InnoSpectra NIRScan

Spectrometer & Module

User Manual

Ver. 1.2

2021/09/06

www.inno-spectra.com

Thank you for choosing InnoSpectra! Please read this manual carefully and follow the operating instructions and application guidelines.

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Chapter 1 Introduction

1.1 Near-infrared Spectroscopy

Near-infrared spectroscopy (NIRS) is a spectroscopic method based on the absorption of electromagnetic radiation at wavelengths from 700 to 2500nm. NIRS is a form of molecular spectroscopy. NIR radiation is absorbed by molecules through a mechanism involving molecular vibration. Not all bonds in a molecule are capable of absorbing infrared radiation. Only those bonds that have a dipole moment that changes as a function of time are capable of absorbing infrared radiation. For example, O–H, N–H, C–H, S–H bonds are strong NIR absorbers. The most prominent absorption bands occurring in the NIR region are related to overtones and combinations of fundamental vibration. In vibrational spectroscopy, an overtone band is the spectral band that occurs in a vibrational spectrum of a molecule when the molecule makes a transition from the ground state (v=0) to the second excited state (v=2), which is called the first overtone, or from the ground state (v=0) to the third excited state (v=3), which is called the second overtone.

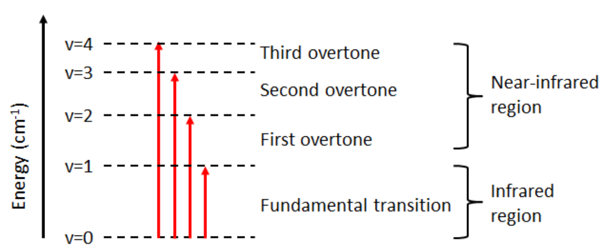


Figure 1.1 Vibrational Transitions

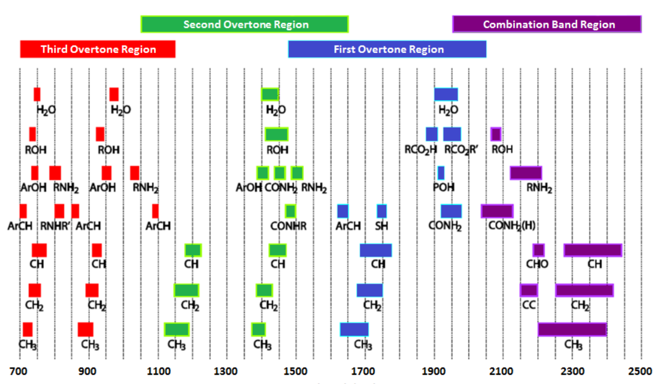


Figure 1.2 NIR Absorption Bands

NIRS has unique properties which makes it very useful for the analysis of most solid, slurry and liquid samples. NIRS in conjunction with chemometrics has revolutionized much of the general area of analyses.

1.2 NIRScan

InnoSpectra Corporation (ISC) is devoted to the development of NIR analysis solution. ISC is committed to providing a series of compact and cost-effective DLP-based NIR spectrometers including fiber input modules, diffuse reflective modules and transmissive modules in different wavelength range to support all sorts of applications. The optical engine of the DLP-based NIR spectrometer adopts a post-dispersive architecture, which is composed of an entrance slit, a set of collimating lenses, a bandpass filter, a diffraction grating, a set of focusing lenses, a DMD (digital micromirror device), a set of light receiving lenses and a single-element InGaAs detector. A DLP-based spectrometer uses a DMD and a single-element InGaAs detector to replace a traditional linear array detector. Compared to the spectrometer with a linear array detector, NIRScan is equivalent to a 128-pixel device at the same wavelength range and spectral resolution.

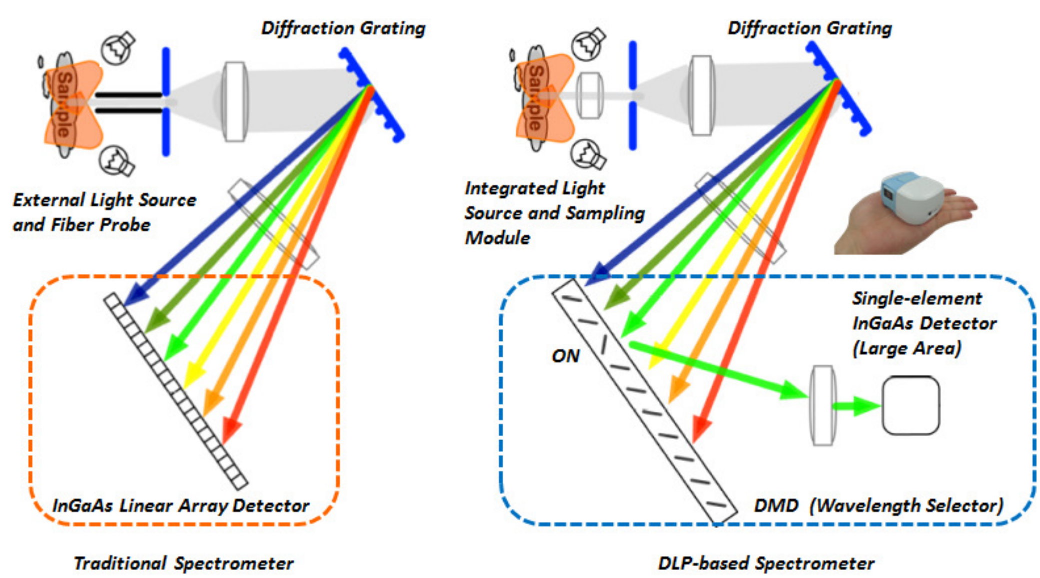


Figure1.3 Traditional vs. DLP-based Spectrometer

DLP technology in NIR spectroscopy provides the following advantages:

1. Higher performance through the use of a larger single-element detector (φ=1mm) in comparison to a linear array with very small pixels (e.g. 50µm).
2. The high resolution DMD (854*480 pixels) allows custom patterns to optimize the optical performance of each individual system.
3. With programmable patterns, a DLP spectrometer can use Hadamard patterns to improve SNR. In Hadamard mode, a wide DMD pattern is displayed, so higher optical energy will be captured by the InGaAs detector.

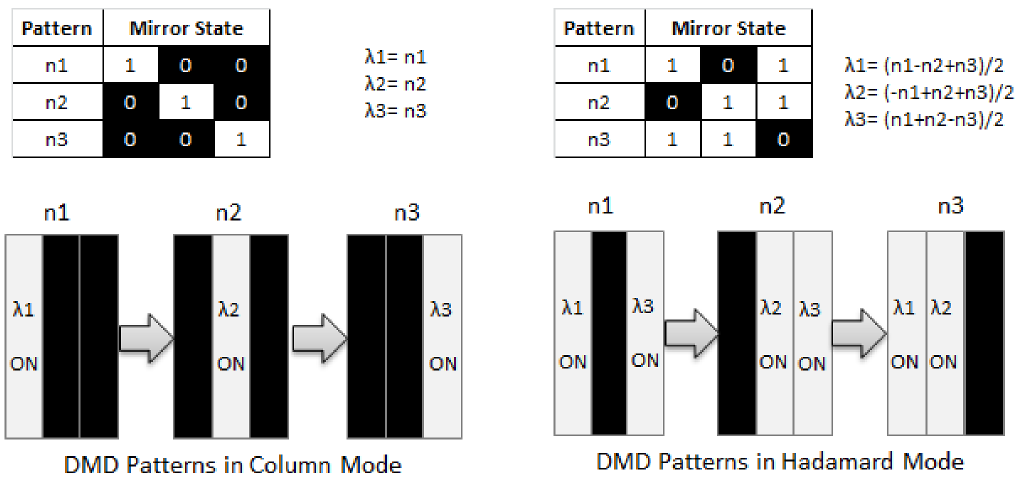


Figure1.4 Column Mode vs. Hadamard Mode

ISC provides high performance and cost-effective DLP-based NIR spectrometers in two wavelength ranges:

1. Standard wavelength range：900-1700 nm (STD)
2. Extended wavelength range：1350-2150 nm (EXT)

Table 1.1 ISC NIRScan Specifications

Specification	Description	
Wavelength Range	900-1700nm (STD)	1350-2150nm (EXT)
Optical Resolution	10nm	12nm
Wavelength Accuracy	≦ +/- 1nm	
Signal-to-Noise Ratio	≧ 5000:1	
Slit Size	1.8mm * 0.025mm	
Detector	1mm InGaAs (non-cooled)	
Scan Capability	Linear (Column) / Hadamard / Slew	
Measurement mode	Fiber Input/ Transmissive / Diffuse Reflective / Transflective	
Interface	USB / BLE / UART	
Sensor	Humidity / Temperature	
Power Supply	USB / Li-ion battery	

1.2.1 Diffuse Reflective Module & Spectrometer

1. NIR-S-G1 (900-1700nm)

NIR-S-G1 is a diffuse reflective spectrometer that integrates two built-in 0.7W tungsten filament lamps as illumination sources, a sampling module with a sapphire scan window, a DLP-based post-dispersive optical engine, a BLE module, an operation panel, a rechargeable lithium-ion battery pack and an EMC shielding case.

- Wavelength Range: 900 to 1700nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 10nm, Max. 12nm
- Wavelength Accuracy: Typ. ±1 nm (verified with SRM2036), Max. ±2 nm
- Detector: 1mm InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Illumination Module: Diffuse reflective with two integrated tungsten filament lamps
- Scan window: Protect and seal with sapphire glass
- Communication Interface: Micro USB / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / Li-ion battery (1000mAh@3.7V)
- Dimensions: 82.2mm * 66mm * 43.5mm
- Weight: < 150 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

Figure 1.5 NIR-S-G1

2. NIR-M-R2 (900-1700nm)

NIR-M-R2 is a diffuse reflective module that integrates two built-in 0.7W tungsten filament lamps as illumination sources, a sampling module with a sapphire scan window, and a DLP-based post-dispersive optical engine. Both power and signal can be transmitted via USB or UART interfaces, while BLE module and operation panel are optional. NIR-M-R2 is suitable for secondary development by system integrators.

- Wavelength Range: 900 to 1700nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 10nm, Max. 12nm
- Wavelength Accuracy: Typ. ±1 nm (verified with SRM2036), Max. ±2 nm
- Detector: 1mm InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Illumination Module: Diffuse reflective with two integrated tungsten filament lamps
- Scan window: Protect and seal with sapphire glass
- Communication Interface: Micro USB / UART / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / UART / Li-ion battery
- Dimensions: 76mm * 57.6mm * 26.8mm
- Weight: < 80 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

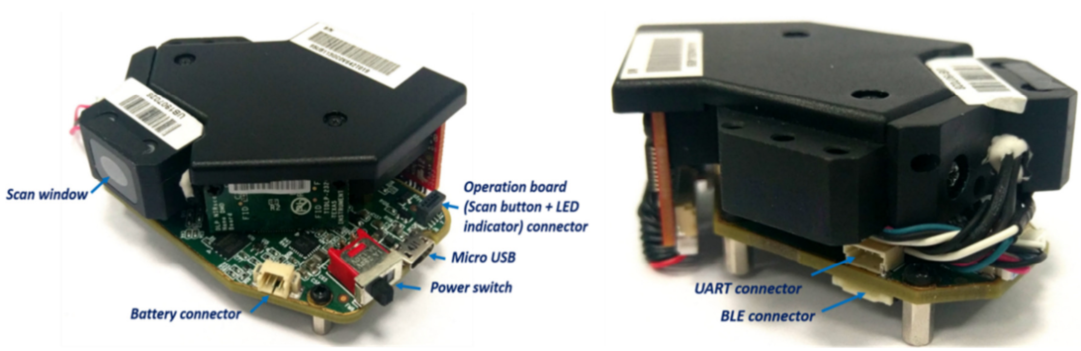


Figure 1.6 NIR-M-R2

1.2.2 Transmissive Module

1. NIR-M-T1(900-1700nm)

NIR-M-T1 is a transmissive module that integrates one built-in 0.7W tungsten filament lamp as illumination source, a sampling module with cuvette holder and receiving lens, and a DLP-based post-dispersive optical engine. Both power and signal can be transmitted via USB or UART interfaces, while BLE module and operation panel are optional. NIR-M-T1 is suitable for secondary development by system integrators.

- Wavelength Range: 900 to 1700nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 10nm, Max. 12nm
- Wavelength Accuracy: Typ. ±1 nm (verified with RM-NIR), Max. ±2 nm
- Detector: 1mm InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Illumination Module: One integrated tungsten filament lamp
- Cuvette Holder: Standard 10 x 10 mm cuvette
- Communication Interface: Micro USB / UART / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / UART / Li-ion battery
- Dimensions: 76mm * 91.8mm * 41.2mm
- Weight: < 106 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

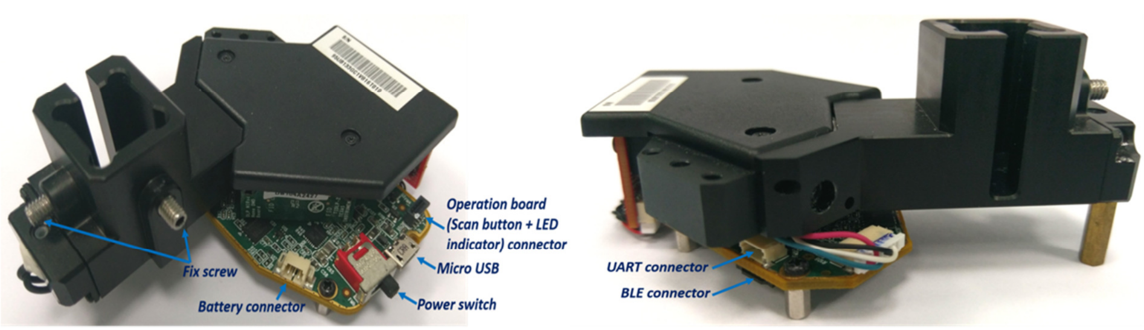


Figure 1.7 NIR-M-T1

2. NIR-M-T11 (1350-2150nm)

NIR-M-T11 is a transmissive module that integrates one built-in 0.7W tungsten filament lamp as illumination source, a sampling module with cuvette holder and receiving lens, and a DLP-based post-dispersive optical engine. Both power and signal can be transmitted via USB or UART interfaces, while BLE module and operation panel are optional. NIR-M-T11 is suitable for secondary development by system integrators.

