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## Fourier Transform Infrared (FT-IR) Spectroscopy in An-Overview

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### ABSTRACT

In the recent years, vibration spectroscopes (infrared spectroscopy) have been developed for all sorts of analysis in life and chemical science. Important features of these methods are the relative ease with which measurements can be performed. Fourier transform infrared spectroscopy (FT-IR) is a technique that has been used over the years in chemical analysis for the identification of substances and is one that may be applied to the characterization of biomolecules. Infrared spectroscopy is based on the measurement of the molecular bond vibration compounds, excited by radiation of a suitable frequency, when given the conditions for energy absorption by the molecules. Here, we review the potential application of vibrational spectroscopies for use in natural product. It can be concluded that vibrational spectroscopy show high potential as novel methods.

**Key words:** Fourier transforms infrared spectroscopy, natural product, identification, classification, discrimination

### INTRODUCTION

Today numerous different near-infrared systems are available on the market, ranging from simple filter systems to scanning systems that are able to scan a complete spectrum in the fraction of a second. After the first applications of the FT-principle to NIR in the late eighties of the 20th century (Mc-Clure and Davis, 1988) spectroscopic methods are so fast that they can generate hundreds of spectra in a few minutes for a sample containing multiple components. Unfortunately, univariate calibration methods are not suitable for this type of data, as they require an interference free system. Multivariate calibration deals with data of instrument responses measured on multiple wavelengths for a sample that usually contains more than one component. FT-IR also used in the natural product chemistry for the identification of new compounds isolated from various plant species (Purohit *et al.*, 1991; Rawat *et al.*, 1989; Sati and Pant, 1985; Joshi *et al.*, 1996; Prasad *et al.*, 1997). In recent years, advances in chemometrics and computers have led to the development of several multivariate calibration methods (Lindberg *et al.*, 1983; Geladi and Kowalski, 1986; Haaland and Thomas, 1988; Wentzell *et al.*, 1997) for the analysis of complex

chemical mixtures. Inverse Least Squares (ILS) is based on the inverse of Beer's Law where the concentration of an analyte is modeled as a function of absorbance. Genetic Inverse Least Squares (GILS) is a modified version of original ILS method in which a small set of wavelengths are selected from a full spectral data matrix. It has evolved to an optimum solution using a Genetic Algorithm (GA) and has been applied to a number of wavelength selection problems (Ozdemir and Dinc, 2004, 2005; Ozdemir and Ozturk, 2004; Ozdemir and Williams, 1999; Paradkar and Williams, 1997). GA's are non-local search and optimization methods that are based upon the principles of natural selection (Sawamura, 2001; Sing *et al.*, 1998). Today FT-IR spectrometers are able to measure in the NIR range. Extraction of quantitative information from the rather featureless NIR-spectra has been a notable success of multivariate calibration techniques.

But today a significant limitation to the use of multivariate regression in the NIR spectrometry is the difficulty of transferring calibrations from one NIR instrument to another. Essential oils are valuable natural products used as raw materials in many fields, including perfumes, cosmetics, aromatherapy, phytotherapy, spices and nutrition (Buchbauer *et al.*, 1993). Aromatherapy is the therapeutic use of fragrances or at least mere volatiles to cure mitigate or prevent diseases, infections and indispositions by means of inhalation (Spricigo *et al.*, 1999). This has recently attracted the attention of many scientists and encouraged them to screen plants to study the biological activities of their oils from chemical and pharmacological investigations to therapeutic aspects. Hopefully, this will lead to new information on plant applications and new perspective on the potential use of these natural products. Interest in specialty oils has revived in recent decades, with the popularity of Aromatherapy, a branch of alternative medicine which claims that the specific aromas carried by specialty oils have curative effects. Although, it being produce in a small quantity compare to other food oil such as cooking oil from palm oil, soybean oil and maize oil but the specialty oil have a very high price in the market. This is because it being use in specific area especially in cosmetic and medical. Specialty oils are generally extracted by distillation. Other processes include solvent extraction which is a very simple method to get the specialty oil. Usually, the specialty oil can be extract from various raw materials from fruit seeds, bark, leaves, roots and flowers.

