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KRZYSZTOF WÓJCICKI

APPLYING NIR SPECTROSCOPY TO EVALUATE QUALITY OF WHEY PROTEIN SUPPLEMENTS AVAILABLE ON THE POLISH MARKET

S u m m a r y

The objective of the research study was to apply near infrared (NIR) spectroscopy to evaluate the quality of protein supplements available in the Polish shops and gyms. The evaluation was performed on the basis of the determination of the protein quantity contained in the individual samples by a Kjeldahl method and then the evaluation results were correlated with the measured NIR spectra using an appropriate chemometric method.

The research material consisted of fifteen protein supplement samples for athletes, which included the following types: WPI (protein isolate), WPC (protein concentrate), WPH (protein hydrolysate), and mixtures thereof.

The obtained NIR spectra of protein supplements were characterized by a similar shape of the bands. Depending on the type of protein, a different intensity of absorption of individual bands could be observed. A Principal Component Analysis (PCA) was used to distinguish the samples based on the spectra measured. Unfortunately, owing to the varying composition of the protein mixtures, it was not possible to find characteristic arrangement of the samples depending on their types. The spectra were correlated with the protein contents determined in the samples using a Partial Least Squares regression method (PLS regression) and various mathematic transformations of the NIR spectral data. The obtained regression models were analysed and the analysis results confirmed that it was possible to apply NIR spectra to estimate the content of proteins in protein supplements. The best result was obtained in a spectrum region between 9401 and 5448 cm^{-1} and after the first derivative was applied with Multiplicate Scatter Correction (MSC) as a mathematical pre-treatment.

On the basis of the results obtained, it was proved that the NIR spectra applied together with the chemometric analysis could be used to quickly evaluate the products studied.

Key words: NIR, spectroscopy, protein, supplements, PLS, PCA

Dr inż. K. Wójcicki, Katedra Technologii i Analizy Instrumentalnej, Wydz. Towaroznawstwa, Uniwersytet Ekonomiczny w Poznaniu, al. Niepodległości 10, 61-875 Poznań.
Kontakt: krzysztof.wojcicki@ue.poznan.pl

Introduction

The consumption of supplements by fitness enthusiasts and athletes to improve exercise performance has been increasing over the recent years. In some cases users expect the supplements to fulfil their nutritional needs created by an incomplete diet and in other cases they expect the supplements to enhance their sports performance [8]. People are continually searching for supplements to help them build muscles, boost energy and lose weight. There are some supplements, which are commonly used, such as: whey protein, branched-chain amino acids (BCAA) and creatine [4].

Protein is the most important nutrient to boost athletic performance. Whey protein (WP) is popular among athletes, bodybuilders, fitness models, as well as the people wanting to improve their performance in the gym. Numerous studies show that it can help increase strength, gain muscle and lose significant amounts of body fat [9, 10, 16]. Some specific types of protein are made for certain scenarios, such as casein protein for a slow-release protein and whey protein for a faster release. The main types of whey protein are concentrate, isolate and hydrolysate.

The amount of protein in whey protein concentrate (WPC) can vary between 25 and 89 % [6]. The rest of the product consists of lactose (3.5 %), fat (7.2 %), minerals (5.3 %) and moisture (4 %) [6]. That type of protein is the cheapest one.

Whey protein isolate (WPI) is the purest form of whey protein available on the market. The protein content in WPI ranges between 90 and 95 % [6]. It is a good source of protein for the individuals with lactose intolerance as it contains little or no lactose. WPIs are also very low in fat. The cost of WPI will be slightly higher than that of WPC owing to the purity and higher protein content in the product [6].

Whey protein hydrolysate (WPH) is more easily absorbed by the body and may reduce the potential for allergic reactions. WPH is often used in the formulas for infants as well as in sports and medical nutrition products. Hydrolysis does not reduce the nutritional quality of the whey protein. WPH contains between 80 and 90 % of protein [6, 10].

There has been a growth in the consumption of sport supplements, therefore it is necessary to find a quick and accurate method to evaluate the quality of those products. The WPs products are particularly exposed to the adulteration that is extremely common in the case of the products derived from powdered milk [8]. In some studies diverse methods are suggested of how to detect adulterants [1, 5, 7, 18]. The protein content prediction in single wheat kernels using hyperspectral imaging was presented by Martin in 2017 [14]. Ingle at al. [12] used NIR spectroscopy to determine the protein content in powder mix products. However, the reference literature contains no research on the quality assessment of sports supplements, especially of WPs by spectroscopic techniques.

