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Classifying the Variety, Production Area and Season of Taiwan Partially Fermented Tea by Near Infrared Spectroscopy

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ABSTRACT

The purpose of this study is to investigate the feasibility of discriminating the different varieties, production areas and seasons of Taiwan partially fermented tea by using Near Infrared Spectroscopy (NIRS). A total of 308 partially fermented tea samples with 6 different tea varieties, 6 production areas and 2 different production seasons were collected and analyzed. The principal component analysis (PCA) result of NIRS spectra data showed that the first three principal components could explain the sample variation up to 95.0%. The ability of classifying different production areas of tea samples by PCA was the best followed by tea varieties. The discriminant model further established by NIRS data with partial least square (PLS) could recognize and identify the varieties, production areas and seasons of tea samples up to 98.4% (299 of 305), 97.4% (296 of 304), and 100%, respectively. Using the established discriminant model, the tea samples with different varieties, production areas and seasons could be correctly predicted and identified at the levels of 96.3%, 94.1% and 99.2%, respectively.

Key words: partially fermented tea, discrimination, NIRS, PCA, PLS

INTRODUCTION

Tea is one of the most popular beverages worldwide. Tea can be classified into non-fermented tea, partially fermented tea and fully fermented tea according to the degree of fermentation during tea making(1). Among them, the partially fermented tea made in Taiwan (as Taiwan Oolong Tea) is famous worldwide due to its unique aroma and taste. Numerous chemical compounds in finished tea leaves are closely associated with sensory characteristics of partially fermented tea. Various kinds of partially fermented tea are created by different degrees of withering and fermentation (enzymatic oxidation) and ways of rolling(2). With well-developed manufacturing techniques, the partially fermented tea becomes the most important kind of tea in Taiwan.

Besides the different ways of tea making, different tea varieties, production areas and seasons of tea leaves are also the major factors influencing the quality, including the physicochemical and sensory characteristics of partially fermented tea(3). Furthermore, the price of different tea is mainly decided according to the quality of tea.

Recently, due to the vigorous competition in tea business, some sellers make profit unethically by taking cheaper, adulterated or fake tea to be high-quality Taiwan tea. In order to prevent such an illegal commercial behavior from occurring in the market, the chemical compositions of tea and DNA markers have been used to discriminate the different categories of teas(4,5). Nevertheless, to clearly classify the variety, production area and season of tea is considerably more urgent and important(6).

Near infrared spectroscopy (NIRS) was developed in 1960s. It was first used in cereal research and became a well-known analytical technique to substitute

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the traditional physicochemical analysis because it is fast, accurate and non-destructive[7,8]. Due to the well-improved instruments, advanced computers and statistical software, NIRS has been extensively used to analyze the components of foods such as cheese[9], milk[10], honey[11], mango[12], chicken[13,14], soy-bean sauce[15] and tea[16,17].

Discrimination of different origins, grades or compositions of food can be achieved by examining the chemical components of food with several chemometric techniques applied to data treatment like principal component analysis (PCA), soft independent modeling of class analogy (SIMCA), hierarchical cluster analysis (HCA), canonical analysis (CA), discriminant analysis (DA), principal component regression (PCR) and partial least square analysis (PLS)[18-23]. Traditional analyses of the chemical components of food are expensive and time consuming. In order to reduce the cost and time for discriminating food, NIRS can also be used in discriminating different categories of foods, like honey[24], herbal medicines[25], citrus oils[26], finishing oils[27] and distilled alcoholic beverages[28]. In terms of tea, Budínová *et al.* have used NIRS to classify the black tea, green tea and partially fermented tea[29], and He *et al.* have also used NIRS to classify different kinds of green tea[30]. However, for the well-known Taiwan Oolong tea, classifying the varieties, production areas and seasons of tea by using NIRS have not been investigated.

Therefore, in this study, the NIRS spectra of tea samples were used and combined with multivariate analysis to establish a ready-to-use model to classify the different production areas, varieties and production season of the partially fermented tea produced in Taiwan. PCA was first applied to ascertain the possibility of classification with NIRS spectra data of tea samples. The discriminant analysis with PLS was then applied to develop a discriminant model and finally the discrimination capability of the established model was evaluated.

