coffee (WET) and 60 samples of adulterated coffee (ADT) (SMD coffee was adulterated with DRY and WET coffee). All samples were extracted using a standard protocol as explained by previous works. A low-cost benchtop UV-visible spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, the USA) was utilized to obtain UV spectral data in the interval of 190-400 nm using transmittance mode. Using the first two principal components (PCs) with a total of 82% of explained variance, there was good separation between samples. The samples were clustered into four possible groups according to different cherry processing methods: dry, semi-dry, wet, and adulterated. Four supervised classification methods, partial least squares-discriminant analysis (PLS-DA), principal component analysis-linear discriminant analysis (PCA-LDA), linear discriminant analysis (LDA), support vector machine classification (SVMC), were selected to classify the Lampung robusta specialty coffee according to differences in cherry processing methods. PCA-LDA is the best classification method with 91.7% classification accuracy in prediction. PLS-DA, LDA and SVMC give accuracy of 56.7%, 80.0% and 85.0%, respectively. The present research suggested that UV spectroscopy combining with chemometrics will be highly useful in Lampung robusta specialty coffee authentication.

Author's Reply to the Review Report (Reviewer 1)

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	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	(x)	( )	( )	( )
Are the results clearly presented?	(x)	( )	( )	( )

Are the conclusions supported by the results?	( )	( )	( )	( )

Comments and Suggestions for Authors	The authors improved and expanded the manuscript based on my recommendation. I got the correct answer to my questions.
Submission Date	28 December 2020
Date of this review	18 Jan 2021 10:31:28

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( ) I don't feel qualified to judge about the English language and style

	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	( )	(x)	( )	( )
Are the results clearly presented?	( )	(x)	( )	( )

Are the conclusions supported by the results?	(x)	( )	( )	( )

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Comments and Suggestions for Authors	The authors answered most of the questions I posed. The variation in the samples still need to be clarified. I was expecting something like 1±0.1 g for average weight of 100 samples. Next to figure 5 of the paper, I'd include the one presented in the answer to the reviewers, as well as the explanation accompaning it, to clarify the results from figure 5.
Submission Date	28 December 2020
Date of this review	18 Jan 2021 22:13:20

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Author's Reply to the Review Report (Reviewer 3)

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	Yes	Can be improved	Must be improved	Not applicable
Does the introduction provide sufficient background and include all relevant references?	(x)	( )	( )	( )
Is the research design appropriate?	(x)	( )	( )	( )
Are the methods adequately described?	(x)	( )	( )	( )
Are the results clearly presented?	(x)	( )	( )	( )

Are the conclusions supported by the results?	(x)	( )	( )	( )

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Comments and Suggestions for Authors	Thank you to the authors for their time in revising the article. The article is improved.

Submission Date	28 December 2020
Date of this review	20 Jan 2021 13:01:08

Response to Reviewer 1 Comments

Point 1: Needless to say, it was measured in transmittance mode. Absorbance is measured with a UV spectrophotometer, so no other phenomenon can be detected

Response 1:
Yes. The authors agree to revise this part. The sentence "it was measured in transmittance mode" was removed in the revised article.

Point 2: Lines 58-64: shows with literature references how the processing method affects other properties (glucose and fructose concentration, amino acid, etc.) Here it is worth explaining this better and e.g. table to present comparative data. It is not known whether these data are given for dry matter or fresh product. Thus, the terms "higher" or "lower" concentration cannot be interpreted.

Response 2:
The authors agree to revise this part.
The authors agree that a fair comparable judgment of cup quality can only be expected, if (1) comparable starting material is used; and (2) the conditions chosen are suitable to produce good-quality coffee with either way of cherry processing. For this reason, the authors agree to show the influence of cherry processing method on final quality of coffee beverages in general way by literature-based comparison.

As it has been mentioned in the third paragraph in introduction section, the postharvest processing factors including cherry processing methods highly influence the final quality of coffee beverages, especially in the composition of several coffee metabolites such as glucose, fructose, the amino acid (glutamic acid), and chlorogenic acids (CGA) as well as trigonelline contents. Several references were provided to support this.

Point 3: Chapter 2.2: Sample preparation for coffee is not clear to me: "Stirred with hot distilled water at 98°C for 10 minutes". How was it ensured that the water temperature was 98°C throughout? Why was the technique of making espresso coffee not used: extraction with high pressure, water vapor? The dissolution of valuable components is thus more efficient

Response 3:
The protocol for sample extraction was performed based on previous works as mentioned in the article. There was no temperature control during stirring the

samples. Each sample was put in 50 mL of hot distilled water (98°C) and well stirred for 10 minutes using CiBlanc magnetic stirrer. However, to avoid misinterpretation, we revised the sentence.

Revised sentence;
For each sample, 50 mL of hot distilled water (98°C) was added and then well stirred for 10 minutes using CiBlanc magnetic stirrer.

Point 4: Chapter 2.3.: the near UV range does start at 190 nm, but we don't really use it below 200 nm anymore - as you can see in the spectra, the signal-to-noise ratio is bad.

Response 4:
The authors agree to revise this part. In fact, the default value for the spectrometer starting from 190 nm. For this reason, the authors performed spectral acquisition starting from 190 to 400 nm.

Point 5: The equation is unnecessary it is evident.

Response 5:
The authors agree to remove the equation. The number of equations were revised.

Point 6: Chapter 2.4.: The difference between the methods must be presented in at least one sentence.

Response 6:
Yes. The authors agree to revise this part. A short explanation of each method has been added in the revised article. The following sentences have been included in the revised article.

PLS-DA works based on a PLS regression algorithm which searches for latent variables (LVs) with a maximum covariance with the Y-variables. It was chosen because it has been satisfactorily applied in the field of food analysis as mentioned in previous works [1-2]. LDA and PCA-LDA is one of popular classical statistical method for feature extraction and dimension reduction and mostly employed among many supervised pattern recognition methods [3]. In LDA and PCA-LDA, the variance between the categories to be maximised and the variance within the categories to be minimised [4]. The main drawback for LDA and PCA-LDA is only well working when the number of variables is fewer than the number of samples. It was mentioned by Harvey et al. [5] that for LDA and PCA-LDA, in order to avoid model over-fitting, it is required that the number of samples have to be at least twice as many as the number of variables. SVM is one of machine learning method that can be operated with relatively small datasets. It has recently become popular and widely used and

investigated because of its ability in prediction for both, classification and regression [6]. Two SVMC types are available in The Unscrambler: type 1 (C-SVMC) and type 2 (nu-SVMC). In this study, the SVM classification type 2 was used as this type minimizes the error function. The nu value (lower bound on correct classified support vectors and an upper bound on misclassified samples) was set to 0.5 (default value), and the linear function kernel was applied as the optimal method. To select the appropriate gamma value (γ), a grid search was used.

The following references have been added in the revised article.

References:

[1] Jiménez-Carvelo, A.M.; González-Casado, A.; Bagur-González, M.G.; Cuadros-Rodríguez, L. Alternative data mining/machine learning methods for the analytical evaluation of food quality and authenticity – A review. *Food Res Int.* **2019**, *122*, 25–39. https://doi.org/10.1016/j.foodres.2019.03.063.

[2] Medina, S.; Perestrelo, R.; Silva, P.; Pereira, J.A.M.; Câmara, J.S. Current trends and recent advances on food authenticity technologies and chemometric approaches. *Trends Food Sci Technol*. **2019**, *85*, 163–176. https://doi.org/10.1016/j.tifs.2019.01.017.

