Optimization of food compositions according to the ideal protein profile in a personalized nutrition system

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Abstract. The article deals with the problem of optimizing food compositions from plant raw materials according to the ideal protein profile. The mathematical formulation of the issue is carried out and the result is obtained by a computer software developed by the authors for this class of issues. Two options were used as criteria for the rationality of the blend being composed: with all essential amino acids of the proteins of the developed mixture components, and with only those essential amino acids, the score of which is less than one. The formation of the optimal blend was carried out for two criteria: the minimum score and the proportion of total protein based on plant materials. The resulting blends from mixtures of plant cultures have a higher biological value and can be used to enrich the composition of functional and specialized products, as well as in the development of products and diets for personalized nutrition.

1. Introduction
The development of a functional and, moreover, individual nutrition, requires balancing nutrients recommended by a nutritionist at the recipe using the nomenclature of real food products [1-8]. One of these nutrients is protein. In the classical triad “proteins-fats-carbohydrates” proteins play a special role, since they, in particular, provide the formation and restoration of human muscle mass [9-12]. However, proteins from different food sources have different biological values. The protein content in the product can be quite high, but if it is of low quality, then the body will experience protein starvation even with a high intake [13]. All proteins are chains of amino acids connected in a certain sequence [14]. Proteins characteristic of the human body is synthesized by the body itself from amino acids supplied with food. Under the action of digestive enzymes in the body, the protein is decomposed to amino acids, their absorption into the bloodstream, followed by use for the synthesis of new proteins inherent in this body.

All amino acids can be conditionally divided into two groups: essential (enter the body from the outside) and nonessential (synthesized in the body). Amino acids are absorbed by the body in a certain proportion. Hence the concept of a reference (ideal) protein. The profile (amino acid composition) of this protein, based on many years of biomedical research, is proposed by the Food and Agriculture Organization (FAO) at the United Nations. Periodically, the profile of the reference protein is revised taking into account the updated scientific knowledge [15].

Based on the concept of a reference (ideal) protein, all proteins can be divided into three groups:
Исходя из концепции эталонного (идеального) белка, все белки можно разделить на три группы:

- Complete protein - the amino acid (AA) profile matches the profile of the reference protein;
- Defective protein - at least one of the essential amino acids is missing;
- Incomplete protein - all essential amino acids are available, but not in proper proportion.

Most plant proteins are incomplete. Of the two incomplete proteins, the better and more valuable is the one with the higher Cm score of the first limiting essential amino acid (taking into account digestibility), i.e. more reference part of the protein. Obviously, in this case, the defective (excess) part of the protein (1-Cm) is definitely less.

It is known that by mixing (blending, combining) certain products, it is possible to adjust the protein profile [16-20].

Animal proteins are complete and do not need supplementation. Plant proteins are generally incomplete and their essential amino acid profile can be improved by the addition of complete or complementary protein.

Recently, there has been an increased attention to the efficiency of using proteins in general and plant proteins in particular. For example, in the European Union, since January 1, 2020, a new Smart Protein project was launched, within the framework of which a number of alternative food proteins derived from plants, mushrooms, processing by-products and industrial waste will be developed.

2. Materials and methods

In the work, the following mathematical formulation of the blending problem was used to obtain a rational mixture for a given profile of the reference protein.

Many ingredients are used as input data:

\[ Ingr(i) = \langle ingr(i, j) \rangle \quad i=1, N \quad j=1, 9 \]  

where, \( ingr(i,1) \) - isoleucine content in the \( i \)-th component, %;
\( ingr(i,2) \) - leucine content in the \( i \)-th component, %;
\( ingr(i,3) \) - lysine content in the \( i \)-th component, %;
\( ingr(i,4) \) - methionine + cystine content in the \( i \)-th component, %;
\( ingr(i,5) \) - phenylalanine + teronisin content in the \( i \)-th component, %;
\( ingr(i,6) \) - trionin content in the \( i \)-th component, %;
\( ingr(i,7) \) - tryptophan content in the \( i \)-th component, %;
\( ingr(i,8) \) - valine content in the \( i \)-th component, %;
\( ingr(i,9) \) - histidine content in the \( i \)-th component, %;
\( ingr(i,10) \) – total protein content in the \( i \)-th component, %.

The content of essential amino acids in the reference (ideal) protein \( Idb \) is also set

\[ Idb = \langle ingr(j) \rangle \quad j=1,9 \]  

where \( idb(j) \) - content of the \( j \)-th amino acid in the reference protein, %.

To solve the problem, it is required to determine the vector \( X(k) \), which determines the \( k \)-th blend option:

\[ X(k) = \langle x(k, i) \rangle \quad i=1, N \]  

where \( x(k, i) \) – proportion of \( i \)-th ingredient in \( k \)-th blend option (%) can take values equal to 0, 1, 2, ..100.

A feasible solution \( X(k) \) for any option \( k \) is determined by the following condition

\[ \forall k \sum_{i=1}^{N} x(k, i) = 100 \]
protein composition \( kp(k,j) \) in blend \( Kp(k) \) is determined by the formula:

\[
Kp(k) = < kp(k,j) > \quad j=1,9
\]  

(5)

where \( kp(k,j) \) – content of essential amino acids in blend \( k \), %

Total protein \( kp(k,10) \) in blend \( k \), %:

\[
kp(k,10) = \sum_{i=1}^{N} ingr(k,10) * x(k,10) / 100
\]  

(6)

The structure of the ideal protein content in the mixture relative to the total protein content in the blend \( k \) is determined by vector \( IKp(k) \):

\[
IKp(k) = < ikp(k,j) >
\]

where \( ikp(k,j) = kp(k,j) / kp(k,10) * 100 \)

Score structure in blend \( k \) is presented by vector \( Score(k) \):

\[
Score(k) = < score(k,j) > \quad j=1,9
\]  

(7)

where \( score(k,j) = ikp(k,j) / idb(j) \)

\( idb(j) \) – proportion of the \( j \)-th essential amino acid in the blend in relation to the reference.

