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## CHAPTER 5

# Compositional analysis and potential of buckwheat and oats as functional food ingredients

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### Abstract

Buckwheat and oats are traditional, though not the most popular, crops with strong environmental adaptability. The bioactive substances in buckwheat and oats have a positive impact on human health, including antioxidant and anti-inflammatory properties and the ability to prevent cancer. In this work, a comprehensive analysis of buckwheat and oat powders was carried out, including sieve analysis, infrared spectroscopy (IR spectroscopy), X-ray fluorescence analysis (XRF) and gas chromatography with mass spectrometry (GC/MS).

According to the results of sieve analysis, the highest content of fractions with a particle diameter of 1.1–0.5 mm was found: 41.76% for buckwheat powder and 52.56% for oat powder. The analysis of the IR spectra showed a similar chemical composition of both samples, including carbohydrates, proteins, fats and minerals. However, the buckwheat powder had a higher content of proteins and carbonyl compounds, and the oat powder had a higher content of polysaccharides. X-ray fluorescence analysis showed that both samples contain mainly C, H, P, S, K, Ca, Mn, Fe, Cu, Zn, but in different proportions. Buckwheat powder is characterized by a higher content of potassium and phosphorus, while oat powder has higher levels of calcium and manganese.

The GC/MS method was used to identify 15 bioactive compounds in buckwheat powder and 18 in oat powder. Sucrose, palmitic acid, linoleic acid and phytosterols (gamma-sitosterol, campesterol) were found in both samples. Buckwheat powder has a higher content of antioxidants, in particular  $\gamma$ -tocopherol, while oat powder contains steroidal compounds and oxazole derivatives that may affect lipid metabolism.

The study confirmed the unique nutritional profile of buckwheat and oat groats grown in Volyn. The results can be used in the field of functional food, pharmacology and nutrition to develop products with high biological activity.

### Keywords

Buckwheat, oats, nutrient, chemical composition, functional food, antioxidants, bioactive compounds, GC-MS, XRF.

## 5.1 Introduction

In the context of current demographic trends, in particular the growth of the world's population by about 1.1% per year (according to the United Nations in 2019), ensuring global food security remains an extremely urgent issue [1, 2]. The modern agricultural industry prefers monoculture cultivation of a limited set of crops [3]. This strategy leads to a narrowing of the range of available nutrients for consumers, as the human diet is based on a small number of plant species [4].

According to researchers [5], 67% of humanity's energy intake comes from four main crops: wheat, rice, corn and soybeans. The dominance of these crops in global agriculture creates global patterns of consumption. Despite the undoubted nutritional value of the aforementioned crops, numerous studies demonstrate their insufficiency in providing the full range of essential nutrients critical for the optimal functioning of the human body [6]. In particular, there is a significant deficiency of essential micronutrients, proteins, essential amino acids and vitamins, which are fundamental components of a balanced diet. This nutritional deficiency can lead to long-term health consequences for the population, including an increased risk of developing chronic diseases and a reduced overall quality of life. In addition, due to global climate change, global production of major consumer crops may decline significantly [7].

Buckwheat and oats are traditional crops grown around the world. It should be noted that these crops have a strong environmental adaptability that allows them to grow in almost all types of extreme environments. In 2023, the global production of buckwheat was 2.2 million tons, and oats 18.8 million tons [8]. The dynamics of changes in buckwheat and oat production and area over the past 5 years are shown in the diagram (**Fig. 5.1**). The main producers of buckwheat grain in 2023 were Russia, China and Ukraine (**Table 5.1**). Russia, Canada and Australia produce the most oats in the world. The level of production of these crops is significantly lower compared to wheat, rice, corn and soybeans.

At the same time, oats and buckwheat have a unique nutritional profile and potentially significant health benefits, which underscores the need to increase the diversity of agricultural production and diets to improve global health and food security.

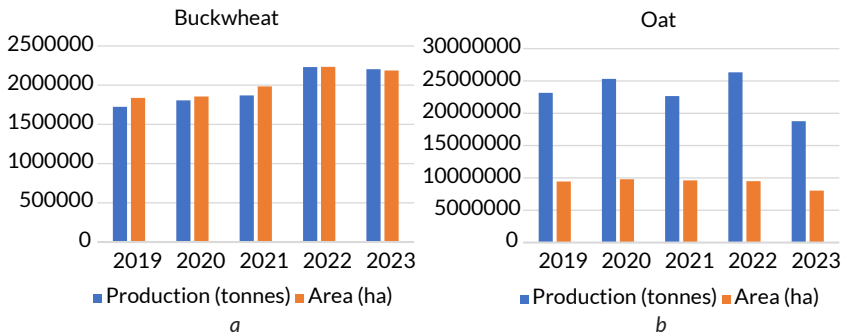


Fig. 5.1 Dynamics of changes in buckwheat (a) and oat (b) production and sown area  
Source: [8]

Table 5.1 World's largest producers of buckwheat and oat (production year 2023)

| Buckwheat          |                   |           | Oats               |                   |           |
|--------------------|-------------------|-----------|--------------------|-------------------|-----------|
| Countries          | Production (tons) | Area (ha) | Countries          | Production (tons) | Area (ha) |
| Russian Federation | 1149066.65        | 1037110   | Russian Federation | 3300000           | 1770000   |
| China              | 504265.75         | 624246    | Canada             | 2635574           | 822500    |
| Ukraine            | 210720.00         | 147900    | Poland             | 1503440           | 497690    |
| USA                | 86679.82          | 83462     | Finland            | 1019720           | 291300    |
| Kazakhstan         | 83491.29          | 114484    | Australia          | 959829            | 569082    |
| Brazil             | 64611.39          | 47490     | Brazil             | 907046            | 528649    |
| Japan              | 35500.00          | 66700     | Great Britain      | 830000            | 167000    |
| Tanzania           | 22190.89          | 21218     | USA                | 828010            | 336300    |
| Belarus            | 16937.05          | 15593     | China              | 600000            | 160511    |
| Nepal              | 15083.49          | 11857     | Spain              | 464140            | 464760    |
| World total        | 2204015           | 2187456   | World total        | 18776760          | 8024447   |

Source: [8]

The aim of the presented study is:

- 1) to analyze the literature data on the biochemical characteristics of buckwheat and oats as important components of functional food;
- 2) to experimentally determine the content of the main micro and macronutrients in powders obtained from buckwheat and oat grains grown in the Volyn region (Ukraine).

