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# Using terahertz spectroscopy to identify transgenic cottonseed oil according to physicochemical quality parameters



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#### ABSTRACT

This study proposed a non-destructive and rapid distinguish methodology for transgenic cottonseed oil according to physicochemical quality parameters applying terahertz spectroscopy and chemometric tools. 50 samples of transgenic cottonseed oils, belong different manufacturers, are used in this paper. The physicochemical quality parameters of cottonseed oils are estimated by GB/T 22223-2008. Terahertz spectra are employed in data preprocessing by of Savitzky–Golay derivative and offset baseline correction after principal component analysis (PCA). The linear discriminant analysis combines with successive projection algorithm (SPA-LDA) and discriminant analysis by partial least squares (PLS-DA) are applied to build identification models. in order to evaluate the performance of these identification models, 50 samples are divided into two groups, including training setsand test sets, by using different selection methods (Kennard-Stone, Duplex and Random). The obtained results show that the terahertz spectra can be apply as an alternative to identify different transgenic cottonseed oil from non-transgenic ones.

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#### 1. Introduction

Edible oil is a complex organic compounds, which mainly about is triglycerides, in which the  $\alpha$ -linolenic acid and linoleic acid cannot be synthesized in body and must obtain from food. It has the very high nutritional value and can reduce blood fat and cholesterol. The quality of an oil can be evaluated by the value of acid, peroxide and so on. Different kinds of oil have different value of fatty acids and n6/n3.

The transgenic oil is an oil distilled from the transgenic plant. The transgenic is a biotechnology focus on increase biological resistance and products by implantation of exogenous gene [1–4]. Although the transgenic technology can ameliorate the production and resistance of plant to some extent, the transgenic food is a huge threat for human health and ecological environment [5–8]. Therefore, it is importance to research a fast and non-destructive method for identify transgenic oil. Several physicochemical analytical methods can be used to distinguish different type of transgenic oils, such as acidity,

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peroxide value, phenols, k232, k270 which depicted by IOC regulation [9–12]. However, these methods are laborious, high costs, time consuming, and need a lot of chemical reagents.

Recently, Other analytical techniques including spectroscopy, Raman scattering have been developed by scholars. Dahlberg et al. using mid-infrared (MIR) and PLS successfully to identified transgenic edible oils from margarines. Catharino, Martin et al. [13,14] using chemometrics method, such as ESI–MS and LDA, to characterizes edible oils. Barthus et al. [15] applied Raman spectroscopy and partial least squares (PLS) to measure the iodine index of edible oils. Luna, Silva et al. [16,17] proposed a method which using near infrared (NIR) spectroscopy combined with chemometrics methods to identify transgenic soybean oil samples from non-transgenicones. Aparicio et al. [18] contrasted spectroscopy with high performance liquid chromatography (HPLC) in the identification of adulteration of olive oil samples. Koidis et al. [19] developed a novel discriminate methodology which coupled spectroscopy to chemometrics technique for correct label vegetable oils. Nunes et al. [20] proposed a novel method to evaluate the authenticity of quality parameters of edible oil and fats by using absorption spectroscopy and chemometrics.

This paper proposed a non-destructive and rapid method which using terahertz spectroscopy couple with SPA-LDA and PLS-DA, respectively to distinguish transgenic cottonseed oil with the physicochemical quality parameters. The result shows that the proposed method can replace the standard analytical methods for fast and nondestructive classification of transgenic cottonseed oil.

#### 2. Materials and methods

#### 2.1. Materials

The transgenic and non-transgenic cottonseed oils are supplied by Sigma-Aldrich Shanghai Trading Co., Ltd. A total of 50 samples (25 transgenic samples and 25 non-transgenic samples) are prepared in this paper. All oil samples are labeled as transgenic and non-transgenic by the manufacturers.

#### 2.2. Physicochemical quality parameters

The physicochemical quality parameters of oils (including Acidity, Polyphenols, Peroxide index, K232 and K270) of cottonseed oil samples is estimated by GB/T 22223-2008. The physicochemical quality parameters of samples are extracted by IOC regulation.

#### 2.3. Spectra acquisition

The spectra of cottonseed oil samples are obtained by using the THz time-domain spectrometer which the center wavelength of the laser is 780 nm. In the experiment, the relative humidity of the internal system should be restricted to 2%

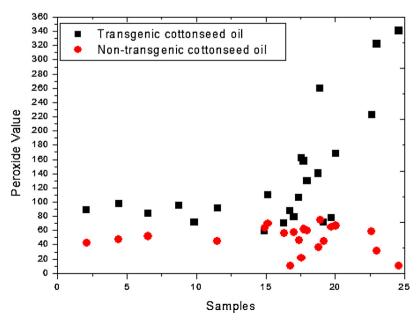


Fig. 1. Peroxide value of transgenic and non-transgenic cottonseed oil samples.

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