

## Analysis of fingerprints features of infrared spectra of various processed products of *Radix Aconiti kusnezoffii*

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### ABSTRACT

Fourier-transform infrared spectroscopy (FTIR) and two-dimensional correlation infrared spectroscopy (2D-IR) are employed to analyze various processed products and ether extracts of *Radix Aconiti kusnezoffii*. There is a resemblance among the spectra of different processed products. The major difference lies in the absorption peak at  $1641\text{ cm}^{-1}$  in the IR spectra, which reflects the transformation of raw aconite to the processed products. There are distinctive differences in the absorption peaks in the range of  $1800\text{--}1500\text{ cm}^{-1}$  in the second derivative spectra, which has better resolution, of different processed products. 2D-IR spectra, which elevate the resolution further, can present even more differences among the products in the range of  $1800\text{--}800\text{ cm}^{-1}$ . Analysis of ether extracts of various processed products proves that there are alcohols, esters, carboxylic acids or ketones in all of them. However, their contents in different samples have obvious differences. With the advantages of high resolution, high-speed and convenience, IR can quickly and precisely distinguish various processed products of *Radix A. kusnezoffii*, and can be applied to predict the tendency of transformation of the complicated chemical mixture systems under heat perturbation.

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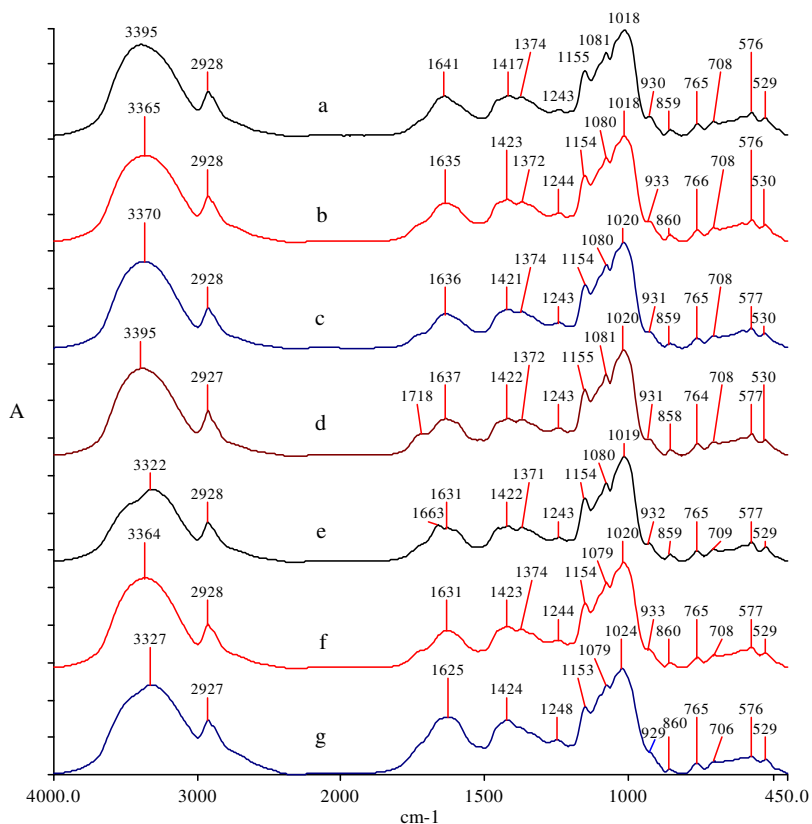
## 1. Introduction

*Radix Aconiti kusnezoffii*, named *CaoWu* in China, is the dry root of *Aconitum kusnezoffii* Reichb., which belongs to the plant family of Ranunculaceae. It has the pharmaceutical functions, in the traditional Chinese medical terminology, of expelling wind, removing dampness and warming the channels to alleviate pain. The principal components of aconitine, hypaconitine and mesaconitine of *CaoWu* are not only efficacious but also poisonous. In order to reduce the toxicity, it is necessary to process raw *CaoWu* before it becomes pharmaceutically acceptable. The toxicities of different processed products vary with the processing methods. Therefore, it is important for the quality control of *CaoWu* to find a method which can quickly and precisely distinguish different processed products. Presently, spectrophotometry, TLC scanning and HPLC are often employed. [1–3] However, it is complicated to prepare samples for such analysis, and limited diagnostic information, difficulty in obtaining quantitative results and high price are obvious deficiencies.

