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Application of terahertz spectroscopy and chemometrics for discrimination of transgenic camellia oil

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ABSTRACT

Discrimination of transgenic edible oil has become the focus of attention in the field of food safety. In this paper, we propose a method for discrimination of transgenic edible oils by using terahertz spectroscopy combine with weighted linear discriminant analysis (WLDA). To evaluate the lustiness of the model, we employ successive projection arithmetic (SPA) and partial least squares (PLS) to verify the discrimination performance through variable selection. The results demonstrate that the SPA-WLDA model has higher classification accuracy than PLS-WLDA. In conclusion, terahertz spectroscopy is coupled with chemometrics is an effective method for discriminating various types of transgenic edible oils.

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1. Introduction

The main goal for transgenic technology of oil crops is to increase oleic acid content at the expense of palmitic acid [1–4]. With the development of biotechnology, more and more transgenic edible oil appears in public. The transgenic technology can promote the development of human society in some ways, but at the same time, it can also pose a threat to human health ecological environment [5–9]. Therefore, how to quickly and effectively identify transgenic oil become very important.

As a nondestructive detection tool, spectroscopy technology has been widely used in the detection of edible oil. Dahlberg et al. combine mid-infrared (MIR) spectroscopy with PLS to measure the chemical parameters (refraction index and viscosity) in different types edible oils and margarines [10]. Nunes using vibrational spectroscopy and chemometrics to develop a methodology based on vibrational spectroscopy and chemometrics to evaluate the quality parameters of edible oil and fats [11]. Luna et al. presents a method which using near-infrared spectroscopy chemometrics methods to identify transgenic soybean oil from non-transgenic soybean oil samples [12]. To evaluate the iodine index of edible oils, the Raman spectroscopy and partial least squares (PLS) were applied by Barthuset [13]. Koidis et al. [14] proposed a

methodology which combine spectroscopy with chemometrics technique to correct label different types vegetable oils.

Terahertz is an electromagnetic wave which local in between the microwave and far-infrared, it has a dual characteristic of electronics and optics. Research shows that rotation and vibration level of many biological molecular is in terahertz band. Due to its unique fingerprint spectrum characteristics, THz spectroscopy has become one of the most dynamic fields of scientific research [15–21].

Therefore, the combination of terahertz spectroscopy with chemometrics is a powerful tool of detection edible oil. It is mainly used for quality control in food science because of its advantage that needs no pretreatment of the sample, fast and excellent results. Based on these characteristics, the purpose of this paper is to propose a novel method for the discrimination of transgenic edible oil samples using terahertz spectroscopy combine with chemometrics.

2. Theory and Algorithm

2.1. Principal Component Analysis (PCA)

PCA is a feature extraction method, it is capable of linear combination of multiple independent variables according to the principle of maximum variances, and replace the original variable with a small number of synthetic variables [22,23]. The datamatrix X is expressed by a linear model in an equation shown below: $X = TP^T + E$. Where,

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T is the scores matrix ($n \times k$), P is the loadings matrix ($m \times k$) and E is the error matrix.

2.2. Weighted Linear Discriminant Analysis (WLDA)

In order to reduce the dominant effect of edge classes on the projection direction, the weight value are introduced in the LDA. This paper develops a simple weighting function. In subspace, the distribution matrix between classes is defined as follows:

$$S_b'' = \sum_{i=1}^{K-1} \sum_{j=i+1}^K P(c_i)P(c_j) \times \omega(d_{ij})(M_i' - M_j')(M_i' - M_j')^T$$

$$\omega(d_{ij}) = \frac{\eta_{bij}d_{ij}^{-4}}{\sum \eta_{bij}d_{ij}^{-4}}$$

In this equation, M_i' is the i -th samples in subspace A; d_{ij} express a Mahalanobis distance between two types of samples (i -th and j -th); $\omega(d_{ij})$ is a decreasing function of about d_{ij} .

According to the above, The S_w'' is redefined as:

$$S_w'' = \sum_{i=1}^K P(c_i)\eta_{wi}E \times \{(x_i' - M_i')(x_i' - M_i')^T | x_i' \in c_i\}$$

In this equation, η_{wi} is the correction coefficient. Under normal circumstances, the fact that $\eta_{wi} = 1$, if you want to improve the classification rate, you can increase the corresponding correction coefficient.

Considering the scatter matrix within a class may be singular, the improved Fisher criterion is described as:

$$J(W') = \left| \frac{W'^T S_b'' W'}{W'^T S_t'' W'} \right|$$

where $S_t'' = S_w'' + S_b''$, because of $S_w'' \geq 0$ and $S_b'' \geq 0$, so $S_t'' \geq 0$.