Infrared spectroscopy has been a workhorse technique for materials analysis in the laboratory for over seventy years. An infrared spectrum represents a fingerprint of a sample with absorption peaks which correspond to the frequencies of vibrations between the bonds of the atoms making up the material. Because each different material is a unique combination of atoms, no two compounds produce the exact same infrared spectrum. Therefore, infrared spectroscopy can result in a positive identification (qualitative analysis) of every different kind of material. In addition, the size of the peaks in the spectrum is a direct indication of the amount of material present. With modern software algorithms, infrared is an excellent tool for quantitative analysis. FT-IR is one of the most widely used methods to identify the chemical constituents and elucidate the compounds structures and has been used as a requisite method to identify Medicines in Pharmacopoeia of many countries. Owing to the fingerprint characters and extensive applicability to the samples, FT-IR has played an important role in pharmaceutical analysis in recent years (Vlachos *et al.*, 2006; Gough *et al.*, 2003). Now days FT-IR is certainly one of the most important analytical techniques available. One of the great advantages of FT-IR is that any sample in any state can be studied and short time to obtain data. Liquid, solutions, pastes, powders, films, fibers, gases and surfaces can all be examined. Infrared (IR) spectroscopy has been recognized as a powerful analytical technique in the food industry for many years (Schultz *et al.*, 2002) and it has been employed to measure

some quality parameters of oils (Schulz *et al.*, 2004). FT-IR is the equipment that based on vibration of atoms of a molecule. An infrared spectrum is commonly obtained by passing infrared radiation through a sample and determining what fraction of the incident radiation is absorbed at a particular energy. The energy at any peak in an absorption spectrum appears correspond to the frequency of a vibration of a part of sample molecule. Fourier transform infrared (FT-IR) spectroscopic instrumentation, the application of this technique expanded in food research and particularly has become a powerful analytical tool in the study of edible oils and fats. FT-IR spectroscopy is a rapid, non-destructive technique with minimum sample preparation necessary. It allows the qualitative determination of organic compounds as the characteristic vibrational mode of each molecular group causes the appearance of bands in the infrared spectrum at a specific frequency, which is further influenced by the surrounding functional groups (Schulz *et al.*, 2003). The basic principle behind the technique is based on the vibrational motions of atoms and chemical bonds within organic molecules. When a beam of light containing the Mid-IR radiation band is passed through a sample, light energy from the photons is absorbed by bonds and transformed into vibrational motions (Baranska *et al.*, 2005). Library searching in the Mid-IR region is a well established and powerful way of classifying and identifying compounds. Computer software compares the measured spectrum with every spectrum in a selected library. Comparison is usually accomplished by subtracting the measured spectrum from each spectrum in the library. The software keeps track of the number of differences found for each library spectrum. The best matches are those with the fewest differences. Computer reports the best match, second match, etc., in order to ensure the quality of essential oils used in fragrances, cosmetic materials and aroma preparations, usually gas chromatography combined with flame ionization or mass spectrometry detection is applied. Goulden, first used Mid-Infrared for milk analysis techniques absorption, the first commercial spectrometer became available allowing direct measurement of fat, protein and lactose in milk using a double beam spectrophotometer with two cells and a diffraction grating. Today, a large number of commercial essential oils have been described by the International Organization for Specification (ISO), the Food Chemical Codex and the European Pharmacopoeia. During the last decades, the economic importance of essential oils has led to systematic breeding activities; in this context numerous new cultivars were obtained by alternation of generations or by vegetative routes. Higher yields of essential oil and particularly changed profiles of the oil are primary targets, leading to deviations from the standardized product quality. Since most of the methods presently applied for quality control purposes and selection of high-quality plants are very time-consuming, some attempts have been made to find alternative analytical options. In this context some new vibrational spectroscopic methods in combination with sophisticated chemometric algorithms were successfully introduced (NIRS, ATR-IR and Raman) for an efficient and mostly non-destructive determination of secondary metabolites occurring in different parts of various medicinal and aromatic plants (Baranska *et al.*, 2004; Strehle *et al.*, 2005).

Whereas NIRS data can be interpreted only by application of statistical methods, IR and Raman spectra in most cases present characteristic key bands of the individual volatile fraction and therefore in principle allow the discrimination of different essential oil profiles of the individual oil plants among the same species (chemotypes) without applying any chemometric algorithms. Infrared and near infrared spectroscopy have been described in this context (Settle, 1997; Jacquinet, 1984; Perkins, 1987; Frost *et al.*, 1993). Based on the spectral data sets, cluster analysis can be established presenting the specific differences of the individual chemotypes as well as quantitative predictions of individual essential oil substances is generally possible.

