JAP&T
TPA-Timisoara

Available online at http://journal-of-agroalimentary.ro

Journal of Agroalimentary Processes and Technologies 2023, *29* (1), 9-15

Journal of Agroalimentary Processes and Technologies

Conformational changes in dough and bread from wheat flour with the addition of oat bran in combination with phospholipids

Anastasiia Shevchenko [1,*], Svitlana Litvynchuk [2], Vira Drobot [1]

[1] Department of Bakery and Confectionery Goods Technologies, National University of Food Technologies, 01601, Volodymyrska Street 68, Ukraine
[2] Department of Physics, National University of Food Technologies, 01601, Volodymyrska Street 68, Ukraine

Abstract

The purpose of the research was to determine the influence of oat bran in combination with sunflower lecithin on conformational changes in the structure of dough semi-finished products and bread made from wheat flour. After kneading the dough, no conformational changes were observed, and during the fermentation process, they deepened with an increase in the percentage of replacement of wheat flour with oat bran. The spectra of bread had a lower reflectance than the dough samples both after kneading and during fermentation. The protein of such bread is more fully used for anabolic needs by the body. The biological value of bread with oat bran is higher, which makes them a promising raw material not only from the point of view of enriching bakery products with valuable nutrients, but also of a higher degree of their digestibility.

Keywords: oat bran; sunflower lecithin; bread, dough; conformational transformations

1. Introduction

Nowadays because of unfavorable environmental situation in the world, diseases of the gastrointestinal tract are becoming more and more common. In recent decades, the number of cases of irritable bowel syndrome has increased, especially among young working population [1]. It is also associated with higher levels of stress [2]. Irritable bowel syndrome is a disease of industrialization and urbanization. The main approach to reducing the incidence of this disease is diet therapy [3]. The FODMAP (fermentable oligosaccharides, disaccharides, monosaccharides, and polyols) diet is based on the elimination or reduction in the diet products with a high content of FODMAP carbohydrates and their replacement [4]. This approach makes it possible to diversify the diet and improve the quality of life [5]. It is important to replace high-FODMAP products with fiber-rich alternatives [6]. One of these products is oat and its processing products, and especially oat bran, which is considered to be food waste. Their use in the recipes of products, in particular the bakery industry as one of the main ones, will promote the sustainable development of production and increase the level of food security.

Oat bran, as a product rich in fiber, can lower the glycemic index of bakery products. It was found that the addition of a mixture of wheat bran and oat bran reduced the specific volume of bread. The oat bran bread had the highest content of slowly digestible starch, while the control sample made from wheat flour had the highest content of rapidly digestible starch. Oat β-glucan reduced α-amylase activity by intertwining with starch, forming a more stable gel network structure that reduced the contact area between amylase and starch. Thus, oat bran β-glucan can be a key component for reducing the glycemic index of bread with this raw material [7].

Extracted oat protein fractions are characterized by a relatively high protein content and a unique amino acid profile compared to other cereals. On the other

* Corresponding author: nastyusha8@ukr.net

hand, oat bran is separated during the production of oat flour, which helps to increase the content of oat proteins in food waste. Modification methods, including chemical, physical and enzymatic, have been proposed to improve the techno-functionality of native oat proteins and their biological activity [8].

The underlying physical mechanism by which bran affects the properties of whole wheat flour dough was elucidated by IR-Fourier spectroscopy by monitoring the state of water and gluten secondary structure in wheat dough and with the addition of bran. The addition of bran to the dough caused a redistribution of water in the dough system with flour and bran, as evidenced by a shift of the OH stretching frequency in the region of 3200 cm^{-1} to higher frequencies and a decrease in monomeric water (free water). [9]. However, no data were found on the study of the influence of oat bran on the conformational transformations in the gluten network of the dough.