MATERIALS AND METHODS

I. *Materials*

A total of 308 partially fermented tea samples were collected from famous tea contests held in Tao-Chu-Miao (TCM), Mu-Jha, Min-Jian, Lu-Ku, Jia-Yi and Tai-Dong in Taiwan during 2002 and 2003 as materials. They were collected from six different areas, including TCM, Mu-Jha, Min-Jian, Lu-Ku, Jia-Yi and Tai-Dong, with 25, 34, 52, 48, 60 and 89 tea samples, respectively; six different varieties, such as Chin-Shin Oolong (CSOolong), Taiwan Tea Experiment Station No.12 (TTES #12), Tieh-Kuan-Yin (TKYin), Chin-Shin Da-Pan (CSDPan), Shy-Jih-Chue (SJChue) and Taiwan Tea Experiment Station No.13 (TTES #13) with 178, 45, 34, 25, 13 and 13 samples, respectively; and two different production season, spring (including spring and summer) and winter, with 211 and 97 samples, respectively. All tea samples were pulverized by mill and screened through a 20-mesh sieve. The tea powders were then packed in the vacuum-packed bag and stored in a -80°C cold cabinet.

II. *Near Infrared Reflectance Spectra*

Samples (20-mesh) were mixed thoroughly before scanning. Spectra were taken by reflectance in a NIRSystem 6500 Spectrometer (Foss NIRSystems Co., MD, USA) with a transport module and acquired with a circular sample cup having a quartz window (38 mm in diameter and 10 mm in thickness). The spectrum for each tea sample was average of 32 scans performed at 2 nm intervals over the wavelength range 400-2500 nm. All spectra were recorded as log (1/R) with respect to a ceramic reference standard. A personal computer with the software WINISI II, from Infrasoft International[31] was utilized for operation of the spectrometer and to store and manage optical data. Each tea sample was scanned 5 times.

III. *Principal Component Analysis of Spectral Data*

The acquired spectral data from the WINISI II were transferred to ASCII file-type and exported into the *Unscrambler* 8.0.5 (CAMO PROCESS AS, Norway) software. Principal component analysis (PCA) was performed by the *Unscrambler* 8.0.5 (CAMO PROCESS AS, Norway). The 1050 spectral data points acquired by NIRS were regarded as 1050 variables. PCA can use a fewer new variables (principal components, PCs) instead of original ones. The samples scattered plots were drawn with PC1, PC2 and PC3 as dimensions x, y and z.

III. *Discriminant Equations for Tea Samples*

In order to discriminate the different production areas, varieties and production seasons of partially fermented tea in Taiwan, discriminant equations were developed by WINISI II with the partial least squares (PLS) regression technique[31]. Each category of different production areas, varieties or production seasons was analyzed by PCA, and sorted to a separated file[31]. The calibration matrices were set up with all the tea samples by creating 'dummy variables'. The tea sample was assigned a value of one if the spectrum belonged to a particular group (according to file name), or zero if it did not belong to that group. Calibration was then developed by regressing optical data on the 'reference values' (zero or one) of the dummy variables. Cross validation was used to test the accuracy of the calibration at each step, as a new PLS factor was added to the equation, until a minimum standard error of cross validation value was attained[14]. These procedures were used to model a discriminant function for categories of tea samples, with six files for production areas (Mu-Jha, TCM, Min-Jian, Lu-Ku, Jia-Yi and Tai-Dong), six files for varieties (CSOolong, TTES #12, TKYin, CSDPan, SJChue and TTES #13) and two files for production seasons (spring and winter).

V. *Prediction Abilities of Discriminant Equations*

Each category of tea samples was divided into training set and testing set(30). The tea samples in the training set were used to establish the discriminant model, and the samples in testing set were used to evaluate the discrimination ability of the established discriminant model. The tea samples in two sets were randomly selected by using the WINISI II software, and the ratio of samples in training set and in testing set was about 6:1. The two steps, to set the training and testing sets and to evaluate the discrimination ability of the established model, were repeated ten times for the evaluation of the prediction ability.