- Wavelength Range: 1350 to 2150nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: 12nm @1530nm LD
- Wavelength Accuracy: Typ. ±1 nm (verified with RM-NIR), Max. ±2 nm
- Detector: 1mm extended InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Illumination Module: One integrated tungsten filament lamp
- Cuvette Holder: Standard 10 x 10 mm cuvette
- Communication Interface: Micro USB / UART / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / UART / Li-ion battery
- Dimensions: 48mm * 96mm * 38.2mm
- Weight: < 100 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

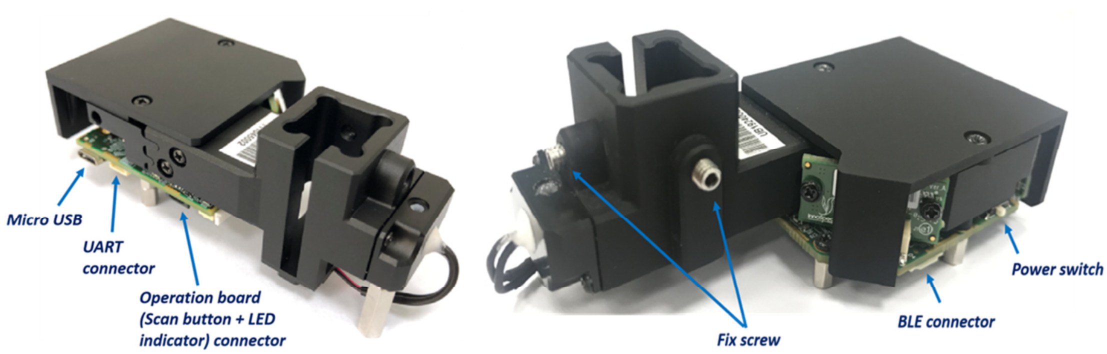


Figure 1.8 NIR-M-T11

1.2.3 Fiber Input Module

1. NIR-M-F1 (900-1700nm)

NIR-M-F1 is a fiber input module that provides a standard SMA905 connector with key slot. Both power and signal can be transmitted via USB or UART interfaces, while BLE module and operation panel are optional. NIR-M-F1 can be integrated with illumination source, optical fiber and sampling module for diffuse reflection, transmission, trans-reflection or interactive measurement.

- Wavelength Range: 900 to 1700nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 10nm, Max. 12nm
- Wavelength Accuracy: Typ. ±1 nm (verified with RM-NIR), Max. ±2 nm
- Detector: 1mm InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Fiber Connector: SMA905
- Communication Interface: Micro USB / UART / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / UART / Li-ion battery
- Dimensions: 76mm * 54.5mm * 26.8mm
- Weight: < 65 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

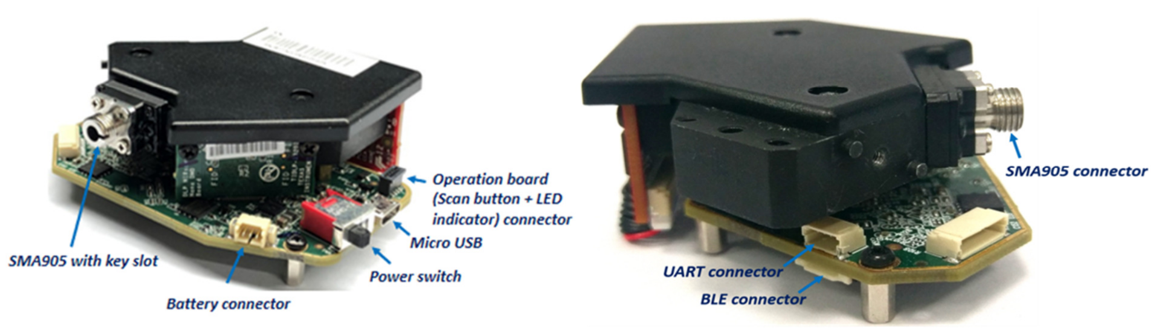


Figure 1.9 NIR-M-F1

2. NIR-M-F11 (1350-2150nm)

NIR-M-F11 is a fiber input module that provides a standard SMA905 connector with key slot. Both power and signal can be transmitted via USB or UART interfaces, while BLE module and operation panel are optional. NIR-M-F11 can be integrated with illumination source, optical fiber and sampling module for diffuse reflection, transmission, trans-reflection or interactive measurement.

- Wavelength Range: 1350 to 2150nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 12nm @1530nm LD
- Wavelength Accuracy: Typ. ±1 nm (verified with RM-NIR), Max. ±2 nm
- Detector: 1mm extended InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Fiber Connector: SMA905
- Communication Interface: Micro USB / UART / Bluetooth Low Energy (BLE)
- Sensors: Humidity and temperature sensor
- Power: Micro USB / UART / Li-ion battery
- Dimensions: 48mm * 59.5mm * 24.6mm
- Weight: < 65 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

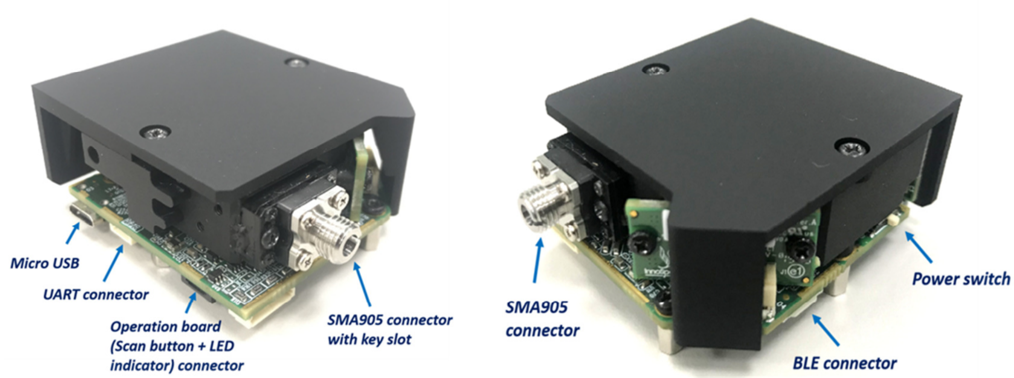


Figure 1.10 NIR-M-F11

1.2.4 Reflective-Transflective Spectrometer

NIR-S-RT1 is a diffuse reflective and transflective spectrometer that integrates two built-in 0.7W tungsten filament lamps as illumination sources, a sampling module with a sapphire scan window, a DLP-based post-dispersive optical engine, a BLE module, 4 LED indicators, a rechargeable lithium-ion battery pack, a 1mm standard glass cuvette holder, a detachable white reference material (NIR-RM-1) pre-installed on the top cover and a case that can make the spectrometer stand stably.

- Wavelength Range: 900 to 1700nm
- Signal-to-Noise Ratio (SNR): 5,000:1 in 1 second scan
- Optical Resolution: Typ. 10nm, Max. 12nm
- Wavelength Accuracy: Typ. ±1 nm (verified with SRM2036), Max. ±2 nm
- Detector: 1mm InGaAs (Uncooled)
- Slit Size: 1.8mm * 0.025mm
- Scan Capability: Linear / Hadamard / Slew Scan
- Illumination Module: Diffuse reflective with two integrated tungsten filament lamps
- Scan Window: Protect and seal with sapphire glass
- Cuvette Holder on Top Cover: support 1mm standard glass cuvette
- Sampling method: diffuse reflective and transflective
- White reference material: NIR-RM-1 included
- Communication Interface: Micro USB / Bluetooth Low Energy (BLE)
- Sensor: Humidity and temperature sensor
- Power: Micro USB / Li-ion battery (1000mAh@3.7V)
- Dimensions: 93mm * 76mm * 73.5mm
- Weight: < 222 g
- Operating Temperature: 0 ~ 40 ℃, RH Max. 85%

