Use of energy dispersive X-ray spectral analysis in a scanning electron microscope system to evaluate the mineral composition of grain bread

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**Abstract.** The concentration of 18 basic elements (in\% by weight) contained in the morphological parts of wheat, rye and triticale grains was studied. It is established that the nature of the distribution of micronutrients is determined by their biological role. The elements are part of enzymes: manganese, iron and zinc prevail in the nucleus. Phosphorus, potassium, magnesium are found in greater quantity in the vital layer of aleurone. Cobalt, nickel, aluminum, calcium, chromium, copper, selenium and cadmium dominate the grain surface. The largest amount of mineral elements in the grain is concentrated in the seed. The distribution of metals in triticale grains is characterized by characteristic patterns of wheat and rye. In the distribution of mineral elements in wheat, rye and triticale grains, differences are observed, which are explained by the specific characteristics of these plants. From the grain studied, cereal bread was prepared unmatched on a thick grain leaven. The analysis of the mineral content of the grain bread showed that it was enriched with all major biogenic mineral elements and contained toxic metals (lead and cadmium) in a quantity not exceeding the CMP. A strong negative correlation has been established between levels of certain biological and toxic elements in grain and in pain. The revealed relationship indicates the possibility of switching from dispersive X-ray spectroscopy in a scanning electron microscope system to predict the quality and safety of grain pain, particularly for predicting of the content heavy metals in finished bakery products.

1. Introduction
Most consumers prefer white bread made from refined flour, while many biologically active compounds found in kernels are concentrated in shells and in the aleurone layer [1]. Therefore, nutritionists recommend the daily inclusion of whole grain bread in the diet, which is a good source of dietary fiber, oligosaccharides, amino acids, minerals, B vitamins, phytosterols and antioxidants, mainly found in cereal husks [2]. Studies show that the use of whole grain cereals in the diet helps reduce the risk of obesity, diabetes, cardiovascular disease and oncology [1].

High antioxidant bread is of great interest because of its role in maintaining and promoting health and protecting against many diseases [3]. To increase antioxidant activity, bread is enriched with natural ingredients with antioxidant properties [4 – 8]. However, whole grain bread is naturally enriched with antioxidants. In general, the antioxidant activity of bread is mainly determined by the...
concentration of phenols [9]. The presence of antioxidant properties in phytic acid has also been established. The researchers suggest that phytate can replace preservatives, many of which pose a potential risk to human health [10]. Phytic acid is found in grains and seeds of many plants, including cereals [11]. Most of the grain-form antioxidants are ester-linked with cell wall components with arabinoxylans [12].

It is known that phytates and phenolic compounds form complexes with mineral elements in plant seeds, thus rendering them inaccessible [13]. Phenolic compounds, phytates and some trace elements in cereals are responsible for overall antioxidant activity [14].

Data on the distribution of mineral elements by the anatomical parts of the grain are contradictory in the literature. The nature of the distribution of heavy metals in organs and tissues is determined by the properties of metals and plant species. Data from many authors indicate significant accumulation of metals in the cell wall [15, 16, 17]. The difficulty of penetration is due to the large amount of ions, hydration and charge [18]. Some authors [19] find the greatest number of toxic elements in the nucleus and the aleurone layer, others [15] - in the shells and the nucleus. The largest quantities of copper, manganese, zinc, lead, cadmium and iron contained in a wheat grain are concentrated in the embryo. The copper content of the endosperm is higher than that of the shells, while manganese, zinc, lead and iron are reversed. The amount of cadmium in membranes and endosperm is approximately the same [16]. According to [20], copper are highly present in cereal grains of embryos (2-18 mg / kg) and in the seed coat (8-23 mg / kg). Other researchers believe that the distribution of copper in the grain is uniform [21].