In his previous research study Wójcicki successfully applied NIR spectroscopy and chemometrics to distinguish various types of sports supplements. The samples were subjected to NIR within a broad range of wavenumbers (12500 ÷ 4000 cm^{-1}). A principal component analysis (PCA) performed on the near infrared spectra made it possible to define three distinctive groups of sports supplements: (1) whey, (2) creatine and (3) BCAA [19].

In this paper a novel application of NIR spectroscopy is suggested to determine the protein content.

Materials and methods

Samples

Whey protein supplements were purchased in local shops and gyms in Poznan, Poland. There were 15 whey protein samples in total: 4 WPI, 1 WPC, 2 WPI + WPC, 4 WPC + WPI, 2 WPC + WPI + WPH, 1 WPC, WPH + WPI and 1 green protein (for vegetarians).

Protein determination

The protein content in whey protein samples was determined by a Kjeldahl method using a conversion factor of total nitrogen to protein equalling 6.25 [2]. The 0.1 g of samples was placed in the mineralization flask with 0.335 g of copper (II) sulphate (VI) and 7.5 g potassium sulphate (VI). The reagents were derived from the Chempur Company (Poland) and they were pure for analysis. Next 15 cm^3 of the concentrated sulphuric acid (VI) (POCH Company, Poland) was added to the tubes and all the samples were mineralized for about 60 min in K-425 SpeedDigester apparatus (Buchi Company, Switzerland). After the mineralization process 20 cm^3 of distiller water was added to the cooled flasks and next, the distillation of ammonia was carried out. The distillation process took 20 - 30 min and was carried out using a steamer model K-350 by Buchi Company. A 4 % boric acid (Chempur Company, Poland) solution was used as the weak acid. Ammonia bound in the boric acid was titrated with 0.1 N hydrochloric acid in the presence of Tashiro indicator (0.02 % methyl alcohol and 0.1 % methylene blue aqueous solution (10:3)) that was the end-of-reaction indicator. The distillation was carried out in the presence of 33 % of potassium hydroxide, pure for analysis (P.P.H. Stanlab Company, Poland). The designation was carried out in three parallel trials for each sample.

The percent rate of protein in Sample (X) was calculated according to the formula [2]:

$$X = \frac{a \cdot n \cdot 1.4 \cdot f}{m}$$

where:

a – amount of standard solution of hydrochloric acid used for titrating ammonia in a given sample [cm^3]; n – molar concentration of hydrochloric acid used for titration; m – sample mass [g]; f – conversion factor of total nitrogen to protein (6.38 as for milk products; 6.25 as for meat products; 5.70 as for vegetables); 1.4 – the amount of nitrogen, which corresponds to 1 ml 0.1 molar solution of hydrochloric acid [mg].

Spectral measurements

The near infrared (NIR) spectra were performed on a MPA\FT-NIR spectrometer (Bruker, USA). Single beam spectra of the samples were collected and rationed against the background of air. For each sample the NIR spectra were recorded from 12500 to 4000 cm^{-1} by co-adding 16 interferograms at a resolution of 4 cm^{-1}. The measurements were performed in triplicate.

Data Analysis

A principal component analysis was performed on the NIR spectra of whey protein supplements to distinguish the samples. PCA is a multivariate technique that linearly transforms an original set of variables into a substantially smaller set of uncorrelated variables that represents most of the information in the original data set. The data for PCA are arranged in a two-way matrix, in which the column vectors represent variables and the row vectors represent the objects of which the variables are measured [17]. The PCA analysis was carried out using Unscrambler 9.7 (CAMO, Norway) software.

To determine the relationship between the spectra of the samples studied and the content of protein a Partial Least Squares (PLS) regression method was used. The selected regions of spectra and data pre-processing options to optimize the model were used. The total number of measured spectra was 45 (15 samples in triplicate). The 20 % of all the samples were selected as the test samples (3 samples in triplicate), the other 12 samples were used to construct a regression model between the spectral data and the concentration of protein. The NIR spectra constituted a set of independent variables X was and the protein contents – a set of dependent variables Y. A full cross-validation was applied to the regression model. The regression models were evaluated using an adjusted R^2 and a Root Mean-Square Error of Cross-Validation (RMSECV) as the term indicating the prediction error of the model. The quality models were evaluated by the ratio of standard deviation of reference data for the validation samples to the RMSEP (RPD). The values predicted were compared to the reference values. A PLS analysis was carried out using an OPUS 7.0 (Bruker, USA) software.

