# **Diversity in NIR instrumentation**

# **Edward Stark and Karen Luchter**

KES Analysis, Inc., 160 West End Ave., New York, N.Y. 10023 USA

# Introduction

Due to editorial requirements, this printed version of the plenary talk for the Instrumentation session of the 2003 ICNIRS meeting is only half of the original version. The complete paper, including additional discussion and Figures, is available on the <u>accompanying CD</u>.

# NIR instrumentation types

NIR instruments may be grouped as general purpose spectrometers, application specific analyzers, or imaging spectrometers. Bench top, on-line, and portable configurations are available. (CD Figures 1–3).

# Instrument selection criteria

The two primary criteria for instrument selection should be that the photometric (energy measurement) and the spectral (wavelength) performance are adequate for the applications of interest. Better performance than that required for the applications may be unduly costly. Therefore, the application's performance requirements should be investigated during the initial development period of a new application. This, and other special techniques, makes successful NIR application development a knowledge intensive and non-trivial exercise.

Good reproducibility among instruments facilitates the transfer of the calibrations from a master or application development instrument to multiple slave instruments. Data processing techniques improve this transfer of calibrations between similar and dissimilar instruments. Some instrument manufacturers now claim the ability to directly transfer calibrations between certain distinctly dissimilar instruments.

The sample handling and presentation to the instrument are critical aspects of NIR analysis. Flexibility of measurement modes, reflection or transmission being the most basic, may be important to the success of a method development. Once the sample presentation and measurement mode have been determined for an application, unused flexibility may add unnecessary cost to the instruments routinely performing the application.

Instruments often co-add many spectral scans to increase the signal to noise ratio. To avoid spectral distortion, it is important that the sample spectrum not change significantly during each individual spectral scan. Sample movement, temperature change, and/or chemical reactions are potential sources of spectral variations that determine the necessary scan rate and limits to scan averaging.

Environmental requirements are particularly stringent in certain (but not all) plant applications therefore; many instruments are available in environmental enclosures and are capable of operation under adverse situations.

The technical support from the instrument manufacturer as well as the extent and functionality of the built-in instrument diagnostic tests are important factors to evaluate carefully in selecting an instrument. Software capabilities, flexibility and ease of use together with the capabilities and training of the intended operator also affect the application's success.

Finally, needed capability should not be compromised for instrument cost. Method development and maintenance costs far exceed the initial cost of the instrument.

#### Photometric specifications

Photometric specifications refer to the optical energy response of the instrument that, in turn, affects the quality of transmittance, reflectance, and absorbance spectra and, ultimately, the quality of the analytical results.

## Instrument noise

The detector and preamplifier are the usual sources of NIR instrument noise; although readout noise from multiplexed array detectors may also be significant. Detector and preamplifier noise are typically random, so averaging of spectra can reduce the effective noise level proportional to the square root of the measurement time. However, readout and digitizing noise are repetitive so averaging in those cases is not effective. NIR instrument noise is usually quoted in micro-absorbance units as measured on the baseline, i.e. with a sample reflectance or transmittance of unity. Under these conditions, 10 micro-absorbance noise represents a signal-to-noise ratio (SNR) of over 43,000:1. Such a high baseline SNR, which is equivalent to low absorbance noise, decreases as sample absorption or other factors reduce the sample signal. A large SNR is critical to enable a multivariate calibration to mathematically separate the spectral interferences caused by absorption of the sample matrix components from the spectral data of the analyte.

#### Stability

Stability is an equally important factor of photometric performance. Drift may arise from a number of causes, some discussed in more detail later. Correcting baseline drift, including the spectral drift component, requires measuring the reference energy at a rate faster than its drift and using the information to correct the baseline. Repeated measurements of a baseline standard or, preferably, dual-beam operation that rapidly and automatically measures the reference energy, are essential to maintaining stability.