It is recommended to combine the use of dietary fiber with products rich in phospholipids for people with irritable bowel syndrome. Sunflower lecithin as a source of lipids important for the body can be an alternative to soy lecithin, as it is considered to be a product without genetically modified organisms [10]. In the technology of bakery products, it helps to improve the elasticity of the dough, increase the gas formation in the dough, the volume and porosity of the bread [11]. It is assumed that lecithin combined with oat bran will be able to improve the digestibility of wheat flour bread and give it increased nutritional value.

The purpose of the research was to determine the effect of oat bran in combination with sunflower lecithin on conformational changes in the structure of wheat flour dough and bread and the completeness of the body's assimilation of products with this raw material.

2. Materials and Method

2.1. Materials

For research such materials were used: wheat flour of the highest grade ("KyivMlyn" LLC, Ukraine), oat bran ("Organic-Eco-Produkt" LLC, Ukraine) and sunflower lecithin (TM Fruity Yummy, Ukraine). Main characteristics of wheat flour are: protein content – 11.3%, fat content – 1.1%, fiber content – 3.5%, gluten content – not less than 25%. Main characteristics of oat bran are: protein content – 17.0%, fat content – 7.0%, fiber content – 15.4%. Dough samples were prepared from wheat flour, baker's pressed yeast in the amount of 3% by weight of flour, salt in the amount of 1.5% by weight of flour. Lecithin was added in the amount of 3% to the mass of flour. This dosage was chosen based on the recommendations of the daily lecithin rate for people with diseases of the gastrointestinal tract [12]. Samples were also prepared with replacement of wheat flour in the recipe with oat bran in the amount of 5%, 7%, 10% and 15%. The control was a sample without additional raw materials.

2.2. Biological value of bread

Biological value is characterized by utilitarian coefficient (the balance of all essential amino acids (EAA) of proteins with respect to physiological norm), redundancy coefficient (the mass fraction of essential amino acids in 100 g product, which is not fully used by the body), DCAS (the average excess of essential amino acids in comparison with the smallest amino acid score of the limiting amino acid) and indicator of biological value.

Redundancy coefficient was calculated by the formula:

$$\sigma_{red} = \frac{\sum_{j=1}^{k}(A_j - C_{min}A_{ej})}{C_{min}}$$

Utilitarian coefficient was calculated by the formula:

$$U = \frac{C_{min} \cdot \sum_{j=1}^{8} A_{ej}}{\sum_{j=1}^{8} A_j}$$

where C_{min} is C_{min} –score of the first limited acid EAA units; A_j is the mass fraction of the j-th of EAA in the product, mg/g protein; A_{ej} is the mass fraction of the j-th of EAA in the protein model, mg/g protein (FAO/WHO scale).

DCAS was calculated by the formula:

$$DCAS = \frac{\sum \Delta DAS}{n}$$

where DAS – the difference in amino acid score for each EAA compared to the AS of a limiting amino acid expresses as %; n – the number of amino acids.

Biological value was calculated by the formula:

$$BV = 100 - DCAS$$

where, BV – Biological value of the protein expresses as % [13].

2.3. Near-infrared reflection spectroscopy

Reflectance spectra of the samples were obtained using Infrapid spectrometer (Labor-Mim, Hungary). The reflection spectra of Samples were grounded to particles with a smooth surface. Measurements were made in the range of wavelengths from 1330 to 2370 nm [14,15]. Reflection spectrum from the sample and the I0 standard was recorded by the spectrometer. The spectra are presented as reflectance R in relative units (ratio of intensities I/I0 = R), depending on the wavelength in nm. The intensity of reflection was measured in bread and in the dough after kneading and after 3.5 hours of fermentation [16].

2.4. Statistical analysis

The data represents the mean of a minimum three replicates ± standard deviation (SD). Graphical presentation of experimental data was performed using standard statistical processing programs – Microsoft Excel 2010.

3. Results and Discussion

Raw materials and their main nutrients play a decisive role in forming the properties of the dough system, particularly the gluten frame and the quality of bread. The chemical composition of wheat flour and oat bran differs significantly. Oat bran has an increased content of protein compared to high grade wheat flour - 17.1% and 11.3%, dietary fiber - 15.4% and 3.5%, respectively. The composition of sunflower lecithin includes lipids, the main of which is phosphatidylcholine.

