

CHAPTER

8

QUALITY CONTROL AND STANDARDIZATION OF HERBAL PRODUCTS USING FTIR

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8.1 INTRODUCTION TO INFRARED SPECTROSCOPY

The region of infrared (IR) radiation ranges from the wavelength between 0.78 μm to 1000 μm . Some IR radiations may absorb, and some may emit by a sample. Absorption happens when radiant energy matches molecular vibration energy. When IR light travels through a sample, the absorption intensity versus wavenumber is recorded to create an infrared spectrum. The band intensity is expressed as absorbance (A) or percentage transmittance (%T). The relationship A and %T can be seen in Equation 8.1. Wavenumber is a more popular unit used for infrared radiation, which is the reciprocal of wavelength (λ) in centimeters (Equation 8.2). A higher absorbance value means more light is absorbed by the sample. Wavenumber represents the number of wave cycles per centimeter. A higher wavenumber means shorter wavelength and higher energy.

$$\text{Absorbance, } A = \log_{10} \frac{1}{\%T} \quad (8.1)$$

$$\text{wavenumber} = \frac{1}{\lambda} \quad (8.2)$$

Infrared (IR) spectroscopy has a high potential for the determination of molecular structures. The spectra of polyatomic molecules are determined by molecular vibrations, which are affected by atomic masses, bond strengths, and interactions between molecules. IR spectroscopy triggers molecular vibrations which are stretching and bending with the change in dipole moment. There are no two molecules having similar spectra, the IR spectrum can act as the fingerprint of a sample.

To solve dispersive instrument limitations such as low speed and sensitivity, IR spectroscopy has been transformed into fourier transform infrared spectroscopy (FTIR). There are some advantages of FTIR over IR which lead to transformation of IR to FTIR. The advantageous features of FTIR include low noise, high repeatability, rapid speed, easy operation, and low expense. All spectral components can be measured simultaneously, and the measurements take seconds rather than minutes in FTIR. The quick scans allow the combination of multiple scans to greatly reduce random measurement noise.

Due to the complexity of chemical structures in herbs, FTIR is considered as a useful technique for analyzing multiple functional groups of the compounds. It is a very simple optical instrument which produces interferogram, a special signal that has all the infrared frequencies encoded into it. Typically, this signal can be swiftly captured within a single second. Subsequently, employing a widely recognized mathematical method known as fourier transformation, the interferogram is decoded to reveal individual frequencies, thereby constructing a frequency spectrum illustrating the intensity at each wave number or frequency.

8.2 TYPES OF INFRARED SPECTROSCOPY

Infrared region can be divided into middle infrared spectroscopy (MIR), near infrared spectroscopy (NIR), and far infrared spectroscopy (FIR). The

MIR region lies at the wavelengths range from 2.5 μm to 25 μm , containing the most fundamental absorptions of molecular vibrations. Fundamental vibrational shifts occurring between the ground state and the initial excited state manifest in the mid-infrared spectrum. The NIR region lies at the wavelengths range from 0.8 μm to 2.5 μm . The transitions from the ground state to the second or third excited states occur in the near-infrared range which is also known as overtones and characterized by notably weak absorption bands. However, FIR is seldom applied due to its low energy or long wavelength.

Near infrared spectroscopy (NIR) is often used for a quick compositional quality testing. Standard NIR bands consist of organic and inorganic compounds, including O–H, C–H, N–H, and S–H bond vibrations. The vibrational transitions occur due to overtone and combination bonds. NIR spectroscopy detects electromagnetic radiation in the NIR spectrum to analyse chemical structures quickly, precisely, and cost effective. The combination of modern NIR spectroscopy and chemometrics enables the verification of herbal species and precise identification of herbal medicine origin (Pei & Zhiguo, 2015). Compared to MIR, NIR requires cheaper materials. Water is visible in the transparent band of NIR, and therefore, sample can be prepared with water as a solvent. Moreover, NIR needs little sample preparation, even samples are stored in glass or plastic containers during analysis (Gonzales et al., 2019). However, NIR has drawbacks. NIR is more likely to misread because it incorporates overtone information and vibration combinations, and thus harder to comprehend. Additionally, NIR scattering makes signal analysis more complicated and unreliable for data interpretation (Gonzales et al., 2019).

Middle infrared spectroscopy (MIR) gives precise composition and chemical structural information on tested samples. MIR spectroscopy is widely used to identify and validate herbal medication. Herbal medicine samples can be swiftly and immediately analysed using MIR spectroscopy without the need for sample extraction. It is considered as non-destructive analytical technique. Its spectrum fingerprint contains all chemical components of herbs. FT-MIR with attenuated total reflectance (ATR) had successfully been used to categorize *Dendrobium officinale*, a Traditional