According to some scientists, zinc is associated with low molecular weight compounds and is highly mobile in plants. In insoluble complexes, zinc is bound to phytin or linked to the cross-links of long-chain components of cell walls [22]. The maximum amount of lead and cadmium accumulates in the peripheral parts of the grain [23]. Nickel is freely absorbed by the outer layers [24]. Cadmium is concentrated in the protein fraction of plants because it has a strong affinity for sulphydryl groups, as well as for the side chains of proteins and phosphate groups [17]. At the same time, it is known that cadmium is bound by sulphydryl groups only if its excess intake is sufficient [21]. There is evidence of the binding of cadmium, zinc and lead by the plant pectin fraction [17, 25]. Seregin [15] estimates that cadmium and lead are located in the cell walls of the seed coat of the cereal seed, strontium and nickel in the cells of the embryo, as well as strontium in the cells of the endosperm, nickel in the shield.

The study of the distribution of mineral elements in the constituent parts of the grain requires the use of high precision methods with digital data processing.

The aim of the study was to study the possibility of using energy dispersive X-ray spectral analysis in an electronic scanning microscope system to predict the quality and safety of grain bread by the mineral composition of individual morphological parts of grain.

2. Methods
We analyzed 6 types of wheat grains (Moskovskaya 39, Mironovskaya Inna 808, Arbatka, Belgorodskaya 12, Mirich) 2 varieties of rye (Orlovskaya 9 and Talovskaya 33) and triticale Talva 100. The studied varieties of cereals were grown under the conditions of one agricultural enterprise in the Oryol region. Agricultural land is located on the same type of soil and had similar agrochemical characteristics. Therefore, the mineral composition of the grain differed slightl. This allowed us to study the average grain sample, composed of several varieties of the same species.

The studies were carried out using a JEOL JSM 6390 scanning electron microscope. Separate grains were selected in a medium sample of wheat, rye and triticale grains weighing 10 g and their cross sections were prepared. The sections were plated with platinum in a vacuum table vacuum unit JEC-3000FC and placed on a carbon dioxide coated tape. An EMF analysis of the chemical composition of the ash components (Na, P, S, K, Mn, Fe, Mg, Ca, Al, Si, Cl, Zn, Se, Mo) was determined by energy dispersion spectrometry. (ESD) on a JEOL JSM scanning electron microscope. 6390. The resolution of the microscope is 4 Nm at an acceleration voltage of 20 kV (secondary
electron image). During the elementary analysis, the working distance (WD) is 10 mm. An energy dispersion spectrometer makes it possible to carry out a quantitative X-ray microanalysis in a given search domain, for example at a specific point, and to obtain microcards of the distribution of the elements. X-ray microanalysis data are presented as standard protocols containing the microstructural image of the sample under study in the form of tables, spectra and atomic correlation. Given the intensity of the spectral lines, it is possible to determine the concentration of the desired element. The fractional precision of the chemical analysis is distributed as follows: when the concentration of elements is between 1 and 5%, the accuracy is less than 10%; from 5 to 10%, the accuracy is less than 5%; with an element concentration greater than 10%, the accuracy is less than 2%. 20 points from each sample were studied.

When baking bread, use whole grain cereals. The grain washed with tap water was soaked in water for 12 hours. A two-time grinding of pre-soaked wheat, rye and triticale grains was performed on a Tekator Homogenizer 1094 dispersant.

The bread dough based on wheat cereals and triticale based on dispersed grain mass was prepared in an irregular manner and with a thick leaven (moisture - 50-52%, acidity - 14-16 degrees). The dough for wheat-rye bakery products was prepared without dough and on a dense grain leaven, for which the scattered rye grain was used. The moisture content of the leaven was 50-52, %, the acidity was 8-10 degrees. The ferment was added at a rate of 40%.

The kneading under laboratory conditions was done manually, then matured in a laboratory fermentation chamber at a temperature of 35 °C and a relative humidity of 75-80%. Cooking dough pieces cut in 0.35 kg in a laboratory oven at a temperature of 220 °C.

