

Full Length Research Paper

Non-destructive measurement of crude fat and crude protein contents of oats from different geographical zones in China using visible and near-infrared spectroscopy

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Oats' geographical origin and internal component contents have great impacts on their flavor, off-flavor, emulsifying and binding properties. Geographical origin identification was done by classical Soft Independent Modeling of Class Analogy (SIMCA) and least squares support vector machine (LS-SVM), respectively. The correct answer rate of the LS-SVM model was 98.3%, better than that of SIMCA (75.0%). LS-SVM models were also established for the content determination of crude fat and crude protein of oats. Eleven and thirteen wavelength variables were selected by successive projections algorithm for crude protein and crude fat analyses, respectively. The correlation coefficients were 0.814 and 0.915, and the root mean square errors of validation were 0.338 and 0.389 for the crude protein and crude fat analyses, respectively. Overall Vis-NIRS is a promising technique for the fast and reliable determination of geographical origins and crude fat content of oats. The determination of crude protein content needs to be further researched.

Key words: Visible and near-infrared spectroscopy, oats, protein, fat.

INTRODUCTION

In recent years, oats (*Avena sativa* L) have received increased interest due to their excellent health-related chemical properties and 'high nutritive' and physiological values. Oats have the good reputation of a good taste 'with dietetic properties', 'serum cholesterol reduction' and an activity stimulating metabolic changes in the body (Mirmoghtadaie et al., 2008; Mohamed and Biresaw, 2008; Gates et al., 2008). In comparison with other cereals, oat contains a larger amount of protein and fat. Oat's protein is considered to be more nutritive than other cereals such as wheat and corn (Wioletta et al., 2009). Oats also which makes oats a good source of energy and contain

higher content of fat than other cereal grains unsaturated fatty acids (Zhou et al., 1999). The average contents of protein and fat of oats are 12.9/100 and 8.7/100 g, compared with 9.4/100 and 3.3/100 g for maize, and 12.7/100 and 2.2/100 g for wheat (Welch, 1995). As the world-wide trade in fresh agricultural products increase year by year, so does the interest by consumers for high quality food products with a clear geographical origin (Dion et al., 2008). Many agricultural products such as potatoes (Rivero et al., 2003), onions (Ariyama et al., 2007) and garlics (Smith, 2005) have been studied. Nowadays, oats have gotten more attention on their geographical origins and composition contents with the development of the modern oat industry. Due to a combination of 'growing conditions' such as soil, temperature and humidity, the nutritive ingredients of oats are different in those from different geographical origins. However, it is difficult to

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distinguish the geographical origins of oats by naked-eyes. As two main components, protein and fat have great impacts on the flavor, off-flavor, emulsifying and binding properties of oats during the production processing. Kjeldahl determination method (Hiller et al., 1948) and Soxhlet extraction method (Robert and Yoshikatsu, 2004) are commonly used methods to determine the crude protein and fat contents, respectively. However, they are destructive, time-consuming and need professional operators.

The use of chemical reagents in these methods is another problem against the needs of sample safety and low cost. So a fast, nondestructive and safety alternative for the determination of oats' geographical origins and chemical composition is needed. Visible and near-infrared spectroscopy (Vis-NIRS) technology is widely used as a simple, fast and non-destructive analyzing method such as in the analysis of drink and pharmaceutical products (Li et al., 2007) and in the identification and components analysis of food (Cen and He, 2007). The method also has been applied on the analysis of crops such as paddy rice (Li et al., 2008), wheat (Dowell et al., 2009) and barley (Miryong et al., 2008). There are two kinds of oats: husked and naked. The yield of naked type accounts for 90% of the total oats production in China (Zhang and Zhai, 2004). The objective of this study is to explore the potential of using Vis-NIRS spectra to distinguish naked oats' geographical origins and determine the contents of crude protein and crude fat. To the authors' knowledge, the current study is the first time Vis-NIRS is used to non-destructively determine the overall quality information of oats such as geographical origins, crude protein and crude fat.

The specific objectives of this research were: 1) to compare the performances of geographical origin discrimination between classical soft independent modeling of class analogy (SIMCA) and least squares support vector machine (LS-SVM), 2) to establish quantitative relationships between Vis-NIR spectra and the contents of crude protein and crude fat in oats by LS-SVM, 3) to do further wavelength selection using successive projections algorithm (SPA), and 4) to find the optimal wavelengths and the best calibration model.

