

# Technical Note 7: Description of NTAS (NIR Technology Analysis Software)

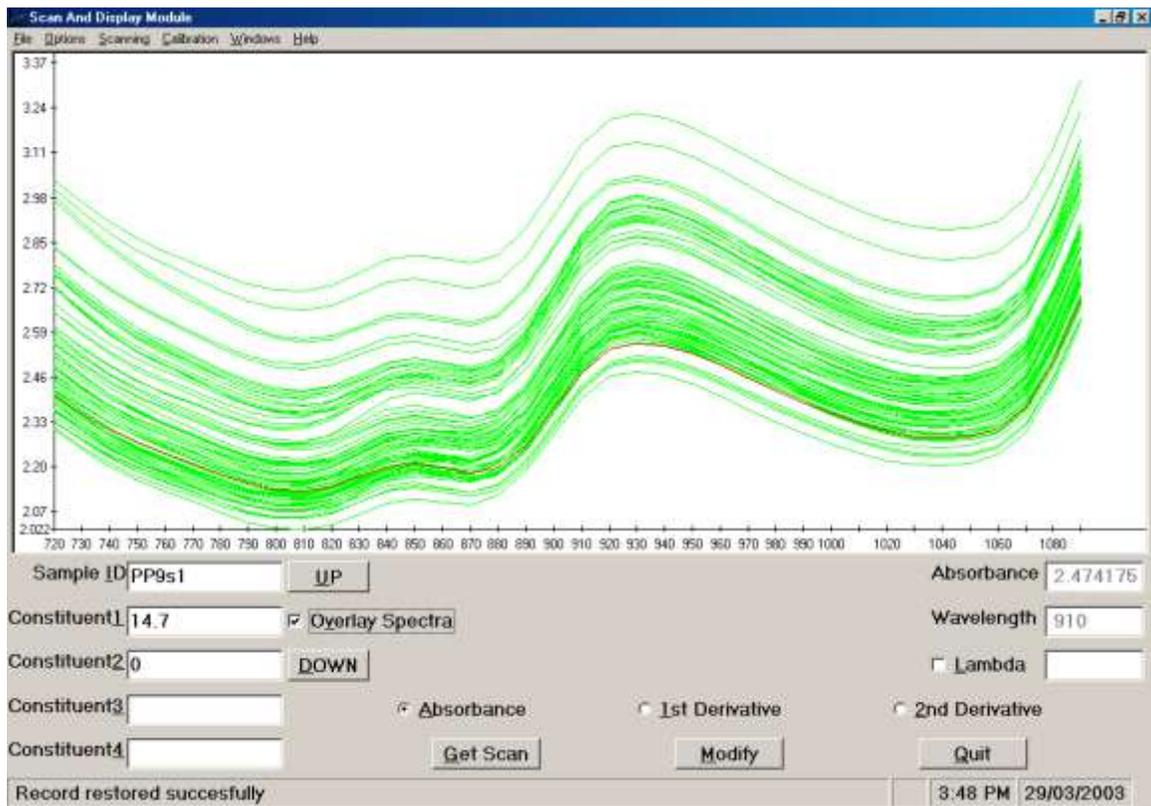


Spectral Analysis and Calibration software package developed in house consisting of the following menus:

- Scan and Display
- Discriminant Analysis
- Analysis
- Calibration Creation
- Spectral Conversion

## *Scan and Display*

This application allows the user to connect NIR Technology Australia products to an external PC for the purpose of:



### 1) *Single Sample Analysis*

- This is useful for:
- Calibration development, i.e. Optimising a particular pathlength to get all spectra within a certain absorbance range
  - Visually distinguishing samples based on spectral characteristics and for the potential determination of outliers.

### 2) *Uploading a data set from an instrument*

Used in a similar way to WGA-Test to upload data, except the data may be viewed instantly as absorbance spectra.

## Features

### 1) Allows spectra to be viewed as:

- Absorbance Spectra
- 1<sup>st</sup> and 2<sup>nd</sup> Derivative Spectra. This is a useful determination whether baseline shifts are affecting the sampling procedure.
- Normalised Spectra. This allows absorbance spectra to be analysed for baseline shifts by normalising multiple spectra to a particular wavelength. This function also allows the user to determine if skew exists if spectra from two instruments are viewed simultaneously.

### 2) Conversion of Regression Models into Binary Files.

- Models generated by regression software packages such as Unscrambler® and Pirouette® must be converted into a format which the instrument can apply the calibration equation to the sample spectral data. LiPS software converts ASCII files into binary files of the correct format for use by NIR Technology Australia instruments.