The determination of the mineral elements in the bread was carried out after dry incineration in a muffle oven at a temperature of 450 °C and dissolution of the ashes in a mixture of 10% hydrochloric and nitric acid by absorption spectrophotometry atomic in an air-acetylene flame on a Hitachi apparatus (Japan), with deuterium background corrector. To calibrate the instrument, standard solutions of elements from Merk (Germany) were used.

The statistical processing of the obtained data was performed using the statistical packages Microsoft Office Excel 2007 and Statgraphics Centurion XVII, with determination of the arithmetic mean value (M), the mean error of the arithmetic mean value (m) and correlation coefficient (r).

3. Results and Discussion
The concentration of 18 basic elements (in wt. %) Contained in the morphological parts of wheat grain (table 1), rye (table 2) and triticale (table 3).

Figure 1 presents microphotographs characterizing the microstructure of the surface of the studied anatomical parts of the grain of cereal crops, which indicate the points of microanalysis.

Using energy dispersive X-ray spectrometry, data were obtained on the diversity of the mineral composition of wheat, rye and triticale grains.

It has been established that in all the studied morphological parts of the native wheat grain, the main chemical elements that make up the organic compounds - carbon, nitrogen and oxygen - prevail. The nature of the distribution of micronutrients is determined by their biological role. Sodium is distributed evenly in the wheat grain. The elements involved in the composition of enzymes: manganese, iron and zinc prevail in the nucleus.

Phosphorus, potassium, magnesium are found in greater quantity in the vital layer of aleurone. Lead and iodine are concentrated in the endosperm. Cobalt, nickel, aluminum, calcium, chromium, copper, selenium and cadmium dominate the surface of the grain and beard. A high percentage of copper is also characteristic of the embryo and peripheral parts of the wheat grain.

The main chemical elements of organic compounds (C + N + O) also prevail in rye grains. However, there are differences in the distribution of mineral elements. Most of them are concentrated in the embryo. Sodium, aluminum, calcium, chromium, cobalt, iodine, lead, cadmium and selenium exist, whereas in wheat grain these elements were concentrated in other parts morphological grain.
The distribution of iron, zinc, phosphorus, magnesium, and potassium is similar to that of wheat, while manganese predominates in the seed coat.

The mineral composition of triticale grains is: the percentage of the sum of the main chemical elements (C + N + O) is lower than that of the basic forms and represents 49.74 - 67.97% in various morphological parts of the grain this amount is 81.08 for wheat grain - 99.18% for rye grain - 69.75 - 98.30%.