The following options are proposed as criteria for the rationality of the blend:

- in the first option, when comparing two vectors, all essential amino acids are involved [10];
- when comparing two vectors of a reference protein and a blend protein, only those essential amino acids are used for which the score is less than one.

Type 2 criterion:

\[
F = \min_{k} \sqrt{\sum_{j=1}^{9} [1 - score(k,j)]^2}, k = 1,K
\]  

(8)

Type 2 criterion:

\[
F = \min_{k} \sqrt{\sum_{j=1}^{9} [1 - score(k,j)]^2}
\]  

(9)

where \( J \) is the set of all \( j \) for which \( 1-score(k,j)>0 \).

3. Results and discussion
In the present study, an algorithm and a program for solving this issue have been developed. The algorithm is based on generating possible options, preliminary screening out of unacceptable and unpromising options. Tables 1 and 2 show the initial data, calculation results for a mixture of beans, flax seeds, peanuts, Poltava groats and dried carrots.
Table 1. Data for solving the problem of optimization along the ideal protein profile.

| Name of raw materials | Isoleucine | Leucine | Lysine | Methionine + cystine | Phenylalanine + tyrosine | Threonine | Tryptophan | Valine | Histidine | Total protein | type 1 criterion | type 2 criterion |
|-----------------------|------------|---------|--------|----------------------|--------------------------|-----------|------------|--------|-----------|---------------|----------------|----------------|
| beans                 | 4.90/1.63  | 8.29/1.36 | 7.57/1.28 | 2.05/0.89            | 8.38/2.04                | 4.14/1.66 | 1.24/1.88 | 1.33/1.70 | -         | 21.00         | -              | -              |
| flax seeds            | 4.00/1.33  | 5.90/0.97 | 3.70/0.77 | 3.70/1.61            | 7.10/1.73                | 3.60/1.44 | 1.60/2.42 | 1.23/1.27 | 1.27/1.27  | 30.90         | -              | -              |
| peanut                | 4.22/1.41  | 3.62/0.59 | 3.82/0.80 | 2.01/0.87            | 9.03/2.20                | 3.17/1.27 | 3.17/4.80 | 3.17/1.25 | 26.30      | -             | -              | -              |
| Poltava grains        | 2.87/0.96  | 5.91/0.97 | 2.43/0.51 | 2.78/1.21            | 7.91/1.93                | 2.63/1.05 | 0.78/1.18 | 3.30/1.36 | 11.50      | -             | -              | -              |
| carrots               | 3.99/1.33  | 4.17/0.68 | 3.89/0.81 | 1.47/0.64            | 5.04/1.23                | 3.69/1.48 | 1.07/1.62 | 4.27/0.97 | 8.10       | -             | -              | -              |
| reference protein     | 3.00       | 6.10     | 4.80    | 2.30                 | 4.10                     | 2.50      | 0.66      | 4.00     | 1.60       | -             | -              | -              |
| mixture 1             | 3.88/1.29  | 5.95/0.98 | 3.94/0.82*| 3.00/1.30            | 7.13/1.74                | 3.48/1.39 | 1.32/2.00 | 1.14      | 17.25**    | 3.621         | -              | -              |
| mixture 2             | 4.10/1.37  | 6.17/1.01 | 4.84/1.01*| 2.32/1.01            | 7.68/1.87                | 3.53/1.42 | 1.42/2.15 | 1.16      | 15.30**    | -             | 0.00           | -              |

* – minimal amino acid score  
** – total protein
Table 2. Optimal solution.

| Name of raw materials | Limitation on the percentage of the mixture in the blend | Optimized version (mixture 1), (%) | Optimized version (mixture 2), (%) |
|-----------------------|--------------------------------------------------------|----------------------------------|----------------------------------|
|                       | Minimum content (%) | Maximum content (%)              |                                  |
| Beans                 | 0                   | 100                              | 10                               | 26                               |
| Flax seeds            | 0                   | 100                              | 30                               | 6                                |
| Peanut                | 0                   | 100                              | 0                                | 8                                |
| Poltava groats        | 0                   | 31                               | 30                               | 30                               |
| Dried carrots         | 0                   | 31                               | 30                               | 30                               |

It can be seen from the data obtained that the second algorithm leads to more acceptable results for obtaining a blend from a mixture of plant crops: the minimum score (1.0 versus 0.82) and the proportion of total protein in the mixture is higher (15.30 versus 14.14). At the same time, when calculating the first mixture, the restrictions on the content of flax seeds were clearly overestimated, and in the second mixture on the content of carrots. However, these points can be adjusted by manually changing the restrictions on these components.

4. Conclusion

The proposed program allows, within the accepted limits on the content of individual components of the mixture, to obtain their rational ratio based on the proximity of the protein of the mixture to the reference protein in accordance with the accepted criteria. The interface panel also displays the total protein and essential amino acid scores of the mixture. In this case, the minimum score of the resulting mixture and the proportion of the reference protein in it should be assessed. The larger they are, the better. Criterion (9), which takes into account only those essential amino acids for which the score is less than one, leads to better results. In addition to the quality of protein, other requirements may be imposed on products (for vitamins, microelements, special nutrients), and such optimization makes sense if the mixture meets other criteria and, first of all, sensory (organoleptic). Currently, work is underway to improve the optimization algorithm. In the future, it is planned to take into account other indicators of product quality, in addition to protein, for which an appropriate modern database on the chemical composition of raw materials is needed.

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