[3] Jia, S.; Yang, L.; An, D.; Liu, Z.; Yan, Y.; Li, S.; Zhang, X.; Zhu, D.; Gu, J. 2016. Feasibility of analysing frost-damaged and non-viable maize kernels based on near infrared spectroscopy and chemometrics. *J. Cereal Sci.* **2016**, *69*, 145–150. https://doi.org/10.1016/j.jcs.2016.02.018.

[4] Kennard, R.W.; Stone, L.A. Computer aided design of experiments. *Technometrics* **1969**, *11*, 137–148.

[5] Harvey, T. J.; Gazi, E.; Henderson, A.; Snook, R. D.; Clarke, N. W.; Brown, M.; Gardner, P. Factors influencing the discrimination and classification of prostate cancer cell lines by FTIR microspectroscopy. *The Analyst*, **2009**, *134(6)*, 1083–1091. https://doi:10.1039/b903249e.

[6] Olivier D.; Cyril R.; Alexandra D.; Ludovic D.; Jean-Pierre H. Support vector machines (SVM) in near infrared (NIR) spectroscopy: Focus on parameters optimization and model interpretation. *Chemometr Intell Lab Syst*. **2009**, *96(1)*, 27–33. https://doi:10.1016/j.chemolab.2008.11.005.

Point 7: If the accuracy is given as a percentage, then Equation 2 is incorrect, it must be multiplied by 100.

Response 7:

Yes. The authors agree to revise the equations.

$$\text{Accuracy (\%)} = \frac{\text{Number of correct classification}}{\text{Number of total samples}} \times 100\%$$

Point 8: Chapter 3.1. these are different data processing operations. It is not mentioned later which pretreatment method and where it was used.

Response 8:

Yes. The authors agree to revise this part. In fact, we combined three spectral pre-treatments of Savitzky-Golay smoothing with smoothing points: 5 segments (SGS), standard normal variate (SNV), and Savitzky-Golay first derivative with a second-order polynomial and a window size of 5 points (SG 1d). We have revised this part to better explain how we use the spectral pre-treatment.

Several different spectral pre-treatments are available to reduce or to remove the effect of several different unwanted interfering phenomena such as particle size influence (baseline different and light scattering), etc. As mentioned by Roger *et al.* (2020) and Bian *et al.* (2020), it is hard to determine which pre-treatments can successfully improve the given original spectral data. For this reason, instead of selecting the best pre-treatments, in order to optimize the effect of spectral pre-treatment, the combination of several spectral pretreatment was often used. In this study, a selective combination pre-treatments strategy was used by combining three different pre-treatments of SGS, SNV and SG 1d. This combination was done sequentially, e.g. SGS followed by SNV and followed by SG 1d.

For example, Qiao *et al.* (2017) reported the best PLSR model using the combination of first order derivative and Savitzky-Golay smoothing of vis-NIR reflectance spectral data for estimating soil organic matter. Bian *et al.* (2020) reported that the combination of several spectral pre-treatments gives the best result compared to individual pre-treatment for quantitative analysis of near infrared spectra.

The caption of Figure 2 has been revised.

References:

Bian, X.; Wang, K.; Tan, E.; Diwu, P.; Zhang, F.; Guo, Y. A selective ensemble preprocessing strategy for near-infrared spectral quantitative analysis of complex samples. *Chemom. Intell. Lab. Syst.* **2020**, *197*, 103916. https://doi:10.1016/j.chemolab.2019.103916.

Qiao, X.; Wang, C.; Feng, M.; Yang, W.; Ding, G.; Sun, H.; Liang, Z.; Shi, C. Hyperspectral estimation of soil organic matter based on different spectral preprocessing techniques. *Spectrosc Lett*. **2017**, *50(3)*, 156–163. https://doi:10.1080/00387010.2017.1297958.

Roger, J.; Biancolillo, A.; Marini, F. Sequential preprocessing through ORThogonalization (SPORT) and its application to near infrared spectroscopy. *Chemom. Intell. Lab. Syst.* **2020**, *199*, 103975. https://doi:10.1016/j.chemolab.2020.103975.

Point 9: Chapter 3.2. For PCA, PC1 and PC2 explain only 82% of the variance. This is not enough; it is too low. In this case, the value of PC3 must also be taken into account

Response 9:
The authors agree to revise this part. The score plot of PC1 and PC2 was removed. PC3 was included in the calculation of PCA score plot. New score plot of the first three PCs (PC1xPC2xPC3) was added in the revised article. The total of three PCs could explain 93% of the total variances of spectral data which meets the general requirements of cumulative percent variance (CPV) > 70-85% for PCA analysis as mentioned by Hu et al. (2019). The authors also revised Figure 4. The x-loadings of three PCs was plotted.

The following reference (Hu et al., 2019) has been added in the revised article.

Reference:
[1] Hu, L.; Yin, C.; Ma, S.; Liu, Z. Vis-NIR spectroscopy combined with wavelengths selection by PSO optimization algorithm for simultaneous determination of four quality parameters and classification of soy sauce. *Food Anal. Methods* **2019**, *12*, 633–643. https://doi:10.1007/s12161-018-01407-1.

Point 10 What percentage was the accuracy of the classification using PCA?

Response 10:
For PCA, no calculation for accuracy. PCA is one of popular unsupervised pattern recognition. In this study, we utilized PCA to show possible separation between samples (using PCA scores) and to examine most influential wavelength responsible for the sampel separation (using PCA x-loadings). The authors have revised the manuscript to avoid misinterpretation of PCA.

Original sentence:
PCA (principal component analysis) was used to perform unsupervised classification

Revised sentence:
PCA (principal component analysis) was used to perform unsupervised pattern recognition.

Point 11: - Chapter 3.3. The accuracy of the calibration is not usually reported because, in fact, the accuracy of the validation is crucial. This is also confusing because for the

PCA-LDA model, the accuracy is once 93.33% and then 91.7% in the table.

Response 11:

The authors agree to revise this part. The authors agree that the accuracy of the validation is crucial. For this reason, the authors reported accuracy both in validation and in prediction. Several previous works also reported both accuracies (calibration/validation and prediction). Bona et al. [1] reported SVM performance using accuracy parameter both in training/validation and prediction. Zhang et al. [2] reported accuracies of calibration and prediction using different spectral pre-treatment method in authentication of Beijing-you chicken (BJY) from four breeds of chickens using near-infrared hyperspectral imaging combined with chemometrics. Hu et al. [3] reported accuracy in calibration set for rapid evaluation of the quality of chestnuts using near-infrared reflectance spectroscopy.

In our study, PLS-DA, SVM, LDA and PCA-LDA was developed using 300 samples of training set. Then, the reliability of each classification model was validated using the validation procedure. In order to evaluate the practical classification abilities of the developed model, classification test was performed using 60 unknown samples in the prediction sample set which had not been used in the model training. In this study, the accuracy obtained in prediction was used in the final evaluation and comparison of the classification models as often reported by several previous works [4-5].

In this study, for example, for PCA-LDA, accuracy of 93.33% was obtained for calibration/validation and accuracy of 91.7% was obtained for prediction. The authors agree to revise this part to avoid misinterpretation of the obtained accuracy.

References:

[1] Bona, E.; Marquetti, I.; Link, J.V.; Makimori, G.Y.F.; Arca, V.C.; Lemes, A.L.G.; Ferreira, J.M.G.; dos Santos Scholz, M.B.; Valderrama, P.; Poppi, R.J. Support vector machines in tandem with infrared spectroscopy for geographical classification of green arabica coffee. *LWT-Food Sci. Technol*. **2017**, *76*, 330–336. https://doi:10.1016/j.lwt.2016.04.048.

[2] Zhang, B.; Gao, S.; Jia, F.; Liu, X.; Li, X. Categorization and authentication of Beijing-you chicken from four breeds of chickens using near-infrared hyperspectral imaging combined with chemometrics. *J. Food Process Eng*. **2020**, *43(12)*, e13553. https://doi:10.1111/jfpe.13553.