## 5.2 Chemical composition and biochemical activity of buckwheat and oat grains

### 5.2.1 Buckwheat

Buckwheat grain contains a balanced complex of macro- and microelements, as well as a wide range of biologically active phytochemicals. Epidemiological and clinical studies show that regular consumption of this grain is associated with significant preventive effects against a number of chronic non-communicable diseases. In particular, there is a reduced risk of developing cancer, metabolic syndrome (including obesity and type 2 diabetes), and cardiovascular disease [9].

Among all the buckwheat species, only two are grown for food grain production: common buckwheat (*Fagopyrum esculentum* Moench) and Tatar buckwheat (*F. tataricum*(L.)Gaertn). Common buckwheat is widespread in Asia, Europe, America and Austria, while the cultivation area of tartaric buckwheat is limited to the Asian region [10].

There are two groups of buckwheat seed dishes: flour and cereals. Other buckwheat products include buckwheat honey, green buckwheat tea, buckwheat sprouts and fresh green parts of the plant used as salad.

Buckwheat grain is a valuable source of protein, starch, fat, dietary fiber, minerals, vitamins and phytochemicals [11]. **Table 5.2** shows the content of the main components in different parts of buckwheat grain [11].

**Table 5.2** Main chemical composition of whole buckwheat seeds, dehulled seeds and husks

| Sample        | Protein<br>(g·100g <sup>-1</sup> ) | Fat<br>(g·100g <sup>-1</sup> ) | Total carbohydrates<br>(g·100g <sup>-1</sup> ) | Starch<br>(g·100g <sup>-1</sup> ) |
|---------------|------------------------------------|--------------------------------|--|-----------------------------------|
| Dehulled seed | 15.29–19.96                        | 2.19–2.48                      | 78.18–79.68                                    | 45.24–55.11                       |
| Whole seed    | 12.28–15.61                        | 1.72–2.24                      | 77.36–81.38                                    | 38.41–43.11                       |
| Hull          | 5.13–5.68                          | 0.50–0.81                      | 91.72–92.19                                    | 0.31–2.26                         |

Source: [11]

Buckwheat is an important source of protein, as the average protein content in its grain can reach 8.5–18.8% [12]. Buckwheat proteins have one of the highest levels of amino acids among vegetable proteins. Buckwheat proteins are well balanced and contain albumin, globulins, prolamins and glutelins and provide the human body with such important amino acids as leucine, phenylalanine, lysine, threonine, isoleucine, asparagine and cysteine [13]. The peculiarity of buckwheat's protein composition is the absence of gluten, which allows expanding the food base for people with gluten

intolerance and celiac disease [14]. Acting similarly to dietary fiber, buckwheat proteins prevent obesity. They have special biological activity in reducing cholesterol and blood pressure.

Work [15] notes that the presence of tannins in buckwheat can lead to a decrease in protein absorption in humans and animals due to their ability to form stable complexes with plant proteins. Tannins form numerous bonds with protein molecules, which disrupts their metabolic activity and nutrient availability. However, the presence of the amino acid lysine in buckwheat increases the digestibility of proteins compared to other cereals.

The total carbohydrate content of buckwheat grain is about 80%. The main carbohydrate in this raw material is starch, with an average content of 54.5% [16]. Buckwheat grain contains 18 different fatty acids with a total content of 1.5–3.7%. The most common higher carboxylic acids are palmitic, oleic and linoleic, which account for about 88% of the total content of these substances [15].

The nutritional potential of buckwheat is significantly increased by the presence of biologically active substances of polyphenolic compounds (bioactive peptides, flavonoids and phenolic acids) [12]. The content of the main biologically active substances is presented in **Table 5.3** [11]. Buckwheat contains a significant amount of flavonoids such as rutin, isoorientin, quercetin, isovitexin, vitexin and orientin. Buckwheat grain is the richest source of rutin and quercetin among pseudo-cereals (maximum 5.186 mg/100 g and 857.625 mg/100 g, respectively) [12, 17], which is 10–100 times higher than in other plants. Buckwheat flavonoids are contained in the grain hull [11]. Bioactive substances have a positive effect on human health, in particular, they exhibit antioxidant and anti-inflammatory properties and are able to prevent cancer [18].

**Table 5.3 Bioactive compounds of whole buckwheat seeds, dehulled seeds and husks**

| Sample        | Dietary fiber (g·100g <sup>-1</sup> ) | Resistant starch (g·100g <sup>-1</sup> ) | Total polyphenols (mg·100g <sup>-1</sup> ) | Antioxidant activity (mmol Trolox·g <sup>-1</sup> ) |
|---------------|---------------------------------------|--|--|---|
| Dehulled seed | 1.16–6.65                             | 6.13–11.35                               | 280.00–328.03                              | 63.20–66.50   |
| Whole seed    | 20.32–25.45                           | 3.29–5.64                                | 311.98–357.14                              | 31.28–34.93   |
| Hull          | 76.52–80.73                           | not found                                | 434.06–525.45                              | 42.93–49.05   |

Source: [11]

Buckwheat grain contains a variety of minerals and vitamins. The concentration of the main macronutrients phosphorus (P), potassium (K), magnesium (Mg) and calcium (Ca) is over 100 mg per kilogram of dry weight. The content of micronutrients

is significantly lower than that of macronutrients, but the concentrations of iron (Fe), manganese (Mn) and zinc (Zn) are higher than other micronutrients [15]. Vitamins A, C, E and B vitamins are found in buckwheat. The average vitamin C content is 5 mg/100 g in grain, and its content in buckwheat sprouts is 5 times higher (25 mg/100 g).