RESULTS AND DISCUSSION

I. *Categories of Partially Fermented Tea Samples*

The partially fermented tea samples included 274 Oolong tea and 34 TKYin tea samples. With regard to the variety of 308 tea samples, CSOolong was the major one among the six varieties (57.6%), while the SJChue and TTES #13 varieties were the least. The variety of the tea samples collected from Jia-Yi and Tai-Dong were exclusively CSOolong and TTES #12, while the variety of tea samples collected from Min-Jian was varied including CSOolong, SJChue, TTES #12 and TTES #13.

II. *NIR Spectra of Partially Fermented Tea Samples*

Averaged absorbance of near infrared radiation for tea samples are shown as log (1/R) in Figure 1, where the spectra of each production area, variety and production season are presented in Figure 1A, 1B and 1C, respectively. These three figures all show strong absorption bands at 1730 nm and 1940 nm. The absorption band at 1730 nm is related to the CH and CH_2 bonds, and at 1940 nm is related with OH bonds of water(32). The differences in the spectra among different production areas, varieties and production seasons were extremely small throughout the near infrared region (1100 nm to 2498 nm). The results were similar to those of He *et al.*(30) and Li *et al.*(33) showing the small differences in the NIR spectra among different varieties of tea and Chinese bayberry, respectively. The differences in the spectra among different categories of tea sample were obvious throughout the visible region (400 nm to 1100 nm). These should be due to the difference in color among different categories of partially fermented tea samples(33,34).

In order to reduce the effects of factors such as size, water content, *etc.* causing baseline shifts, to increase the resolution of over-lapping peaks, and to emphasize the useful spectral information, a mathematic treatment of "2-5-5" was used with the raw spectral data. The first numeral "2" meant that the differential treatment of spectrum was second derivative, the second numeral "5" meant the number of data points over which the derivative was calculated was 5 data points over a gap, and the third numeral "5" meant the number of data points to be averaged for data smoothing was 5 data points(31). The new spectra with the mathematic treatment mentioned above were shown as Figure 2 (400-2498 nm). It can be seen that the baseline shift had been almost eliminated. The tea samples of different production areas and varieties were better classified with the absorption peak at 720 nm (Figures 2A and 2B). He *et al.* also observed the small difference between the 2nd NIR spectra of different varieties of tea(30). For different production seasons, the tea samples were better classified with the absorption peak at 1404 nm (Figure 2C).