Among the trace elements, the most important by weight in the endosperm of wheat grains are lead and iodine, in the endosperm of rye - iodine, zinc and potassium, in the endosperm of triticale - lead and sulfur. In the aleuron layer of wheat and rye kernels, phosphorus, magnesium, and potassium predominate by weight. Sulfur, copper and lead predominate in the aleurone layer of triticale grains. In the integument of the trace elements of the grain of wheat and rye, potassium is more than other elements of the grain of triticale: the lead. Calcium and copper predominate in coatings of wheat: for rye, the spectrum of these elements is wider and is represented by copper, potassium, phosphorus, calcium, sulfur and for triticale, calcium, potassium, sulfur, copper and lead.
| Chemical element | Embryo | The surface of the fruit shell | Fruit shell | Seedcoat | Aleuronlayer | Endosperm | Beard |
|------------------|--------|-------------------------------|-------------|----------|--------------|-----------|-------|
| C + N + O        | 93.39 ± 0.472 | 98.41 ± 0.521 | 99.18 ± 0.283 | 93.98 ± 0.544 | 81.08 ± 0.582 | 99.00 ± 0.343 | 93.02 ± 0.467 |
| Na               | 0.03 ± 0.002 | 0.01 ± 0.001 | 0.03 ± 0.002 | 0.01 ± 0.001 | – | 0.02 ± 0.003 | 0.03 ± 0.002 |
| Mg               | 0.10 ± 0.006 | 0.12 ± 0.014 | 0.06 ± 0.003 | 0.08 ± 0.004 | 2.03 ± 0.096 | 0.05 ± 0.007 | 0.20 ± 0.013 |
| Al               | 0.06 ± 0.003 | 0.06 ± 0.004 | 0.03 ± 0.002 | – | – | 0.01 ± 0.002 | 0.33 ± 0.021 |
| P                | 0.31 ± 0.017 | 0.15 ± 0.014 | 0.06 ± 0.004 | 0.04 ± 0.003 | 3.95 ± 0.108 | 0.02 ± 0.001 | 0.30 ± 0.019 |
| S                | 0.16 ± 0.011 | 0.18 ± 0.012 | 0.07 ± 0.005 | 0.13 ± 0.011 | 0.13 ± 0.017 | 0.03 ± 0.002 | 0.06 ± 0.003 |
| K                | 0.55 ± 0.022 | 0.10 ± 0.005 | 0.08 ± 0.003 | 0.21 ± 0.019 | 2.71 ± 0.103 | 0.09 ± 0.008 | 0.03 ± 0.002 |
| Ca               | 0.15 ± 0.006 | 0.33 ± 0.012 | 0.10 ± 0.004 | 0.18 ± 0.016 | 0.05 ± 0.003 | 0.01 ± 0.002 | 0.49 ± 0.024 |
| Cr               | 0.01 ± 0.002 | 0.12 ± 0.010 | 0.01 ± 0.001 | 0.01 ± 0.002 | – | 0.05 ± 0.003 | 0.84 ± 0.031 |
| Mn               | 0.92 ± 0.034 | – | – | 0.01 ± 0.001 | 0.02 ± 0.003 | – | – |
| Fe               | 0.89 ± 0.036 | 0.04 ± 0.002 | 0.02 ± 0.001 | 0.01 ± 0.002 | 0.11 ± 0.010 | – | – |
| Co               | 0.02 ± 0.002 | 0.08 ± 0.004 | – | 0.01 ± 0.001 | 0.03 ± 0.002 | 0.03 ± 0.003 | 1.19 ± 0.082 |
| Ni               | 0.02 ± 0.003 | 0.03 ± 0.002 | 0.01 ± 0.001 | 0.06 ± 0.003 | 0.05 ± 0.002 | 0.07 ± 0.004 | 0.14 ± 0.011 |
| Cu               | 1.71 ± 0.087 | 0.12 ± 0.014 | 0.10 ± 0.004 | 0.15 ± 0.018 | 0.07 ± 0.003 | 0.10 ± 0.009 | 2.36 ± 0.098 |
| Zn               | 1.41 ± 0.079 | 0.05 ± 0.004 | 0.03 ± 0.002 | 0.03 ± 0.002 | 0.01 ± 0.002 | – | – |
| Se               | 0.17 ± 0.012 | 0.20 ± 0.017 | 0.05 ± 0.003 | 0.05 ± 0.004 | 0.11 ± 0.014 | 0.06 ± 0.005 | 0.88 ± 0.031 |
| Cd               | 0.01 ± 0.002 | 0.03 ± 0.002 | 0.02 ± 0.002 | – | 0.01 ± 0.002 | – | 0.05 ± 0.004 |
| I                | – | – | – | 0.05 ± 0.003 | 0.04 ± 0.002 | 0.11 ± 0.017 | 0.06 ± 0.002 |
| Pb               | 0.17 ± 0.013 | 0.09 ± 0.005 | – | – | – | 0.28 ± 0.013 | – |
Table 2 - Distribution of chemical elements by morphological parts of rye grain, mass\%  