[3] Hu, J.; Ma, X.; Liu, L.; Wu, Y.; Ouyang, J. Rapid evaluation of the quality of chestnuts using near-infrared reflectance spectroscopy. *Food Chem*. **2017**, *231*, 141–147. https://doi:10.1016/j.foodchem.2017.03.127.

[4] Diniz, P.H.G.D.; Barbosa, M.F.; de Melo Milanez, K.D.T.; Pistonesi, M.F.; de Araújo, M.C.U. (2016). Using UV–Vis spectroscopy for simultaneous geographical and varietal classification of tea infusions simulating a home-made tea cup. *Food Chem*. **2016**, *192*, 374–379. https://doi:10.1016/j.foodchem.2015.07.022.

[5] Soares, S.F.C.; Gomes, A.A.; Galvão Filho, A.R.; Araújo, M.C.U.; Galvão, R.K.H. The successive projections algorithm. *Trends Anal. Chem*. **2013**, *42*, 84–98. https://doi.org/10.1016/j.trac.2012.09.006.

Point 12: What is the difference between the LDA and the PCA-LDA model?

Response 12:
The authors agree to revise this part. The following sentences were added in the revised article.

In general, LDA and PCA-LDA is belong to supervised classification technique where the number of variables is smaller than the number of samples. In this study, the variable selection for LDA and PCA-LDA was performed in different way. For the LDA classification model, 6 wavelengths with high x-loadings from PCA results were selected as input variables: 255 nm, 270 nm, 290 nm, 310 nm, 315 nm, and 320 nm. For PCA-LDA, the input variables were the PCA sample scores on 10 principal components (PC1 to PC10).

Point 13: During LDA, the data are previously subjected to PCA data reduction in all cases. I do not understand. This also shows that 2.4. Chapter 2 lacks a description and explanation of the methods.

Response 13:
As mentioned in previous response, for the LDA classification model, 6 wavelengths with high x-loadings from PCA results were selected as input variables: 255 nm, 270 nm, 290 nm, 310 nm, 315 nm, and 320 nm. The authors agree to revise section 2.4. More explanation on chemometrics used in this study was presented.

Point 14: In the end, for the classification models, were only the absorbance values of the designated wavelengths used?

Response 14:
Yes. For LDA, absorbance values of six designated wavelengths were used as input variabels. However, for PCA-LDA, the PCA score of samples using 10 PCs were used as input variables.

Point 15: It would have been worth considering the entire spectral data set, precisely because of the overlaps.

Response 15:
For PLS-DA and SVM, the entire spectral data in the interval of 230-350 nm was used as input variables. However, the obtained accuracy for those models was low. Using fewer input variables, LDA and PCA-LDA resulted in higher accuracy.

Point 16: Chapter 4 The Conclusion chapter is very short.

Response 16:
Yes. The authors agree to revise this part. Conclusion was extended.
The following sentences were added in the Conclusion in the revised article.

In term of the number of variables, it was mentioned that LDA and PCA-LDA model with fewer variables tend to produce more robust classification model. In term of the delta accuracy between training and prediction (delta accuracy=accuracy in training-accuracy in prediction), LDA and PCA-LDA model also resulted in a smaller delta accuracy of 1% and 1.63% comparing to SVMC and PLS-DA model.

Point 17: Lines 38 and 39: the name of the coffee plant must be written in italics

Response 17:
Yes. The authors agree to revise this part. The name of the coffee plant was written in italics (*Coffea arabica*) (*Coffea canephora*).

Point 18: Line 99: Lampung Robusta – italics

Response 18:
Yes. The authors agree to revise this part. *Lampung Robusta* was written in italic.

Response to Reviewer 2 Comments

Point 1: I believe the ranges of the values, such as grain size and sample weight should be informed, instead of the average value only.

Response 1:
In this study, all Lampung Robusta coffee samples were collected from same harvest season, same location and same grade as mentioned in the article (The samples were collected from the same harvest season in Sumber Jaya coffee plantation, West Lampung, Lampung (5°00'28.5"S 104°28'37.4"E). The samples were belonging to premium grade (first grade) by maintaining the number of defective beans as low as 11 scores according to Indonesian National Standard for coffee bean (ISN No. 01-2907: 2008). Unfortunately, we did not measure the bean (grain) size. However, all samples were roasted in same roasting profile (200°C for 20 minutes using a portable roasting machine), grinded and sieved using same parameter (50 mesh), we believe that the source of variability within the samples mostly influenced by differences in cherry processing methods.

Each sample has 1 gram weight. The composition of each samples was described in Table 1.

The total sample are 360 samples: 100 samples of pure dry coffee (DRY), 100 samples of pure semi-dry coffee (SMD), 100 samples of pure wet coffee (WET) and 60 samples of adulterated coffee (ADT) (SMD coffee was adulterated with DRY and WET coffee).

For this reason, we have revised Table 1. The number of samples for 20% adulteration is 20 not 10.

Point 2: Authors should address better the differences between Fig. 1 and Fig. 2, where some peaks seems to be appeared. Is it an artifact of the pre-treatment?

Response 2:
The authors agree to revise this part. Figure 1 is original spectra obtained directly from spectral acquisition system. It is raw spectra. The typical feature of original spectra is rich in unrelated information such as background information and systematic noise coming from the influences of light scattering, different in path length, sample particle size, and other factors [1]. For this reason, we improve the quality of spectral data by applying spectral pre-treatment. In general, standard normal variate or SNV was used as similar to MSC to cancel the influence of light scattering effect. Savitzky-Golay first

derivative with a second-order polynomial and a window size of 5 points (SG 1d) was used to cancel the baseline drifts and to enhance small spectral differences [1]. Due to similarity in cherry processing methods especially for wet and semi-dry method, it was expected that the spectral difference in coffee samples due to differences in cherry processing methods was small. This is the main reason to use SG 1d: to enhance those small spectral differences. However, at the same time, as a consequence of derivation, the noises were also enhanced. To avoid this, the spectra were first smoothed using SG smoothing pre-treatment as recommended by previous work [1]. Therefore, in this present study we utilized three sequentially spectral pre-treatments: SGS, SNV and SG 1d (SGS+SNV+SG 1d). Our approach was previously used by Shawky and Selim [1] and Zhang et al. [2]. Figure 2 is modified spectra obtained by subjecting combination of three spectral pre-treatments and it is an artifact of spectral pre-treatments. The authors agree to put more highlights of the difference between Figure 1 and Figure 2.

The following references has been added in the revised article.