## Photometric linearity and stray light

Photometric linearity refers to the ability of the detector and electronics to generate a linear response to the incoming energy. Linearity of better than 1% is readily achievable although it is difficult for a user to independently determine.



Figure 4. Stray light non-linearity

Stray light is any extraneous energy included in the measurement that does not represent the effects of absorption by the sample within the spectral bandpass of the instrument. Sources may include spectral stray light, discussed later, ambient illumination, energy leakage around the sample, and, in reflection measurements, the significant specular component reflected from the surface of the sample. Stray light limits the maximum apparent absorbance to the value caused by the stray light alone (Figure 4) and causes significant non-linearity in the response starting approximately one absorbance unit before saturation.

#### Dynamic range

Dynamic range, the ratio of the maximum allowable signal to the minimum detectable signal, defines the ability to measure a small signal in the presence of a much larger one as well as the range of signal strengths that are measurable. Dynamic range limitations may arise from several sources. Stray light, as discussed previously, limits the absorbance dynamic range. The analog to digital converter (A/D) requires a minimum signal, which is the value of the least significant digital bit (LSB), to produce an output other than zero. The number of digitizing levels, or bits, establishes the maximum signal allowed therefore control of either the optical energy or the electronic gain is necessary to avoid A/D saturation. The maximum absorbance supported by 16-bit digital resolution is the negative log of 1/65536, or about 4.8. Larger absorbance values require either an optical or electronic absorbance offset or additional digital resolution.

Instrument noise may limit the dynamic range of the energy measurement by establishing a minimum detectable signal threshold that is greater than the LSB. In this case, additional optical signal energy or averaging of multiple scans is required to increase the SNR and dynamic range. For averaging of spectra to be effective, the noise level must exceed the LSB of the A/D and the digital word length must support any resulting increase in the dynamic range.

Charge coupled devices (CCD) and many diode-array detectors integrate the photocurrent before readout and digitization thereby introducing the possibility of analog saturation. In these systems, adjusting the light level or varying the integration time and scan rate can keep the signal below saturation.

#### Spectral performance

#### Wavelength range

The realistic upper wavelength cut-off of an NIR instrument is largely determined by the choice of detector material, hence 1100 nm for silicon, 1700 nm for normal indium gallium arsenide, and 2500 nm for lead sulfide. NIR spectral information consists of repeating overtone and combination bands providing several orders containing the same information but with diminishing signal intensity as wavelength decreases. Offsetting the diminished signal strength is the higher detectivity of detectors with shorter cut-off wavelengths. The low-cost silicon detector has the shortest cut-off wavelength and the highest detectivity of the three detector types. The wavelength range, sensitivity and cost tradeoffs among detectors allow for the often-successful use of different detectors for the same application. Fourier transform instruments generally do not cover the visible, as silicon detectors do, but with appropriate detectors and beam splitters, they can provide combined NIR and mid-infrared coverage.

#### Wavelength reproducibility and precision

The performance requirements on wavelength reproducibility and precision are application specific. Wavelength reproducibility among instruments of  $\pm 0.5$  nm ( $\sim 1$  cm<sup>-1</sup>) and wavelength precision of  $\pm 0.05$  nm ( $\sim 0.1$  cm<sup>-1</sup>), available with many filter and grating instruments, is sufficient for most applications. Reproducibility among instruments is particularly important for successful transfer of calibrations. Laser referenced interferometer (FTNIR) instruments excel in wavelength reproducibility and precision although their full capability is rarely needed.