The following serves as a demonstration of how to convert an ASCII file to a binary file.

- Four files should be generated by the regression software for two constituents:
  - a. Cal.1b0
  - b. Cal.1bn
  - c. Cal.2b0
  - d. Cal.2bn

Where: Cal denotes the name of the model generated  
 1 and 2b0 denotes the ASCII files containing the b0 regression coefficients of the two constituents respectively.  
 1 and 2bn denotes the ASCII files containing the regression coefficients for the constituents respectively.

- Under the Calibration menu, select the convert cal file option and:
  - The user is asked to name the calibration for display on the instrument.
  - Using the browse option, the name of the Cal file is placed in the PC file box. The WGA file box instantly displays the name of the binary file to be generated and the data path it is to be saved to.
  - Click on the Convert button and then proceed to the Parameters menu.
  
- The Parameters menu lets the user:
  - View the number of constituents in the calibration,
  - Allows the number of scans to be set
  - Allows the cell code option to be utilised (although this function is rarely used).
  - Click on Convert and proceed to the Options menu.
  
- The Options menu is used to:
  - Name the constituents, which make up the calibration.
  - Set the limits for the calibration range.
  - Set the mode of calibration, i.e. Absorbance or derivative.
  - Set the temperature correction, (if required).
  - Allows the calibration to set up for constant moisture calculations.
  - Click on convert for each individual constituent and proceed to the Information menu (optional).
  
- The Information menu allows for individual users to:
  - Add information about the calibration including:
    - Authors name.
    - Any special modifications.
    - Date of calibration.
  - This is optional and is used at the discretion of the operator.
  - Click on Convert and proceed to the Summary menu.
  
- The Summary menu allows the user to check for any errors and is used to check that all information is present before downloading the calibration to the instrument.
  - The last part of the Summary file shows four columns. The first two show the b0 and bn regression coefficients.

- The third and fourth columns are for a future feature involving a spectral rejection algorithm based on the average and standard deviation of a set of measurements.
- Click on Convert and the file is now ready for downloading to the instrument.

### 3) Wavelength Calibration

NTAS is used routinely for the wavelength calibration of slave instruments to a master. The process involves measuring a packed wheat sample in the master instrument and then measuring it in the slave. Calibration is usually performed in 1<sup>st</sup> derivative mode where zero points are aligned using the gratings adjustment screw.

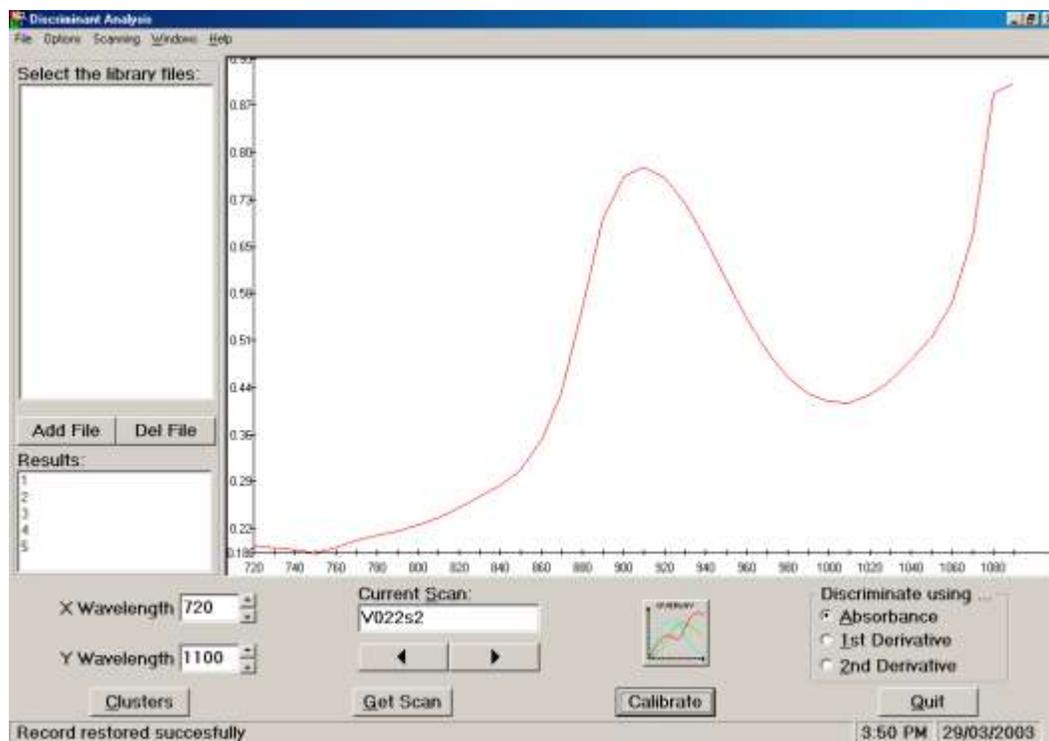
### 4) Modification of existing Calibration files and .ini files.