3. Experimental

3.1. Samples

The transgenic and non-transgenic camellia oils with the purity of above 99% are supplied by Sigma-Aldrich Shanghai Trading Co., Ltd. A total of 100 samples (50 transgenic samples and 50 non-transgenic samples) of similar size are prepared in this paper. All transgenic camellia oil samples are distinguished and labeled as transgenic and non-transgenic by the manufacturers. The physicochemical quality parameters of samples are extracted by the standard physicochemical analytical methods. The parameters of samples are shown in Table 1.

Table 1
The parameters of 100 camellia oil samples.

Category/samples	Parameters		
	Acidity in %	Polyphenols (g/L)	Peroxide index (meq O ₂ /kg)
Transgenic camellia oil, 50 samples			
Min	0.36	3.67	8.61
Max	0.58	2.49	16.36
Mean	0.47	6.78	6.97
STD	0.29	3.60	7.83
Non-transgenic camellia oil, 50 samples			
Min	0.45	4.57	2.71
Max	0.59	7.39	14.36
Mean	0.38	4.58	8.97
STD	0.31	5.50	4.39

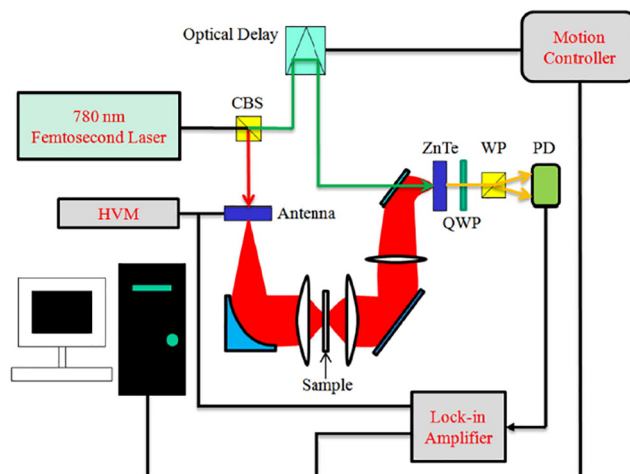


Fig. 1. Experimental setup of the THz-TDS system.

3.2. Spectra Acquisition and Data Analysis

Terahertz spectra are obtained by using the THz time-domain spectrometer (Zomega Terahertz Corp., USA), where the center wavelength as the laser is 780 nm. To ensure the accuracy of the experiment, in the system, dry air is injected until the internal relative humidity to 2% below. Indoor relative humidity is 25%, and the temperature is 292 K. The standard spectrum is gathered before measure each sample. Fig. 1 shows the Z-3 THz time-domain spectrometer.

The absorbance spectra of samples ranged from 0.1 THz–1.5 THz is shown in Fig. 2(a), (b) and (c), respectively. As can be seen from Fig. 2, there are associated information with functional groups, such as C–C, CH₂, CH₃, C–O and C=O, directly involved with camellia oil's oxidation process in terahertz range (the scope of this paper focuses on 0.1 THz–1.5 THz). This suggests that the terahertz spectrum data contains a large number of physical and chemical information of camellia oils and can, which can be evaluated by a multivariate method.

3.3. Principal Component Analysis (PCA)

The score plot of PC1 × PC2 which resulting from application PCA to different spectrum data (such as raw, offset and derivative), respectively, are shown in Fig. 3a–c. It can be seen from Fig. 2 that most samples are divided into two groups (transgenic and non-transgenic)

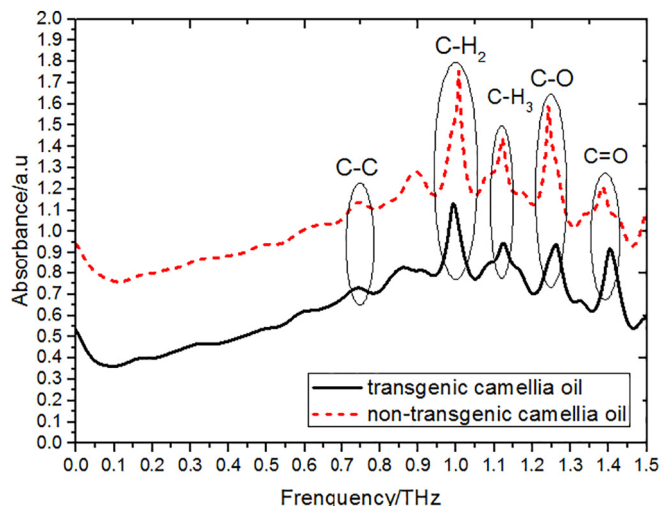


Fig. 2. The absorbance spectra of samples.

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