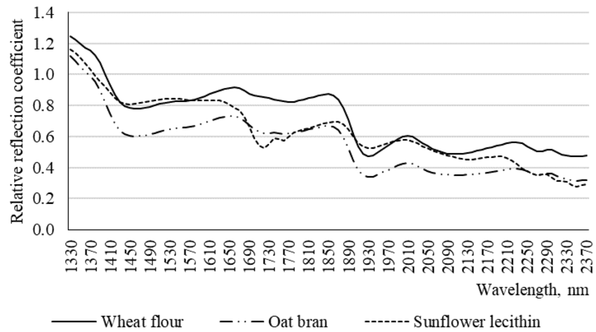

Figure 1. Reflection spectra of raw material samples in the near-infrared region

To identify and analyze different components such as proteins, lipids etc., it is advisable to use the reflection spectrum in the near-infrared region [17]. The infrared reflectance spectra of wheat flour, oat bran, and sunflower lecithin are shown in Figure 1.

As the obtained results showed, the spectra of wheat flour and oat bran have a similar character: they are located parallel to each other, but differ in the intensity of reflection. At the same time, the main extrema of these spectra are observed at the same wavelengths. Wheat flour has a higher relative reflection coefficient, so its spectrum is placed higher than the spectrum of oat bran. Accordingly, the initial reflection intensity of the wheat flour sample was higher than the initial reflection intensity of the oat bran sample.

Sunflower lecithin is a raw material of lipid nature, so this was also reflected in its spectrum curve. The curve is significantly different from the reflection spectrum of oat bran and wheat flour. Additional extremes appear on its spectrum. For example, at wavelengths of 1720 and 1760 nm, clear minima of reflection intensity are observed, which were not previously observed in the spectra of wheat flour and oat bran. Similar minima of reflection intensity also occur at wavelengths of 2310 and 2350 nm. Extremes at these lengths characterize lipid groups, which are clearly manifested in lecithin due to its lipid nature.

Also, when comparing the three specified spectra at some wavelengths a shift of the reflection minima on the spectrum of sunflower lecithin to the short-wave range (from 1460 to 1450 nm) and to the long-wave range (from 2110 to 2140 nm) is noticeable. At the wavelength of 2100 nm, which characterizes protein groups, there is no extremum on the spectrum of lecithin, which indicates the absence of protein in its composition, which is present in flour and bran samples [18]. At the wavelength of 1930 nm, which characterizes the moisture content of the product, the highest moisture content in the oat bran sample is observed, a little less content is in wheat flour, and the lowest is in lecithin.

The obtained results confirm the different chemical composition of the studied raw materials, and therefore it is possible to predict a significant influence of oat bran and lecithin on the change of the main structural units of dough and bread with these components in the recipe. The obtained reflection spectra of dough samples immediately after mixing were compared (Figure 2).

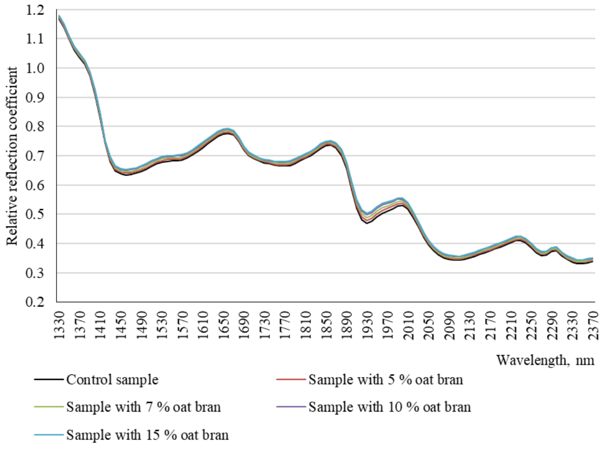

Figure 2. Reflection spectra of dough samples with oat bran (5, 7, 10 and 15% replacement) after kneading