#### Spectral resolution

Resolution, or spectral bandpass, is defined as the full width at half height (FWHH) of the instrument response function (Figure 5). It is important to differentiate instrument resolution,

defined as the spectral bandpass, from the spectral sampling or data point interval, often incorrectly called resolution. Both the width and the shape of the spectral response of the instrument



#### Figure 5. Spectral resolution.

significantly affect the measured spectrum. In general, there are tradeoffs between resolution and signal-to-noise ratio that result in an optimum resolution for a given application.<sup>1</sup>

For Fourier transform spectrometers, the maximum pathlength difference of the mirror scan establishes the minimum FWHH of the response function. The response function is modified by a mathematical apodisation, or weighting, function applied to the interferogram prior to the transform operation. Gaussian apodisation is one of several functions that perform well. Other apodisation functions

(frequency in cm<sup>-1</sup>), which is proportional to the

reciprocal of the wavelength  $\lambda$  in nanometers.

The v axis on the right and the v cm-1 curve in

Figure 6 show the non-linear relationship

wavelength

transform instruments have a resolution that is

constant with wavenumber. The non-linear

relationship between the  $\Delta\lambda$  and  $\Delta\nu$  resolution is illustrated with the  $\Delta\lambda$  axis on the left and the

Grating instrument resolution tends to be

while

Fourier

between these spectral scales.

with

four  $\Delta v$  curves of Figure 6.

produce a smaller FWHH but result in large ripples in the response function producing a form of spectral stray light. The apodization used should be consistent throughout calibration and prediction to avoid errors.

A triangle is the idealized shape of the instrument response function for a grating spectrometer with the optimum matched entrance and exit slits. Optical effects may diminish the sharpness of the response so that it is similar to the Gaussian FT response. Aberrations may also result in an asymmetric response, particularly in the tails. These optical effects may vary from unit to unit, adversely affecting transferability of calibration.

#### Spectral scale conversions

Spectral scale conversions are often confusing. Grating instrument spectra have an approximately linear wavelength scale while Fourier transform spectra are linear in wavenumber v

constant



Figure 6. Spectral scale conversions.

Spectral stray light

Spectral stray light refers to the energy measured by the instrument that is outside the fundamental spectral response, generally considered 2 to 3 times the FWHH. Such energy may produce optical non-linearity and, if it varies among instruments, problems in the transfer of calibrations will occur. For filters, blocking is the specification relating to spectral stray light and

the blocking must extend over the entire spectral region of detector sensitivity. Grating spectrometers may have spectral stray light due to inadequate rejection of unwanted orders of the grating diffraction as well as internal scattering and reflections. Due to non-linearity of the electronics or laser energy leakage, Fourier transform instruments may have spectral artifacts that have effects similar to spectral stray light.

# Other considerations

Additional parameters are important in the selection of an appropriate instrument, for example:

- Physical layout of sampling area
- Shock and Vibration
- Ambient temperature range
- Clean-in-place requirements

Based on these considerations to begin with, examine each specific instrument for use in either the development or implementation of the specific applications. The success of an installation, particularly for in-plant use, may well depend on a correct evaluation of these factors.

# Diversity in spectrometer technology

NIR spectrometers exist in pre-dispersive and post-dispersive configurations depending on the location of the sample relative to the wavelength selection device. (CD Figure 7)

# **Development of diversity**

The development of new techniques for selecting the measurement wavelength has been the

driving force in the increasing diversity of NIR instrumentation (Figure 8). Because each technique has unique features, all continue in use and their growth has paralleled that of NIR spectroscopy in general.

Until recently, NIR instruments measured the average spectrum of a single defined sample area. With the availability of commercialised focal plane array detectors, hyperspectral imaging can provide simultaneous parallel spectral measurements of many smaller areas of the sample opening a myriad of new applications.



Regulatory requirements

Safety requirements

Portability

Figure 8. Growth of diversity in technology.

# Wavelength selection technologies

The methods for selection of the measurement wavelengths primarily determine the diverse capabilities of modern NIR instruments. Wavelength selection technologies include narrow passband fixed or variable filters, diffraction gratings, and interferometers; each technology implemented in several ways. The filter techniques and the scanning grating are limited to one wavelength at a time, although filtered LEDs, AOTF, and LCTF feature rapid wavelength switching or sequential scanning. Dispersive photodiode array, dispersive Hadamard multiplexed instruments

59

and interferometer multiplexed instruments (FT) have the advantage of simultaneous measurement of the entire wavelength range.