Results and discussion

Protein determination

The contents of protein in the whey protein samples (determined by the Kjeldahl method) are given in Tab. 1. The results show that the producers declare protein contents similar to those marked. For the majority of producers the differences between the declared and measured protein contents do not exceed 5 g/100 g of protein and are considered acceptable. In the three samples the highest differences were reported between the determined protein content and those as declared on the package. Whey protein from producer 9 should have 84.7 g/100g of protein, whereas its protein content determined by the Kjeldahl method was 73.87 g/100 g. The producer 8 declared the protein content to be 82 g/100 g in the sample and the actual protein content was 75.92 g/100 g. Producer 15 was the third to have the difference between the declared and the measured protein content. This producer declared 85 g/100 g of protein and the actual protein content was 76.73 g/100 g. Moreover, based on the results obtained, it

Table 1. Protein content in whey protein samples as determined by Kjeldahl method
Tabela 1. Zawartość protein w odżywkach białkowych wyznaczona metodą Kjeldahla

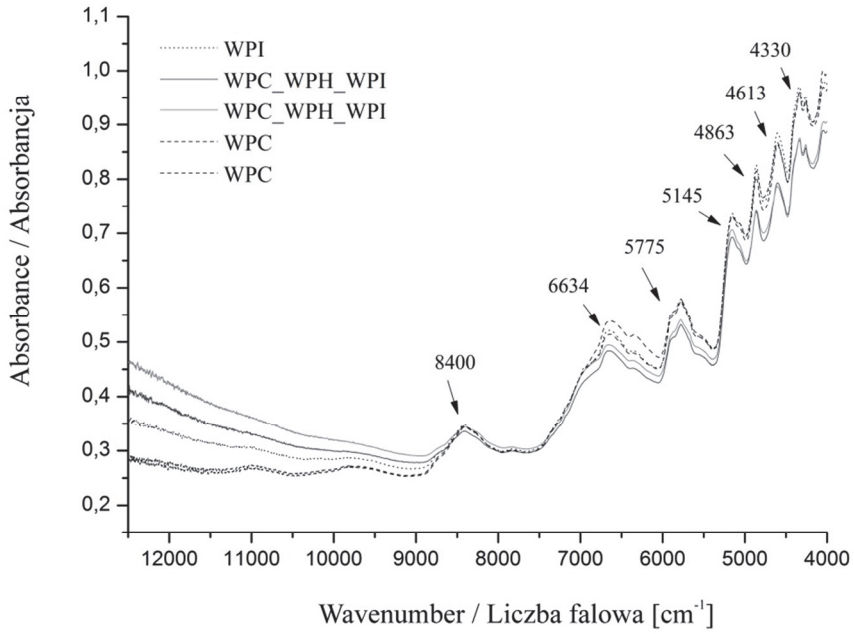
Producer Producent	Type of protein Rodzaj białka	Declaration Deklaracja [g]	Measured value Wartość zmierzona [g]	Standard deviation Odchylenie standardowe
1	WPC + WPH + WPI	72.72	72.72	1.98
2 (vegetarian)	-	56.7	54.72	0.29
3	WPI	85	86.30	4.39
4	WPI + WPC	78.5	81.49	0.28
5	WPC + WPI + WPH	71	74.18	1.25
6	WPC + WPI	71	73.04	1.08
7	WPC + WPI + WPH	63	65.31	1.67
8	WPC + WPI	82	75.92	2.48
9	WPI	84.7	73.87	0.91
10	WPI + WPC	79.2	78.02	1.45
11	WPC + WPI	71	68.69	0.31
12	WPC	70	71.08	0.36
13	WPC + WPI	80	78.21	0.52
14	WPI	88	85.32	0.81
15	WPI	85	76.73	0.87

Explanatory notes / Objaśnienia:
WPI – whey protein isolate / izolat białkowy; WPC – whey protein concentrate / koncentrat białkowy; WPH – whey protein hydrolysate / hydrolizat białkowy.

can be said that most producers declare correct protein contents in their products and show them the packages thereof.