The analysis of the results showed the similarity of all the studied samples and the overlap of the reflectance spectra. However, there is a direct regularity in the location of the spectra of the dough samples with different concentrations of oat bran to replace wheat flour: the lowest is the control sample of the dough, above it - with 5, 7, 10, and 15% replacement, although this regularity is hardly noticeable. This can be explained by the absence of conformational transformations in the dough system due to the fact that the biopolymers of the raw materials did not have time to interact with each other. At the wavelength of 1930 nm, which characterizes the presence of moisture in the samples, there is a minimum extremum for all samples, at which the difference in spectra is most noticeable. This is explained by the fact that bran has a higher water absorption capacity than flour, due to which, with the same dosage of water in the dough, its absorption and binding will be higher. That is, from a technological point of view, at the stage of mixing, the samples do not differ significantly. At the wavelengths of 1720, 1760 nm, 2310 and 2350 nm, which characterize the lipid groups and at which the extrema of the lecithin sample were present, no extrema were detected in the spectra of the dough samples. This is explained by the fact that the main properties of the dough system are determined by the properties of flour, as its content is the largest in the recipe, and lecithin loses its individual characteristics in the process of kneading the dough.

However, in the process of fermentation of the dough, the components of the recipe enter into stronger bonds, the structure of the dough is formed. This indicates the course of conformational processes that will be affected by the added oat bran in combination with lecithin (Figure 3). The samples were analyzed after 3.5 hours of fermentation (the total time of fermentation and proofing of the dough).

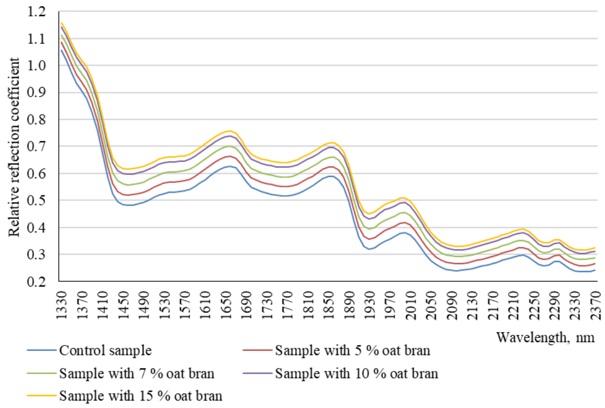

Figure 3. Reflection spectra of dough samples with oat bran (5, 7, 10 and 15% replacement) after fermentation

In contrast to the reflection spectra obtained immediately after kneading the dough, after fermentation there were noticeable changes in each of the analyzed spectra: their intensity differs depending on the percentage of replacement of wheat flour with oat bran, although the spectra retained their regularity of location. This indicates that the nature of the influence of different amounts added raw materials on the processes that occur in the dough during fermentation is the same, regardless of their amount. However, quantitatively, the difference is significant. Thus, the greater the replacement of wheat flour with oat bran is, the more the reflection coefficient increased, and, accordingly, the spectrum was located higher than the control sample of the dough. At a wavelength of 2100 nm, which characterizes protein structural groups, there is a minimum extremum for all samples, the value of the relative reflectance of the control sample is 0.24, of samples with 5, 7, 10, and 15% substitution is 0.6, 0.95, 0.1, and 0.2, respectively. Such a position of minimums can be explained by the fact that oat bran does not participate in the formation of gluten, as it has a globular protein structure. Instead, they are incorporated into the gluten framework formed by gliadins and glutenins of wheat flour and delay its development [19]. Due to the presence of a large amount of dietary fiber, it can be predicted that the structure of the protein matrix of the dough with oat bran will weaken.

Since changes in the dough during fermentation were established, they should also be expected in the process of baking bread. All the reflectance spectra of the obtained bread samples (both control and with 5%, 7%, 10%, and 15% replacement) after baking have the same character and almost overlap each other in the investigated wavelength range (Figure 4).