MATERIALS AND METHODS

Sample preparation and spectral measurement

In this study, naked oats were obtained from four main geographical origins: Inner Mongolia, Jilin, Gansu, and Hebei provinces in China, all of which are located in northern China and are about 2000 km apart from each other. These samples were harvested once per year from 2009 to 2010, and came from three different points per origin. A total of 160 intact samples (40 for each origin) were obtained without germination and mold. Vis-NIR reflectance spectra in the 325 to 1075 nm region were measured using an ASD FieldSpec® Handheld spectroradiometer (Analytical Spectral Devices, Inc., Boulder, CO). For the spectral measurement, a uniform glass vessel (diameter = 65 mm, height = 140 mm) was filled with

oats. The probe with the visual angle of 15° was positioned at a distance of approximately 120 mm from the surface of the oats. The light source, a Lowell pro-lam 14.5 V Bulb/128690 tungsten (Ushio Lighting Inc., Japan) was positioned at a distance of 100 mm from the surface of the sample, to make sure that the probe did not interrupt the lighting pathway. The average spectral distribution for each sample was the average of 30 scans which were collected at the same position of the measurement point. All experiments were conducted at ambient temperature (about 25°C) during the spectral measurement. For spectral analysis, the reflectance spectrum (R) for each sample was first transformed into an absorbance spectrum by $\log(1/R)$. To avoid a low signal-to-noise ratio, only the wavelength region from 400 to 1000 nm was used for the calculations.

Software from Unscrambler V9.7 (CAMO, Process AS, OSLO, Norway) and Matlab 7.8.0 R2009a (The Math Works, Natick, USA) were used for data analysis.

Reference measurement of crude fat and protein

Fat content was measured by the Soxhlet extraction method following GB/T 14772-2008 (National Standard of P. R. China). The samples were milled and sieved. About 10 g of every sample were placed in the extraction cartridge made of filter paper. The cartridge was placed in the Soxhlet chamber. The pre-tared distillation flask contained 100 ml of analytical grade absolute ethyl-ether which was used as the solvent. After extracted for 8 h, the solvent was released in a water path, then any traces remaining were removed by placing the flask in an oven at $103 \pm 2^\circ\text{C}$. The fat content value was the weight of fat per 100 g of oats. Crude protein content was measured by Dumas combustion method (Sader et al., 2004). Rapid N Cube (Elementar Analysensysteme) was used for the measurement. The protein measurement process includes complete combustion, reduction, purification and detection. Finally, the Rapid N Software V 3.4.0 (Elementar Analysensysteme) outputs the protein content which was calculated as the value of total nitrogen content multiplied by 6.25. The 160 samples obtained were divided into a calibration set and a validation set. All samples have been sorted according to their respective y-value (namely, the reference measurement values). Three spectra of every eight samples were selected into the validation set. Finally, the calibration set contained 100 spectra and another 60 spectra constitute the validation set.

Spectra preprocessing

Spectra preprocessing sometimes can improve the model's performance. Several spectral pre-processing algorithms including Savitzky-Golay smoothing (SGS), multiplicative scatter correction (MSC), 1st derivatives (1st D) and standard normal variate (SNV) were implemented using "The Unscrambler V9.7" (CAMO PROCESS AS, Oslo, Norway). SGS is an averaging algorithm that fits a polynomial to the data points (Savitzky and Golay, 1964). MSC is a transformation method used to compensate for additive and/or multiplicative effects in spectral data (Helland et al., 1995). 1st D attempts to correct for baseline effects in spectra. SNV is a row-oriented transformation which centers and scales individual spectra (Barnes et al., 1989).

SIMCA

SIMCA is an extension of principal component analysis to include supervised modeling (Nils et al., 1987) for classifying in which the goal is to obtain a classification rule about a set of k groups denoted by X^j , $j = 1, 2, \dots, k$. We label this set X^j as the training set

(Branden and Hubert, 2005). The training set is modeled by principal component analysis (PCA) that is utilized to perform dimension reduction. As PCA is applied to each group separately, SIMCA provides additional information on the different groups such as the relevance of the different variables (Flåtén et al., 2004).