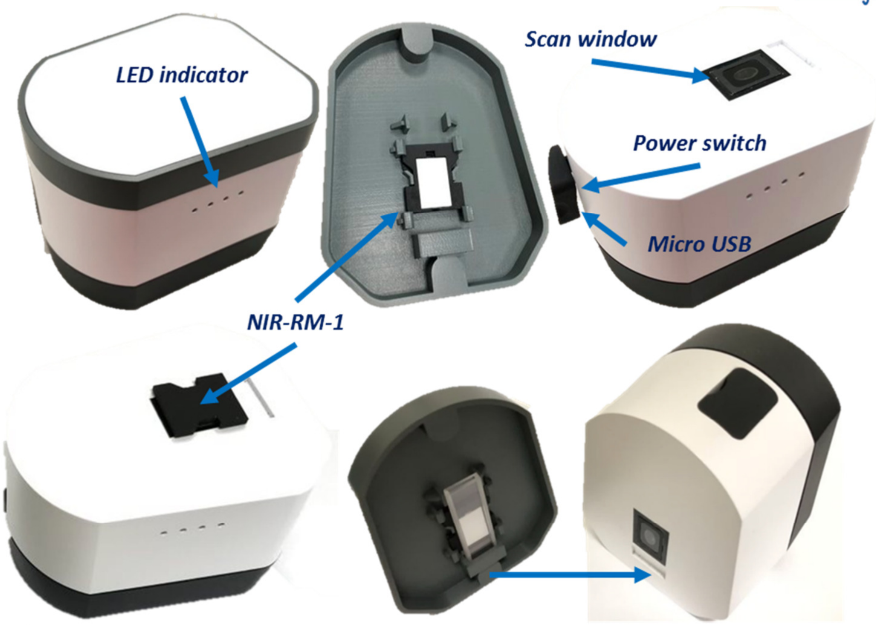


Figure 1.11 NIR-S-RT1

1.3 NIR Measurement

Karl Norris, the Father of Near-Infrared Spectroscopy, discovered that the NIR region had a convenient combination of useful properties that caused it to be uniquely suited to being used for various applications to chemical analysis. The advantages of the use of NIR are speed, cost, range of applicability, non-destructive, environmental benefits due to non-use of chemicals, and simultaneously multi-component analysis. NIR analysis can be used successfully when sample is not in a clear solution (e.g. a powdered solid, an emulsion, a suspension, etc.). Spectral measurement can be taken using diffuse reflection rather than transmission. NIR analysis has been rapidly and widely applied in agriculture, petroleum, pharmaceuticals, biometrics, soil analysis, and so on. The advent of NIR analysis in conjunction with chemometrics has revolutionized much of the general area of analyses. There are four standard measurement modes for the acquisition of NIR spectra from a sample: transmission, reflectance, transflectance, and interaction.

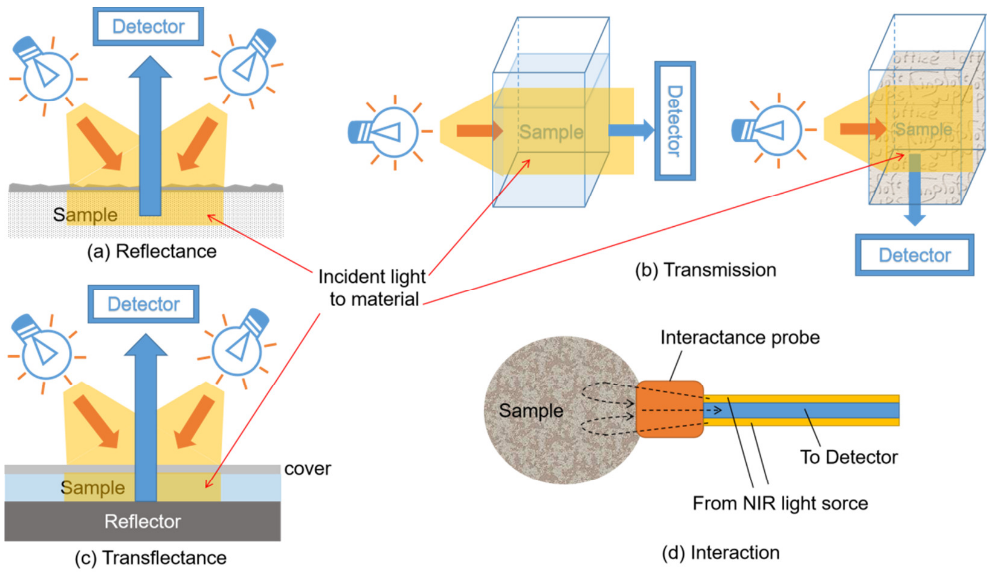


Figure 1.12 Measurement Modes for NIR Spectroscopy

Chapter 2 Getting Started and Software Operation

2.1 Getting Started

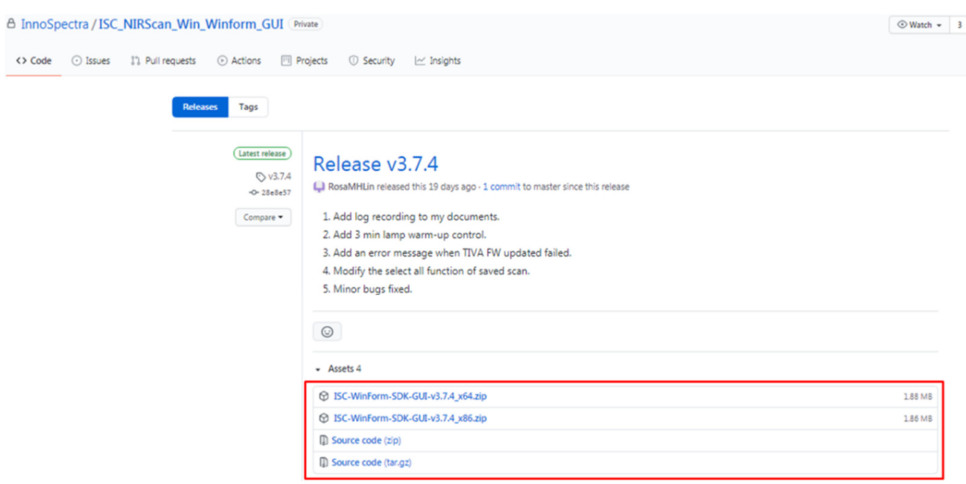
2.1.1 System Requirement

Please check the following system requirements.

- OS: Microsoft Windows 7/8/10
- Microsoft Visual C++ Redistributable (x86/x64): 2010 or 2017

2.1.2 Download Software

ISC provides WinForms GUI and SDK, which supports 32bit or 64bit Windows via USB interface. Please provide your GitHub account, we will invite you to access our repository and you will be able to download software and user guides from https://github.com/innospectra.



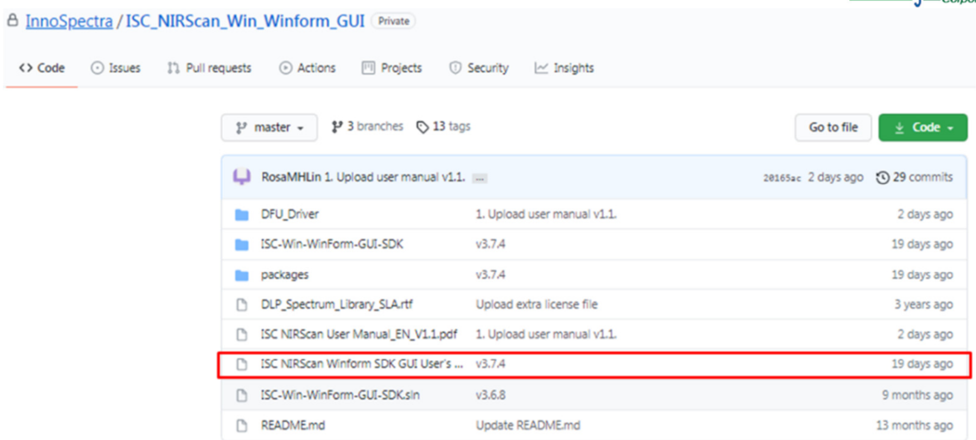


Figure 2.1 Download WinForms GUI and User Guide from Github

2.1.3 Install Software

After downloading the software package from GitHub, you can unzip it and run the executable file directly. Please note that for some reasons, antivirus software may quarantine executable files. When the executable file is found to be quarantined, please try to restore it through the antivirus program settings.

