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Review of the doctoral dissertation
'The composition of triacylglycerols as an indicator of edible oil adulteration'
by Qian Ying, M.Sc.

written under the supervision of prof. Magdalena Rudzińska

Formal comments

The basis for this review is the Resolution of the Scientific Council of the Food and Nutrition Technology Faculty of Poznań University of Life Sciences adopted on July 13, 2022, pursuant to which I was appointed a reviewer of the above-mentioned doctoral dissertation. According to the letter by prof. Magdalena Rudzińska, Chairwoman of the Scientific Council of the Food and Nutrition Technology Faculty, the dissertation submitted for review falls within the discipline of food and nutrition technology. The dissertation meets the formal requirements for this type of work presented in the procedure for the obtainment of a doctoral degree, i.e. it is experimental and contains all the necessary chapters arranged in a typical sequence. The study constitutes a coherent whole and is correctly written in a clear and understandable language.

Structure and layout of the work

The doctoral dissertation submitted for evaluation is 126 pages long. It includes summaries in English and Polish, a list of abbreviations, an introduction, theoretical preliminaries, a formulation of the research objective, a discussion of the study methods and material, a presentation of results and appraisal, a summary, conclusions, a list of tables and figures, and appendices (43 pages). The list of literature includes 90 items, mainly English-language scientific articles from recent years. In addition, the work contains 20 tables, 15 figures, and numerous appendices. The layout of the work is logical and typical for this type of research and scientific studies.

Substantive evaluation of the doctoral dissertation

The subject matter chosen by the PhD candidate has a very significant and practical meaning. In recent years, the issues of the authenticity of food products have increasingly attracted the attention of the economic environment as well as various national and international law-making bodies. The term covers both adulterated products as well as counterfeit, tampered, and imitated products. Ensuring the



authenticity of the product is important both from the consumer's point of view (economic security and health) and the producer's (ensuring fair market competition). The consumer expects that the quality of the products declared by the manufacturer or distributor is not debased. Detection of potential threats resulting from deliberate counterfeiting of food products is primarily predicated on the advanced examination of the chemical composition, as well as on the monitoring of physico-chemical properties determining the quality of a product, and lastly on the correct interpretation of the collected analytical data. Effective supervision of compliance with food laws, especially in terms of product adulteration, requires the development of analytical methods that can be used by food control authorities. In the doctoral dissertation presented for evaluation, the PhD candidate focuses her research on verifying the usefulness of chromatographic methods in combination with artificial neural networks in terms of ensuring effective characterization of the chemical composition of vegetable oil samples. At the same time, the PhD candidate shows the great potential of chromatographic methods in combination with methods of artificial neural networks in confirming the authenticity of edible oils. Artificial neural networks are currently one of the most actively developing branches of artificial intelligence. An artificial neural network is a computational tool that simulates, in a simplified way, the operation of the human brain. However, an extreme simplification of the neuron model does not result in a loss of the most important feature of real neural networks, i.e. the ability to learn. Currently, neural networks are a tool that makes it possible to map very complex functions. Compared to the existing methods of linear modeling, neural networks have much greater potential due to their non-linear nature. They allow for quick and efficient solving of problems from various fields of knowledge. In recent years, there has been a rapid increase in research on learning algorithms derived from artificial intelligence and neural networks. This development resulted in numerous applications of the above-mentioned algorithms in many fields of science, such as physics, medicine, and chemistry. Their application in the analysis of data related to food quality can significantly improve the effectiveness of food quality control methods. I believe it a very important task to develop, improve and test analytical methods in combination with new chemometric methods. They should be used by government bodies and various industries when the subject of analysis are multidimensional data, in order to monitor the quality of food, raw materials, and processes. I consider the choice of the dissertation subject by the PhD candidate to be fully justified both from the scientific point of view and taking into account potential applications.

The doctoral dissertation consists of 7 chapters. Chapter 1 '*Introduction*' is a short introduction into the topic of the dissertation. It justifies the choice of the research objective, pointing to the high nutritional role of vegetable oils, the problem of quality assurance and establishing the authenticity of these food products. It indicates the methods of artificial neural networks as those which, when combined with chromatographic methods, can significantly boost quality control. Some doubts may



arouse the information that with the existing instrumental methods it is possible to detect mixtures of no more than two or three oils. Perhaps we are not able to find out the exact quantitative composition of the mixtures, but with the use of appropriate analytical and chemometric methods, we are able to conclude that the tested sample (including consisting of more than three components) is an adulterated product.