Whey protein spectrum within the near infrared range

In the NIR spectroscopy there are some typical bands derived from the overtones and combination vibrations. Those bands are attributed to the overtones vibration of C-H, N-H and O-H groups [13]. The spectral range between 4000 and 4545 cm^{-1} corresponds to the combination of C-H stretching vibrations. The bands within the range between 4545 and 5000 cm^{-1} are assigned to the combination of N-H stretching and O-H stretching vibrations, while the range between 5555 and 6060 cm^{-1} corresponds to the first overtone of C-H stretching vibrations. The first overtone of N-H and O-H stretching vibrations is found within the range of 6666 ÷ 7142 cm^{-1}. The absorptions bands within the range of 7142 ÷ 7692 cm^{-1} are derived from the combination of C-H stretching vibrations, while the bands within the range of 8163 ÷ 9090 cm^{-1} are assigned to the second overtone of C-H stretching vibrations [13].



Explanatory notes as in Tab. 1. / Objaśnienia jak pod tab. 1.

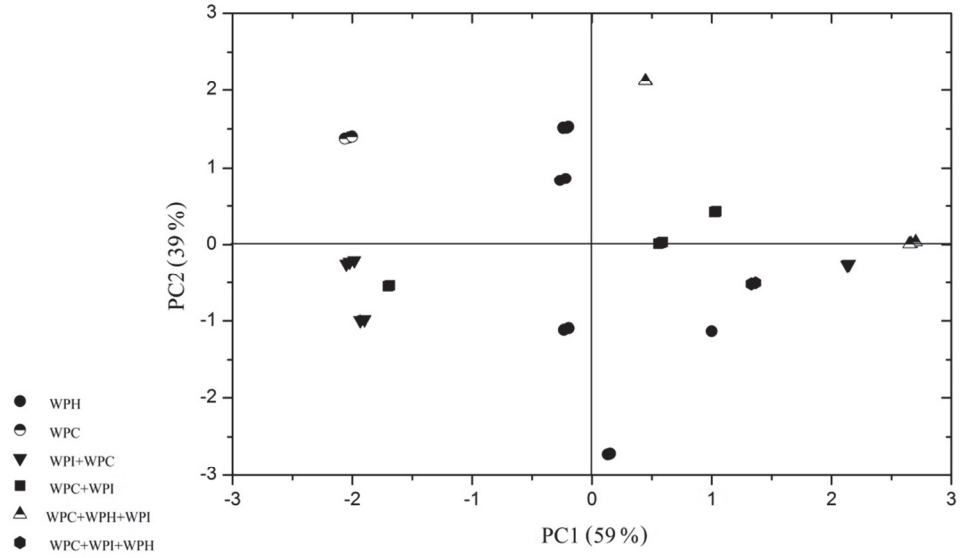
Fig. 1. Absorption spectra of whey protein supplements samples in near-infrared region (12500 ÷ 4000 cm^{-1})

Rys. 1. Widma absorpcji odżywek białkowych w zakresie bliskiej podczerwieni (12500 ÷ 4000 cm^{-1})

The NIR absorption spectra of the studied whey supplements measured against air are shown in Fig. 1. The absorption spectra of the whey product are similar to those of milk. The bands at about 6580 ÷ 6490 cm^{-1} and 6670 ÷ 6580 cm^{-1} correspond to the first overtone of NH_2 symmetric and antisymmetric stretching vibrations, respectively [3, 15]. Based on the reference literature the band with the maximum absorption at about 4854 cm^{-1} and 4587 cm^{-1} corresponds to the protein, while the band with the maximum absorption at about 5076 cm^{-1} and 5636 cm^{-1} corresponds probably to the lactose and protein, respectively [3]. As seen in Fig. 1, those bands also occur in the measured samples. The absorption bands of protein are seen at 4863 cm^{-1}, 4613 cm^{-1} and 5775 cm^{-1}, while those of lactose at 5145 cm^{-1}. The intensity of the spectrum differs depending on the type of protein.

Principal Component Analysis (PCA)

PCA was used to distinguish the near infrared spectra obtained from the different types of whey protein samples. It was applied to the spectra acquired from the fourteen samples measured in triplicate. The sample from producer 2 (green protein) was deliberately omitted. After PCA was performed, the data were plotted on a graph of the first principal component (PC1) vs. second principal component (PC2) as shown in Fig. 2.



Explanatory notes as in Tab. 1. / Objaśnienia jak pod tab. 1.