| Chemical element | Morphological parts of the grain | Embryo | The surface of the fruit shell | Fruit shell | Seed coat | Aleuronlayer | Endosperm | Beard |
|------------------|----------------------------------|--------|--------------------------------|------------|-----------|--------------|-----------|-------|
| C + N + O        | 69.75 ± 0.446                    | 94.36 ± 0.523 | 96.83 ± 0.371 | 98.30 ± 0.487 | 85.74 ± 0.458 | 98.25 ± 0.406 | 88.37 ± 0.394 |
| Na               | 0.71 ± 0.036                     | 0.08 ± 0.004 | 0.08 ± 0.003 | 0.02 ± 0.002 | 0.02 ± 0.002 | 0.05 ± 0.003 | 0.02 ± 0.003 |
| Mg               | 0.35 ± 0.022                     | 0.11 ± 0.009 | 0.05 ± 0.004 | 0.06 ± 0.005 | 0.05 ± 0.005 | 0.05 ± 0.005 | 0.05 ± 0.005 |
| Al               | 0.19 ± 0.017                     | 0.07 ± 0.002 | 0.01 ± 0.001 | 0.05 ± 0.005 | 2.38 ± 0.117 | 0.05 ± 0.003 | 0.02 ± 0.003 |
| P                | 0.10 ± 0.004                     | 0.10 ± 0.012 | 0.48 ± 0.026 | 0.07 ± 0.006 | 5.99 ± 0.131 | 0.13 ± 0.014 | 0.04 ± 0.003 |
| S                | 0.26 ± 0.020                     | 0.22 ± 0.027 | 0.40 ± 0.024 | 0.30 ± 0.021 | 0.35 ± 0.020 | 0.07 ± 0.009 | 0.03 ± 0.002 |
| K                | 4.81 ± 0.132                     | 0.51 ± 0.029 | 0.53 ± 0.021 | 0.40 ± 0.025 | 5.08 ± 0.076 | 0.23 ± 0.015 | 0.03 ± 0.002 |
| Ca               | 2.08 ± 0.103                     | 0.47 ± 0.025 | 0.41 ± 0.023 | 0.02 ± 0.001 | 0.02 ± 0.003 | 0.06 ± 0.004 | 0.06 ± 0.004 |
| Cr               | 0.81 ± 0.029                     | 0.08 ± 0.006 | 0.07 ± 0.003 | 0.07 ± 0.004 | 0.03 ± 0.002 | 0.01 ± 0.002 | 0.01 ± 0.002 |
| Mn               | 0.07 ± 0.003                     | 0.04 ± 0.002 | 0.10 ± 0.003 | 0.05 ± 0.002 | 0.02 ± 0.002 | 0.06 ± 0.005 | 0.06 ± 0.005 |
| Fe               | 0.95 ± 0.023                     | 0.06 ± 0.002 | 0.05 ± 0.002 | 0.04 ± 0.002 | 0.09 ± 0.007 | 0.01 ± 0.002 | 0.01 ± 0.002 |
| Co               | 0.08 ± 0.005                     | 0.02 ± 0.002 | 0.07 ± 0.003 | 0.04 ± 0.003 | 0.06 ± 0.005 | 0.04 ± 0.003 | 0.04 ± 0.003 |
| Ni               | 0.21 ± 0.013                     | 0.04 ± 0.002 | 0.04 ± 0.002 | 0.06 ± 0.003 | 0.13 ± 0.012 | 0.07 ± 0.004 | 0.07 ± 0.004 |
| Cu               | 2.84 ± 0.115                     | 0.05 ± 0.003 | 0.75 ± 0.031 | 0.10 ± 0.005 | 0.07 ± 0.005 | 0.11 ± 0.014 | 0.08 ± 0.004 |
| Zn               | 1.29 ± 0.051                     | 0.09 ± 0.004 | 0.02 ± 0.002 | 0.02 ± 0.002 | 0.22 ± 0.016 | 0.01 ± 0.014 | 0.01 ± 0.014 |
| Se               | 1.56 ± 0.063                     | 0.34 ± 0.018 | 0.03 ± 0.002 | 0.22 ± 0.012 | 0.04 ± 0.006 | 0.01 ± 0.002 | 0.01 ± 0.002 |
| Cd               | 1.81 ± 0.084                     | 0.07 ± 0.003 | 0.02 ± 0.002 | 0.02 ± 0.002 | 0.02 ± 0.002 | 0.02 ± 0.002 | 0.02 ± 0.002 |
| I                | 2.37 ± 0.103                     | 0.24 ± 0.019 | 0.08 ± 0.004 | 0.25 ± 0.018 | 0.01 ± 0.002 | 0.01 ± 0.002 | 0.01 ± 0.002 |
| Pb               | 4.42 ± 0.126                     | 0.12 ± 0.018 | 0.08 ± 0.003 | 0.12 ± 0.014 | 0.12 ± 0.014 | 0.12 ± 0.014 | 0.12 ± 0.014 |
Table 3 - Distribution of chemical elements by morphological parts of triticale grain, mass %