In Chapter 2 '*Literature review*', the author, in a synthetic way, describes the main ingredients of edible oils, such as triacylglycerols, fatty acids and sterols. Moreover, discussed are the processes of obtaining edible oils, economic data on edible oils, the methods of their counterfeiting and the methods of counterfeiting detection, as well as the basics of artificial neural networks (ANN). The issues discussed in this chapter have been correctly selected and logically presented, providing a good introduction to the subsequent chapters. The title of section 2.4 '*Methods of adulteration of edible oils*' could be extended as it does not fully cover all the content. Apart from the methods of counterfeiting, this section describes also the methods of detecting adulteration. In this chapter, the author of the dissertation has undoubtedly proved that she possesses a general theoretical knowledge in the discipline of food and nutrition technology.

Chapter 3 '*Aims of the thesis*' presents the main objective of the doctoral dissertation, which is to assess the usefulness of artificial neural networks for identifying vegetable oils on the basis of components such as triacylglycerols, fatty acids and sterols. There is some inaccuracy here, as the objective stated in the introduction (Chapter 1 '*Introduction*': 'The objective of this study is to provide a method employing ANNs to detect adulteration by most kinds of edible vegetable oils') slightly differs from that of Chapter 3 (Chapter 3 '*Aims of the thesis*': 'The main goal of this thesis is to evaluate the ability of artificial neural network to identify vegetable oil making use of the composition and the content of endogenous components such as triacylglycerols, fatty acids and sterols'). In my opinion, it would be better to standardize the wording related to the research goal throughout the work, and to connect it more closely with the subject of adulteration. Also, in Chapter 3, the PhD candidate writes that the detection of adulteration in edible oils is a way to strengthen *food defence*. I think it would be called for, first of all, to mention the prevention of *food fraud*. The term *food defence* is understood in the literature as the prevention of deliberate contamination with various chemical, biological or other harmful substances, in the context of terrorist activities, while the term *food fraud* is understood as the deliberate replacement, improper labeling, adulteration or counterfeiting of food, raw materials, ingredients or packaging placed on the market in order to obtain economic benefits. There are certainly more cases of actions aimed at obtaining economic benefits than cases related to activities aimed at intimidation. In addition, in this chapter, the PhD candidate presents the main research tasks, which include:



- evaluation of the HTGC-FID method for the determination of triacylglycerols in vegetable oils
- evaluation of the HPLC-ELSD method also for the determination of triacylglycerols in vegetable oils
- collecting samples of vegetable oils
- determination of triacylglycerols, fatty acids and sterols in nearly 50 samples of each of the 8 types of oils
- the use of PCA to reduce the dimensionality of data entered into artificial neural networks (ANNs)
- choosing the best ANN model
- testing artificial neural network models and defining detection thresholds.

The formulated aim of the work and the presented research tasks correspond to the topic of the work as closely as possible. The research tasks were planned in a correct and logical manner, thanks to which they were used to collect research data, select the variables containing most information about the tested samples, and to develop the ANN model for the identification of edible oils. The implementation of the chosen goal and planned research tasks required conducting numerous empirical studies preceded by the selection of research material and research methods. The large quantity of research analyses carried out is certainly noteworthy. The research scheme presented on p. 24 shows the outline of the work carried out, which makes it easier to read the doctoral dissertation. In my opinion, the presented diagram does not fully do justice to the enormity of the work done by the author, in relation to the rich methodological arsenal, the number of samples tested, repetitions and statistical analyses.

The research methods and research material used in the work are presented in detail in Chapter 4 *'Materials and Methods'*. The research material consists in 8 types of vegetable oils (corn, linseed, rapeseed, sunflower, soybean, pumpkin seed, black cumin seeds and olive oil) obtained directly from producers or purchased in a retail chain. The number of samples ranged from 35 to 50 depending on the type of oil. I did not find information whether the tested oils were cold pressed or refined. During the refining process, sterols are removed from the oil, which could have influenced the choice of variables for statistical analysis. The content of triacylglycerols in the analyzed oil samples was determined using the HTGC-FID and HPLC-ELSD methods, as well as the composition of fatty acids (GC-FID) and sterols (GC-FID).

In total, as many as 59 parameters have been marked for each oil. The presence of C16: 0, C18: 1, C18: 2, OPP, POL, OOL, LOL, campesterol, campestanol, stigmasterol, β -sitosterol and sitastanol was detected in all tested oils. The set of experimental data was subjected to principal components analysis (PCA), as a result of which the most important variables were selected. The selected variables, based on



principal components analysis, constituted input data for artificial neural networks. I consider the selection of the statistical methods of artificial neural networks used in the doctoral thesis to be very accurate. These are the methods with very high potential, which have already been proven to be highly effective in many areas of the food industry, and whose possible applications in detecting adulteration have not yet been well known and studied.