References:

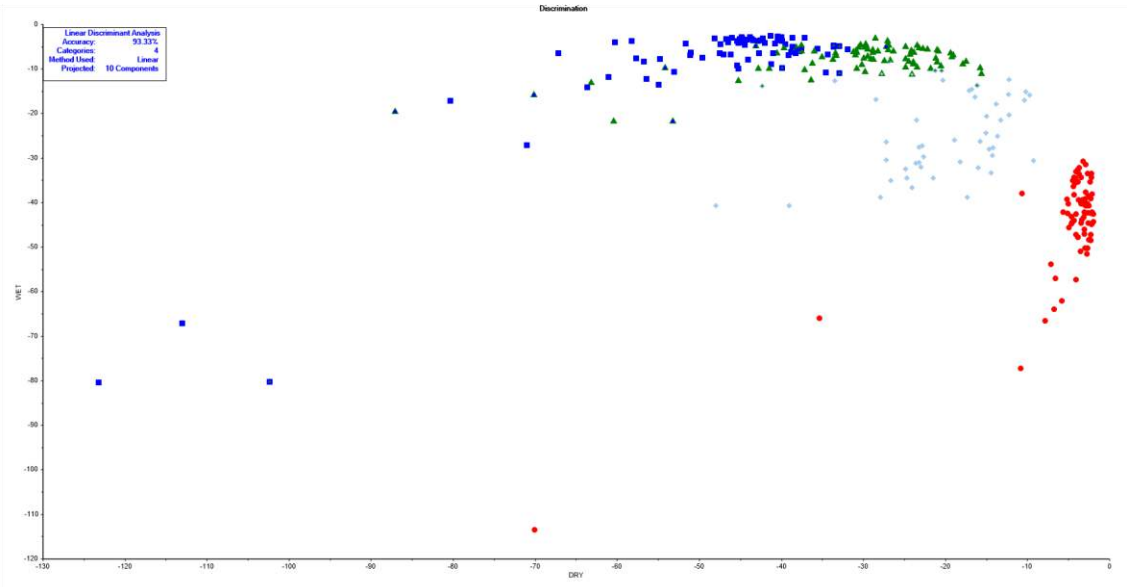
[1] Shawky, E; Selim, D.A. NIR spectroscopy-multivariate analysis for discrimination and bioactive compounds prediction of different Citrus species peels. *Spectrochim. Acta A Mol. Biomol. Spectrosc*. **2019**, *219*, 1–7. https://doi:10.1016/j.saa.2019.04.026.

[2] Zhang, Z.; Wang, Y.; Yan, H.; Chang, X.; Zhou, G.; Zhu, L.; Liu, P.; Guo, S.; Dong, T.T.X.; Duan, J. Rapid geographical origin identification and quality assessment of angelicae sinensis radix by FT-NIR spectroscopy. *J Anal Methods Chem*. **2021**, *2021*, 1–12. https://doi.org/10.1155/2021/8875876.

Point 3: In Fig. 5, the training and validation points for dry and adulterated are mixed, not supporting the claim that the samples were correctly classified.

Response 3:

The authors agree to revise this part. There was a mistake in labelling the plot. The original plot of PCA-LDA from The Unscrambler was shown here. There was a clear separation of the most samples according to differences in cherry processing methods. Some of wet and semi-dry samples are overlapped.



Original plot of PCA-LDA model obtained from the Unscrambler.

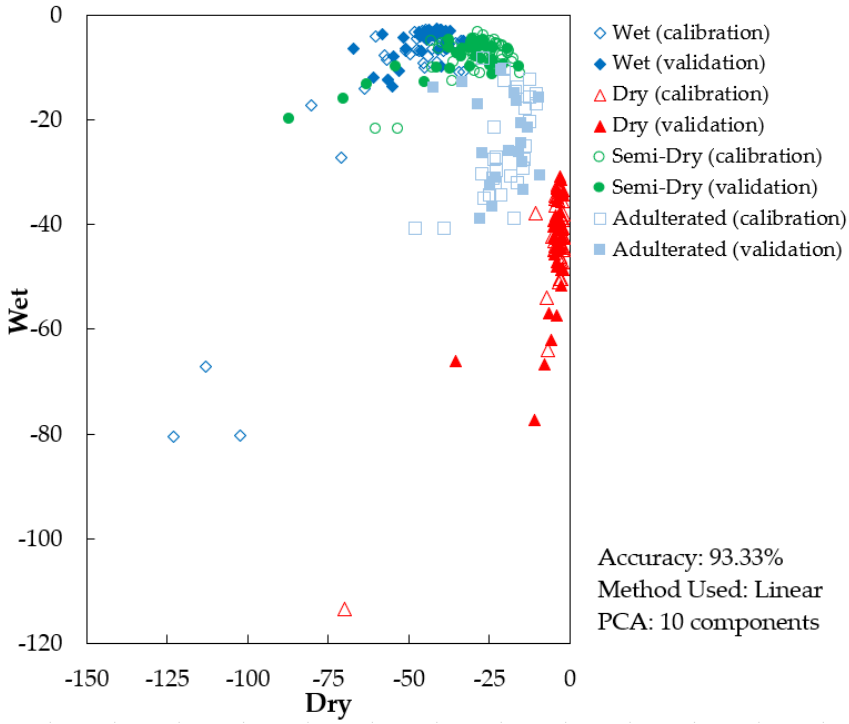
PCA-LDA model was developed using training sample set (total 300 samples). During PCA-LDA training, the calibration set was composed of 180 samples (including 51 dry, 50 wet, 49 semi-dry and 30 adulterated samples). The model was verified with the validation set of 120 samples (including 33 dry, 33 wet, 34 semi-dry and 20 adulterated samples) after the establishment of the PCA-LDA model.
The confusion matrix of training samples generated by the Unscrambler was shown here and resulted in (280/300) x100%=93.33% of accuracy.

File Edit View Insert Plot Tasks Tools Help

Line Plot(1)
PCA
SVM(10)
SVM(11)
PCA(1)
LDA(2)
LDA(3)

Confusion m	Actual	DRY	WET	SEMI-DRY	ADULTERAT
Predicted		1	2	3	4
DRY	1	84	0	0	0
WET	2	0	76	6	0
SEMI-DRY	3	0	7	75	5
ADULTERAT	4	0	0	2	45

We have revised Figure 5 with proper labelling of calibration and validation.



The revised Figure 5

Response to Reviewer 3 Comments

Point 1: Subjective language used throughout, such as “good”, “better”, or “best” and should be reworded.

Response 1:
The authors agree to revise this part. Several sentences having subjective language were reworded.

Section Abstract
Original sentence:
Using the first two principal components (PCs) with a total of 82% of explained variance, there was good separation between samples.
Revised sentence:
Using the first three principal components (PCs) with a total of 93% of explained variance, there was a clear separation between samples.

Section 3.2.
Original sentence:
Using these two PCs, there was good separation between samples.
Revised sentence:
Using these three PCs, there was a clear separation between samples.

Section 3.3.
Original sentence:
As expected, it is noted that variables selection using PCA scores was better to improve classification accuracy.
Revised sentence:
As expected, it is noted that variables selection using PCA scores was appropriate to improve classification accuracy.

Section 3.3.
Original sentence:
It was reported that PCA-LDA significantly gave better results with 92% and 100% accuracy rate.
Revised sentence:
It was reported that PCA-LDA significantly gave acceptable results with 92% and 100% accuracy rate.

Several sentences with subjective language of "the best" have been kept in the revised article to show the superiority of PCA-LDA among the tested classification models.

Point 2: Sample division into cal, val, test is well constructed.

Response 2: OK

Point 3: Should list the explained variance for the selected 10 PCs.

Response 3:
The authors agree to revised this part. The authors listed the explained variance for the selected 10 PCs and insert 1 new table in the revised article. The cumulative percent variance (CPV) for 10 PCs are presented in Table 1.