| Chemical element | Morphological parts of the grain | Embryo | The surface of the fruit shell | Fruit shell | Seed coat | Aleuronlayer | Endosperm | Beard |
|------------------|--------------------------------|--------|-------------------------------|-------------|-----------|-------------|-----------|-------|
| C + N + O        |                                | 49.74 ± 0.394 | 62.24 ± 0.563 | 58.67 ± 0.571 | 67.97 ± 0.494 | 62.52 ± 0.698 | 66.88 ± 0.676 | 62.99 ± 0.613 |
| Na               |                                | 0.57 ± 0.029 | 1.07 ± 0.076 | 1.06 ± 0.091 | 1.02 ± 0.089 | 0.68 ± 0.021 | 1.49 ± 0.087 | 1.46 ± 0.082 |
| Mg               |                                | 1.07 ± 0.072 | 1.29 ± 0.108 | 2.21 ± 0.119 | 2.05 ± 0.114 | 1.25 ± 0.106 | 1.44 ± 0.082 | 0.48 ± 0.019 |
| Al               |                                | 0.09 ± 0.003 | 0.08 ± 0.003 | –              | –           | –           | 0.05 ± 0.004 | 0.02 ± 0.003 |
| P                |                                | 0.63 ± 0.032 | –              | –              | 1.07 ± 0.096 | 2.04 ± 0.117 | 0.16 ± 0.019 | 0.13 ± 0.015 |
| S                |                                | 5.52 ± 0.143 | 2.44 ± 0.116 | 5.39 ± 0.135 | 5.45 ± 0.127 | 6.92 ± 0.141 | 5.51 ± 0.138 | 6.55 ± 0.138 |
| K                |                                | 6.75 ± 0.129 | 5.16 ± 0.123 | 6.57 ± 0.142 | 4.41 ± 0.139 | 3.05 ± 0.119 | 0.79 ± 0.033 | 6.84 ± 0.131 |
| Ca               |                                | 2.02 ± 0.101 | 3.50 ± 0.138 | 7.52 ± 0.139 | 5.12 ± 0.122 | 2.85 ± 0.113 | –           | 6.20 ± 0.129 |
| Cr               |                                | 0.91 ± 0.078 | –              | 0.18 ± 0.007 | 0.27 ± 0.009 | 0.25 ± 0.018 | 0.23 ± 0.015 | –       |
| Mn               |                                | –           | 0.12 ± 0.006  | –             | –           | –           | 0.23 ± 0.012 | 0.63 ± 0.035 |
| Fe               |                                | 0.58 ± 0.027 | –              | 1.14 ± 0.103 | 0.32 ± 0.013 | 0.38 ± 0.017 | 0.25 ± 0.018 | –       |
| Co               |                                | 1.65 ± 0.092 | 1.63 ± 0.088  | –             | 0.17 ± 0.008 | 0.22 ± 0.011 | –           | 0.17 ± 0.007 |
| Ni               |                                | 3.17 ± 0.131 | 4.34 ± 0.163  | 0.11 ± 0.012 | 0.32 ± 0.021 | 0.51 ± 0.029 | –           | 0.98 ± 0.016 |
| Cu               |                                | 9.78 ± 0.146 | –              | 4.63 ± 0.130 | 3.10 ± 0.128 | 9.65 ± 0.172 | 2.44 ± 0.114 | –       |
| Zn               |                                | 6.78 ± 0.159 | –              | 0.73 ± 0.028 | 1.44 ± 0.116 | 2.36 ± 0.122 | 2.85 ± 0.123 | –       |
| Se               |                                | 0.38 ± 0.022 | 3.25 ± 0.126  | 1.12 ± 0.106 | 1.21 ± 0.103 | 0.18 ± 0.014 | 0.60 ± 0.019 | –       |
| Cd               |                                | –           | –              | 2.34 ± 0.111 | –           | 0.37 ± 0.016 | –           | –       |
| I                |                                | 5.28 ± 0.126 | –              | –              | –           | –           | 0.70 ± 0.019 | –       |
| Pb               |                                | –           | 13.96 ± 0.184 | 6.36 ± 0.132 | 6.08 ± 0.148 | 6.61 ± 0.145 | 10.64 ± 0.163 | 10.13 ± 0.171 |
From an average grain sample, grain bread was prepared. Table 4 presents the results of the analysis of mineral content by atomic absorption spectrophotometry of wheat, rye and triticale.

