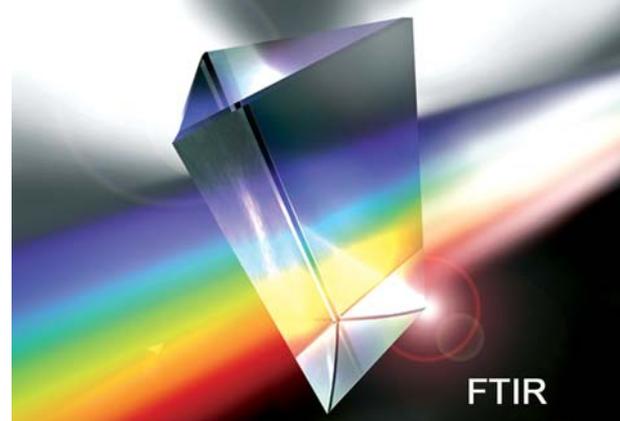


Application Note

Chinese drug library measured with diffuse reflectance accessory as an example for FT-NIR Spectroscopy



FT-NIR Spectroscopy is one method available for the identification of materials, within this application even identification from same material in different shapes is done. The classical identification technique is the MIR but in some cases it is too sensitive overall details. A search in a MIR library will result in a much worse hit quality. The benefit of the NIR measurement range is that the spectra are more smoothed, the signals are more broad and not so sensitive reacting on stray light phenomena related to the sample surface. A rough look to the spectra will result in nearly same spectrum view but even though the spectra of several substances are looking comparable smooth there are still enough differences visible in the derivative spectra which make it possible to use library for the identification.

In this example different samples of drugs were measured. The check of the reproducibility and the comparison of the derivative spectra gave confidence in this quality control tool of a NIR-Library. The used Chinese drugs are listed in table 1.

Latin	English	Chinese
Salviae miltiorrhiza radix	Sage root	Dan Shen
Scutellariae radix		Huang Qin
Zingiberis rhizoma	Ginger root #Powder and root	Gan Jiang
Paeoniae albae radix	Paony root	Bai Shao
Pinelliae rhizoma		Fa Ban Xia
Rehmanniae praep. radix	Rehmannia root	Shu Di Huang
Angelicae sinensis radix	Angelica	Dang Gui
Uncariae ramulus		Gou Teng

Table 1: Drugs used to test a simple library model in FT-NIR



Fig. 1: View to the seven drug samples with different shapes.

More and more the alternative drugs like homeopathic style are requested in the pharmacies. The natural based materials are claimed as more smooth and healthy than the designed drugs from industrial plants for the so called classical medicine. Even though the Chinese drugs are by age well known since ever they are now a days defined as modern and alternative in our European regions.

Very important for the suppliers of such material is the quality control of these drugs. Prepared as natural products from roots, leaves or wood the content of the drug can vary by the presence of the natural filler material like cellulose, etc. So, a quality control or minimum identification should be possible.

The FT-NIR technique is a tool for quick analysis, less sample preparation and simple cleaning of analysis tools. It is highly effective to work with different aggregations of samples with one analysis tool. The Chinese drugs are possible to get in powder form or as dried material from a root as it is by nature. See the ginger samples in the picture which

shows a part of a root and a powder from ginger root.

Sample preparation

Powder – it was used as it is to see in the figure 1, without any treatment filled into the glass tube and pushed for homogeneous packaging of powder particles.

Root – small pieces were manually prepared and filled into the glass tube, pushed to have as much material as possible touching the bottom of the glass tube. At all sample preparation time was approx. 1 min.

Measurement technique

Diffuse Reflection measurement is by definition a penetration of the beam of 3 mm into the surface of the sample. The beam will be transmitted, reflected and refracted, doing this picking up spectral information from the sample material.



Fig. 2: IntegratIR, a diffuse reflectance sphere for the FT-NIR measurement

The diffuse reflectance is collected in an integrating sphere made with a rough surface from gold, which is also the mirror coating for the reference measurement. The most sensitive InGaAs detector will collect the spectral information. The integrating sphere opening is protected with a quartz window plate.

Measurements

Reproducibility- to have a good confidence with the measurements the reproducibility of the measurement has to be controlled.

Repetition measurement and library search are two check criteria to get a confidence level in the analysis.

Comparison of the two spectra of ginger powder and ginger root shows the sensitivity of the measurement. The spectra are not the same. The cellulose, lignin and remaining water in the root are visible in the spectra of the root in comparison to the powder. Same will be reflected in a search of both, were the system finds easily the ginger root and not ginger powder for the root material.



Fig. 3: Ginger root and powder, two samples for the check of the method

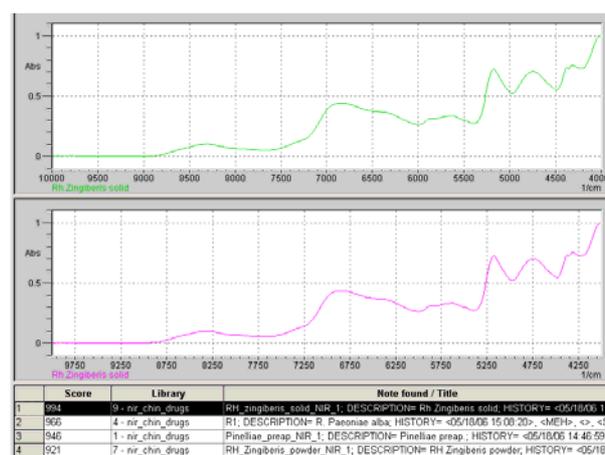


Fig. 4: search result from the Chinese drug library

Other criteria for proofing are the derivative spectra which show very easily differences in both materials. These are all necessary tests to proof the reliability/confidence in a method. Naturally more spectra in a library and different materials will improve the quality of the results.

Instrument

IRPrestige-21, FT-NIR Kit, IntegratIR
 Range: 4000 – 10000 cm⁻¹ (2.5 μm to 1 μm)
 Resolution: 8 cm⁻¹

The given specifications serve purely as technical information for the user. No guarantee is given on technical specification of the described product and/or procedures.