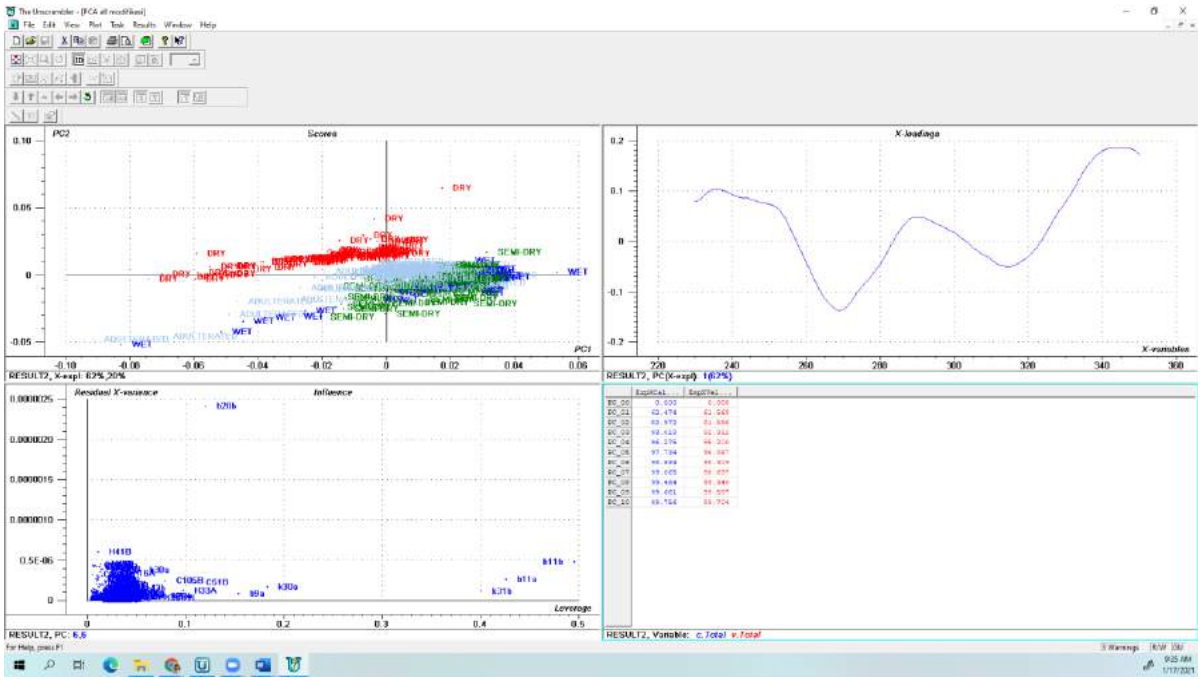


Table 1 Number of principal components and its cumulative percent variance (CPV) chosen for PCA analysis using combined pre-treated spectral data in the interval of 230-350 nm.

Principal Components (PCs)	Cumulative Percent Variance (%)	
	Calibration	Validation
PC1	62.474	61.569
PC2	82.972	81.596
PC3	93.018	92.312
PC4	96.275	95.200
PC5	97.734	96.867
PC6	98.634	98.309
PC7	99.065	98.697

PC8	99.464	99.340
PC9	99.661	99.587
PC10	99.756	99.704

Point 4: P3, L128: is not correct. It states that "PCA is used for unsupervised classification". PCA is not a classification method, but rather a visualization tool that does not explicitly calculate classification. This should be reworded.

Response 4:
The authors agree to revise this part. PCA is one of popular unsupervised pattern recognition. In this study, we utilized PCA to show possible separation between samples (using PCA scores) and to examine most influential wavelength responsible for the sampel separation (using PCA x-loadings). The authors have revised the article to avoid misinterpretation of PCA. Sentence has been reworded.

Original sentence:
PCA (principal component analysis) was used to perform unsupervised classification

Revised sentence:
PCA (principal component analysis) was used to perform unsupervised pattern recognition.

Point 5: There is not enough information given on the four supervised classification approaches. Stating that "A detailed explanation of those methods can be found …" is not enough information to tell the reader any details of those approaches for this dataset. For example: there are many different parameters that are needed to run a SVMC such as the gamma, kernel type, cost-of-classification… Info is listed for SVMC in results and discussion, but there is no justification to why these were selected. Was a grid search performed to identify optimal SVMC parameters in Unscrambler? If so, that should be listed in materials and methods.

Response 5:
The authors agree to revise this part. An additional explanation was included in the revised article.
The following sentences have been included in the revised article.

PLS-DA works based on a PLS regression algorithm which searches for latent variables (LVs) with a maximum covariance with the Y-variables. It was chosen because it has been satisfactorily applied in the field of food analysis as mentioned in previous works [1-2]. LDA and PCA-LDA is one of popular classical statistical method for feature extraction and dimension reduction and mostly employed among many

supervised pattern recognition methods [3]. In LDA and PCA-LDA, the variance between the categories to be maximised and the variance within the categories to be minimised [4]. The main drawback for LDA and PCA-LDA is only well working when the number of variables is fewer than the number of samples. It was mentioned by Harvey et al. [5] that for LDA and PCA-LDA, in order to avoid model over-fitting, it is required that the number of samples have to be at least twice as many as the number of variables. SVM is one of machine learning method that can be operated with relatively small datasets. It has recently become popular and widely used and investigated because of its ability in prediction for both, classification and regression [6]. Two SVMC types are available in The Unscrambler: type 1 (C-SVMC) and type 2 (nu-SVMC). In this study, the SVM classification type 2 was used as this type minimizes the error function. The nu value (lower bound on correct classified support vectors and an upper bound on misclassified samples) was set to 0.5 (default value), and the linear function kernel was applied as the optimal method. To select the appropriate gamma value (γ), a grid search was used.

The following references have been added in the revised article.

References:

[1] Jiménez-Carvelo, A.M.; González-Casado, A.; Bagur-González, M.G.; Cuadros-Rodríguez, L. Alternative data mining/machine learning methods for the analytical evaluation of food quality and authenticity – A review. Food Res Int. 2019, 122, 25–39. https://doi.org/10.1016/j.foodres.2019.03.063.

[2] Medina, S.; Perestrelo, R.; Silva, P.; Pereira, J.A.M.; Câmara, J.S. Current trends and recent advances on food authenticity technologies and chemometric approaches. Trends Food Sci Technol. 2019, 85, 163–176. https://doi.org/10.1016/j.tifs.2019.01.017.

[3] Jia, S.; Yang, L.; An, D.; Liu, Z.; Yan, Y.; Li, S.; Zhang, X.; Zhu, D.; Gu, J. 2016. Feasibility of analysing frost-damaged and non-viable maize kernels based on near infrared spectroscopy and chemometrics. J. Cereal Sci. 2016, 69, 145–150. https://doi.org/10.1016/j.jcs.2016.02.018.

[4] Kennard, R.W.; Stone, L.A. Computer aided design of experiments. Technometrics 1969, 11, 137–148.

[5] Harvey, T. J.; Gazi, E.; Henderson, A.; Snook, R. D.; Clarke, N. W.; Brown, M.; Gardner, P. Factors influencing the discrimination and classification of prostate cancer cell lines by FTIR microspectroscopy. The Analyst, 2009, 134(6), 1083–1091. https://doi:10.1039/b903249e.

[6] Olivier D.; Cyril R.; Alexandra D.; Ludovic D.; Jean-Pierre H. Support vector machines (SVM) in near infrared (NIR) spectroscopy: Focus on parameters optimization and model interpretation. Chemometr Intell Lab Syst. 2009, 96(1), 27–33. https://doi:10.1016/j.chemolab.2008.11.005.

Point 6: Should justify why a PC-LDA/LDA was chosen over QDA or Mahalanobis DA which are options that can be selected in the Unscrambler software as well,

dealing with non-linearity or scaling issues. Was there a pattern in the covariance of the data structure that justified LDA or was the accuracy simply higher for that approach?

Response 6:
The authors agree to revise this part. The author has revised the Section. 2.4. Chemometrics to enhance the reason laid on the selection of PCA-LDA and LDA.

LDA and PCA-LDA is one of popular classical statistical method for feature extraction and dimension reduction and mostly employed among many supervised pattern recognition methods [1]. In LDA and PCA-LDA, the variance between the categories to be maximised and the variance within the categories to be minimised [2]. The main drawback for LDA and PCA-LDA is only well working when the number of variables is fewer than the number of samples. It was mentioned by Harvey et al. [3] that for LDA and PCA-LDA, in order to avoid model over-fitting, it is required that the number of samples have to be at least twice as many as the number of variables.