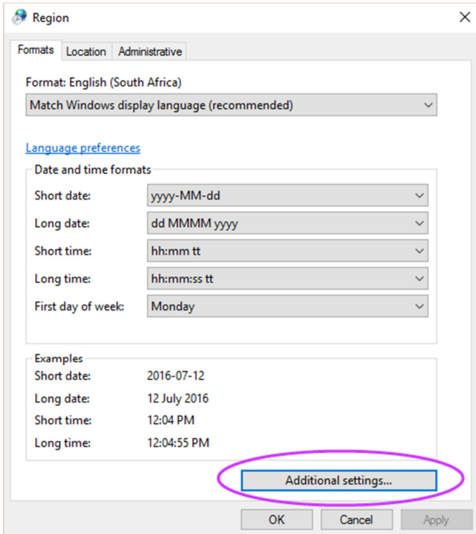
2.1.4 Regional Settings

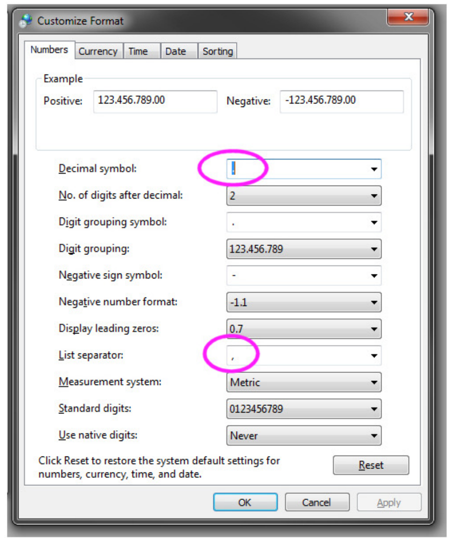
The software will store spectrum data into a CSV file which is a delimited text file that uses a comma to separate values. Please ensure the regional settings of Windows as follows:

- Decimal symbol → dot (.)
- List separator → comma (,)

You can refer to the following website to learn how to set decimal symbol and list separator properly.

https://resrequest.helpspot.com/index.php?pg=kb.page&id=279

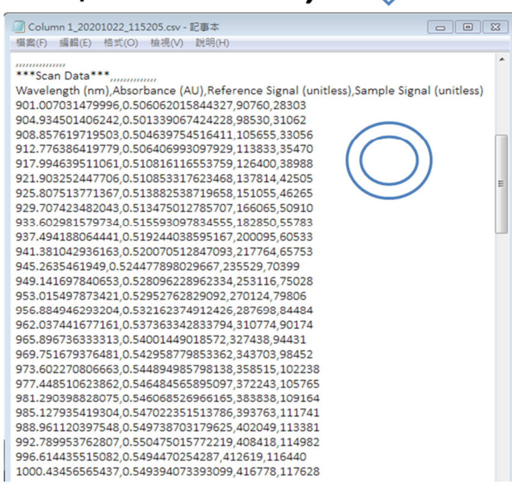




If you use a comma as the decimal point symbol, an error will occur when opening the CSV file in Excel.

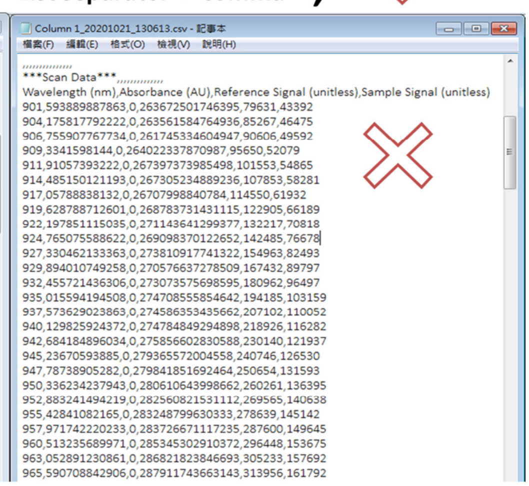
Decimal symbol -> dot .

List separator -> comma ,



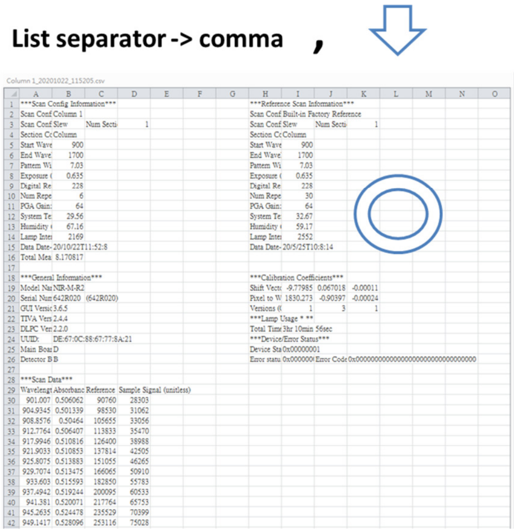
Decimal symbol -> comma ,

List separator -> comma ,



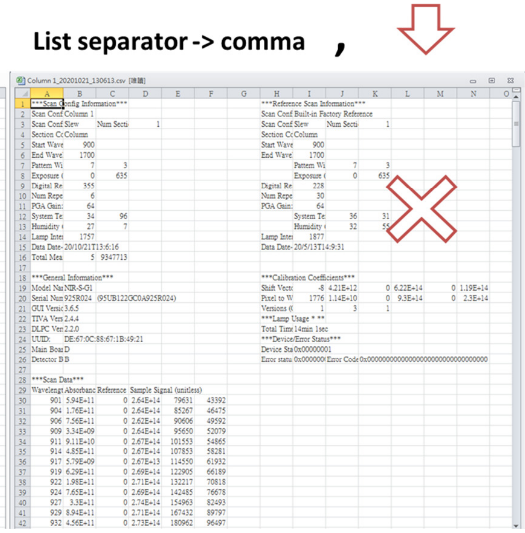
Decimal symbol -> dot .

List separator -> comma ,



Decimal symbol -> comma ,

List separator -> comma ,

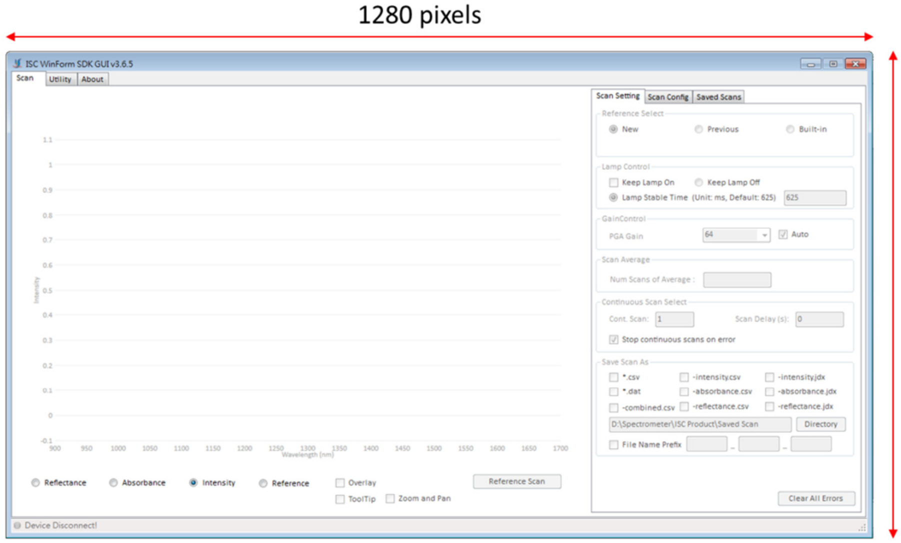


2.1.5 Font Size vs. Text Overlay

Whether your monitor is 1366x768, 1920x1080, or any higher resolution, whether you're running Windows 7 or 10, please set the default font size (100%) to obtain the correct GUI display. If you set a larger font size (125%), the text in the screen will overlap without being clearly distinguished.