Methodology of LS-SVM

Support vector machines (SVM) is a powerful methodology developed within the area of statistical learning theory and structural risk minimization. Standard SVM is used for solving problems in nonlinear classification, function estimation and density estimation in a relatively fast way (Liu et al., 2008), and least squares support vector machines (LS-SVM) have been developed for recurrent models and use in optimal control problems (Suykens and Vandewalle, 1999; Wu et al., 2008). LS-SVM is closely related to regularization networks and Gaussian processes but additionally emphasizes and exploits primal-dual formulations. As it gives good performance under general smoothness assumptions on handling the nonlinear relationships between the spectra and target attributes, a radial basis function (RBF) kernel was used in this study. In order to find out the optimal parameter values which include regularization parameter γ and the RBF kernel function parameter σ^2 , a grid-search technique was applied. In this study, these parameters were optimized with values of γ in the range of 2^{-1} to 2^{10} and σ^2 in the range of 2 to 2^{15} with increments chosen from previous studies where the magnitude of parameters to be optimized was established. For each combination of γ and σ^2 parameters, the root mean square error of cross-validation (RMSECV) was calculated and the optimum parameters were selected.

Successive projections algorithm (SPA)

SPA is a new popular tool for variable selection. The goal of SPA consists of finding a small, representative set of spectral variables with an emphasis on the minimization of collinearity (Márcio et al., 2005). SPA can provide more reproducible results than genetic algorithm. It comprises two phases. The principle of variable selection by SPA is that, it starts with one wavelength, then incorporates a new one at each iteration, the new variable selected is the one among all the remaining variables which has the maximum projection value on the orthogonal subspace of the previous selected variable, until a specified number of wavelengths is reached (Mário et al., 2001). SPA was coded in Matlab 7.8.0 R2009a (The MathWorks, Natick, USA).

Model evaluation

The predictive performance of the model was evaluated by the following standards. For geographical origin identification, the correct answer rate (CAR, %) was used. When the crude protein and crude fat analysis were evaluated, several standards listed as follows were used: the root mean square error of calibration (RMSEC), the root mean square error of validation (RMSEV) and residual predictive deviation (RPD). The correlation coefficient (r) was used in all the processes including calibration (r_{cal}) and validation (r_{val}). RPD is the standard deviation of reference data for the validation samples divided by the standard error of validation (SEV) and provides a standardization of SEV (Williams and Norris, 1987). Generally, a good model should have high r_{cal} , r_{val} and RPD value, with low RMSEC and RMSEV values (Wu et al., 2010). The ratio of the standard deviation of the response variable to the

RMSEV (RPD) was calculated to evaluate the model's success rate and accuracy. According to some authors (Nicolai et al., 2007), an RPD value between 1.5 to 2.0 means that the model can discriminate between low and high values of the response variable; 2.0 to 2.5 indicates that coarse quantitative predictions are possible; over 2.5 corresponds to excellent prediction accuracy.

RESULTS AND DISCUSSION

Overview of the spectra

The absorbance spectra of the oat samples of four varieties are shown in Figure 1. There is no remarkable difference between these four varieties of oats. All the curves appear as a gradually increasing absorbance from 450 to 900 nm. The spectral reflectance decreased after 850 nm. It was not feasible to quantify the spectral profiles to oats' geographical origins and determine the contents of crude protein and crude fat. Therefore, during calibration we tell the software what to identify, some chemometric algorithms were needed for the spectral data mining.

Geographical origin discrimination

SIMCA was performed on the spectra after spectral preprocessing. In the SIMCA process, principal components analysis was carried out on the spectra of samples from each geographical origin first. For the four varieties, the first 20 PCs were obtained from PCA, respectively. Then, SIMCA was operated for the geographical origin discrimination based on the principal components obtained. The average CAR of the validation process was 71.66%. The best result (75% CAR) was obtained when SGS was used as the preprocessing step. However, the CAR of SIMCA of 75% was not high enough for our use of the application. LS-SVM was also used for the geographical origin discrimination. Table 1 shows the results of SIMCA and LS-SVM models based on different preprocessing methods. The average CAR of validation process was 92.64%. The best result (98.3% CAR) was obtained when MSC, SNV or 1st D was used for preprocessing. The CAR result increased 23.3% for LS-SVM compared to the CAR of SIMCA. Therefore, LS-SVM was better suited than SIMCA to the discrimination of geographical origin of naked oats.