### 5.2.2 Oats

Coated oats (*Avena sativa L.*) and naked oats (*Avena nuda*) are among the most valuable cereal crops in the world due to the optimal organoleptic properties of the grain and its ability to stimulate metabolic processes in the body [18]. Oat grain is an important source of carbohydrates, dietary soluble fiber, balanced protein, lipids, various phenolic compounds, vitamins and minerals. The basic chemical composition of different types of oat grains is shown in **Table 5.4** [19].

Oat grain stands out among other cereal crops due to its high protein content (mainly globulin fraction) of 7.4 to 14.9% of dry weight [19]. Proteins extracted from oatmeal are characterized by a high degree of digestibility (90.3–94.2% of dry weight) and significant biological value (74.5–79.6% of dry weight), which indicates their significant nutritional value.

**Table 5.4** Main chemical composition of whole oats seeds, dehulled oats seeds, naked oat and husks

| Sample        | Protein<br>(g·100g <sup>-1</sup> ) | Fat<br>(g·100g <sup>-1</sup> ) | Total carbohydrates<br>(g·100g <sup>-1</sup> ) | Starch<br>(g·100g <sup>-1</sup> ) |
|---------------|------------------------------------|--------------------------------|--|-----------------------------------|
| Dehulled seed | 12.93–14.86                        | 4.33–7.64                      | 62.03–69.80                                    | 48.08–49.17                       |
| Whole seed    | 9.91–10.95                         | 1.72–2.24                      | 53.02–65.81                                    | 57.92–64.21                       |
| Naked oat     | 11.91–13.62                        | 7.53–9.51                      | 70.11–72.14                                    | 31.55–35.27                       |
| Hull          | 1.42–7.40                          | 0.50–1.51                      | 63.32–82.74                                    | 2.52–16.33                        |

Source: [19]

The amino acid composition of oat grain is quite diverse compared to other cereals, and the concentration of essential amino acids (lysine, methionine, threonine, tyrosine, leucine, valine, and phenylalanine) is higher [19]. Oats do not contain gluten. Studies show that people with celiac disease can consume foods containing oat protein. While most celiac patients tolerate oats, a small proportion may be sensitive because they react to avenin, an oat protein that is structurally similar to gluten.

The starch content of oat grain is lower than that of other cereals (30–60%) [19, 20]. In addition, oat starch has a small granule size, higher amylose content, high viscosity and high water retention capacity. Due to these characteristics, oats are widely used in the food industry as a thickener and gelling agent.

The content of the main bioactive substances is presented in **Table 5.5** according to [21]. The content of higher carboxylic acids in oat grain is 2.2–11%. Unsaturated higher carboxylic acids make up 80% of all fatty acids present in oat grain. The most common are linoleic oleic, docosahexaenoic, eicosapentaenoic and arachidonic. Among the saturated higher carboxylic acids, palmitic acid prevails with a content of 21.4–22.7% of the total amount of higher fatty acids in oat grain.

**Table 5.5** Bioactive compounds of whole oats seeds, dehulled oats seeds, naked oat and husks

| Sample        | Dietary fiber (g·100g <sup>-1</sup> ) | $\beta$ -glucan (g·100g <sup>-1</sup> ) | Total polyphenols (mg·100g <sup>-1</sup> ) |
|---------------|---------------------------------------|---|--|
| Dehulled seed | 1.16–6.65                             | 4.31–5.1                                | 20.9–29.7                                  |
| Whole seed    | 20.12–38.20                           | 2.70–3.54                               | 23.8–29.8                                  |
| Naked oat     | 8.6–12.11                             | 3.92–4.64                               | 10.2–18.2                                  |
| Hull          | 70.16–71.33                           | 0.003–0.006                             | 19.3–30.6                                  |

Source: [21]

Oats have a high content of soluble dietary fiber, in particular  $\beta$ -glucans, which make up 3% to 5% of the dry weight of the grain. Numerous scientific studies have shown that  $\beta$ -glucans have a pronounced hypolipidemic activity, helping to reduce the level of total cholesterol and low-density lipoprotein in the blood. In addition, due to their ability to slow down the breakdown and absorption of carbohydrates,  $\beta$ -glucans effectively stabilize blood glucose levels, making them useful for the prevention and treatment of diabetes. Recent scientific studies have also pointed to the anti-cancer and anti-inflammatory properties of  $\beta$ -glucans, which may be related to their immunomodulatory activity [22].

Oat grain is an important source of many minerals essential for human health. All the main macro- and microelements are present in the grain of this crop, including Ca, Mg, Fe, Mn, Cu, Zn, P and K. The high content of phosphorus and potassium, more than 300 mg/100 g, makes oat products a valuable source of minerals in the diet [23]. Oatmeal is rich in B vitamins (B1, B2, B3 and B5) [24]. In addition, oat products also contain vitamin E, which has high antioxidant properties. The spectrum of biologically active polyphenolic compounds in oats is similar to buckwheat, but the content of these compounds, in particular rutin and quercetin, is significantly lower (maximum 0.48 mg/100 g and 8.9 mg/100 g, respectively) than in oats [12].

### 5.3 Materials and methods

For the study, samples of buckwheat and oat groats produced by Zemledar-Info LLC were selected. To obtain buckwheat and oat powders, the respective cereals were ground using a BOSCH TSM6A013B coffee grinder. The bulk density of the crushed oat and buckwheat raw materials was determined as the ratio of the weight of the raw material to its volume.