III. *Principal Component Analysis with NIR Spectra of Partially Fermented Tea Samples*

As the NIRS data of different categories of tea

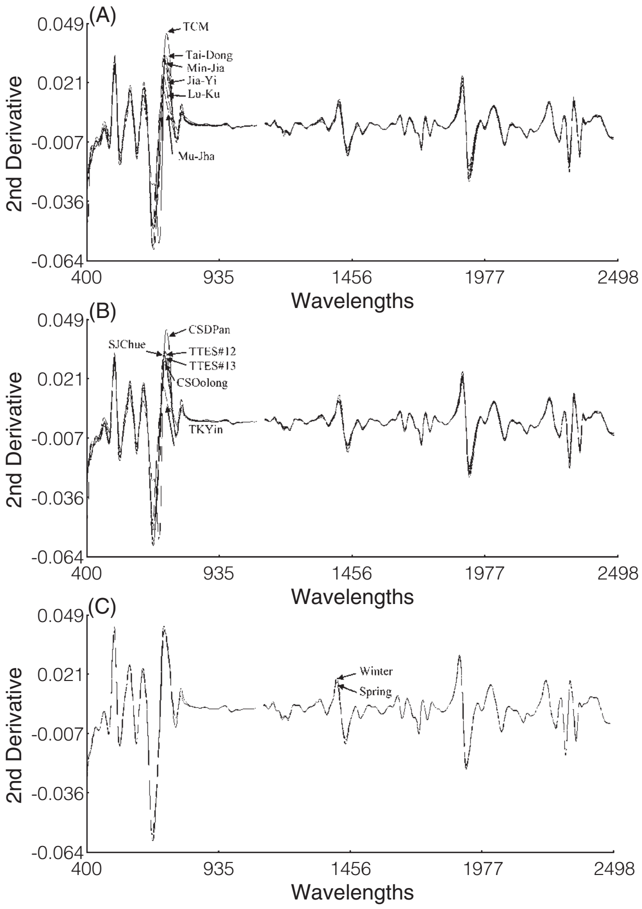

Figure 1. The averaged NIR spectra, as log (1 / R), for tea samples. Samples from (A) different production areas, (B) different varieties and (C) different production seasons.

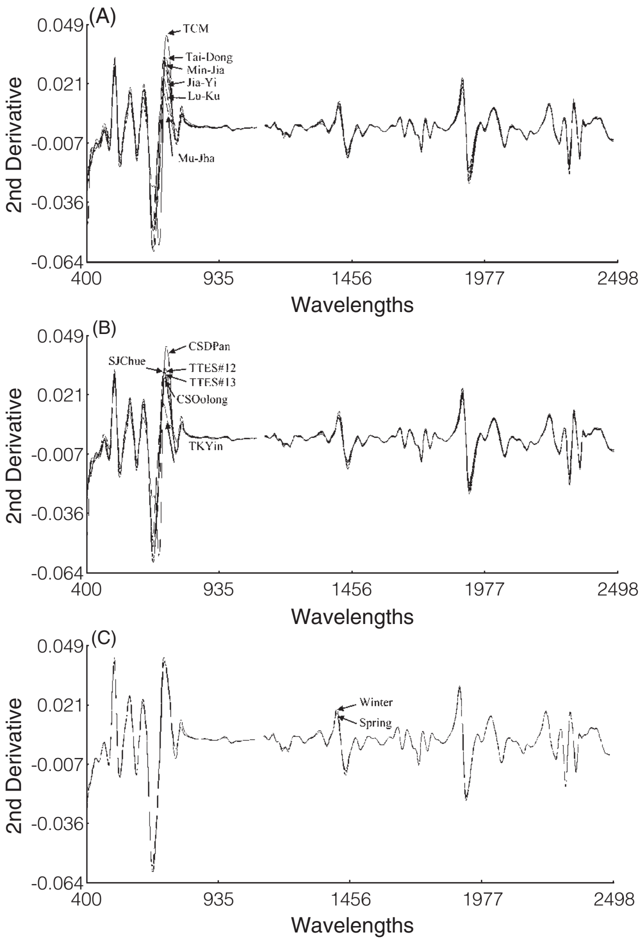

Figure 2. The averaged NIR spectra, as second derivative, for tea samples.
Samples from (A) different production areas, (B) different varieties and (C) different production seasons.

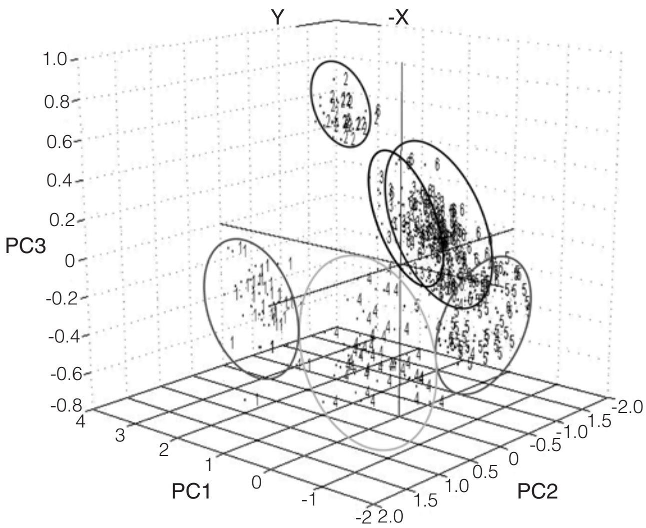

Figure 3. Principal component analytical results for the partially fermented tea samples with six different production areas.
1: Mu-Jha, 2: TCM, 3: Min-Jian, 4: Lu-Ku, 5: Jia-Yi and 6: Tai-Dong.