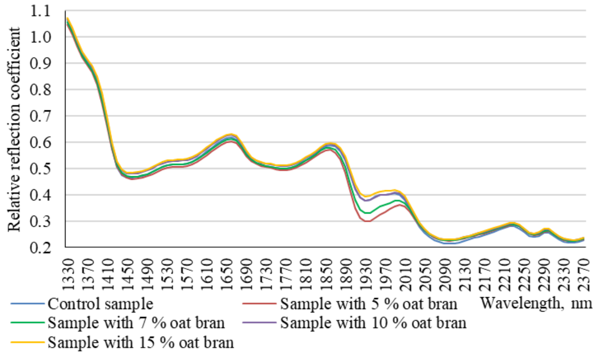

Figure 4. Reflection spectra bread with oat bran (5, 7, 10 and 15% replacement)

In contrast to the spectra of the dough samples after kneading, where a significant difference between the reflection intensity was observed, for the bread samples there are almost no differences in the reflection index. This is explained by the fact that in the process of baking, dough samples are subjected to thermal effects at high temperatures (220°C), which leads to the splitting of peptide bonds and the destruction of protein macromolecules [20].

At the same time, the obtained spectra have a lower reflection coefficient than the dough samples both after kneading and during the fermentation process. For example, at a wavelength of 2100 nm, the reflectance coefficient for bread is 0.22, while for dough samples after fermentation it is higher than 0.25, and after kneading it is higher than 0.35.

The obtained data on the conformational transformations of the structural elements of the dough with oat bran and sunflower lecithin allow predicting better assimilation of bakery products with this raw material in the recipe. To confirm this hypothesis, the utilitarian coefficient was calculated, which characterizes the balance of essential amino acids (EAA) in relation to the physiologically necessary norm. To characterize the total amount of EAA that the body uses for anabolic needs, the indicator of the comparative excess of EAA (redundancy coefficient) and the amount of the excess amino acid composition of EAA (the coefficient of difference in the amino acid score of DCAS) and the biological value (BV) were calculated (Table 1).

The analysis of the utilitarian coefficient showed that the degree of balance of essential amino acids in relation to the physiologically necessary norm is the highest in the sample with the replacement of 15% of wheat flour with oat bran. The redundancy coefficients of the samples showed that the protein of bread with 15% replacement is more fully used by the body for anabolic needs. As the replacement percentage increased, the DCAS indicator decreased slightly. This indicates that the amino acids contained in the bread with the additive are more fully used by the body than in the control sample. That is, the introduction of oat bran contributes to a more complete use of the product's protein. These conclusions confirm the above-mentioned studies of conformational transformations in dough and bread with the addition of oat bran in combination with phospholipids. In general, the biological value of the control sample is lower than the samples of bread with oat bran in combination with lecithin, which makes them a promising raw materials not only from the point of view of enriching bakery products with valuable nutrients, but also from the point of view of a higher degree of their digestibility.

4. Conclusions

As the obtained results showed, the spectra of wheat flour and oat bran have a similar character: they are located parallel to each other, but differ in the intensity of reflection. Sunflower lecithin is a raw material of lipid nature, so this was also reflected in its spectrum curve. After kneading the dough, no conformational changes were observed, and during the fermentation process, they deepened with an increase in the percentage of replacement of wheat flour with oat bran, and the reflection coefficient increased. For the bread samples, there were almost no differences in reflectance, but the obtained spectra had a lower reflectance than the dough samples both after kneading and during fermentation. It was established that bread with oat bran will be better absorbed, since the degree of balance of essential amino acids in relation to the physiologically necessary norm increased with an

Table 1. Utilitarian coefficient, redundancy coefficient, DCAS, BV of products when replacing part of wheat flour with oat bran

Indicators	Control sample	Sample with lecithin	Oat bran to replace wheat flour, %			
			5	7	10	15
Utilitarian coefficient	0.49±0.01	0.49±0.01	0.55±0.01	0.57±0.01	0.60±0.01	0.64±0.01
Redundancy coefficient	37.25±1.11	37.25±1.11	29.45±1.07	27.03±1.01	23.93±0.95	19.82±0.90
DCAS	0.47±0.01	0.47±0.01	0.45±0.01	0.45±0.01	0.44±0.01	0.42±0.01
Biological value (%)	99.53±2.49	99.53±2.49	99.55±2.49	99.55±2.49	99.56±2.49	99.58±2.49