The fractional content of the studied powders by size was determined by sieve analysis. The essence of the analysis is the mechanical distribution of particles by size [25]. The test material (50 g) was sieved through a set of sieves of different mesh diameters. The percentage of each fraction ( $A$ ) was calculated by the formula

$$A = \frac{m_i}{m} \times 100,$$

where  $m_i$  – the mass of the  $i$ -th fraction,  $m$  – the total mass of the mixture.

The average particle size  $\bar{d}_i$  of the  $i$ -th fraction was calculated as the arithmetic mean between the hole sizes  $d_j$  of the sieve on which the fraction was retained and the hole sizes  $d_{j-1}$  of the previous sieve

$$\bar{d}_i = 0.5(d_j + d_{j-1}),$$

where  $\bar{d}_i$  – the average particle size of the  $i$ -th fraction, mm;  $d_j$  – the diameter of the holes of the lower sieve, mm;  $d_{j-1}$  – the diameter of the holes of the upper sieve, mm. At least 3 sievings of samples of the same weight were carried out, and the results of the fraction with a relative deviation from the mean value of no more than 5% were taken into account.

The infrared (IR) spectra were recorded using an IRAffinity-1S spectrophotometer (Japan) in the frequency range of 4000–400  $\text{cm}^{-1}$  using the single-beam method in reflected light. The material under study was mixed in an agate mortar with KBr powder. Then, samples were formed on a hydraulic press with a force of 20 MPa in the ratio: test material – 1 mg, KBr – 300 mg. A Nicolet iS10 FT-IR spectrometer was used to determine the functional composition of the samples.

The relative content of chemical elements in the raw material samples was determined using confocal micro-X-ray fluorescence spectroscopy (high-performance micro-X-ray fluorescence ( $\mu$ -XRF) spectrometer M4 TORNADO). The conditions of the study are shown in **Table 5.6**.

**Table 5.6 Conditions for XRD analysis**

| Parameter              | Value       | Unit          |
|------------------------|-------------|---------------|
| Real-time              | 42,908      | ms            |
| Live-time              | 30,000      | ms            |
| Detector type          | XFlash 430  | -             |
| Si sead layer          | 0.029       | $\mu\text{m}$ |
| Detector thickness     | 0.45        | mm            |
| Window type            | Custom type | -             |
| Fano factor            | 0.114       | -             |
| Mn FWHM                | 142.43      | eV            |
| Calibration (linear)   | 10          | eV            |
| Calibration (absolute) | -955.9      | eV            |
| Channels               | 4095        | -             |

In order to confirm the qualitative composition of buckwheat and oat powders, a study was conducted by gas chromatography with mass spectrometry (GC/MS) [26]. For the analysis, 0.6 g of the respective powders were placed in tubes with 5 ml of  $\text{CH}_3\text{OH}$ , extracted in an ultrasonic washer for 30 min (ultrasonic washer "WUC-A02H"), then centrifuged for 5 min (centrifuge laboratory "80-1"), and the extract was taken and analyzed under the conditions given in **Table 5.7**. Identical measurement results were obtained for three samples of each material, and the accuracy of the measurements corresponds to the technical characteristics of the equipment used.

**Table 5.7 Conditions of the study by chromatography-mass spectrometry**

| Parameter                | Value   | Unit                   |
|--------------------------|---|------------------------|
| 1                        | 2   | 3                      |
| Column type              | Rxi@-5ms  | -                      |
| Column dimensions        | 30 m $\times$ 0.25 mm $\times$ 0.25 $\mu\text{m}$ | -                      |
| Carrier gas              | Helium  | -                      |
| Carrier gas flow rate    | 1.18  | ml/min (constant flow) |
| Oven temperature program | <b>Start:</b> 80°C (hold 1 min)                   | °C                     |
|                          | <b>Ramp:</b> 15°C/min to 250°C (hold 8 min)       | °C/min                 |
|                          | <b>Ramp:</b> 20°C/min to 310°C (hold 10 min)      | °C/min                 |
| Injection mode           | Autosampler AOC-20i+s                             | -                      |

Continuation of Table 5.7

| 1                      | 2                        | 3                  |
|------------------------|--------------------------|--------------------|
| Split ratio            | 20:1                     | -                  |
| Injection volume       | 1                        | $\mu\text{l}$      |
| Detector type          | MSD QP2020NX EI          | -                  |
| Operation mode         | Scan, range 40–900 amu   | -                  |
| Solvent delay          | 2.5                      | min                |
| Multiplier voltage     | According to tuning file | -                  |
| Ion source temperature | 250                      | $^{\circ}\text{C}$ |
| Injector temperature   | 250                      | $^{\circ}\text{C}$ |
| Interface temperature  | 300                      | $^{\circ}\text{C}$ |
| Control substance      | Methanol                 | -                  |

The study was conducted in the laboratory of the Lutsk National Technical University (Ukraine). The micro-X-ray fluorescence spectroscopy study was conducted in the laboratory of the Institute of Analytical Chemistry at TU Bergakademie Freiberg as part of the international educational project "SUUUpoRT – Structural support of Ukrainian Universities in Upkeep and Rebuilding of Higher Education".

#### 5.4 Results of experimental studies

The results of the sieve analysis of buckwheat and oat powders are shown in **Table 5.8**. The differential curves of the particle size distribution of the powders are shown in **Fig. 5.2**. According to the results of sieve analysis, the highest content of fractions with a particle diameter of 1.1 to 0.5 mm was found: for buckwheat powder – 41.76%, for oatmeal – 52.56%.