samples exhibited small difference, using univariate analysis was not appropriate to analyze the data sets. Multivariate analysis techniques such as PCA made it possible to extract information related to the NIR data[25,35]. In this study, PCA was used to visualize the categories of the tea samples, and to develop criteria for selecting variables to classify the categories of tea samples. The spectra of 308 tea samples were analyzed by PCA. The 67, 22 and 6% of variation in tea samples were explained by the first three PCs, respectively. Figures 3, 4 and 5 showed the score plots of the first

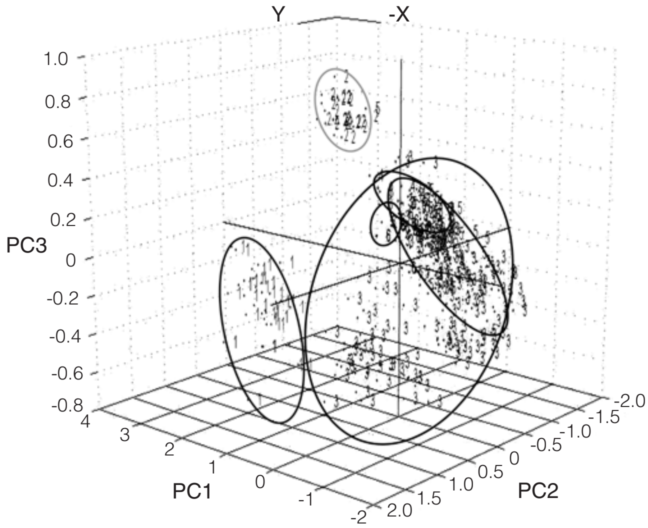

Figure 4. Principal component analytical results for the partially fermented tea samples with six different varieties.
1: TKYin, 2: CSDPan, 3: CSOolong, 4: SJChue, 5: TTES #12 and 6: TTES #13.

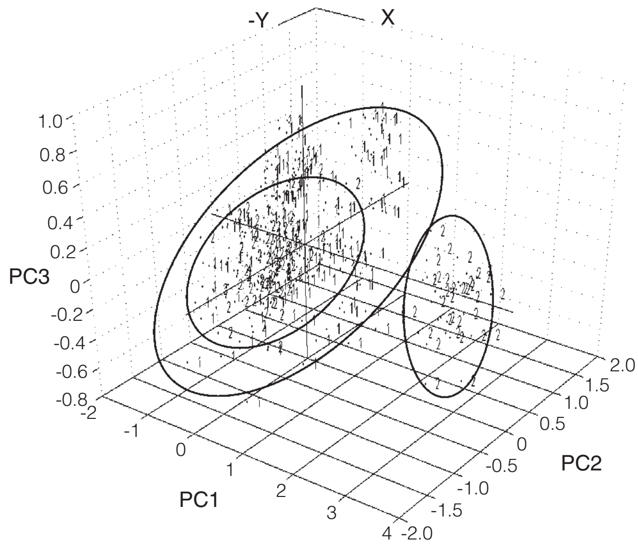

Figure 5. Principal component analytical results for the partially fermented tea samples with different production seasons.
1: spring and 2: winter.

three PCs in different classification of tea samples with production areas, varieties and production seasons, respectively. It was shown the score plots could display the information of categories from multiple wavelengths.

In Figure 3, six different production areas were grouped into 6 loops. The tea samples from either Mu-Jha (#1) or TCM (#2) were well separated from others. It is due to the variety of tea samples from Mu-Jha and TCM was thoroughly TKYin and CSDPan, respectively, which were different from those of other production areas. The majority of tea samples in Lu-Ku (#4) seems like also well separated from others, but some of them were still mis-located in other areas and the other way around as well.