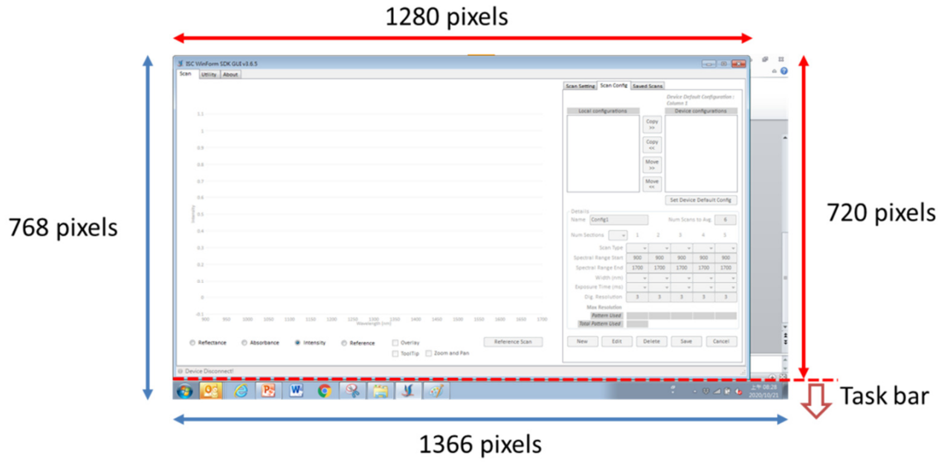
GUI resolution: 1280 x 720 (fix)

1280 pixels

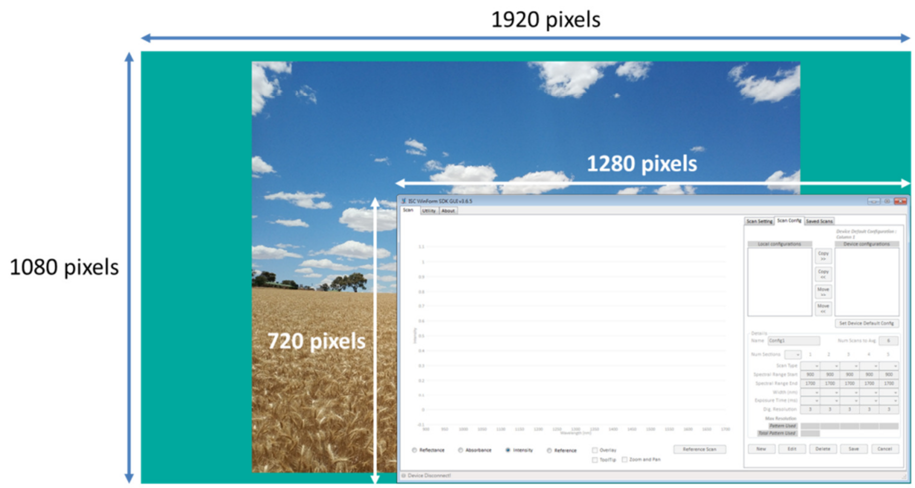


720 pixels

Display resolution: 1366 x 768 and Windows font size: default (100%)

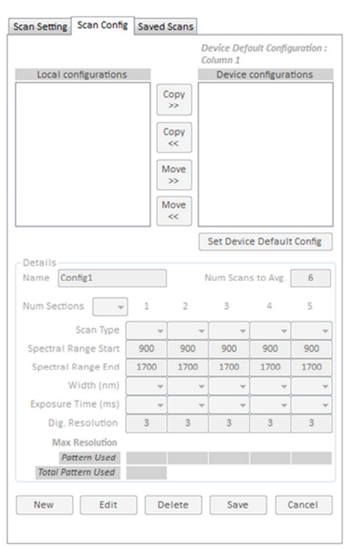


Display resolution: 1920 x 1080 and Windows font size: default (100%)

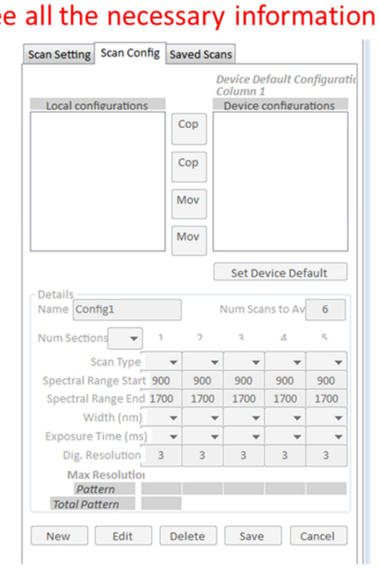


Windows font size: 100% -> **125%**

100% font size (default) => normal display



125% font size => text overlay, cannot see all the necessary information



2.1.6 USB Requirement

All ISC NIRScan can be powered by USB cable. The USB specification is as below:

- USB 2.0: 5V (4.75-5.25V) / Minimum of 0.5A (1A is preferred for diffuse reflective modules)
- USB A male to micro-USB B male

2.1.7 LED Indication

For products with an operation panel (OP) and BLE module, such as NIR-S-G1, NIR-S-RT1 and NIR-M-R2-OB, you can check the device status through the LED indicator. As shown in the following figure, when you power on the NIR-S-G1, the green and blue LEDs will light up, indicating that the NIR-S-G1 is ready for BLE or USB connection. If the NIR-S-G1 is connected to the ISC WinForms GUI via a USB cable, the BLE function will be turned off and the blue LED will also be turned off.

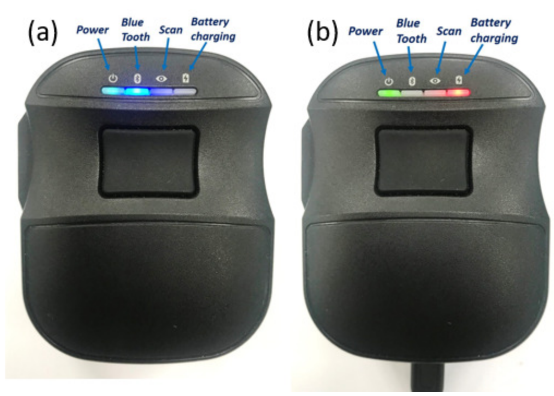


Figure 2.2 LED indicator of ISC NIRScan Device

For all the details of the LED indications, please refer to the following table.

Table 2.1 ISC NIRScan LED indicators

LED	Condition	Description
Green	ON	Indicates system is powered and active

	Pulse on and off, twice per second	Indicates any of the following errors occurred: ADC data access error Tiva EEPROM access error Spectrum data calculation error Hardware error Temperature & humidity sensor access error Insufficient memory error System error
Blue	ON	Bluetooth circuits are active and advertising *OFF: When USB connection or no BLE function
	Pulse on and off, once per second	Bluetooth Low Energy connection has been established
	Pulse on and off, twice per second	Bluetooth communications error
Yellow	ON	Scan is being performed
	Pulse on and off, twice per second	Scan error
Red	ON	System is charging a battery
	Pulse on and off, every 250 milliseconds	Battery Low

2.2 Software Operation

After connecting ISC NIRScan via USB, turning on the power switch and executing the ISC-NIRScan-GUI.exe, the software will check ISC NIRScan automatically. In order to get the best GUI display effect, we recommend using a screen resolution of 1366 x 768. There are three tabs in the upper left corner of the GUI.

- Scan: You can edit the scan configuration and scan settings, perform reference scans and sample scans, and view the saved scan data.
- Utility: You can check device information and sensor readings, manage calibration coefficients and built-in reference data, update firmware, and activate advanced functions.
- About: You can view the license agreement and obtain ISC contact information.