Analysis on reference crude fat and crude protein content

The reference contents of the crude fat and crude protein of oats from each geographical origin (every origin contains 40 samples) are shown in Table 2. The content range of crude fat was from 5.82 to 9.10%. The highest value was from the samples of Inner Mongolia, while

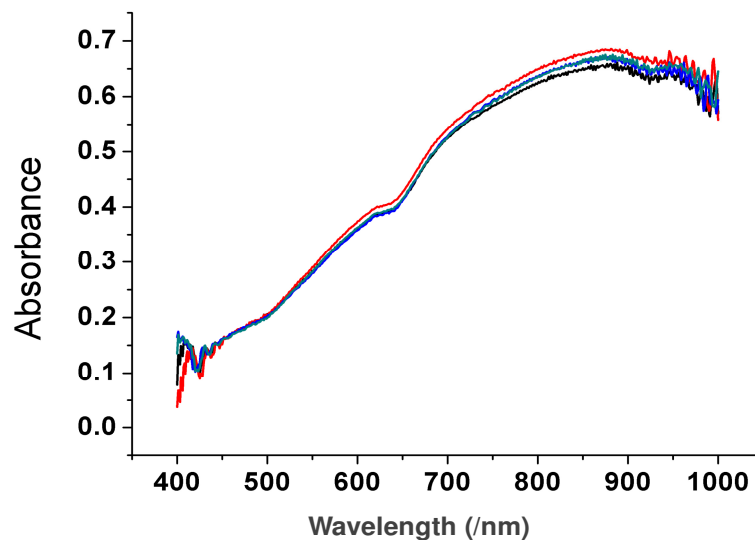


Figure 1. Original visible and near-infrared spectra of oat.

Table 1. Classification and validation accuracy rate of the SIMCA and LS-SVM model based on different pretreatment.

Model	Pretreatment	Classification			Validation		
		No.	Misclassified	CAR (%)	No.	Misclassified	CAR (%)
SIMCA	1 ^a	100	9	91.0	60	16	73.3
	2 ^b	100	12	88.0	60	15	75.0
	3 ^c	100	4	96.0	60	18	70.0
	4 ^d	100	5	95.0	60	19	68.3
	5 ^e	100	7	93.0	60	17	71.7
LS-SVM	1 ^a	100	0	100.0	60	3	95.0
	2 ^b	100	0	100.0	60	10	83.3
	3 ^c	100	0	100.0	60	1	98.3
	4 ^d	100	0	100.0	60	1	98.3
	5 ^e	100	0	100.0	60	1	98.3

^a Raw spectra with no pretreatment, ^b Savitzky-Golay smoothing, ^c multiplicative scatter correction (MSC), ^d standard normal variate (SNV) and ^e Savitzky-Golay 1st derivative (1st D).

samples from Jilin had the lowest value. The contents of crude protein ranged from 10.03 to 12.67%. The mean value of the geographical origin from Inner Mongolia was the highest while the lowest mean value was from Gansu. As the contents, the flavor, off-flavor, emulsifying and binding properties of oats are different during the production processing and finally that will have an effect on the price of the oats products. What's more, in this work, the different contents of each component lead to different effects on the Vis-NIR spectra.

Determination of crude fat and crude protein content using full-range spectra

Table 3 show the results of the LS-SVM models with

different preprocessing for the crude fat and crude protein analyses. For the crude fat analysis, the original spectra obtained the best result with the r_{cal} value of 0.978 and the r_{val} value of 0.931. The absolute value of the difference between RMSEC and RMSEV was 0.124, which was the smallest compared to those of other models. This result shows that the model based on the original spectra has less overfitting. Moreover, the RPD of 2.341 indicates that coarse quantitative predictions are possible (Nicolai et al., 2007). For the crude protein analysis, the models based on the original spectra and SGS pretreated spectra produced better results than other models, but the differences from the other models were very small. Considering that the performance of the

Table 2. Contents of the crude protein and crude fat in four regions of oats.