The tea samples collected in the famous tea contest held in Lu-Ku were exclusively the Dongding-Oolong tea. For this kind of tea, both enzymatic oxidation in withering and non-enzymatic oxidation in roasting during the process of tea making are very important, and roasting is the key procedure in the formation of its special sensory attributes[36]. It caused the Lu-Ku loop well separated from others. However, the varieties of tea samples collected from Lu-Ku was exclusively the CSOolong while the varieties of tea samples collected from Min-Jian, Jia-Yi and Tai-Dong were either TTES #12, TTES #13, SJChue, CSOolong or mixed. The loops of Min-Jian (#3), Jia-Yi (#5) and Tai-Dong (#6) were found not well separated. It is because the methods of tea-making for their partially fermented tea were quite similar and the tea varieties they used were mixed.

Using NIRS to classify the production areas of Riesling wines, Liu *et al.* pointed out that the wines were all over-lapped in the plots of PCA[37]. The results of He *et al.* also showed that the PCA score plots for eight kinds of green tea were slightly over-lapped[30]. By comparison, the separation among the production areas of tea samples in this study was better than those by Liu *et al.*[37] and comparable with the results of He *et al.*[30]. Basically, the regionally special teas in every different production areas of Taiwan are well established. The particular characteristics of each tea are almost unique in different production areas[38]. It is well reflected on the use of NIR spectra of different areas of tea samples to separate them.

The results shown in Figure 4 for varieties were closely related to that in Figure 3. The tea samples with varieties of TKYin (#1) and CSDPan (#2) were thoroughly collected from Mu-Jha and TCM, respectively. Therefore, these two groups were well separated from others. The groups of TTES #12 (#5), TTES #13 (#6) and SJChue (#4) were separated roughly, but some tea samples were slightly over-lapped one another. The loop of CSOolong (#3) tea samples covered those of TTES #12, TTES #13 and SJChue. It was just because some of tea samples collected from Min-Jian, Lu-Ku, Jia-Yi and Tai-Dong were also made by CSOolong variety.

In terms of production season, only TKYin tea samples collected in winter were well separated from that in spring as shown in Figure 5. However, other tea samples collected in spring or winter were mixed together. It was caused by the interaction of different varieties and production areas.

In brief, the classification ability of PCA with NIR spectra for different production area of tea samples was better than those for varieties and production seasons.

IV. *Discrimination of Partially Fermented Tea Samples with NIR Spectra*

The discriminant analysis based on PLS was utilized with NIR spectra. Spectra files for calibration with the information of PCA were established by the ISI software[31]. The discriminant method utilized not only the spectral data itself but also the external information of the origin of tea samples based on different production areas, varieties and production seasons[22,25]. In order to increase the discriminant abilities of equations, the outlier samples were first purged from the calibration set by WINISI II software. Total six calibrations were developed by applying several mathematic treatments to obtain discriminant equations, in order to recognize tea samples to a particular production area, variety or season. The two spectral pre-treatments included "no pre-treatment" and "standard normal variate (SNV) with detrend". After spectral pre-treatments, the derivations of spectra including non-derivative, first and second derivative were carried out. The results were shown in Table 1.

The results showed the best model developed for recognizing production area was able to correctly identify 97.4% (296 of 304, 4 out of 308 samples were purged as outlier) of the tea samples (Table 1). The spectral pretreatment was "no pre-treatment" with spectral data. The second derivative were used in the mathematic treatment with a gap of 5 data points and 5 data points averaged for data smoothing (2-5-5). The PLS terms of the model was 15.

The best model developed for recognizing the variety was able to correctly identify 98.4% (299 of 305, 3 out of 308 samples were purged as outlier) of tea samples. The condition terms of the model were the same as the model of production area except the PLS term which was 14. The percentage of correct identification of model with different condition terms developed for recognizing production season of tea samples listed in Table 1 were all 100%.