Table 5.8 Sieve analysis results

| Sieve size | $\bar{d}, \text{mm}$ | Buckwheat powder, A (%) | Oat powder, A (%) |
|------------|----------------------|-------------------------|-------------------|
| < 2.0      | 2.5                  | 0.96                    | 3.34              |
| 2.0–1.1    | 1.55                 | 5.52                    | 20.36             |
| 1.1–0.5    | 0.8                  | 41.76                   | 52.56             |
| 0.5–0.25   | 0.375                | 35.84                   | 16.90             |
| > 0.25     | 0.2                  | 15.92                   | 6.84              |

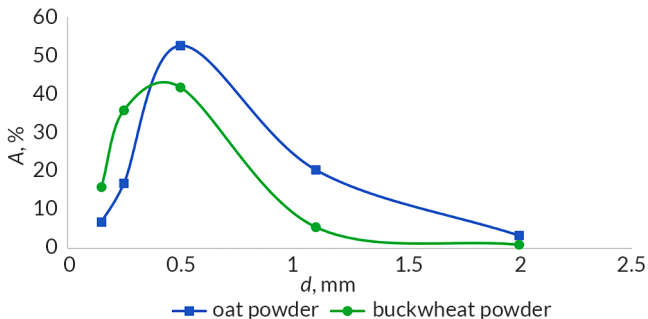


Fig. 5.2 Differential curves of buckwheat and oat powders particle size distribution

The analysis of the infrared spectra of oat and buckwheat powders (Fig. 5.3) shows that both samples have a similar chemical composition, typical of plant-based products. The main components are carbohydrates, proteins, fats, water and mineral compounds. However, there are significant differences in the intensity and location of individual bands, which allows to identify the specific characteristics of each sample.

Characteristic C-O valence bands in the range of  $1000\text{--}1300\text{ cm}^{-1}$  ( $1238\text{--}1076\text{ cm}^{-1}$  in oatmeal and  $1237\text{--}1077\text{ cm}^{-1}$  in buckwheat powder) are observed in both powders. This indicates the presence of polysaccharides (starch, fiber) as the main components. Low-frequency bands ( $500\text{--}800\text{ cm}^{-1}$ ) indicate the structural features of these carbohydrates.

Amide bands in the range of  $1500\text{--}1600\text{ cm}^{-1}$  (amide I and amide II) confirm the presence of proteins. In both samples, these bands are clearly defined, although in buckwheat powder they have a higher intensity, which may indicate a higher content of protein compounds. The C-H valence vibrations in the range of  $2800\text{--}3000\text{ cm}^{-1}$  ( $2920\text{--}2852\text{ cm}^{-1}$  in oatmeal powder and  $2929\text{--}2852\text{ cm}^{-1}$  in buckwheat powder) demonstrate the presence of methyl and methylene groups characteristic of fatty acids.

The broad O-H vibrational bands in the range of  $3200\text{--}3600\text{ cm}^{-1}$  ( $3276\text{ cm}^{-1}$  in both powders) indicate residual moisture as well as alcohols that are part of carbohydrates. In buckwheat powder, there is a band of  $1743.00\text{ cm}^{-1}$ , which indicates a significant presence of carbonyl compounds. These can be fatty acid esters, aldehydes or ketones, which are metabolic products. In oat powder, this area is less pronounced.

More intense amide bands ( $1587.85$ ,  $1562.26$ ,  $1530.76\text{ cm}^{-1}$ ) were observed in buckwheat powder, indicating a higher protein content. This is consistent with the general composition of buckwheat, which is known for its high content of amino acids and proteins.