NTAS may be used in preference to WGA-Test to perform routine operations such as:

- File uploading/downloading
- Editing .ini files
- Setting up general instrument settings

## Discriminant Analysis

The Discriminant analysis function of the LiPS software package requires a pre-collected library of spectra in order to classify new objects based on a distance measure known as the *Mahalanobis Distance*.



- Such pattern recognition is known as Unsupervised Analysis, (classes are found during the course of the learning process).
- In general, discrimination is usually performed using correlation coefficients (sometimes called similarity measures) or using distance measures.

The correlation coefficient can sometimes be too limiting in its application in cluster analysis as it is a measure of the co linearity between variates and takes no account of non-linear relationships. Instead, distance measures are more commonly used.

***The common point between the two methods of analysis is that the greater the distance between objects, the less their similarity.***

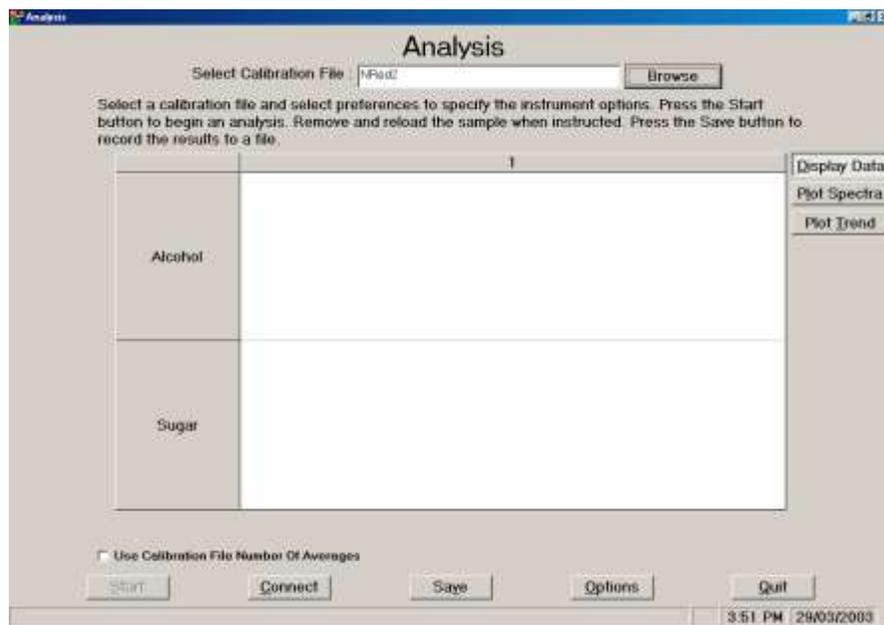
An unknown sample, when presented to the discriminant function, is classified into a particular cluster of spectra using statistical analysis. The closer the distance an object is to a cluster, the higher its membership is to that cluster. Such measures provide a means of developing quality control libraries of spectra in which routine batch analyses can be performed.

## Analysis

The Analysis tool allows the operator to analyse samples directly from a personal computer.

To use the Analysis tool, the following procedure is required:

- A calibration file is chosen from a list of pre-existing calibrations.
- Click on Get Scan and wait for the PC to prompt the user to insert the sample.
- The Cropscan will then scan the sample in the usual way.
- After each scan, the results will be displayed on the screen.
- Allows NIR Spectrum to be displayed on the screen
- Allows Trend Plots to be displayed of the data collected.