In the dissertation, three types of statistical models were built, depending on the adopted variable selection criterion:

- First type models: the variables were marked with triacylglycerols, fatty acids and sterols selected on the basis of a literature review and experimental data
- Second type models: the variables were marked with triacylglycerols, fatty acids and sterols selected on the basis of the principal components analysis
- Type three models: only triacylglycerols selected on the basis of principal components analysis were the variables.

The results of laboratory tests and statistical analyzes, presented in Chapter 5 '*Results and Discussion*' have been presented in a correct and logical manner. The use of principal components analysis allowed for the selection of significant primary variables, on the basis of which models of artificial neural networks were then built, allowing for the identification of vegetable oils. In the final stage of the research, the original samples of soybean oil and black cumin oil were mixed in a controlled manner in order to obtain adulterated samples and to test the previously obtained model of artificial neural networks. The research results obtained by the PhD candidate were subject to scientific discussion in view of results obtained by other authors, and the probable reasons for the results were explained. The in-depth discussion of the results proves once again the great theoretical knowledge of the PhD candidate. The obtained results increase the knowledge in the field and are of great practical importance in developing methods of quality and authenticity control of edible oils. Conducting the research planned by the PhD candidate allowed for the achievement of the aim set in the work.

In Chapters 6 '*Summary*' and 7 '*Conclusions*', the obtained research results is summarized and the achievement of the research goal is demonstrated. Ten final conclusions are formulated. The presented research results are very valuable from the cognitive point of view as well as indicate the direction of further research and, as a result, their potential practical applications.

The significant achievements of the evaluated doctoral dissertation include, among others :



1. The determination of significant primary variables constituting input data for statistical models aimed at subsequent identification of edible oils.
2. The optimization of the artificial neural network topology for the detection of adulteration of edible oils. The higher efficiency of MLP neural networks over RFB in solving this type of problems has been demonstrated.
3. Conducting analyses to conclude that the AR model based solely on triacylglycerols allows for similar results as statistical models based on additional data following from fatty acid and sterol determinations. It has been shown that there is no need to carry out additional, more time-consuming determinations and building a statistical model on the basis of triacylglycerols is sufficient.

The assessed doctoral dissertation is usually written carefully and in a correct language. There are, however, some editorial errors related to, for example, punctuation, letter replacement, or the use of unfortunate phrases, as well as minor grammatical errors, which, however, do not in any way reduce the substantive value of the presented work. Examples:

- p. 12, unfinished sentence: ‘Some unconventional seed oils have total phytosterols’
- p. 17, some inaccuracies stemming from ignoring the fact that Ukraine is in Europe, as is part of Russia: ‘Russia, Ukraine and Europe were the main producers of sunflowers’
- p. 17, The inaccuracy stemming from ignoring the fact that the Mediterranean countries and the European Union countries are not two independent groups of countries: ‘...especially in Mediterranean countries and in the EU countries’
- p. 18, there are no markers when listing the methods of adulterating olive oil, making it difficult to read
- p. 20, the author probably meant ‘machine-learning’ and not ‘machine - earning’
- p. 20, minor linguistic errors: ‘Fureri had to development the software’.

In reading the dissertation by Qian Ying, M.Sc., some issues arise of a more debatable character:

1. Perhaps it would be more advantageous to look for an answer to the question whether the tested oils are authentic in the first stage, instead of looking for information about what they are adulterated with. I believe that the most consumers are interested in the question of whether the product is adulterated or not in the first place.
2. In the chapter on research methods and research material, there is no information as to whether the oils used in the research were cold pressed or refined,



or maybe they were oils from different production processes. The choice of oils could have had a significant impact, e.g. on the selection of variables for further analysis. For example sterols are, at least partially, removed during the refining process.

3. It would be interesting to check whether the inclusion in the model of characteristic variables typical only for selected oils (e.g. brassicasterol) and not just relying on those found in all oils could not improve efficacy. I am thinking especially about the situation where we seek an answer to the question of whether a given oil is authentic and not whether it is adulterated. I believe that such a study could be very valuable.

The comments I formulate here are typically debatable, and do not detract from to my positive evaluation of the work.

Final conclusion

In conclusion, I would like to state that the research carried out by Qian Ying, M. Sc., has both cognitive value and potential application value. Moreover, the obtained results constitute a significant contribution to the development of the food and nutrition technology discipline, and the conducted research and analyses prove the PhD candidate's ability to conduct scientific work independently. They contribute to a significant expansion of knowledge on the possibility of using chromatographic methods in combination with artificial neural networks to monitor the quality of edible oils, including their authenticity. I declare that the dissertation 'The composition of triacylglycerols as an indicator of edible oil adulteration' fully meets the requirements for doctoral dissertations and I am applying to the Scientific Council of the Food and Nutrition Technology Faculty of Poznań University of Life Sciences for the acceptance of the dissertation and the admission of Qian Ying, M. Sc., to the next stages of the doctoral procedure.

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