The infrared spectroscopy spectrum displayed characteristic bands corresponding to aromatic CH bonds, between 3000 and 3100  $\text{cm}^{-1}$ ; to CH alkenes, between 3020 and 3080  $\text{cm}^{-1}$ ; to C = C, between 1640 and 1680  $\text{cm}^{-1}$  and to the aldehydes C = O group between 1690 and 1760  $\text{cm}^{-1}$ . The spectra similarity of the cinnamon essential oil and a cinnamaldehyde (SDBSWeb) comparing infrared spectrum of cinnamon essential oil and the individual spectra of the main compounds such as cinnamaldehyde and eugenol (database of SDDBS) superimposed, both spectra are notoriously similar. This could result from the high content of cinnamaldehyde as well as from the presence of eugenol in the essential oil analyzed.

**Limitations of FT-IR:** Given the power of FT-IR spectroscopy, one has to question why it is not used more and more effectively. One of the key limitations in this regard is that the currently accepted methodology is qualitative rather than quantitative. At issue is the complexity and variability of formulated lubricants, making unambiguous quantitative IR data difficult to obtain. At present, FT-IR spectroscopy is mostly used to track relative changes in essential oil, the baseline being the fresh or new oil. By subtracting the spectrum of the fresh oil from its used or in-service oil counterpart, one can spectrally visualize what has changed at a molecular level, including moisture ingress, additive depletion, oxidation, soot buildup etc. Hence the JOAP protocols attempt to standardize the measurement of these changes in terms of absorbance or arbitrary units that can be correlated with machine faults, wear or failure. This type of spectral information can be rapidly collected on an ongoing basis and via trending can be associated with specific lubricant changes (oxidation, soot buildup). With the correct interpretation, lubricant replacement or additive replenishment can be made on the basis of oil condition monitoring rather than simply on the basis of time, thereby reducing oil consumption and machine wear caused by the use of oils which have exceeded their useful life. One of the main limitations of this approach is that the results may be completely off-track if the base oil formulation changes or the reservoir has been topped up with another oil formulation.

**Chemometrics:** The combination of FT-IR spectroscopy and multivariate techniques such as Partial Least Squares (PLS) and Principal Component Regression (PCR) provides a powerful tool for interpretation and spectra. Chemometric data analysis is therefore required to extract the information about quality attributes which is hidden in near infrared spectrum. Chemometrics age of met cover quit a broad range of methods such as exploratory data analysis, patterns reorganization and statistical experiments. The most common used multivariate data analysis techniques applied to principal component analysis.

**Advantages and disadvantages of fourier transform spectrometric techniques compared to traditional analytical methods:** The advantages of Fourier transform techniques over dispersive instruments have resulted in almost total replacement of the dispersive instruments in spectroscopy.

**The multiplex or Fellgett advantage:** In a dispersive spectrometer, wave numbers are observed sequentially. In an FT-IR and FT-NIR spectrometer, all the wave numbers of light are observed simultaneously. Therefore, when spectra are collected under identical conditions the signal to noise (S/N) ratio of the FT-IR spectrum will be greater than that of the dispersive IR spectrum (Hill *et al.*, 1997).

**The throughput or jacquinot advantage:** In FT-IR instruments there is no need to limit the beam width in order to obtain an adequate resolution. In fact, a circular optical aperture is used in Fourier transform instruments and the beam area is 75 to 100 times larger than the slit area of dispersive instruments. As a consequence, there is an advantage of increased beam intensity going through the sample and therefore a much higher throughput with a FT-IR than with a dispersive instrument (Jacquinot, 1984).

**Wave number accuracy or conne's advantage:** In FT instruments, e.g., in FT-IR Bomem spectrometers, a wavelength accuracy of  $0.04 \text{ cm}^{-1}$  can be obtained, which is much higher than the traditional wavelength accuracy obtained with dispersive instruments (only about  $1.5 \text{ cm}^{-1}$ ) (Settle, 1997). This difference is due to the fact that the frequency-stabilised helium. Neon laser is used as internal wavelength standard. Therefore the frequency precision is 18 determined by the frequency stability of the laser, which leads to precise and reproducible wavelengths (Perkins, 1987; Frost *et al.*, 1993).

**High and constant resolution:** Spectral resolution is a measure of how well a spectrometer can distinguish closely spaced spectral features. Filter instruments cannot offer high resolution because, in dispersive instruments, resolution decreases as lower frequencies are scanned. In FT- IR, the resolution depends on the Optical Path Difference (OPD) that can be achieved. Thus it is constant across the scanning range (Wilks, 1986).