Component	Varieties*	Maximum	Minimum	Mean	SD
Fat (%)	1	8.17	7.08	7.59	0.24
	2	8.55	8.21	8.37	0.08
	3	6.92	5.82	6.41	0.25
	4	9.10	7.20	8.47	0.43
Protein (%)	1	11.70	10.03	10.85	0.35
	2	12.28	11.51	11.90	0.16
	3	12.67	11.03	11.83	0.40
	4	12.52	11.52	12.15	0.24

*The numbers represent different origins in China: 1-Gansu, 2-Hebei, 3-Jilin, 4-Inner Mongolia.

Table 3. Comparison of classification and prediction of the content of crude protein based on different pretreatment with the LS-SVM model.

Property	Pretreatment	Calibration		Validation		
		r_{cal}	RMSEC	r_{val}	RMSEV	RPD
Crude fat	1 ^a	0.978	0.187	0.931	0.311	2.341
	2 ^b	0.976	0.195	0.917	0.336	2.176
	3 ^c	0.994	0.098	0.899	0.357	2.206
	4 ^d	0.994	0.090	0.899	0.357	2.206
	5 ^e	0.997	0.070	0.917	0.336	2.202
Crude protein	1 ^a	0.908	0.257	0.789	0.361	1.140
	2 ^b	0.915	0.246	0.791	0.361	1.133
	3 ^c	0.942	0.213	0.740	0.391	1.047
	4 ^d	0.945	0.214	0.742	0.390	1.047
	5 ^e	0.960	0.181	0.731	0.399	1.021

^aOriginal spectra with no pretreatment, ^bSavitzky-Golay smoothing, ^cSavitzky-Golay smoothing and MSC, ^dSavitzky-Golay smoothing and SNV, ^eSavitzky-Golay smoothing and 1st D.

models based on the original spectra and pretreated spectra are similar and that the spectral analysis procedure should be simple, the model based on the original spectra was considered the best. The original spectral model also obtained the smallest absolute value of the difference between RMSEC and RMSEV, demonstrating that the model based on the original spectra has less overfitting. However, the low RPD values between 1.021 and 1.140 showed that the determination of crude protein was not very successful. A comprehensive analysis of the LS-SVM models of protein and fat indicated that the results of using the original spectral data were better, probably because that effective information became weak after pretreatment. As a conclusion, the predictive ability of Vis-NIRS technique for the determination of crude fat was better than that for crude protein. Nortvedt et al. (1998) and Šašić and Ozaki (2001) found that fat was modeled with greater success than protein in the Atlantic halibut fillets and milk studies

respectively. The same findings are true in this work. There might be two reasons to cause these results.

First of all, the spectral signal of protein was not as intense as that for the fat in oats over the Vis-NIR spectral range. Secondly, the oat grains are not uniform enough, and that might be one of the reasons that the analysis on the crude protein had low RPD values. Some papers have demonstrated that the particle size of samples would have a great effect on the spectroscopy and therefore the prediction accuracy of the spectral quantitative model (Casler and Shenk, 1985; Windam, 1987).

Determination of crude fat and crude protein content using the spectra of selected variable

In order to reduce the complexity of the model, SPA was carried out for selecting effective wavelength variables from the full-range spectra. Figure 2 shows the RMSE