# Fixed and variable filters

## Interference filters

NIR narrow bandpass interference filters typically have a bandwidth of  $10\pm 2$  nm and a peak transmission of approximately 40% and are usually mounted in a rotating filter wheel (CD Figure 9).

#### Multiple filtered light emitting diodes (LEDs)

LEDs combined with filters are efficient, rugged, and inexpensive sources making them ideal for portable, low cost instruments without moving parts. LEDs emit relatively broadband energy so an auxiliary filter is required to obtain sufficient resolution for NIR spectroscopy. (CD Figure 10)

#### Acousto-optic tunable filter (AOTF)

The acousto-optical tunable filter (CD Figure 11) depends on the interaction of optical energy and a traveling acoustic wave in a  $TeO_2$  crystal. The transmitted wavelength is electronically tunable. Crystals up to 1 cm in size are available which may limit the energy transmitted.

## Liquid crystal tunable filter (LCTF)

The liquid crystal tunable filter (CD Figure 12) is fundamentally a multiple stage Lyot filter, each stage consisting of birefringent material placed between linear polarisers. The LCTF provides better image quality than an AOTF but the maximum commercially available wavelength is limited by the liquid crystal and by the polarizer materials to less than 1800 nm.

#### Diffraction gratings

The aberration corrected concave holographic diffraction grating forms the basis of most NIR dispersive instruments although some instruments rely on flat gratings. By adjusting the recording parameters during the generation of a concave holographic grating, the spectral focus can be moved to a location near the astigmatic focus where the focal plane is nearly flat. This configuration is common for instruments using flat diode-array detectors. Alternative recording parameters result in the constant deviation grating, the basis of most NIR scanning monochromators. (CD Figure 13)

#### Scanning monochromator

The scanning monochromator based on a near constant deviation concave holographic grating is a mature technology providing sufficient resolution for most applications. This optical design (CD Figure 14) is not complex but very good control of the grating mechanical motion over the life of the instrument is critical to the wavelength performance and ensuring the stability of calibrations.

#### **Diode-array spectrometers**

Low cost miniature diode-array spectrometers that use a fiber-optic input exhibit low optical throughput that is partially compensated by the high sensitivity of silicon CCD array detectors. (CD Figure 15) A fiber-optic illuminator and sample interface are required to complete the system.

Other diode-array instruments utilizing concave holographic gratings with silicon and/or InGaAs photodiode array detectors are integrated units that combine the source, sample interface, and sensor (CD Figure 16). Both fiber optic and remote viewing interfaces are available.

## Interferometer technology

The laser referenced wavenumber scale is the primary advantage of interferometer technology for wavelength selection. The accurate spectral reproducibility among units allows the transfer of calibrations without mathematical wavenumber corrections. However, NIR condensed phase spectra rarely benefit from the high spectral resolution possible from an interferometer. Jacquinot's optical throughput advantage and Fellget's multiplex advantage are of limited value in the NIR due to the high intensity of NIR sources and the dynamic range limitations of the multiplexed signal.

#### The Michaelson interferometer

The Michaelson interferometer is the basis of the majority of interferometer systems. (CD Figure 17) The rapid-scan interferometer modulates the energy at a frequency proportional to the frequency of the light producing an interferogram which is converted to a spectrum by the Fourier transform.

In some applications, such as hyperspectral imaging, the mirror position is stepped slowly while images are collected and the interferogram is reconstructed and processed after data collection is completed.

#### Crystal polarization interferometer

The crystal polarization interferometer (CD Figure 18) utilises a moving prism and differential retardation of perpendicular light polarizations to produce phase shift (equivalent to path length difference) between collinear beams of energy. Interference at the detector generates an interferogram similar to that from a Michaelson interferometer.