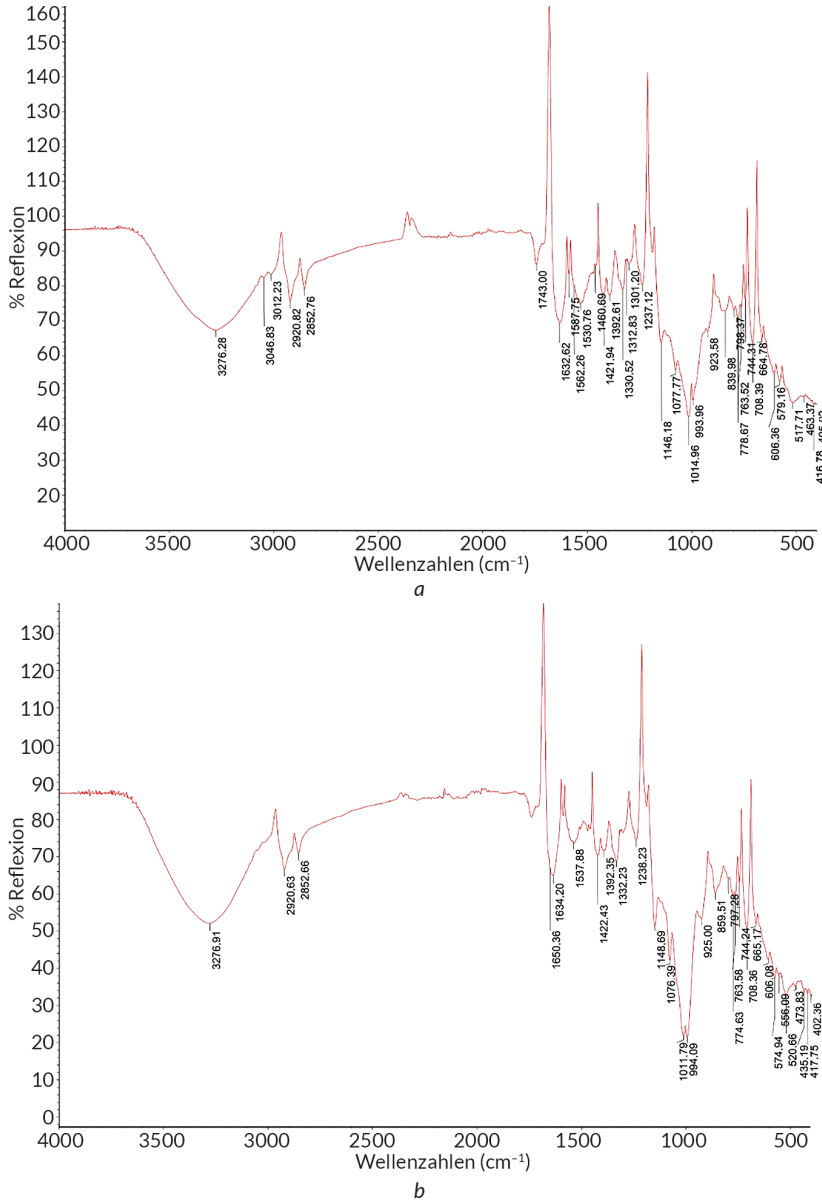


Fig. 5.3 Infrared absorption spectra of buckwheat (a) and oat (b) powders

A unique band of  $839.98\text{ cm}^{-1}$  is present in buckwheat powder, which is not found in oat powder. This may be due to the peculiarities of the starch structure or aromatic compounds inherent in buckwheat. Additional bands in the region of  $3000\text{--}3100\text{ cm}^{-1}$  ( $3046.83, 3012.23\text{ cm}^{-1}$ ) were observed in buckwheat powder, which may indicate the presence of unsaturated fatty acids, while they are absent in oat powder.

Thus, oat powder is characterized by a high content of polysaccharides, as evidenced by strong C-O vibrations, and less pronounced carbonyl groups, indicating a low content of fats and simple sugars. This makes it a more neutral product with a high carbohydrate content. Buckwheat powder has a more pronounced protein profile (powerful amide bands), a significant content of fats and carbonyl compounds, which confirms its richer chemical composition.

The X-ray spectral analysis of the buckwheat and oat powders under study was carried out. **Table 5.9** shows the results of the quantitative determination of the relative content of elements in the studied samples: sample 1 – the average relative content of elements in buckwheat powder, sample 2 – the average relative content of elements in oat powder. The study was carried out in triplicate. The X-ray fluorescence analysis showed that both samples contain mainly C, H, P, S, K, Ca, Mn, Fe, Cu, Zn, but in different proportions. Buckwheat powder is characterized by a higher content of potassium and phosphorus, while oat powder has an increased level of calcium and manganese. The X-ray fluorescence spectra for the samples under study are shown in **Fig. 5.4**. The maximum peak in the spectra corresponds to an intensity of 35000.

**Table 5.9 Results of quantification of the relative content of elements**

| Buckwheat powder, wt. % |                      |                      |                        |                      |
|-------------------------|----------------------|----------------------|------------------------|----------------------|
| H                       | C                    | P                    | S                      | K                    |
| $14.24037 \pm 0.06$     | $84.84687 \pm 0.4$   | $0.46452 \pm 0.2$    | $0.13848 \pm 0.08$     | $0.29713 \pm 0.1$    |
| Ca                      | Mn                   | Fe                   | Cu                     | Zn                   |
| $0.00863 \pm 0.003$     | $0.00086 \pm 0.0003$ | $0.00130 \pm 0.0004$ | $0.00031 \pm 0.00009$  | $0.00130 \pm 0.001$  |
| Oat powder, wt. %       |                      |                      |                        |                      |
| H                       | C                    | P                    | S                      | K                    |
| $14.31301 \pm 0.03$     | $85.27965 \pm 0.2$   | $0.10123 \pm 0.05$   | $0.05630 \pm 0.01$     | $0.22803 \pm 0.2$    |
| Ca                      | Mn                   | Fe                   | Cu                     | Zn                   |
| $0.04575 \pm 0.02$      | $0.00324 \pm 0.002$  | $0.00162 \pm 0.0006$ | $0.00015 \pm 0.000004$ | $0.00149 \pm 0.0004$ |

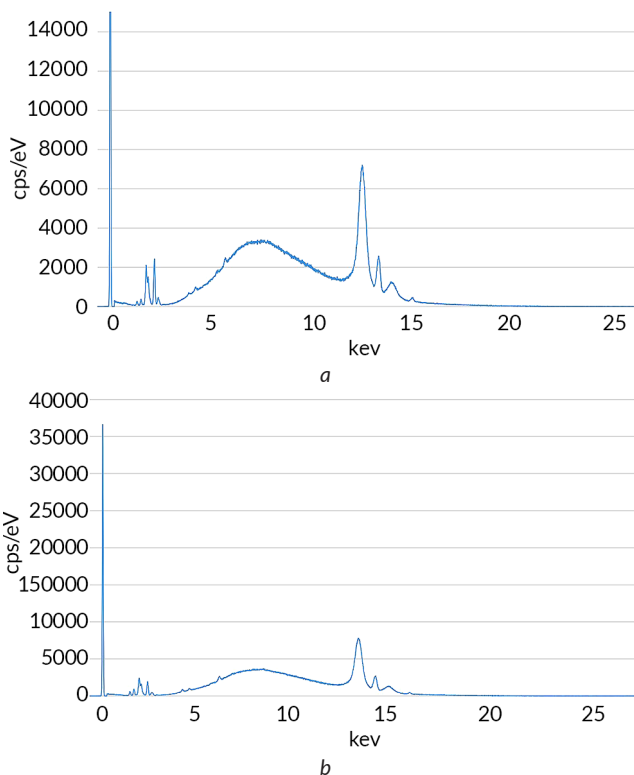


Fig. 5.4 X-ray fluorescence spectra of buckwheat (a) and oat (b) powders

In order to clarify the qualitative composition of buckwheat and oat powders, a study was carried out by gas chromatography with mass spectrometry (GC/MS). The obtained chromatograms are shown in **Fig. 5.5**. The peaks were processed and identified based on the comparison of chromatographic and mass spectral data with open source library data (NIST 2017 and Wiley 5th Edition).

In the studied samples of buckwheat and oat powders, 15 and 18 characteristic components were found, respectively, as shown in **Table 5.10**.