**Practical and powerful data station:** FT-IR or FT-NIR instruments are normally equipped with a powerful computer capable of carrying out the Fast Fourier Transformation needed to obtain the spectrum. Additionally, the instrument computer uses software that can perform data processing such as baseline correction, smoothing, derivatisation or library searching and therefore improve data information. The most attractive advantage of FT-NIR spectroscopy over traditional analytical tools and any other spectroscopic method is probably that the measurements are non destructive and non invasive and that it is possible to use solid.

Samples without pre treatment and therefore without solvents. This leads to a large increase in the analysis speed compared to traditional analysis methods and decreases the risk of errors due to weighing and dilution operations (Trafford *et al.*, 1999; Han and Faulkner, 1996). The variety in sampling technologies is another attractive feature of NIR spectroscopy. Several accessories are adaptable to a number of situations and can be used with different scanning modes. For instance, fibre optic probes were used already ten years ago for real time analysis (Williams and Mac-Peters, 1991) and are nowadays often used in the diffuse reflectance mode for routine qualitative and quantitative applications (Blanco *et al.*, 1999, 2000a, b). Diffuse reflectance is also easily used for off-line analysis for samples contained in simple glass vials (Wargo and Drennen, 1996; Frarake *et al.*, 1998). The transmittance mode is more and more widely used for recording spectra from intact 19 tablets (Schilling *et al.*, 1996). It gives results with a better repeatability and a smaller prediction error than reflectance measurements (Corti *et al.*, 1999; Thosar *et al.*, 2001). The transflectance mode, which is a variant of the diffuse reflectance mode, has also been investigated recently. In this case, incident light crosses the sample, is reflected by a reflectance material such as stainless steel or PTFE (Polytetrafluoroethylene) located on the opposite side and travels back through the sample before reaching the detector (Blanco and Villarroya, 2002). An important

property of the NIR signal is that, because it depends on both the chemical composition and the physical properties of the sample, analysis of these two characteristics can be performed by the same technique (Chen and Sørensen, 2000). NIR also has the potential to be used for developing on-line methods, leading to real time control systems (Rantanen *et al.*, 2000). This advantage can be well used in the pharmaceutical or chemical industry to give real time information about processes. On the other hand, there are three main disadvantages of NIR spectroscopy over traditional techniques. First, the development of a NIR method is time consuming because it is necessary to analyse several representative samples by a time consuming reference analysis method (HPLC or Karl Fisher titration for example). Secondly, NIR methods lack robustness: calibrations often need to be updated, e.g., when a sample is provided by a new supplier, or when the manufacturing process of the sample is modified (Candolfi and Massart, 2001). This is especially problematic with raw material whose quality may vary from time to time leading to false identification of the material. Furthermore, NIR spectroscopy is not very sensitive and it can usually be satisfactorily applied to major components (Blanco and Romero, 2002) but not to impurities or low dose substances. Other minor disadvantages are the following: First, in contrast to IR spectra, NIR raw spectra exhibit low specificity. They do not show clear peaks characteristic to a specific compound of interest. Thus, extensive statistical calculations are required to extract useful qualitative or quantitative information (Lowry *et al.*, 2000). Second, NIR spectroscopy methods are developed using the reference analysis results of the calibration samples. Thus, the accuracy of the NIR method cannot be better than the accuracy of the 20 reference method. Furthermore, the transferability of NIR methods from one instrument to another is limited due to the frequent need for updating calibrations after routine maintenance or repair of the instrument (Wang *et al.*, 1998). Finally, the absence of NIR training in pharmacy schools is one of the major obstacles to the acceptance of NIR spectroscopy by pharmacists. The specialized vocabulary used in the chemometrics world makes things even less accessible for pharmacists.

## CONCLUSIONS

The quality control of natural products such as essential oils, alkaloids phenolic and other biological samples is one of the most challenging tasks in modern analytics. Vibrational spectroscopy such as FT-IR and NIR has proven to be a non-destructive and fast method requiring both minimal sample preparation and minimum amount of analyte as compared to traditional chromatographic techniques like HPLC, HPTLC and GC. Recent advancement in analytical instrumentation of NIR principal components analysis and multivariate data processing open new area of application in biological samples. The ability to monitor rapidly various essential oils, biological samples it possible to efficiently select high-quality single plants from wild populations as well as progenies of crossing experiments. It is very clear that FT-IR routinely used in quality control of food, nutraceutical, cosmetic pharmaceutical microbiological samples in order to perform fast quality checks of incoming raw materials and continuous controlling of rapid quality parameters.

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