Combining modern FTIR, which has higher signal-to-noise ratio and reproducibility, with 2D-IR offering higher resolution and enriched information, we can accomplish the macro fingerprinting approach for the appraisal of complicated mixture systems. 2D-IR not only improves the resolution but also provides the dynamic micro structure information to probe the interactions of different chemical functional groups [4–9]. Controlled heating is used as the perturbation to provide 2D correlation spectra. Heating induces characteristic and surprisingly reproducible changes in both physical and chemical nature of the complex natural product sample, which can be most effectively depicted in the form of 2D correlation spectra.

At present, there are a great many of research efforts on the processing of *CaoWu*. However, FTIR and 2D-IR are rarely used in the study of this important system. Sun's group has been studying on the quality analysis and discrimination of the real and fake products of traditional Chinese medicine (TCM), and has made many useful achievements [10–16]. In this paper, we have analyzed seven processed aconite products, raw and extracts of raw and processed products of *CaoWu*, through three-step appraisal method of infrared spectra. We have identified the fingerprint characteristic peaks and established the macro quality control criterion for processed products of this TCM system.

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**Fig. 1.** FTIR spectra for different processed products of *CaoWu*. (a) Raw; (b) glutinous rice wine processed; (c) clear spirits processed; (d) yogurt processed; (e) *Urina Hominis* processed; (f) baked; and (g) stewed.

## 2. Experiment

### 2.1. Apparatus and accessories

Spectrum GX FTIR spectrometer (Perkin–Elmer), equipped with a DTGS detector, was used with a resolution of  $4\text{ cm}^{-1}$ , measuring range of  $4000\text{--}400\text{ cm}^{-1}$ , and co-addition of 16 scans and OPD speed of  $0.2\text{ cm}^{-1}/\text{s}$ . The interference of  $\text{H}_2\text{O}$  and  $\text{CO}_2$  was minimized when scanning. The 50–886 Temperature Controller (Love Control Corporation) was used at the temperature-rising speed of  $2\text{ }^\circ\text{C}/\text{min}$  and temperature range of  $50\text{--}120\text{ }^\circ\text{C}$ , with the sampling frequency of scanning every  $10\text{ }^\circ\text{C}$ .

### 2.2. Samples and reagents

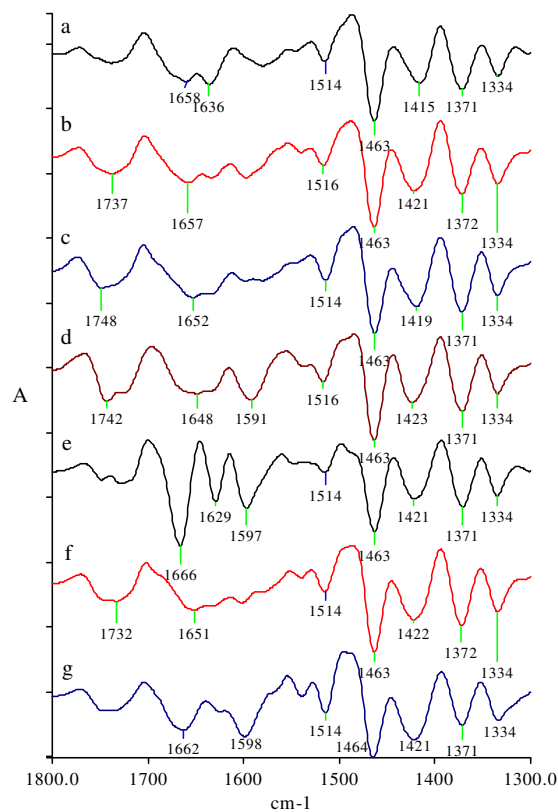
Raw and processed products of *CaoWu* were provided and appraised by Professor Bate Buhe of Inner Mongolia University for Nationalities. All the reagents involved in the experiments are of the analytical grade.

### 2.3. Sample preparation

Seven different dried and crumbled *CaoWu* materials (i.e., raw, glutinous rice wine processed, clear spirits processed, yogurt processed, *Urina Hominis* processed, baked and stewed) were examined. Extract samples were prepared from  $10\text{ g}$  each of them with ether. The KBr tablets of the original sample materials and their extracts of ether were then used to obtain their FTIR spectra.

### 2.4. Data processing

The spectral data were processed with the software of Spectrum v3.02 of Perkin Elmer Company to compare the similarity between



**Fig. 2.** The second derivative spectra of different processed products of *CaoWu*. (a) Raw; (b) glutinous rice wine processed; (c) clear spirits processed; (d) yogurt processed; (e) *Urina Hominis* processed; (f) baked; and (g) stewed.

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