The discrimination results of 304 partially fermented tea samples from different production areas by NIR spectra data with best PLS model in Table 1 were shown in Table 2. 100% of tea samples from Mu-Jha, TCM and Min-Jian were classified correctly. Four tea samples collected from Lu-Ku were misclassified into different production areas (three were misclassified as Jia-Yi, and one was misclassified as Tai-Dong). The

Table 1. Classification of partially fermented tea samples with production area, variety and production season by NIR discriminant equations with 6 different mathematic treatments

Category		Area				Variety				Season			
Pre-treatment	Derivative	PLS[c] terms	No. of samples	No. of Correctly classified	% of correctly classified	PLS terms	No. of samples	No. of Correctly classified	% of correctly classified	PLS terms	No. of samples	No. of Correctly classified	% of correctly classified
No [a]	0	15	304	276	90.79	15	305	279	91.80	15	274	274	100
	1	15	304	289	95.07	15	305	297	97.70	10	274	274	100
	2	15	304	296	97.37	14	305	299	98.36	10	274	274	100
SNV[b] & Detrend	0	12	304	281	92.43	15	305	286	94.10	12	274	274	100
	1	13	304	289	95.07	14	305	295	97.05	12	274	274	100
	2	14	304	293	96.38	14	305	298	98.03	9	274	274	100

[a] no pre-treatment.
[b] standard normal variate.
[c] partial least square.

percentage of incorrect discrimination was 8.5%. Three tea samples collected from Jia-Yi were misclassified as Tai-Dong, and one tea sample collected from Tai-Dong was misclassified as Jia-Yi. The percentage of incorrect discrimination was 5.1% and 1.1%, respectively. Totally 97.4% of the tea samples were correctly identified as the particular areas with PLS model.

For variety, the discrimination results of 305 partially fermented tea samples from different varieties by NIR spectra data with best PLS model in Table 1 were also shown in Table 3. All the tea samples with variety of TKYin, CSDPan and SJChue were classified correctly. Only one TTES #12 tea sample was misclassified as SJChue variety, one TTES #13 tea sample was misclassified as TTES #12 variety, and three CSOolong tea samples were misclassified as TTES #12 variety. The percentage of incorrect discrimination for TTES #12, TTES #13 and CSOolong varieties was 2.3%, 8.3% and 1.7%, respectively. Totally 98.4% of the tea samples with PLS model were correctly identified as the particular variety. Chen *et al.* classified the black tea, green tea and Oolong tea samples by using NIRS. Their results showed that the percentage of correct discrimination reached to 95.0%[(39)].The information of misclassified tea samples were shown in Table 4. In term of production area for tea samples, Jia-Yi and Tai-Dong were both in the high-altitude production areas and misclassified. The variety of tea samples collected from Lu-Ku was exclusively CSOolong. The majority of tea samples from Jia-Yi and Tai-Dong were CSOolong too. Because the characteristics of NIR spectra were similar among the tea samples of the same variety, it is understandable that the tea samples collected from Lu-Ku, Jia-Yi and Tai-Dong were misclassified more easily.

The tea samples in our study were collected from famous tea contests, and the grades were judged[(40)]. In term of varieties, 4 of the 5 tea samples that were misclassified in Table 4 were low-grade tea. It indicated that the uniformity of the tea sample quality was very important for the discriminant model.

The classification results of the PCA (Figures 3 to 5) and PLS (Tables 2 and 3) of partially fermented tea samples exhibited small difference just due to the variation of different production areas, varieties and production seasons. The PCA may use a few new synthetic variables (principal components, PCs) instead of original ones[(25)]. In order to increase the separation ability of PCA, category variables are usually added with PCA. The score plots of PCA with and without categories were different because of the participation of category variables[(41)]. The PCA results obtained in this study did not include the category variables while the discriminant analysis based on PLS to obtain the discriminant model did. It carried out not only the spectral data itself but also the external information about the origin of tea samples based on different production areas, varieties and production seasons which were equal to the information

Table 2. Classification results of 304 partially fermented tea samples with different production areas by NIR spectra with PLS model

From \ To	Mu-Jha	TCM	Min-Jian	LuKu	Jia-Yi	Tai-Dong	Total error	Error (%)
Mu-Jha	34[a]	0	0	0	0	0	0	0
TCM	0	25	0	0	0	0	0	0
Min-Jian	0	0	51	0	0	0	0	0
LuKu	0	0	0	43	3	1	4	8.51
Jia-Yi	0	0	0	0	56	3	3	5.08
Tai-Dong	0	0	0	0	1	87	1	1.14
The percentage of successful discrimination: 97.37%								

[a] number of samples classified.