The following references have been added in the revised article.
References:
[1] Jia, S.; Yang, L.; An, D.; Liu, Z.; Yan, Y.; Li, S.; Zhang, X.; Zhu, D.; Gu, J. 2016. Feasibility of analysing frost-damaged and non-viable maize kernels based on near infrared spectroscopy and chemometrics. *J. Cereal Sci.* **2016**, *69*, 145–150. https://doi.org/10.1016/j.jcs.2016.02.018.
[2] Kennard, R.W.; Stone, L.A. Computer aided design of experiments. *Technometrics* **1969**, *11*, 137–148.
[3] Harvey, T. J.; Gazi, E.; Henderson, A.; Snook, R. D.; Clarke, N. W.; Brown, M.; Gardner, P. Factors influencing the discrimination and classification of prostate cancer cell lines by FTIR microspectroscopy. *The Analyst*, **2009**, *134(6)*, 1083–1091. https://doi:10.1039/b903249e.

It was calculated that LDA and PCA-LDA with linear method was higher accuracy than quadratic and Mahalanobis one.

Point 7: Preprocessing spectral data – SNV is appropriate, but was derivative processing necessary? If so, the authors should state classification results of the raw data to justify the use of Savitzky-Golay (SG). Baseline correction is addressed with (SG), but less invasive adjustments can also be used for baseline correction.

Response 7:
The authors agree to revise this part. The authors give more explanation of the reason laid on the selection of spectral pre-treatment. In general, standard normal variate or SNV was used as similar to MSC to cancel the influence of light scattering effect. Savitzky-Golay first derivative with a second-order polynomial and a window size of

5 points (SG 1d) was used to cancel the baseline drifts and to enhance small spectral differences [1]. Due to similarity in cherry processing methods especially for wet and semi-dry method, it was expected that the spectral difference in coffee samples due to differences in cherry processing methods was small. This is the main reason to use SG 1d: to enhance those small spectral differences. However, at the same time, as a consequence of derivation, the noises were also enhanced. To avoid this, the spectra were first smoothed using SG smoothing pre-treatment as recommended by previous work [1]. Therefore, in this present study we utilized three sequentially spectral pre-treatments: SGS, SNV and SG 1d (SGS+SNV+SG 1d). Our approach was previously used by Shawky and Selim [1] and Zhang et al. [2].

The following two references have been added in the revised article.
References:

[1] Shawky, E; Selim, D.A. NIR spectroscopy-multivariate analysis for discrimination and bioactive compounds prediction of different Citrus species peels. *Spectrochim. Acta A Mol. Biomol. Spectrosc*. **2019**, *219*, 1–7. https://doi:10.1016/j.saa.2019.04.026.
[2] Zhang, Z.; Wang, Y.; Yan, H.; Chang, X.; Zhou, G.; Zhu, L.; Liu, P.; Guo, S.; Dong, T.T.X.; Duan, J. Rapid geographical origin identification and quality assessment of angelicae sinensis radix by FT-NIR spectroscopy. *J Anal Methods Chem*. **2021**, *2021*, 1–12. https://doi.org/10.1155/2021/8875876.

Point 8: P6, L184: should state "…differences in cherry processing methods.", not "different"

Response 8:
The authors agree to revise this part. The sentence has been revised.

Original sentence:
The samples were clustered into four possible groups according to different in cherry processing methods: dry, wet, semi-dry, and adulterated.
Revised sentence:
The samples were clustered into four possible groups according to differences in cherry processing methods: dry, wet, semi-dry, and adulterated.

Section Abstract
Original sentence:
The samples were clustered into four possible groups according to different in cherry processing methods: dry, wet, semi-dry, and adulterated.
Revised sentence:
The samples were clustered into four possible groups according to differences in cherry processing methods: dry, wet, semi-dry, and adulterated.

Point 9: Good job from authors in noting the PC-LDA benefit over LDA for highly correlated spectral data.

Response 9: OK

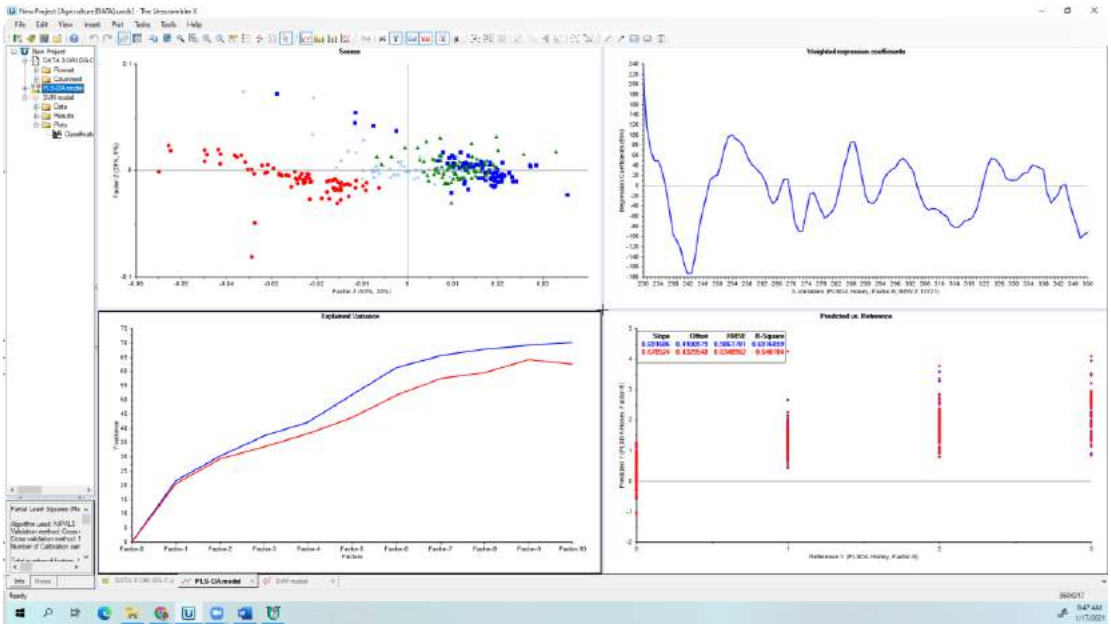
Point 10: Chemometric results: What about the downside of PC-LDA / LDA? These methods may give improved accuracy by forcing classification into a group but may not be realistic. Whereas PLS-DA or SVMC do not force a sample into a classification group.

Response 10:
The main downside for LDA and PCA-LDA is only well working when the number of variables is fewer than the number of samples. It was mentioned by Harvey et al. [1] that for LDA and PCA-LDA, in order to avoid model over-fitting, it required that the number of samples have to be at least twice as many as the number of variables. In our study, the number of samples are 360 samples. The number of input variables for LDA and PCA-LDA is 6 variables (6 wavelengths) and 10 variables (10 PCs). In general, in LDA and PCA-LDA, the variance between the categories to be maximised and the variance within the categories to be minimised [2].