All determinations were done in triplicate, the results were reported as average value ± standard deviation (SD)

increase in the additive. The protein of such bread is more fully used by the body for anabolic needs. In general, the biological value of the control sample is lower than the samples of bread with oat bran and lecithin, which makes them a promising raw materials not only from the point of view of enriching bakery products with valuable nutrients, but also from the point of view of a higher degree of their digestibility.

Compliance with Ethics Requirements. Authors declare that they respect the journal's ethics requirements. Authors declare that they have no conflict of interest and all procedures involving human or animal subjects (if exist) respect the specific regulation and standards.

References

1. Böhn, L.; Störsrud, S.; Törnblom, H.; Bengtsson, U.; Simrén, M., Self-reported food-related gastrointestinal symptoms in IBS are common and associated with more severe symptoms and reduced quality of life, *American Journal of Gastroenterology* **2013**, *108*, 634–641. https://doi.org/10.1038/ajg.2013.105.

2. Gwee, K.A., Irritable bowel syndrome in developing countries: a disorder of civilization or colonization? *Neurogastroenterology & Motility* **2005**, *17*(3), 317–324. https://doi.org/10.1111/j.1365-2982.2005.00627.x.

3. Canavan, C.; West, J.; Card, T., The epidemiology of irritable bowel syndrome, *Clinical Epidemiology* 2015, *6*, 71–80. https://doi.org/10.2147/CLEP.S40245.

4. Bellini, M.; Tonarelli, S.; Nagy, A. G.; Pancetti, A.; Costa, F.; Ricchiuti, A.; de Bortoli, N.; Mosca, M.; Marchi, S.; Rossi, A., Low FODMAP Diet: Evidence, Doubts, and Hopes, *Nutrients* **2015**, *12*(1), 148. https://doi.org/10.3390/nu12010148.

5. Kortlever, T.L.; Ten Bokkel Huinink, S.; Offereins, M.; Hebblethwaite, C.; O'Brien, L.; Leeper, J.; Mulder, C.; Barrett, J. S.; Gearry, R., Low-FODMAP diet is associated with improved quality of life in ibs patients-a prospective observational study, *Nutrition in Clinical Practice* **2019**, 34(4), 623-630. https://doi.org/10.1002/ncp.10233.

6. Gibson, G.R.; Hutkins, R.; Sanders, M.E.; Prescott, S.L.; Reimer, R.A.; Salminen, S.J.; Scott, K.; Stanton, C.; Swanson, K.S.; Cani, P.D.; Verbeke, K.; Reid, G., Expert consensus document: The International Scientific Association for Probiotics and Prebiotics (ISAPP) consensus statement on the definition and scope of prebiotics, *Nature reviews gastroenterology & hepatology* **2017**, *14*, 491–502. https://doi.org/10.1038/nrgastro.2017.75.

7. Hu, H.; Lin, H.; Xiao, L.; Guo, M.; Yan, X.; Su, X.; Liu, L.; Sang, S., Impact of Native Form Oat β-Glucan on the Physical and Starch Digestive Properties of Whole Oat Bread, *Foods* **2022**, *11*, 2622. https://doi.org/10.3390/foods11172622.

8. Ibrahim, M.; Aav, A.; Jõudu, I., The potential and limitations for applications of oat proteins in the food industry, *Agronomy Research* **2022**, *20*(1), 161–173. https://doi.org/10.15159/AR.22.008.

9. Bock, J. E.; Damodaran, S., Bran-induced changes in water structure and gluten conformation in model gluten dough studied by Fourier transform infrared spectroscopy, *Food Hydrocolloids* 2013, *31*(2), 146–155. https://doi.org/10.1016/j.foodhyd.2012.10.014.

