to Editor

Prof. Slavica Ražić

Journal of Serbian Chemical Society

Dear Editor,

The authors would like to thank the Editor and Reviewer for a quick and professional review. It is obvious that Reviewer is an expert in this field. All Reviewer's remarks are accepted and the paper is changed according to Reviewer's comments. The authors believe that the changed paper would satisfy Reviewer's criteria and that it is going to be interesting enough for publishing in the Journal of Serbian Chemical Society.

We decided to revise the manuscript according to reviewer’s remarks, highlighting the changes directly on the revised manuscript.

**Reviewer A:**

Does the manuscript contain enough significant original material?:

    yes

Is the manuscript clearly and concisely written?:

    yes

Are the conclusions adequately supported by the data?:

    yes

Does the manuscript give appropriate credit to related recent publications?:

    yes

Are the references appropriate and free of important omissions?:

    yes

Is the length of the manuscript appropriate?:

    yes

Does the manuscript need condensation or extension?:

    no

Is the quality of the figures (including legends and axes labelling)

satisfactory?:

    yes

Are the nomenclature and units in accordance with SI?:

    yes

Are the English grammar and syntax satisfactory?:

    yes

ADDITIONAL COMMENTS

Please indicate the page numbers for suggested corrections.

AUTHORS: Corrected, according to Reviewer's comment.

Please, be as specific as possible if major correction by the author(s) is recommended! :

    The authors are proposing an analytical method for food quality control, in this particular case, the cereal and pseudocereal types of flour that might be used for adulteration of various bakery products. The method involves the extraction of lipids and their qualitative GC-MS analysis. The data obtained are of binary nature, i.e. describing the presence (annotated with 1) or the absence (annotated with 0) of a particular lipid component. The work is rather interesting, and I hope it will gain an international attention. It raises an important question regarding the use of qualitative metabolomic data for quality control of food and natural products. I am very enthusiastic and happy to see such sort of research. The article is well written and present the research in a nice methodological way, which most certainly warrants its publication in the Journal of the Serbian Chemical Society. However, before the publication, several minor issues should be properly addressed.

The authors would like to thank the Reviewer on professional and helpful comments. Reviewer`s comments contribute to better quality of the paper that was submitted. All remarks are accepted and the paper is changed according to these comments.

REPORT:

    Minor issues

1.    In the introduction part, the authors are extensively reporting on the methods used for tracing authenticity of various food and natural products, such as those involving PCR and NMR, which are not in the focus of the presented work. In order to keep introduction neat and focused, is it possible to entirely remove the following lines: 60 – 69 (marked in yellow color in the attached PDF)?

AUTHORS: This section is removed from the revised version of the text, according to Reviewer's comment.

2.    Table 1 covers the literature describing GC-MS methods combined with various chemometric approaches. However, no reference to any chemometric method is provided in the table. Please add a column with abbreviations of chemometric methods applied in each study. Abbreviations can be further explained in the Table footnote.

AUTHORS: A column with abbreviations of applied pattern recognition methods together with appropriate explanations were added.

3.    The scientific problems are not adequately addressed in the introduction section. Why should someone use binary qualitative data, if continuous chromatographic signals contain more information? Also, knowing a chromatographic signal does not necessary requires knowing exact

concentrations of any particular analyte. Sometimes even peak ratios can be used instead. Also, in majority of reported methods the entire chromatographic signals are used. So, basically the authors should emphasize the disadvantages and major drawbacks of such approaches. I think that the parts reported in the results and discussion (lines 207-204, and 220-223) are perfectly suitable to be incorporated in the introduction part instead (for example after the line 85, or whatever the authors may find suitable).

AUTHORS: Two sections mentioned in the Reviewer's comment are placed beneath the Table I (line 84 in the revised manuscript).

4.    Please refrain from the use of a term chemometrics. Chemometrics is a general term that covers many areas and very specific subareas such as pattern recognition, classification, regression, machine learning etc. Please be specific.

AUTHORS: The term "chemometrics" was changed to more appropriate terms throughout the text, according to Reviewer's comment.

5.    PCA is not the best or the most adequate method for analysis of binary data, but it can be used, especially if, like in the present case, provides meaningful and coherent results. However, for your future works I would recommend the use of correspondence analysis instead, or the use of various binary similarity and dissimilarity measures, tetrachoric correlation matrices etc.

AUTHORS: The similarity of data taken from the samples lead the Authors to the idea to apply the PCA in this investigation, rather then using, for instance: Multiple Correspondence Analysis, Boolean Factor Analysis or the Polychoric Correlation Matrix Analysis. However, this is a good idea for our future investigations.

Some additional remarks you may find annotated in red color in the attached PDF file. I hope that you will find them useful.

AUTHORS: Many corrections were performed in the text, according to Reviewer's comments.

In my opinion, this manuscript should:

    be published after major revision with additional review

If manuscript is suitable for publishing, referees recommendation :

    Original scientific paper