## NIR sources

#### Tungsten-halogen lamps

The tungsten-halogen lamp remains the overwhelming favorite choice among NIR sources due to its good performance characteristics at reasonable cost. Lamps for low voltage operation are particularly rugged and reliable, although the filament may be vibration sensitive.

## Lamp life

Tungsten-halogen lamps are filled with a halogen gas to extend the life by recycling evaporated tungsten back to the filament, thereby avoiding premature bulb blackening and failure. The quartz envelope must operate at sufficiently high temperature to maintain this cycle. The life of a lamp is a function of filament design and operating temperature. Increasing the voltage 10% increases the output and shifts the energy peak to shorter wavelengths while reducing the lamp life to approximately 30% of the rated life. Decreasing the voltage 10% may increase the lamp life by a factor of four at the cost of reduced output intensity, particularly in the visible region. Further voltage reduction may cause failure of the halogen cycle and reduce lamp life.

#### Filament spectra

The tungsten filament spectra (Figure 19), which are a function of both the temperature of the filament and the emissivity of tungsten, peak in the VNIR dropping rapidly towards the blue and more slowly towards longer NIR wavelengths. Lamp temperature variation is a potential source of



Figure 19. Tungsten filament spectra.

Figure 20. Tungsten lamp temperature drift.

significant baseline drift in the measurement (Figure 20). Temperature stabilization or frequent baseline reference measurements can minimize this drift.

# Alternative NIR sources

## Light emitting diodes

Light emitting diodes (LEDs) are an attractive source because of their efficiency, small size, and cool operation. More extensive use of LED sources has been limited by the unavailability of longer NIR wavelengths, thus, this technology is primarily useful in the very near infrared (VNIR) silicon detector region below 1100 nm. Technology exists to fabricate diodes covering much, if not all, of the NIR but at present, insufficient demand exists to prompt commercial availability. Laser diodes, operate at higher power and generate narrow band radiation, also have potential as a NIR source.

## Tunable lasers

As a source, tunable lasers provide very high intensity, narrow band radiation, particularly useful for in-vivo multi-spectral imaging. The spectral range of a specific laser is limited, which may present problems in some applications. The high cost and complexity of such sources has restricted their use primarily to research applications.

# **NIR detectors**

The detectors used in NIR instruments are semiconductors that generate carriers (holes and/or electrons) by absorbing photons of the incident radiation. PbS detectors, commonly used in instruments with response extending to 2500 nm, operate by changing resistance and are known as photoconductive mode detectors. Si and InGaAs detectors are p-n junction diodes. For spectroscopic use, they usually operate in the photovoltaic mode, generating an electrical photocurrent in response to the absorbed photons.

# Detectivity

Detectivity (D\*) of detectors is a normalized quantity describing the performance of detectors of different types on a comparable basis (Figure 21). It is the reciprocal of a detector's noise equivalent power normalized for a one square cm active area and one Hertz noise bandwidth. Noise equivalent power is the incident light power required for the signal to equal the detector noise.



Figure 21. NIR detector detectivity D\*.

The peak response wavelength identifies the various extended wavelength InGaAs detectors. Operating temperatures are given in parentheses. The convenience and hardware advantage of Si, InGaAs, and PbS operation at room temperature (300K) is evident. In all these cases, cooling somewhat improves the detector performance. Operation at 233K (-40°C) with a thermoelectric Peltier cooler is optimum for extended cut-off InGaAs detectors. The detectivity at 233K of selected single element extended wavelength InGaAs detectors with 1.83 µm and 2.11 µm peak response is near the theoretical maximum. However, the 2.48 µm

peak response detectors do not reach this performance level. Longer wavelength cut-off detectors, such as InAs, InSb, and HgCdTe (sometimes used in FT instruments), operate best at 77 K, the temperature of liquid nitrogen. Operation of InAs with a Peltier cooler but still below 300K yields a lower, but still useful, D\*.