Fig. 2. PCA results of principal components (PC1 vs. PC2) of NIR spectra of whey protein samples. Full range of 12500 ÷ 4000 cm^{-1}

Rys. 2. Wyniki analizy głównych składowych (PCA) widm NIR odżywek białkowych. Pełny zakres 12500 ÷ 4000 cm^{-1}

The first and the second main component (PC1 and PC2) describe 98 % of the total variation. PC1 describes 59 % of the total variability, while PC2 39 % (for the spectral range of 12500 ÷ 4000 cm^{-1}). The selection of individual spectral ranges does not improve the results of the analysis. There was not any significant distinction between the samples analyzed. Only WPI samples lay along the PC2 axis near 0 (Fig. 2). The reason of such results is in the fact that mix-WPs (WPI + WPC, WPC + WPI, WPC + WPH + WPI, WPC + WPI + WPH) consist of various concentration for each WP, thus it is hard to distinguish them and arrange them in separate groups.

Regression models for protein determination

PLS was applied to quantitatively evaluate the concentration of protein in whey protein supplements based on their spectral characteristics. Different types of mathematical pre-processing were applied to the spectra before building the model. Complete spectra were analyzed as the first step in all the spectral regions. Next, specific sub-regions were chosen, which relied on the regression coefficients obtained for the complete spectra and the chemical information contained in the specific sub-regions.

The PLS regression results for the complete spectra within the range of 12500 ÷ 4000 cm^{-1} without any pre-treatment indicated the correlation between the spectra and the whey composition. The R^2 of the calibration model equalled 76.9, while that of the validation was 40.65. The regression results improved where the specific spectral regions were used instead of the complete spectra. The mathematical pre-processing of spectra has a significant effect on the regressions results. In Tab. 2 the top ten results of the models obtained were demonstrated (in the order from the most to the least accurate).

The adjusted R^2 for the calibration models were within the range of 66.89 ÷ 96.27 and those for the validation models ranged 62.76 ÷ 67.13; this means that the models built are able to properly predict the protein content in the whey supplements. RMSECV for the validation models were also low (4.8 ÷ 5.1 %); this confirms that the quality of the models obtained was good (Tab. 2).

RPD for the calibration models were within the range of 1.74 ÷ 5.18 and those for the validation models ranged from 1.66 to 1.74. According to Huang et al. [11] the models with RPD values of 3.1 ÷ 4.9 are suitable for screening analysis; those with 5.0 ÷ 6.4 are adequate for quality control; those with 6.5 ÷ 8.0 for process control; and finally RPD > 8.0 indicate models adequate for any application.

The best PLS model was obtained for the analysis of the first derivative + MSC in the region between 9401 and 5448 cm^{-1}. For that model the validation R^2 was the highest (and it equalled 67.13), whereas RMSECV was the lowest (it equalled 4.8 %). The lowest R^2 and RPD values (and the highest RMSECV) for the validation model was

reported for the constant offset elimination and the region of 4601 ÷ 4248 cm^{-1} (Tab. 2).

Table 2. Results of Partial Least Squares (PLS) statistics for calibration and validation models
Tabela 2. Wyniki analizy najmniejszych kwadratów (PLS) dla modeli kalibracyjnych i walidacyjnych

Data pre-treatment Przekształcenie danych	Spectral range Zakres widma [cm^{-1}]	Calibration Kalibracja		Validation / Walidacja		
		R^2	RPD	R^2	RPD	RMSECV [%]
First derivative + MSC	9401 ÷ 5448	78.62	2.16	67.13	1.74	4.8
First derivative + MSC	7500 ÷ 5448	66.89	1.74	66.89	1.74	4.81
First derivative + MSC	7425 ÷ 5448	78.14	2.14	66.89	1.74	4.81
First derivative + SNV	9401 ÷ 5448	78.67	2.17	66.28	1.72	4.86
First derivative + SNV	7500 ÷ 5448	78.17	2.14	66	1.72	4.88
SNV	6100 ÷ 5448, 4601 ÷ 4248	88.39	2.93	64.17	1.73	5.01
MSC	6100 ÷ 5448	80.83	2.28	63.77	1.66	5.03
SNV	6100 ÷ 5448	80.82	2.28	63.62	1.66	5.05
SNV	4601 ÷ 4248	96.27	5.18	62.88	1.68	5.1
Constant offset elimination	4601 ÷ 4248	91.42	3.41	62.76	1.66	5.1

Explanatory notes / Objaśnienia:
MSC – Multiplicative Scatter Correction / multiplikatywna korekcja rozproszenia; SNV – Standard Vector Normalization / standardowa normalizacja wektorowa; first derivative / pierwsza pochodna.