Table 4 – The Chemical composition of grain bakery products

| Elements | Wheat Bread | Rye-wheat bread | Triticale Bread |
|----------|-------------|-----------------|-----------------|
| Na       | 38.80 ± 0.670 | 31.80 ± 0.623 | 39.40 ± 0.564 |
| K        | 23.58 ± 0.342 | 26.42 ± 0.297 | 26.98 ± 0.284 |
| P        | 38.29 ± 0.316 | 41.26 ± 0.349 | 43.12 ± 0.336 |
| Mg       | 35.86 ± 0.328 | 36.84 ± 0.294 | 38.82 ± 0.274 |
| Ca       | 17.90 ± 0.096 | 21.87 ± 0.101 | 24.52 ± 0.113 |
| Mn       | 0.34 ± 0.003  | 0.46 ± 0.004  | 0.49 ± 0.003  |
| Fe       | 3.17 ± 0.051  | 4.87 ± 0.064  | 5.95 ± 0.048  |
| Cu       | 0.34 ± 0.026  | 0.44 ± 0.019  | 0.64 ± 0.013  |
| Zn       | 0.75 ± 0.012  | 0.87 ± 0.016  | 1.12 ± 0.020  |
| Co       | 0.48 ± 0.007  | 0.67 ± 0.009  | 0.75 ± 0.014  |
| Pb       | 0.05 ± 0.002  | 0.11 ± 0.003  | 0.04 ± 0.002  |
| Cd       | 0.06 ± 0.003  | 0.05 ± 0.002  | 0.03 ± 0.002  |

The results of the study show that grain bread is enriched in all major biogenic mineral elements and contains toxic metals (lead and cadmium) in a quantity not exceeding the MPC. Since grain bread was prepared from whole grains of cereal crops, the transition of mineral elements from raw materials to bread was 100%.

A correlation analysis revealed a strong correlation between the content of certain mineral elements in individual morphological parts of the grain of cereals and bakery products based on this grain. In particular, a strong negative correlation was observed between zinc levels in triticale and cadmium grain germ in triticale grain bread (r = -0.84), calcium content in triticale and seeds of lead grain in bread from triticale grains (r = -0.79), zinc content in singer grain embryo and cadmium content in wheat grain bread (r = -0.73).

4. Conclusions

The revealed relationship between the levels of bioelements in the cereal germ and the levels of toxic microelements - cadmium and lead in bakery products made from the grains of these cereals indicates the possibility of using X-ray spectral analysis at energy dispersal in a scanning electron microscope system to predict the quality and safety of grain bread in particular, to predict the level of heavy metals in finished bakery products.

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