Table 3. Classification results of 305 partially fermented tea samples with different varieties by NIR spectra with PLS model

From \ To	TKYin	CSDPan	CSOolong	SJChue	TTES #12	TTES #13	Total error	Error (%)
TKYin	34[a]	0	0	0	0	0	0	0
CSDPan	0	25	0	0	0	0	0	0
CSOolong	0	0	174	0	3	0	3	1.69
SJChue	0	0	0	13	0	0	0	0
TTES #12	0	0	0	1	43	0	1	2.27
TTES #13	0	0	0	0	1	11	1	8.33
The percentage of successfully classfied: 98.36%								

[a] number of samples classified.

Table 4. Information of misclassified partially fermented tea samples

Category	Sample ID	Production area	Variety	Production season	Grading rank[a]	misclassified into
Production area	IIS076	LuKu	CSOolong	Spring	1	Jia-Yi
	IIS077	LuKu	CSOolong	Spring	1	Jia-Yi
	IIS078	LuKu	CSOolong	Spring	1	Jia-Yi
	IIS080	LuKu	CSOolong	Spring	1	Tai-Dong
	IIS061	Jia-Yi	CSOolong	Spring	1	Tai-Dong
	IIS070	Jia-Yi	TTES 12	Spring	1	Tai-Dong
	IIS074	Jia-Yi	TTES 12	Spring	1	Tai-Dong
	IS054	Tai-Dong	CSOolong	Spring	2	Jia-Yi
Variety	IWO031	Tai-Dong	TTES 12	Winter	3	SJChue
	IIS054	Min-Jian	TTES 13	Spring	1	TTES #12
	IS029	Tai-Dong	CSOolong	Spring	4	TTES #12
	IS030	Tai-Dong	CSOolong	Spring	4	TTES #12
	IS031	Tai-Dong	CSOolong	Spring	4	TTES #12

[a] grade 1 is the highest while grade 4 is the lowest.

Table 5. Prediction results of 10 testing sets with established discriminant model for partially fermented tea samples with different categories

Category	No. in training set[a]	No. in test set[b]	No. of misclassified	% of classified
Area	2600	440	26	94.10
Variety	2590	460	17	96.30
Season	2350	390	3	99.23

[a] tea samples in training set were selected to establish the discriminant model and repeated ten times.
[b] tea samples in test set were selected randomly from all the tea samples and repeated ten times.

of category variables(22,25).

It was summarized that the condition terms of the best identification model developed for recognizing production area, variety and production season for tea samples were "no pre-treatment" with spectral data and second derivative (2) in the mathematic treatment with a gap of 5 data points and 5 data points averaged for data smoothing (2-5-5).

V. *Prediction Ability of the Discriminant Model for Partially Fermented Tea Samples*

In previous section, the discriminant model established with NIRS using the established condition and procedure was found useful to identify the categories of tea samples. In order to evaluate the discrimination ability of the discriminant model further, and to confirm the feasibility of the established model, the prediction test was carried out. The evaluation results for predicting different production areas, varieties and production seasons were shown in Table 5.

The percentages of correct discrimination of the production areas, varieties and production seasons were 94.1%, 96.3% and 99.2%, respectively. They were close enough to the results from the discriminant model established in previous section. It indicated that the condition terms of discriminant equations were useful to establish the effective discriminant model, and the discriminant model established in this study had a good ability to discriminate the partially fermented tea samples among different production areas, varieties and production seasons.

CONCLUSION

The study indicates that near infrared spectroscopy has significant potential for discrimination of different production areas, varieties and production seasons of Taiwan partially fermented tea samples. The discriminant model with principal component and partial least square analyses by NIRS was able to discriminate the different categories of Taiwan partially fermented tea samples with accuracy up to 94%-99%. These results were higher than those in other studies and more detail of tea samples could be discriminated using our model. However, in order to improve the calibration specificity, accuracy and robustness of the model, it still requires more tea samples of different categories for further development.

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