Buckwheat and oat powders contain similar groups of compounds, including Sucrose, Palmitic acid, 9,12-octadecadienoic acid (and its derivatives), Campesterol and Gamma-sitosterol. However, buckwheat powder is noted for its high content of antioxidants, such as Gamma-tocopherol (vitamin E), and macrocyclic lipids, which may indicate its strong antioxidant and bioactive properties. In contrast, oat powder

contains a wider range of sterols (Stigmasterol, Fucosterol), oxazole derivatives and steroidal compounds, including 11( $\alpha$ ),17( $\alpha$ )-dihydroxyprogesterone, which may contribute to its metabolic and hormonal benefits. In addition, Linoleyl palmitate was found in oat powder, which indicates a higher content of complex lipids that may increase its nutritional value.

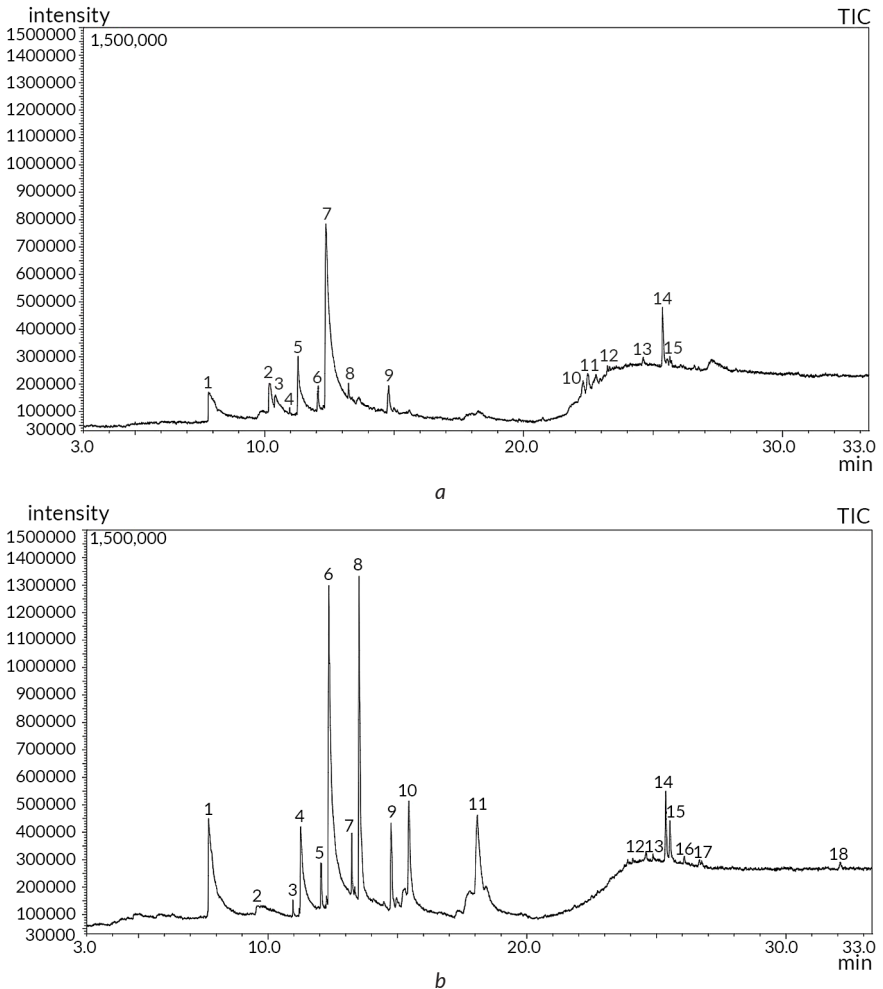


Fig. 5.5 Chromatograms of buckwheat (a) and oat (b) powder extracts

Table 5.10 Results of the chromatography-mass spectrometry study

| Peak                    | R. Time | I. Time | F. Time | Area     | Height  | Name  |
|-------------------------|---------|---------|---------|----------|---------|---|
| 1                       | 2       | 3       | 4       | 5        | 6       | 7   |
| <b>Buckwheat powder</b> |         |         |         |          |         |   |
| 1                       | 7.841   | 7.810   | 7.913   | 292347   | 77324   | Sucrose   |
| 2                       | 10.193  | 10.130  | 10.280  | 628117   | 100663  | Hexanamide  |
| 3                       | 10.423  | 10.377  | 10.440  | 117553   | 37192   | 13-Docosenamide, (Z)-                                     |
| 4                       | 10.965  | 10.937  | 11.000  | 32388    | 22951   | Methyl Palmitate  |
| 5                       | 11.288  | 11.253  | 11.473  | 1138304  | 206451  | Palmitic Acid   |
| 6                       | 12.040  | 12.010  | 12.050  | 77571    | 65284   | 9,12-Octadecadienoic acid (Z, Z)-, methyl ester           |
| 7                       | 12.363  | 12.317  | 12.753  | 7339446  | 664846  | 9,12-Octadecadienoic acid (Z, Z)-                         |
| 8                       | 13.240  | 13.207  | 13.297  | 110185   | 56059   | Octadecanoic acid, 2-(dimethylamino)ethyl ester           |
| 9                       | 14.783  | 14.710  | 14.883  | 456477   | 96959   | 2-(Dimethylamino)ethyl vaccenoate                         |
| 10                      | 22.292  | 22.203  | 22.340  | 248211   | 52280   | Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy- |
| 11                      | 22.475  | 22.390  | 22.547  | 333855   | 62795   | Trilinolein   |
| 12                      | 23.238  | 23.200  | 23.267  | 49458    | 26526   | Gamma-Tocopherol  |
| 13                      | 24.618  | 24.563  | 24.653  | 70201    | 23900   | Campesterol   |
| 14                      | 25.367  | 25.313  | 25.487  | 769366   | 215153  | Gamma-Sitosterol  |
| 15                      | 25.648  | 25.603  | 25.680  | 101920   | 38063   | Germanicol  |
| <b>Oat powder</b>       |         |         |         |          |         |   |
| 1                       | 7.710   | 7.630   | 8.123   | 3648291  | 347997  | Sucrose   |
| 2                       | 9.577   | 9.503   | 9.690   | 236986   | 28314   | 3-Deoxy-d-mannonic lactone                                |
| 3                       | 10.965  | 10.903  | 11.030  | 110556   | 59107   | Methyl Palmitate  |
| 4                       | 11.264  | 11.183  | 11.737  | 3234057  | 322832  | Palmitic Acid   |
| 5                       | 12.040  | 12.010  | 12.190  | 542558   | 160288  | 9,12-Octadecadienoic acid, methyl ester                   |
| 6                       | 12.350  | 12.310  | 12.937  | 10269548 | 1161975 | 9,12-Octadecadienoic acid (Z, Z)-                         |
| 7                       | 13.240  | 13.183  | 13.330  | 425544   | 212373  | Octadecanoic acid, 2-(dimethylamino)ethyl ester           |
| 8                       | 13.518  | 13.457  | 13.910  | 4921115  | 1174524 | 2-((8Z,11Z)-Heptadeca-8,11-dien-1-yl)-4,5-dihydrooxazole  |