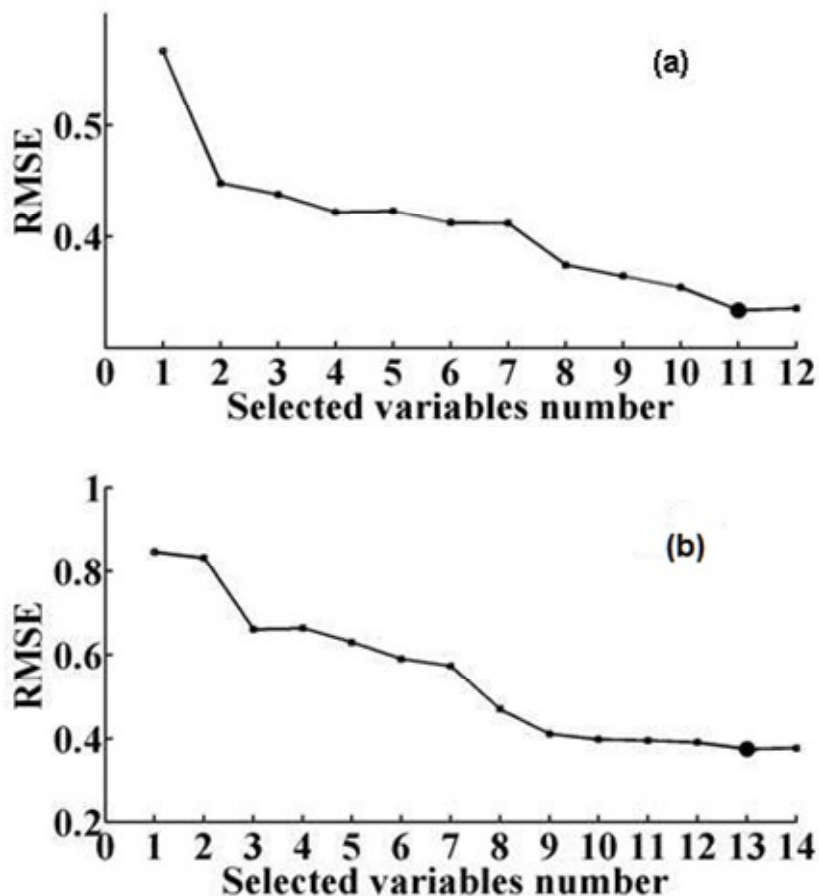


Figure 2. RMSE screen plot of SPA operated based on the whole spectra for crude protein (a) and crude fat (b) in oats samples.

screen plot obtained by SPA based on the whole spectra for crude fat and crude protein, respectively. As can be seen, a sharp fall is shown in the starting part of the RMSE curve as the number of selected variables rises from 2 to 11 for crude protein and from 2 to 9 for crude fat, respectively. Then the trends of RMSE curves become marginal with further increasing number of selected variables. The selected wavelength variables were 411, 421, 474, 935, 937, 945, 962, 980, 986, 992 and 998 nm for the analysis of crude fat, and 423, 443, 488, 916, 932, 940, 943, 954, 959, 962, 989, 992 and 999 nm for crude protein. Most of the wavelengths selected were in the range from 900 to 1000 nm, and some differences in the spectra occurred in the special visible regions. A study has shown that using the 800 to 1100 nm region for fat and proteins to build the determination models can get reliable results (Šašić and Ozaki, 2001). However, this result does not mean that fat or protein is the component which causes these differences. There are other components which can influent the spectrum. The wavelength variables selected by SPA were set as the input variables of LS-SVM. Table 4 shows the validation

results for crude fat and crude protein analysis before and after the variable selection. The performance of full-spectra-LS-SVM and SPA-LS-SVM models was similar for both fat and protein analysis. However, the full-spectra-LS-SVM had more than six hundred variables while the SPA-LS-SVM model only had about ten variables. Therefore, the results show that the variables selected by SPA processing had the same useful information but with fewer variables than full-spectra.

As the fewer variables for calibration, less time was consumed for model establishment. Hence, the SPA-LS-SVM could be used effectively for application, with a small number of samples used for model establishment.

Conclusions

This study evaluated the feasibility of using Vis-NIRS technique as a fast and nondestructive method for the geographical origin discrimination and the component content prediction of oats. Geographical origin

Table 4. Predictive results of crude protein and fat determination in oats by full spectra-LS-SVM and SPA-LV-SVM models.

Component	Model	Variable	Calibration		Validation		
			r_{cal}	RMSEC	r_{val}	RMSEV	RPD
Crude fat	Full spectra-LS-SVM	601	0.978	0.187	0.931	0.311	2.341
	SPA-LS-SVM	13	0.930	0.323	0.915	0.389	2.309
Crude protein	Full spectra-LS-SVM	601	0.908	0.257	0.789	0.355	1.140
	SPA-LS-SVM	11	0.829	0.327	0.814	0.338	1.312

identifications were achieved using SIMCA and LS-SVM algorithms, respectively. The CAR of the SIMCA model was 75.0% and the LS-SVM model reached a higher CAR value of 98.3%. Thirteen and eleven wavelength variables were selected by SPA for crude fat and crude protein analyses. The correlation coefficients were 0.915 and 0.814, and the root mean square errors of validation were 0.389 and 0.338 for crude fat and crude protein, respectively. The result of crude fat validation was acceptable, while the crude protein determination still needs to be improved.

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