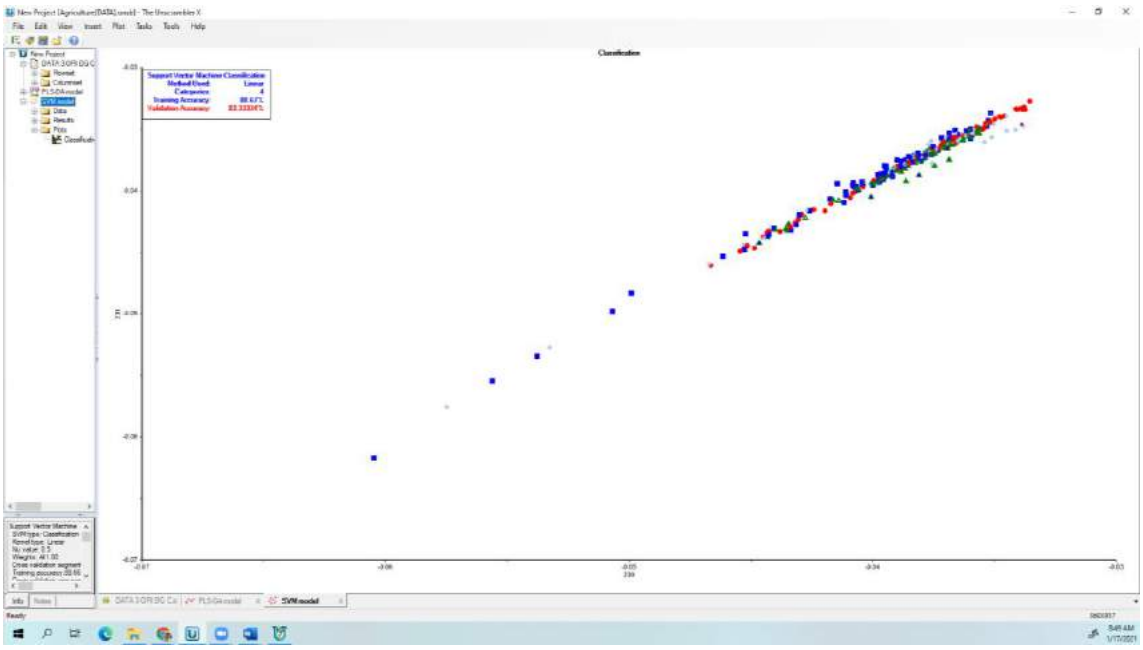
Reference:
[1] Harvey, T. J.; Gazi, E.; Henderson, A.; Snook, R. D.; Clarke, N. W.; Brown, M.; Gardner, P. Factors influencing the discrimination and classification of prostate cancer cell lines by FTIR microspectroscopy. *The Analyst*, **2009**, *134(6)*, 1083–1091. https://doi:10.1039/b903249e.
[2] Kennard, R.W.; Stone, L.A. Computer aided design of experiments. *Technometrics* **1969**, *11*, 137–148.

Point 11: Chemometric results: What does the model fit look like for each of the four approaches?

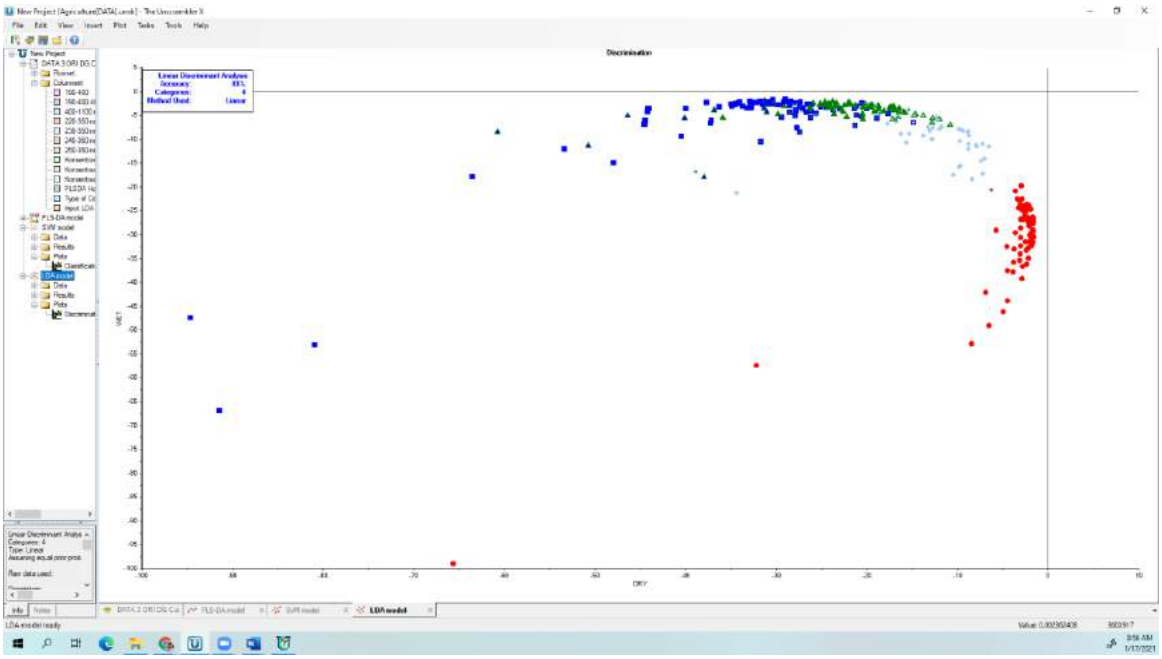
Response 11:
The authors agree to show the all models here. However, in the revised article we visually reported only the plot of PCA-LDA model.



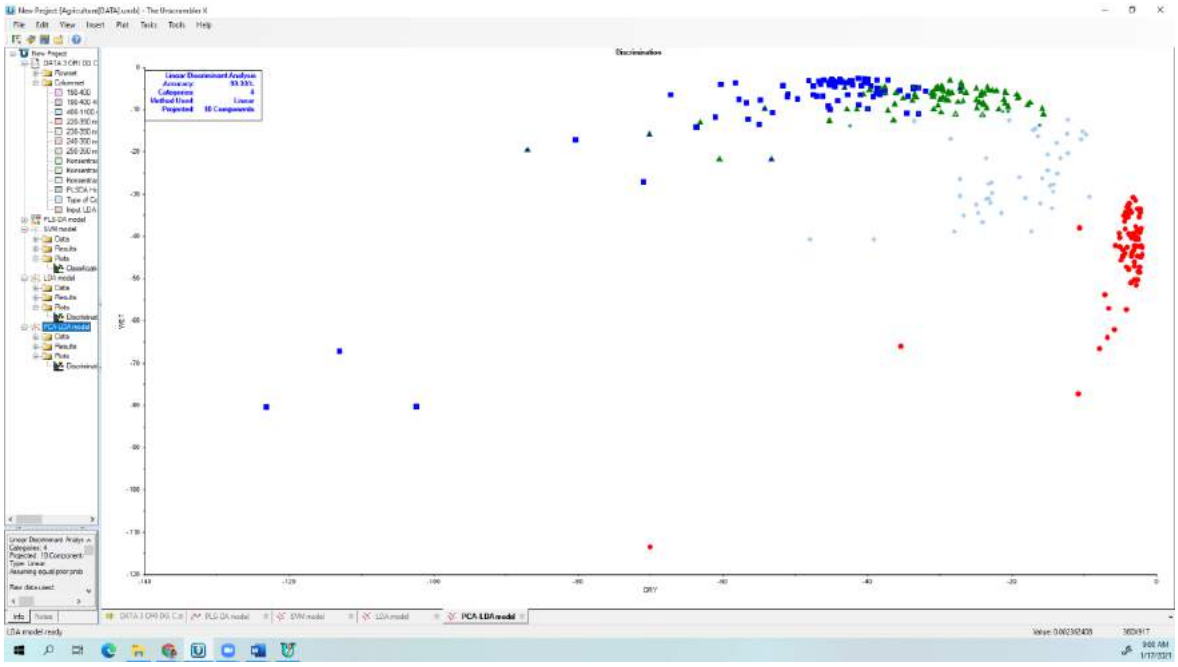
PLS-DA model with 9 latent variables (LVs)



SVMC model using nu-SVM with linear kernel function



LDA model using 6 wavelengths as input variables.