## Detector wavelength ranges

The wavelength of the sharp long-wavelength cut-off in the response of photon detectors varies as a function of detector temperature. Therefore, operation below the peak wavelength  $\lambda_{P}$  yields the best real-life performance (CD Figure 22). In certain applications, useful results may be obtained beyond the peak, particularly if baseline measurements are made repeatedly at short intervals.

#### Detector arrays

Most diode-array spectrometers use linear arrays of Si and InGaAs detectors. InGaAs arrays have extended the wavelength range of detector arrays to 1700 nm and beyond (for the less sensitive extended wavelength InGaAs material). Many InGaAs and Si diode-array instruments use a multiplexed array with an integrating buffer amplifier and multiplexer chip separate from the detector array. Saturation of the integrating buffer circuit may limit the dynamic range of the system.<sup>2</sup> Parallel channel arrays replace the integrating buffer and multiplexer with a transimpedance preamplifier, multiplexer, and variable gain control to increase dynamic range and to utilize larger area detector elements that increase sensitivity.

Two-dimensional charge coupled (CCD) silicon imaging arrays are low-cost devices that are commercially used in quantity by digital cameras and camcorders. They offer high resolution and high sensitivity in the visible and very near infrared (VNIR) up to approximately 900 nm. Scientific CCDs are available at higher cost providing enhanced photometric performance in the same spectral range. Two-dimensional InGaAs imaging arrays have recently become commercially available.

# Sample interface optics

The measurement mode is defined by the specific nature and configuration of the optics used to transmit energy between the sample and the spectrometer. This optical sample interface portion of the NIR instrument is the most application dependent and therefore, may benefit from custom design. Fiber optic probe interfaces allow insertion into or use in close proximity to the sample.

## Regular transmission and regular transflection

The regular transmission mode is a standard approach, useful for non-scattering materials that can be presented in a not too highly absorbing thickness. In this mode, the source energy enters one side of the sample and the energy to be detected exits on the opposite side. In-line regular transmission measurements may be made across a pipe. In cases where only a single point of entry to the process is desirable, fiber optic probes configured to provide a double pass through the sample using a reflector to redirect the energy back towards the incident direction are available. This regular transflection geometry, often called transmission, is particularly useful in cases where the desired pathlength cannot be obtained in straight-through transmission.

## Diffuse reflection and diffuse transflection

In diffuse reflection and transflection, the measured energy returns from the irradiated surface of the sample. Diffuse reflection is appropriate for "infinitely thick" samples with sufficient scattering, so that only an insignificant amount of energy, if any, transmits through the sample. Diffuse transflection may be used for clear or scattering samples that are not "infinitely thick". For diffuse transflection, a diffuse reflector backs the sample thus, providing a double pass through the sample and diffuse return of the energy for measurement similar to diffuse reflection.

#### Near-sample diffuse reflection interface optics

Three configurations of sample interface optics, the integrating sphere, close proximity detectors, and fiber-optics, are common for diffuse reflection and transflection measurements near the sample (CD Figure 23).

#### Remote sample diffuse reflection interfaces

For on-line reflectance measurements, it is often necessary or desirable to separate the instrument from the sample by a significant distance. Many units are based on rotating filter wheel and projection optics (CD Figure 24). A larger remote viewing area and continuous spectral information from 400 to 1700 nm is provided by a simple diode-array system. (CD Figure 25)

#### Interaction interfaces

Interaction involves a probe actually in contact with the surface of a sample. The probe defines an area of the sample illuminated by the source separated by some distance from the area of the sample where returned energy is detected. This separation of source and detection areas eliminates the surface reflection component from the measurement and forces a geometrically determined minimum pathlength for the detected radiation passing through the sample.

# Fibre-optics

Transmission, transflection, diffuse reflection, and interaction are all available measurement modes using fiber optic probes.