10. Guiotto, E. N.; Tomás, M. C.; Diehl, B. W.K., Sunflower Lecithin. In: *Polar Lipids*, Academic Press and AOCS Press, USA, 2015, pp. 57–75. https://doi.org/10.1016/b978-1-63067-044-3.50007-8.

11. Cabezas, D. M.; Madoery, R.; Diehl, B. W. K.; Tomás, M. C., Emulsifying Properties of Different Modified Sunflower Lecithins, *Journal of the American Oil Chemists' Society* **2012**, *89*(2), 355–361. https://doi.org/10.1007/s11746-011-1915-8.

12. Partridge, D.; Lloyd, K. A.; Rhodes, J. M.; Walker, A. W.; Johnstone, A. M.; Campbell, B.J., Food additives: Assessing the impact of exposure to permitted emulsifiers on bowel and metabolic health – introducing the FADiets study, *Nutrition Bulletin* **2019**, *44*(4), 329–349. https://doi.org/10.1111/nbu.12408.
13. Shevchenko, A.; Litvynchuk, S., Influence of rice flour on conformational changes in the structure of wheat bread and its nutritional value, *Food and Environment Safety* **2023**, *22*(1), 5-14. https://doi.org/10.4316/fens.2023.001.
14. Litvynchuk, S.; Galenko, O.; Cavicchi, A.; Ceccanti, C.; Mignani, C.; Guidi, L.; Shevchenko, A., Conformational Changes in the Structure of Dough and Bread Enriched with Pumpkin Seed Flour, *Plants* **2022**, *11*, 2762. https://doi.org/10.3390/plants11202762.
15. Niewitetzki, O.; Tillmann, P.; Becker, H.C.; Mollers, C., A new near-infrared reflectance spectroscopy method for high-throughput analysis of oleic acid and linolenic acid content of single seeds in oilseed rape (*Brassica napus L.*), *Journal of Agricultural and Food Chemistry* **2010**, *58,* 94–100. https://doi.org/10.1021/jf9028199.
16. Yip, W.L.; Gausemel, I.; Sande, S.A.; Dyrstad, K., Strategies for multivariate modeling of moisture content in freeze-dried mannitol-containing products by near-infrared spectroscopy, *Journal of Pharmaceutical and Biomedical Analysis* **2012**, *70*, 202–211. https://doi.org/10.1016/j.jpba.2012.06.043.
17. Baslar, M.; Ertugay, M.F., Determination of protein and gluten quality-related parameters of wheat flour using near-infrared reflectance spectroscopy (NIRS), *Turkish Journal of Agriculture and Forestry* **2011**, *35*(2), 139–144. https://doi.org/10.3906/tar-0912-507.
18. Beć, K.B.; Karczmit, D.; Kwaśniewicz, M.; Ozaki, Y.; Czarnecki, M.A., Overtones of νC≡N Vibration as a Probe of Structure of Liquid CH3CN, CD3CN, and CCl3CN: Combined Infrared, Near-Infrared, and Raman Spectroscopic Studies with Anhar-monic Density Functional Theory Calculations, *The Journal of Physical Chemistry* **2019**, *123*(20), 4431–4442. https://doi.org/10.1021/acs.jpca.9b02170.
19. Alfaris, N. A.; Gupta, A. K.; Khan, D.; Khan, M.; Wabaidur, S. M.; Altamimi, J. Z.; Alothman, Z. A.; Aldayel, T. S., Impacts of wheat bran on the structure of the gluten network as studied through the production of dough and factors affecting gluten network, *Food Science and Technology (Campinas)* **2022**, *42*(3). https://doi.org/10.1590/fst.37021.
20. Zhou, Y.; Dhital, S.; Zhao, C.; Ye, F.; Chen, J.; Zhao, G., Dietary fiber-gluten protein interaction in wheat flour dough: Analysis, consequences and proposed mechanisms, *Food Hydrocolloids* **2021**, *111*, 106203. https://doi.org/10.1016/j.foodhyd.2020.106203.