PCA-LDA model using 10 PCs score as input variables

Point 12: Reporting an accuracy is not enough information. How do we know that approach is the most robust? Possibly reporting the delta accuracy between training and prediction of each method would help.

Response 12:

The authors agree to revise this part. In term of the number of variables, it was mentioned that LDA and PCA-LDA model with fewer variables tend to produce more robust classification model. In term of the delta accuracy between training and prediction (delta accuracy=accuracy in training-accuracy in prediction), LDA and PCA-LDA model also resulted in smaller delta accuracy of 1% and 1.63% comparing to SVMC and PLS-DA model.

The following sentence has been added in the revised article (in Conclusion):

In term of the number of variables, it was mentioned that LDA and PCA-LDA model with fewer variables tend to produce more robust classification model. In term of the delta accuracy between training and prediction (delta accuracy=accuracy in training-accuracy in prediction), LDA and PCA-LDA model also resulted in smaller delta accuracy of 1% and 1.63% comparing to SVMC and PLS-DA model.

Response to Reviewer 2 Comments

Point 1: The authors answered most of the questions I posed. The variation in the samples still need to be clarified. I was expecting something like 1±0.1 g for average weight of 100 samples.

Response 1:
The authors agree to revise this part.

The composition of each samples was described in Table 1. We prepared the weight of each samples and its composition using analytical balances. It can show us data with four decimal places to the right of decimal point (up to 0.0001 g). We have calculated its standard deviation for dry, wet, semi-dry and adulterated samples.

For this reason, we have revised Table 1. The average of weight was shown along with its standard deviation. It was shown that samples have a small variation in term of sample weight.

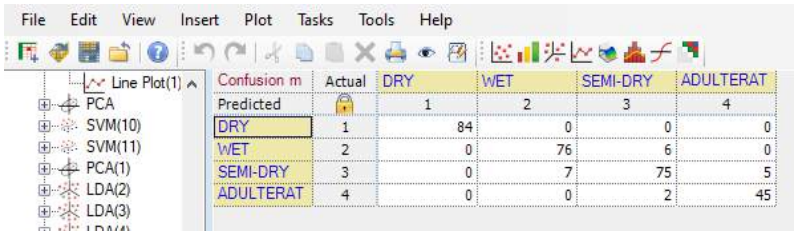
Point 2: Next to figure 5 of the paper, I'd include the one presented in the answer to the reviewers, as well as the explanation accompanying it, to clarify the results from figure 5.

Response 2:
The authors agree to revise this part.

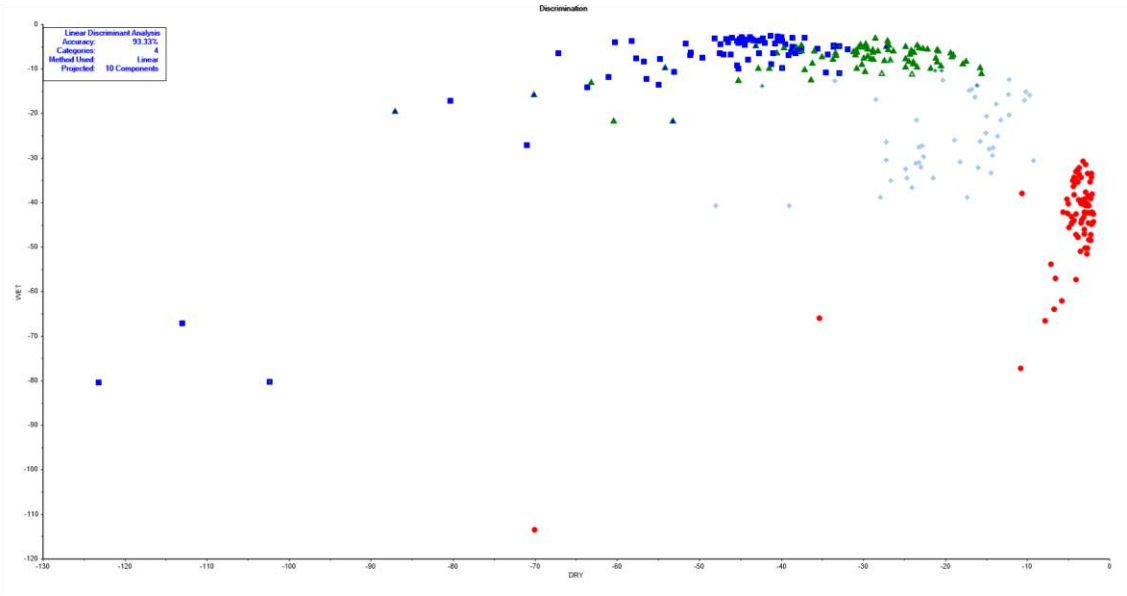
The following sentences were included in the revised article to clarify the obtained accuracy of 93.33% using PCA-LDA (not 100%) due to some overlapping samples.

There was a clear separation of the most samples according to differences in cherry processing methods. However, as seen in Figure 5, some of wet, semi-dry and adulterated samples are still overlapped and fail to be discriminated by using the developed PCA-LDA model. In this model, 7 wet samples were misclassified as semi-dry, 6 semi-dry samples were misclassified as wet, 2 semi-dry samples were misclassified as adulterated and 5 adulterated samples were misclassified as semi-dry samples resulted in 93.33% of accuracy.

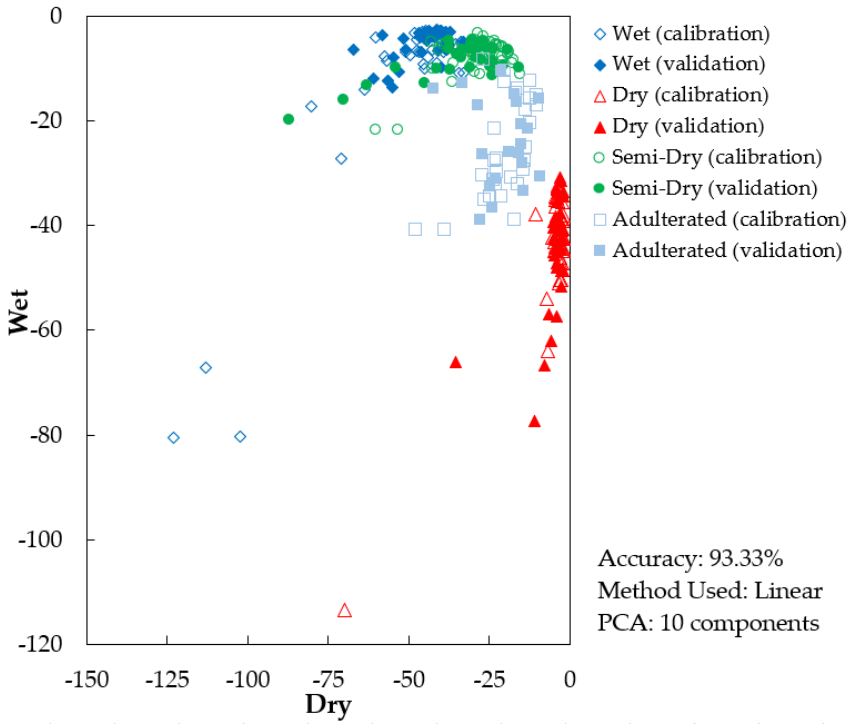
Confusion matrix obtained for PCA-LDA model development.



Confusion m	Actual	DRY	WET	SEMI-DRY	ADULTERAT
Predicted		1	2	3	4
DRY	1	84	0	0	0
WET	2	0	76	6	0
SEMI-DRY	3	0	7	75	5
ADULTERAT	4	0	0	2	45



Original plot of PCA-LDA model obtained from the Unscrambler.



The revised Figure 5