Accepted Manuscript

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PII:	S1386-1425(18)30710-8
DOI:	doi:10.1016/j.saa.2018.07.056
Reference:	SAA 16325
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	28 May 2018
Revised date:	12 July 2018
Accepted date:	18 July 2018

Please cite this article as: Xiaodong Yang, Guanglin Li, Jie Song, Mingju Gao, Shengling Zhou , Rapid discrimination of Notoginseng powder adulteration of different grades using FT-MIR spectroscopy combined with chemometrics. Saa (2018), doi:10.1016/j.saa.2018.07.056

Rapid discrimination of Notoginseng powder adulteration of different grades using FT-MIR spectroscopy combined with chemometrics

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Abstract: Panax notoginseng is a kind of herb material with high medicinal value, which requires adaptive planting environment, and not can be continuously cultivated in the same ground. Those reasons lead to a large number of low-grade Notoginseng appears in the market. The objective of this study is to discriminate adulterant of Notoginseng of different grades by FT-MIR spectroscopy couple with chemometrics. In the experiment, high-grade Notoginseng was adulterated with 14 blend ratios: 0%, 1%, 3%, 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, and 100% of low-grade Notoginseng. All samples were scanned in the range of 4000-400cm^{-1} by FT-MIR spectra instrument in absorption mode. Baseline, standard normal variate (SNV), multiplicative scatter correction (MSC), orthogonal signal correction (OSC), first derivative (D1) with 11-points smoothing and second derivative (D2) with 11-points smoothing were used to preprocess the spectral data, in which Baseline combined with SNV and D1 with 11-points performed best. The spectral data in the range of 1485-405cm^{-1} were selected by interval partial least squares (iPLS) for modeling. Then, Support vector machine (SVM) and linear discriminant analysis (LDA) were applied for modeling analysis. The best result was achieved by SVM, as the classification accuracy was 100%, which indicated that FT-MIR spectroscopy combined with chemometrics was an effective approach to identify Notoginseng powder adulteration. It could detect the blend ratio of 5% (w/w) as well as the blend ratio of over 5%.

Keywords: Panax notoginseng; FT-MIR; PLS; PCA; SVM; LDA

1. Introduction

Notoginseng (the root of Panax notoginseng (Burk) F. H. Chen), a species of the genus Panax, is a renowned and precious traditional herb in China. According to the records, it has been used in China for 600 years [1]. Notoginseng has a long history, and human beings are also rich in the experience of using it as a traditional herb material. However, the planting is still very difficult to fulfill stringent environmental conditions (temperature, humidity, altitude, etc.) [2]. Notoginseng is mainly cultivated in the southwest of China, especially in the Yunnan province [3]. The root, stem, leaf, and flower of Panax notoginseng are commonly used to cure a variety of civilization diseases [4]. And the root of Panax notoginseng is bigger, which is more expensive as a part of primarily medicinal value. Normally, it is distinguished by "Tou" (T, the number of Notoginseng in every 500g). The price of 20T Notoginseng is more than 3 times as expensive as the Notoginseng of greater than 100T.

Due to its high medicinal value and cost, there are a large number of counterfeit Notoginseng in the market, which has an adverse effect on the safety of clinical medicine and the health of consumer. However, not only the color but also the taste of counterfeit Notoginseng is

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