## Calibration Creation

**NTAS provides the ability to develop Partial Least Squares(PLS) calibration models and then to combine them with information, such as, Product name, constituent names, ranges etc into a binary file. The binary file can then be downloaded into the analyser.**

NTAS has been designed to be simple and intuitive. Only those functions which are considered necessary to develop a calibration, are included. NTAS is not intended to be a research grade

statistics software suite but a dedicated NIR applications package which is powerful yet easy to use. The features of NTAS are;



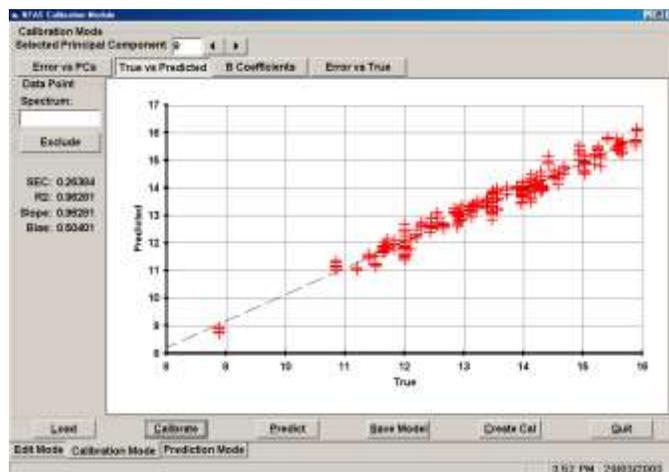
**Edit Mode:** On screen editing of constituent data, Exclusion and Inclusion of samples and wavelengths using an active marquee.

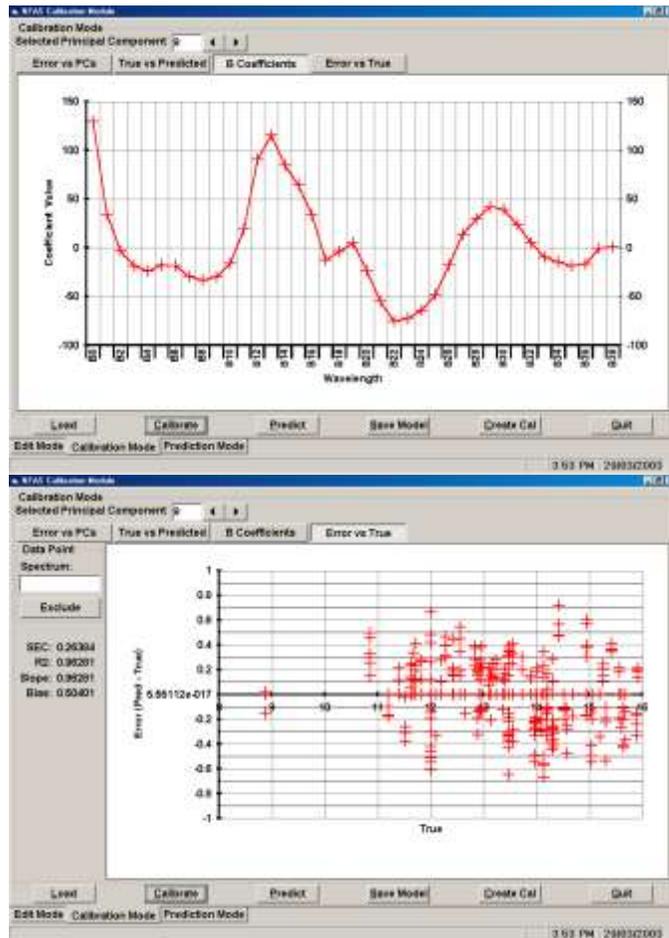
**Error vs PC(Principle Components):** Shows the exponential decay of the SEC as the number of PC's increases.

**True vs Predicted:** An XY plot of the NIR Predicted data vs the True data. Allows interactive exclusion of outliers. Shows labels and values. Allows data to be copied and exported to other programs.

**B Coefficients:** Displays the B0 and B1-B38 coefficients developed in the modelling process. On screen refresh by changing the number of PC's.

**Error vs True:** Displays the plot of the difference between the NIR and the True data vs the True data. Shows any skew or bias on the calibration data.





## Spectral Conversion

This routine allows the user to convert Infratec Spectra into Cropsan domain spectra. A set of samples are scanned on both the Infratec and Cropsan. A wavelength alignment is performed and the software then develops an algorithm to convert the 100 wavelength spectra from the Infratec into 21 wavelengths in the Cropsan domain. Then a large set of Infratec spectra can be converted into Cropsan domain and saved as an unique file name. This file can then be Loaded into the Calibration Creation module and a PLS calibration developed. This calibration can then be downloaded into a Cropsan.

The advantage of this module is that an organization which has a large database of Infratec spectra, can develop calibrations for the Cropsan without the need to rescan all the samples.