Quantification of protein in whey supplement samples

To check the applicability of the calibration models for the prediction of protein content in the whey supplements, the best PLS model was utilized for the quantification of protein content in the prediction set consisting of 3 samples (9 measured spectra). The samples were subjected to the same mathematical pre-treatment as those in the calibration set for the particular model (Tab. 2).

The objective was to validate the best prediction model using a sample set not included in the calibration.

As seen in Tab. 3 the values predicted by the Kjeldahl method and by the NIR spectroscopy coupled with chemometrics are rather similar. This means that the spectroscopic measurements could be used to predict the content of protein in whey supplements instead of time-consuming conventional methods.

Table 3. Predicted and reference concentration of protein in whey supplement samples obtained by PLS calibration/validation model

Tabela 3. Wartość przewidywana i referencyjna zawartości białka w odżywkach proteinowych otrzymana na podstawie modelu kalibracyjnego/walidacyjnego PLS

Name of sample Nazwa próbki	Declared concentration Wartość deklarowana [g]	Measured concentration by Kjeldahl method Wartość oznaczona metodą Kjeldahla [g]	Predicted concentration by NIR Wartość przewidywana na podstawie widm NIR [g]
X1	70	71.08	70.77
X1	70	71.08	72.79
X1	70	71.08	72.50
X2	82	75.92	75.75
X2	82	75.92	76.90
X2	82	75.92	76.22
X3	77.72	77.72	74.48
X3	77.72	77.72	78.78
X3	77.72	77.72	78.94

Conclusions

1. Most producers of whey supplements declare correct protein concentrates on the package of the product.
2. The analysis of the respective spectra using multivariate regression method enabled the quantification of protein content with results similar to that obtained by the conventional method.
3. The results indicate that NIR spectroscopy could replace the time-consuming Kjeldahl method used to predict the concentrate of protein in whey supplements for it is much faster and does not need any reagents.

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ZASTOTOWANIE SPEKTROSKOPII W BLISKIEJ PODCZERWIENI DO OCENY JAKOŚCI ODŻYWEK BIAŁKOWYCH DOSTĘPNYCH NA POLSKIM RYNKU

S t r e s z c z e n i e

Celem pracy było zastosowanie spektroskopii w zakresie bliskiej podczerwieni (NIR) do oceny jakości odżywek białkowych dostępnych w polskich sklepach i siłowniach. Oceny tej dokonano na podstawie wyznaczenia zawartości protein w poszczególnych odżywkach metodą Kjeldahla, a następnie skorelowaniu jej ze zmierzonymi widmami NIR, stosując odpowiednią metodę chemometryczną.

Materiał do badań stanowiło piętnaście białkowych odżywek dla sportowców różnego typu: WPI (izolat białka), WPC (koncentrat białka) i WPH (hydrolizat białka) oraz ich mieszanki.

Otrzymane widma NIR odżywek białkowych charakteryzowały się zbliżonym do siebie kształtem pasm. W zależności od rodzaju odżywki można było zaobserwować różną intensywność absorpcji poszczególnych pasm. Przeprowadzona analiza głównych składowych (PCA) wykorzystana została do rozróżnienia próbek na podstawie zmierzonych widm. Niestety ze względu na różny skład mieszanek białkowych nie udało się zaobserwować charakterystycznego rozmieszczenia próbek w zależności od ich rodzaju. Korelację widm z wyznaczoną zawartością protein w próbkach przeprowadzono stosując metodę regresji najmniejszych kwadratów (PLS) oraz różne przekształcenia matematyczne danych spektralnych. Analiza otrzymanych modeli regresji wykazała, że możliwe jest wykorzystane widm w bliskiej podczerwieni do przewidywania zawartości protein w odżywkach białkowych. Najlepszy rezultat otrzymano w zakresie widma 9401 ÷ 5548 cm^{-1} oraz po zastosowaniu pierwszej pochodnej wraz z multiplikatywną korektą rozproszenia (MSC) jako przekształcenie matematyczne.

Na podstawie otrzymanych wyników udowodniono, że zastosowanie widm NIR wraz z chemometryczną analizą pozwala na szybką ocenę jakości omawianych produktów.

Słowa kluczowe: NIR, spektroskopia, białko, odżywki, PLS, PCA