Purpose: To provide a quick reference to the basic functions of uploading spectral data, calibration development and calibration downloading.

Uploading Spectral Data.

There are two ways of doing this:

1) Using the **WGA_Test** program.

   a. Using the null modem cable, connect the instrument to a PC, double click on the **WGA_Test** icon and wait for the program to start. A window should appear with a number of functions. The **File Downloading** Button should be clicked to upload and download data.

   b. If the warning box, *"No response, Is WGA connected"* appears, click on **NO** and the program window will appear, but in this case, there will be no connection to the instrument. Click on *Com port set-up* and select the COM port the instrument is connected to. The baud rate must also be set to **38400**. Once set-up, exit the program and restart it the make a connection with the instrument.

   c. In the **File Downloading** menu, the first box asks for the **WGA File**. In all cases, the results are stored in a directory called *results.csv*. This should be typed into this box and in the **PC File** box, the directory and the name the file is to be called is placed here. *For example*, if the file is to be saved to floppy with the name *data.csv*, the structure should be as follows:
            a:\data.csv
   d. The data is now in a format for **NTAS** to read.

2) Using **NTAS.**

   a. Double click on the **NTAS** icon to start the program and make a connection to the instrument using the null modem cable. Select the **Scan and Display** button and a dialog box will appear asking the user if they want to connect to the instrument. Click on *Connect* and the computer will make a connection to the instrument. If no connection can be made, select the **Scanning** menu and then the **Preferences** menu. From here set-up the correct COM port and baud rate (38400). This menu also allows the user to select the instrument to connect to, i.e. Cropscan, NIT, FOP etc.

   b. Once connected, select the **File** menu and click on *Upload Results File*. Use the **Browse** option to name the file and the directory you want the results to be saved to and then click on **Upload Results**.

c. When uploading is complete, exit the program and the results are saved in the directory specified as a .csv format.

Entering Laboratory Data to Results File

The easiest way to add laboratory data is to open the results file using Microsoft Excel. Under Cal1, Cal2 etc, enter the laboratory data to the corresponding samples and save the file as a csv file.

Calibration.

1) Double click on the **NTAS** program icon and select **Calibration Creation**. Then click on the Load button to load the results file obtained from the instrument. The spectral data should appear on the computer screen along with the sample ID numbers. To view the laboratory data, click on the Constituent Data button.

2) Using the mouse, select the columns of data to be excluded and using the right hand button of the mouse, select **Exclude Columns**.

3) The data is now ready for calibration. Click on the **Calibrate button** and a dialog box will appear asking the user to enter the maximum number of principal components and which component to calibrate on. Select the appropriate settings and **Start** the calibration.

4) A plot will appear showing the *Standard Error of Calibration (SEC)* vs. Principal Components. This gives an indication of the quality of the calibration and shows where the optimal Principal component is. Some understanding of the basic principles of calibration are required at this stage to optimise the model developed, which may include sample deleting etc.

5) Once a constituent has been calibrated, it must be saved before calibrating on the next. To do this, click on **Save Model** and a box will appear asking the user what directory to save the file to. Select the directory and save the model, then return to the spectral data, click the **Calibrate** button and the computer will ask the user, do you want to recalibrate, select *Yes* and the dialog box will appear. Select constituent 2 (or whatever constituent required) and **Start** the calibration.

6) After the calibration has been optimised, it must be saved. Click on **Save Model** and the computer will ask the user, *"Do you want to add this to the existing calibration"*. Click on **Yes** and the other constituents (if any) are calibrated in the same way.

Converting a Calibration Model into a Binary File.

The models saved in the chosen directory are in a particular format, which NTAS can read in order for conversion of the data to a binary file. The files are saved as the name of the spectral data file, but have extensions of the form *1bn, 1b0, 2bn, 2b0* etc. A file extension 1bn relates to the first constituent (*hence 1*) **b** relates to the term *b-factor*, which is associated with the

regression coefficients of the equation and *n*, relates to the number of spectral points of the instrument. For the NIT-38 instrument, n=38. The ***1b0*** file contains a single calibration value associated with the calibration offset.

To create a calibration:

1) Click on the Create Cal button, the first dialog box to appear (***labelled Filenames***) will firstly ask for the name of the calibration. Type in the name of the calibration (this will be the name to appear on the LCD display). The next box asks the user to enter the name of the model files, including the directory path it is stored under. Beside this box is a button, which when clicked on allows the user to browse the computer for the files. **NTAS** looks only for file types ***1bn*** etc and automatically locates the rest of the files to develop a calibration. If, for example, four constituents have been calibrated for, NTAS will find all files up to a maximum of ***4bn*** and ***4b0*** to convert. If files are missing, a calibration cannot be developed.

2) After the appropriate file has been found, double click on it and the screen returns to the original dialog box showing the calibration name etc. If all files are present and no errors can be found, the **Convert** button becomes active. Click on this button to convert the first part of the calibration.

3) Click on the next menu tab titled **Parameters.** This menu shows the number of constituents in the calibration, the number of scans to perform per measurement (usually set to 5), and the cell to use with the calibration (this does not have to be changed from 20mm). When satisfied with this information, click on **Convert** to store this data.

4) Click on the next menu tab called Options. This menu allows the user to name the individual constituents to be displayed on the screen. If, for example, the calibration consists of four constituents, Protein, Moisture, Colour and Starch, use the mouse to click on the box-containing Con 0. In the box called Constituent name, type in protein (if this was the first constituent calibrated) then click on the update button. The box-containing Con 0 now should read Protein. The next step is to set the calibration limits. If the range of protein values in the calibration set is between, for example 8.3-14.7%, set the minimum limit to 8.0% and the maximum limit to 15.0%. The rest of the parameters are set as default and do not need to be adjusted unless a first derivate calibration is being developed, in which case, the **1**st button is clicked on. The same procedure is followed for the rest of the constituents. When this process is completed, click on the Convert button and the complete calibration is set-up.

5) The next menu, titled **Information**, is an optional step where the author of the calibration, time, date and additional remarks can be added.

6) The next menu, titled **Summary**, allows the user to check that all the data entered is correct and that no errors have occurred.

Downloading a Calibration to the Instrument.

There are two methods for downloading a calibration.

Using **WGA-Test**:

1) Double click on the **WGA_Test** program to make a connection to the instrument and click on the **File Downloading** button. In the **WGA File** box, type in the following:
   c:\wga\calibr*cal name*.bin   The cal name is the one named in the NTAS file with the bin extension, for example, if the calibration is called ***wheat.bin***, the path is ***c:\wga\calibr\wheat.bin***.

2) In the **PC File** box, enter the calibration file name along with the directory it came from, for example, if the calibration file ***wheat.bin*** is on a floppy disk, the following should be typed: ***a:\wheat.bin.*** When this is completed, click on **Download to WGA**. When complete, the computer will show a box ***"File Successfully Downloaded"***. Click on **OK** and then exit from the program. The calibration file is now downloaded to the instrument and is ready for fine-tuning to the new instrument using a minimum of five (5) reference samples.

Using **NTAS**

1) Make a connection to the instrument as described above for **NTAS** in the *Scan and Display Mode*. Click on the **Calibration** menu and then click on **Download Calibration File**. The program will bring up a browse window and allow the user to find the directory where the calibration file is located. Double click on the file and a menu box will appear with a button, **Download Calibration File**. Click on this button and the calibration will be downloaded to the instrument. Exit the program and the calibration is ready for fine-tuning.