#### Fiber optic fundamentals



#### Figure 26. Fiber optic energy propagation.

fibres ranges from 0.37 to 0.66.

### Fiber optic losses

Fiber optics have a central transparent core surrounded by a cladding with a lower refractive index and an external protective buffer (Figure 26). Fibre-optics guide the input optical energy down the central core by total internal reflection at the core-cladding interface. The maximum acceptance angle of the fiber depends on the index of refraction of core and cladding materials. the The numerical aperture (NA) of the fiber equals the sine of the maximum acceptance angle. The energy throughput is proportional to the product of the squares of the core diameter and of the NA. Low -OH quartz fibers have an NA of about 0.22 while the NA of glass

Reflection losses at the input and output faces of the fiber depend on the index of refraction mismatch between the core and the surroundings, usually air (n=1) but sometimes the sample. Antireflection coating can reduce this loss. For maximum efficiency, it is important to match the NA of the illumination optics to the fiber NA. Optical aberrations can disturb the focusing of energy into the core and introduce a loss due to NA mismatch.

For fiber optic bundles, the cladding and, in some cases, a buffer separates the core of each individual fiber from the adjacent fibers. The theoretical geometric packing density of fibers with the buffer stripped is 0.91. The fractional core area is equal to the square of the ratio of the core diameter to the cladding outside diameter. For short fibers, the energy entering the cladding may be transmitted and exhibit different spectral characteristics than the desired core energy.

Bending of the fiber may cause wavelength dependent changes in the NA and the optical

throughput of the fiber. In this way, vibration of the fiber can introduce extraneous spectral and intensity noise into the analytical signal.

Core absorption and scattering due to fiber defects is another source of signal energy loss. For example, OH in the core material is a strong absorber of NIR radiation. Even low OH quartz fiber (Figure 27) shows water-like absorption at 1450 nm and beyond 2000 nm Glass fibers contain higher levels of OH, which limits their use beyond 2000 nm.



Figure 27. Low OH quartz fiber attenuation.

# Hyperspectral imaging

Hyperspectral imaging is a recent extension of the capabilities of NIR spectroscopy. A digital visible light picture image may show little of the distribution of materials in a sample but a chemical image provides additional essential information (Figure 28). Processing the NIR spectral data from

each picture element (pixel) to qualitatively identify the material within that pixel forms a chemical image. Manv different have been instrumentation approaches developed for imaging (CD Figures 29 to 37). Presently pharmaceutical and industrial applications extensively use this capability (CD Figure 38).



NIR Magnified Image NIR log 1/R spectrum Pictures courtesy of ChemImage, Inc.

# Figure 28. Hyperspectral chemical imaging.

The applications of NIR hyperspectral imaging in medicine seem to be the most exciting and potentially important directions. The ability to identify the composition and structure of tissues at the molecular level is adding a new dimension to biological research and medical diagnosis (CD Figure 39)

# Acknowledgements

The authors thank the organizing committee for the invitation to make this presentation and our colleagues at many of the over 60 NIR instrument manufacturing companies for providing material. Inclusion of pictures or diagrams does not represent endorsement of any specific instrumentation.

<sup>&</sup>lt;sup>1</sup> E.W. Stark, "Near-Infrared Spectroscopy: The New FT Frontier – Spectroscopic and Chemometric Considerations", in 8<sup>th</sup> International Conference on Fourier Transform Spectroscopy, Ed by H.M. Heise, E.H. Korte, and H.W. Siesler, Proc. SPIE 1575, pp. 70-86 (1992)

<sup>&</sup>lt;sup>2</sup> E.W. Stark, "Near-infrared Array Spectrometers", in *Handbook of Vibrational Spectroscopy*, *Vol.1, Theory and Instrumentation*, Ed by J.M. Chalmers and P.R. Griffiths, John Wiley & Sons Ltd., Chichester, UK, pp. 393–422 (2002)