Continuation of Table 5.10

| 1  | 2      | 3      | 4      | 5       | 6      | 7   |
|----|--------|--------|--------|---------|--------|---|
| 9  | 14.753 | 14.683 | 14.903 | 1299566 | 312563 | 2-(Dimethylamino)ethyl vaccenoate   |
| 10 | 15.441 | 15.343 | 15.777 | 2494207 | 378531 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester                 |
| 11 | 18.087 | 17.943 | 18.330 | 3082328 | 291700 | 9,12-Octadecadienoic acid (Z, Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester |
| 12 | 24.598 | 24.523 | 24.670 | 108019  | 31778  | Campesterol   |
| 13 | 24.868 | 24.830 | 24.897 | 35842   | 19445  | Stigmasterol  |
| 14 | 25.362 | 25.283 | 25.477 | 853751  | 256939 | Gamma-Sitosterol  |
| 15 | 25.525 | 25.477 | 25.683 | 560112  | 148904 | Fucosterol  |
| 16 | 26.080 | 26.037 | 26.150 | 93279   | 27221  | Stigmasta-7,24(28)-dien-3-ol, (3.beta, 5.alpha)-                          |
| 17 | 26.745 | 26.697 | 26.783 | 72169   | 20750  | 11(alpha),17(alpha)-Dihydroxy-progesterone                                |
| 18 | 32.108 | 32.030 | 32.203 | 99768   | 22052  | Linoleyl palmitate  |

Analysis of the chemical composition of buckwheat and oatmeal powders by chromatography-mass spectrometry revealed the presence of common and unique bioactive compounds. Buckwheat powder is a promising source of antioxidants, while oat powder contains a significant amount of bioactive lipids and sterols that may have a regulatory effect on lipid metabolism. The results obtained can be used for further research on the use of these products in functional food and pharmacology.

## 5.5 Conclusions

Buckwheat and oats are important components of functional foods due to their unique chemical composition and beneficial properties. This conclusion was confirmed by a comprehensive analysis of buckwheat and oat powders, including sieve analysis, infrared spectroscopy (IR spectroscopy), X-ray fluorescence analysis (XRF) and gas chromatography with mass spectrometry (GC/MS). Buckwheat contains high quality vegetable protein (compared to oatmeal powder, more intense amide bands of IR spectra at 1587.85, 1562.26, 1530.76  $\text{cm}^{-1}$ ) with an optimal amino acid

balance, which promotes tissue growth and repair. It is rich in flavonoids, which strengthen blood vessels and reduce the risk of cardiovascular disease. Buckwheat also contains iron (0.00130%), calcium (0.00863%) and zinc (0.00130%), which improve blood formation and support the nervous system. Buckwheat's dietary fiber helps to normalize digestion and reduce cholesterol levels.

Oats are a source of beta-glucans, a soluble dietary fiber that reduces blood glucose and cholesterol levels. Oat groats contain a significant amount of avenantramides, polyphenols (stigmasterol, fucosterol, 11( $\alpha$ ),17( $\alpha$ )-dihydroxyprogesterone) with antioxidant and anti-inflammatory activity. Thanks to its low glycaemic index, oats help stabilize blood sugar levels, making them beneficial for people with diabetes. Magnesium and B vitamins in oats have a positive effect on the functioning of the nervous system and energy metabolism. Oats are also a source of potassium (0.22803%), calcium (0.04575%) and iron (0.00162%), and are high in manganese (0.00324%), which is important for bone health. Regular consumption of buckwheat and oats as part of a functional diet helps to promote health, improve metabolism and prevent chronic diseases.

Oatmeal powder may be preferred for the manufacture of dietary products rich in fiber and carbohydrates, but with a reduced fat content. Buckwheat powder is suitable for products with a high nutritional value, focused on enhanced protein and fatty acid composition. Grinding buckwheat and oat groats improves their digestibility and reduces cooking time. This also allows them to be used in the production of flour, instant cereals and baby food. In addition, crushed cereals give dishes a softer texture and better uniformity. The synergy of buckwheat/oat mixtures and the impact of cereal processing will be the subject of further experimental research.

The comparative analysis of the biochemical characteristics of buckwheat and oat cereals in this article aims to expand the scientific understanding of their potential as functional foods, to assess their potential impact on human health and to determine the possibilities of their integration into a balanced diet. In addition, such an analysis contributes to the diversification of agricultural production by offering an alternative to monoculture farming. The authors hope that the analysis presented in this article will be useful for food producers, nutritionists and consumers, highlighting the benefits of including these crops in the daily diet.

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