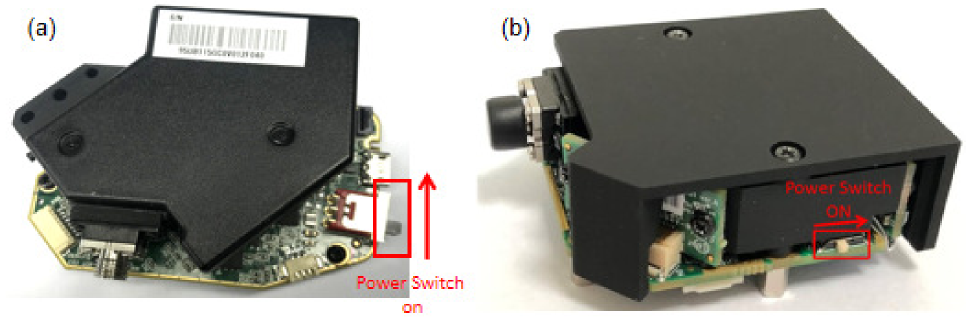


Figure 2.3 Power Switch Location (a) STD Module (b) EXT Module

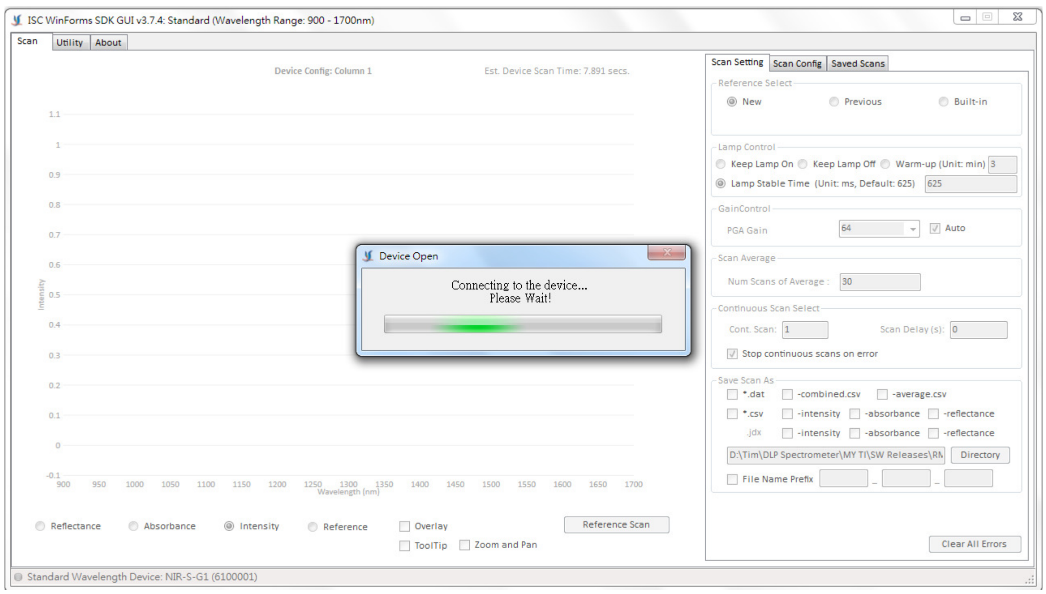


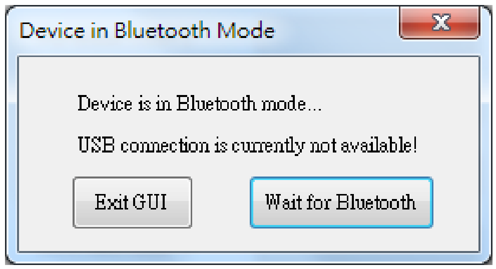
Figure 2.4 ISC WinForms GUI Connecting to NIRScan Device

If you are not able to operate NIRScan device via WinForms GUI, please check the following guidelines:

- If it's the first time for a NIRScan device to connect to the computer, it will take a little time for driver installation. The driver will be installed automatically by Windows.
- After installing the driver, please use the Device Manager to check whether the NIRScan device has been correctly identified as HID compatible device (HID \ VID_0451 & PID_4200) and USB input devices (USB \ VID_0451 and PID_4200).
- If WinForms GUI cannot connect NIRScan properly, but the computer can recognize NIRScan as HID-compliant and USB input devices, please use device

manager to uninstall NIRScan driver and then reboot computer. After rebooting the computer, please insert NIRScan, Windows will try to recognize and install the driver for NIRScan. Once the driver is installed correctly, WinForms GUI will be able to connect with NIRScan.

◆ If the device is in Bluetooth mode, but you connect it to the PC, WinForms GUI will pop up a message box to remind you. You need to close the Bluetooth session before running the WinForms GUI.



2.2.1 Scan Configuration

You need to select or create a new scan configuration before scanning. The ISC NIRScan device is pre-built with one or two scan configurations. You can customize the following parameters in the scan configuration dialog box according to your application.

◆ Name: Type the name of the scan configuration.

◆ Num Scans to Avg: Enter the number of scans to average for corresponding amount of back-to-back scans averaged together. Increasing this amount results in longer scan with the noise averaged out through several back-to-back scans.

◆ Num Sections: Use one section for a scan with the same pattern width and digital resolution in the desired wavelength range. Use more than one section to perform a fast scan with less resolution on wavelengths with little information and a slow scan with higher resolution on wavelengths with areas of interest. A scan can be broken up into 1-5 sections.

◆ Scan Type: Select “Column” or “Hadamard” for each section.

◆ Spectral Range: The desired spectral range can be 900nm to 1700 nm or 1350nm to 2150 nm.

◆ Width (nm): Pattern width corresponds to the smallest wavelength content that you want to resolve.

- Exposure time (ms): The exposure time can be set in the range of 0.635 to 60.960 ms.
- Dig. Resolution: This number defines how many wavelength points (number of sampling points) are captured across the defined spectral range. In general, the recommend digital resolution is (wavelength range/pattern width) x2 or 2.5 (oversampling). For example, (1700-900)/7.03x2=228.

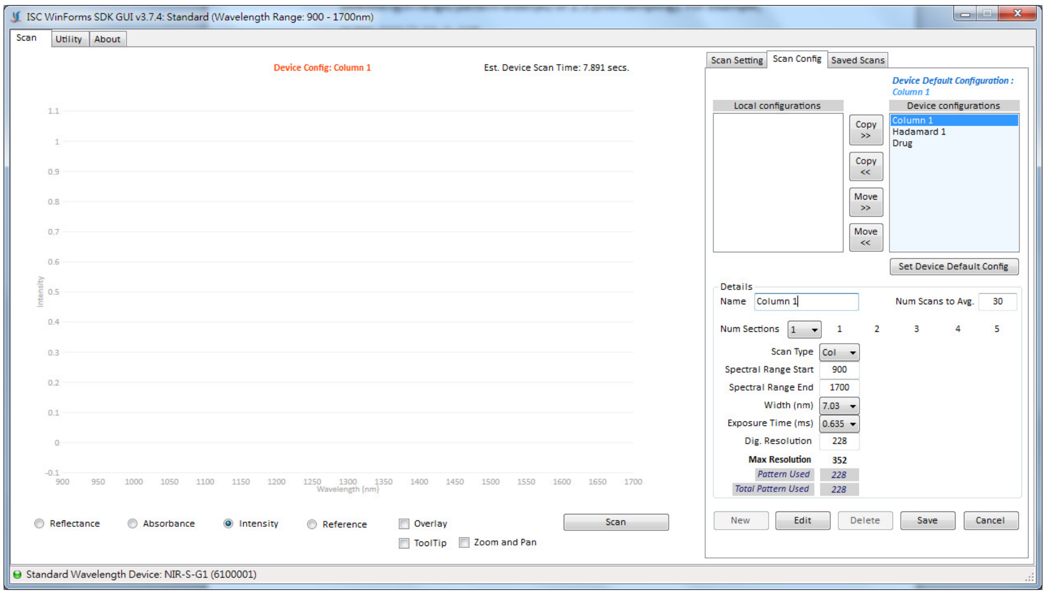


Figure 2.5 Scan Configuration Dialog Box

2.2.2 Scan Setting

After selecting the scan configuration, you can start to scan the sample through the “Scan Setting” tab as shown below. Take diffuse reflective measurement as an example:

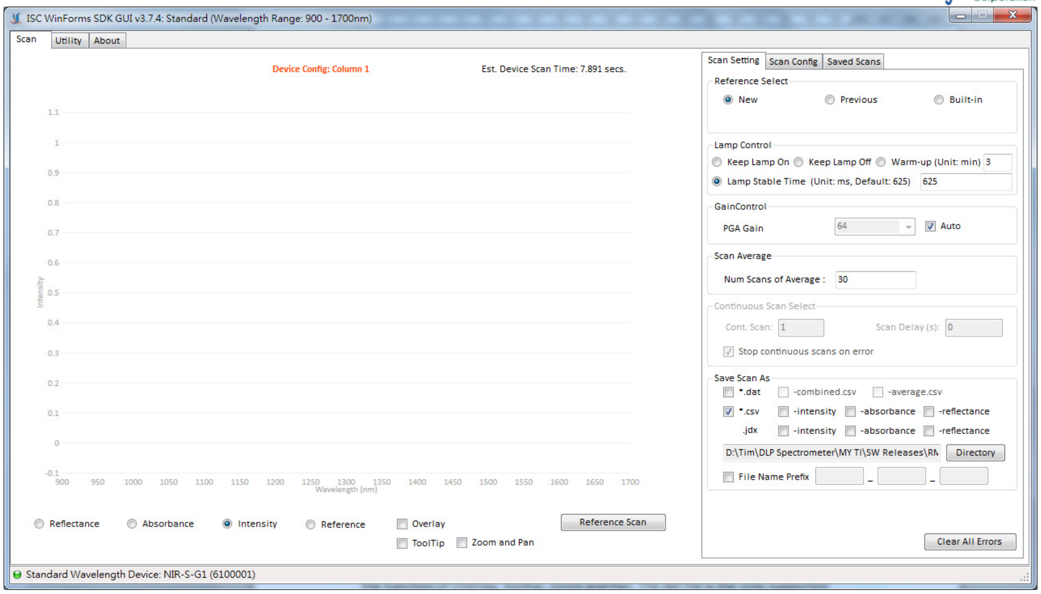


Figure 2.6 Scan Setting

- Reference Select: This option allows users to select the source of reference data, including:

  (a) New: Place a high diffuse reflectance material (such as Spectralon® or NIR-RM-1/2) on the sample window and perform a new reference scan, which will be stored in the Users folder (C:\Users\User Name\ Documents\InnoSpectra\Reference Data) in your computer.

  (b) Previous: Select the reference data previously created using the "New" option.

  (c) Built-in: The reference data stored in the internal memory of the NIRScan device will be interpolated to match the current scan configuration parameters.

- Lamp control: This function allows users to control the ON/OFF/Warm-up of the lamp and change the “Lamp Stable Time”.
- Gain control: This function allows users to select Auto or Fixed PGA (Programmable Gain Amplifier) Gain.

  (a) Auto: When set to Auto, each scan performs a quick scan to set the programmable gain amplifier to the highest possible amount that does not cause overflow. When scanning a new material, please choose “Auto” setting first.

(b) Fixed PGA Gain: When set to a specific number, the PGA is set to that value for all scans. This avoids the quick scan. Care must be taken to not set the PGA to a value that causes overflow. An overflow would show a flat scan with the highest possible intensity value. This option is useful when scanning a material with an intensity that lies at the border of two PGA settings where some scans might select a PGA setting while other scans select the next higher PGA setting. After you are experienced with your device or sample condition, you can choose “Fixed PGA Gain” setting.

- Scan Average: This function allows users to quickly set the number of scans to average to check the spectrum quality. SNR can be improved by increasing this number.
- Continuous Scan Select: This function allows users to set the back-to-back scans to be completed once the Scan button is pressed. The “Scan Delay(s)” indicates the amount of seconds to wait between consecutive scans.
- Save Scan As: This function allows the user to select the data format and file directory to save the spectrum. We recommend that you at least choose the CSV file format to avoid data loss. In order to view the saved scan data under the "Saved Scans" tab, you also need to save the scan data in the *.dat file format.
- File Name Prefix: Before starting the scan, the user can set a file name prefix, which will help the management of spectrum data. For example, select “Column 1” scan configuration to perform a scan. The saved file name could be with or without prefix as follows:

  Without prefix: Column 1_20210712_160057

  Append prefix: 001_MEXILETINE100_MELETIN_Column 1_20210712_160057

2.2.3 Saved Scans

Under the "Saved Scans" tab, users can view the scan data which is save in the *.dat file format.

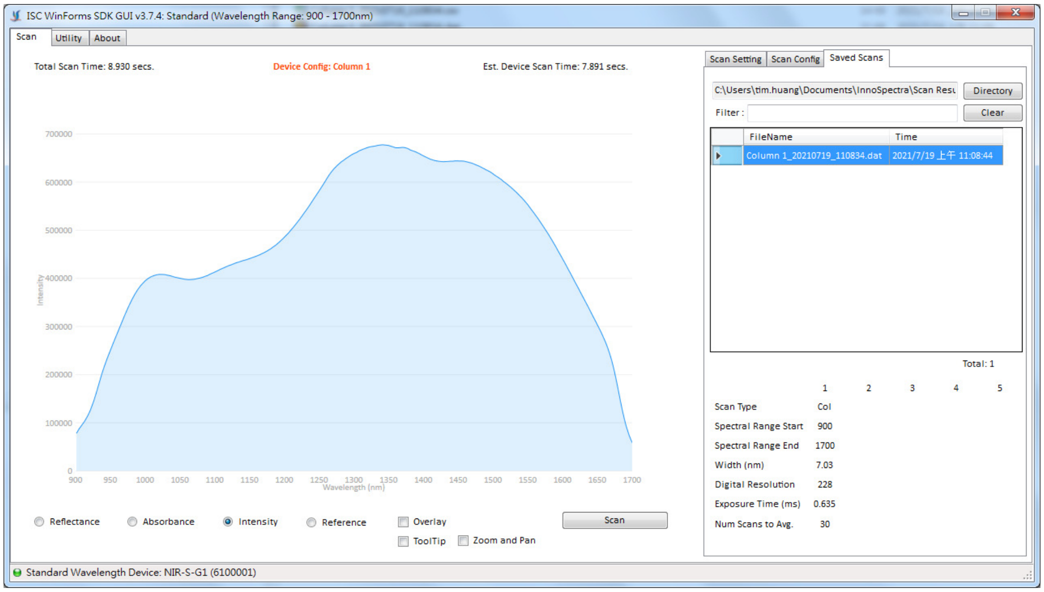


Figure 2.7 Saved Scans

2.2.4 Utility

The Utility screen provides tools to manage the NIRScan device.

- Model Name: get or set the model name
- Serial Number: get or set the serial number.
- Date and Time: get or synchronize date and time.
- Lamp Usage: get or set lamp usage.
- Sensors: read and display sensor data.
  - Battery charger status and battery capacity (only when lithium-ion battery is connected).
  - System Humidity: Ambient humidity read from the main board.
  - System Temp: Ambient temperature read from the main board.
  - Tiva Temp: Tiva internal temperature read by the Tiva internal sensor.
  - Lamp Intensity: ADC reading of lamp output.
- TIVA Firmware Update: search TIVA firmware file and update it.
- DLPC150 Firmware Update: search DLPC firmware file and update it.

- Calibration Coefficients: read or write calibration coefficients (Pixel-to-Wavelength and Shift Vector).
- Device information: displays GUI Version, Tiva SW Version, DLPC Flash Version, Main Board Version, Detector Board Version, Model Name, Device Serial Number, Manufacturing Serial Number, Device UUID, Lamp Usage and BLE Advertising Name.
- Activation Key: input and set activation key.
- Bluetooth LE Advertising Name: get or set BLE advertising name.
- Device: restore or update the built-in reference, reset system, lock or unlock the scan button.
- Log File: Enable or disable the log function. After enabling this function, the GUI will record the running status in the log file. When you find any errors, please provide both log files and CSV files for further analysis.

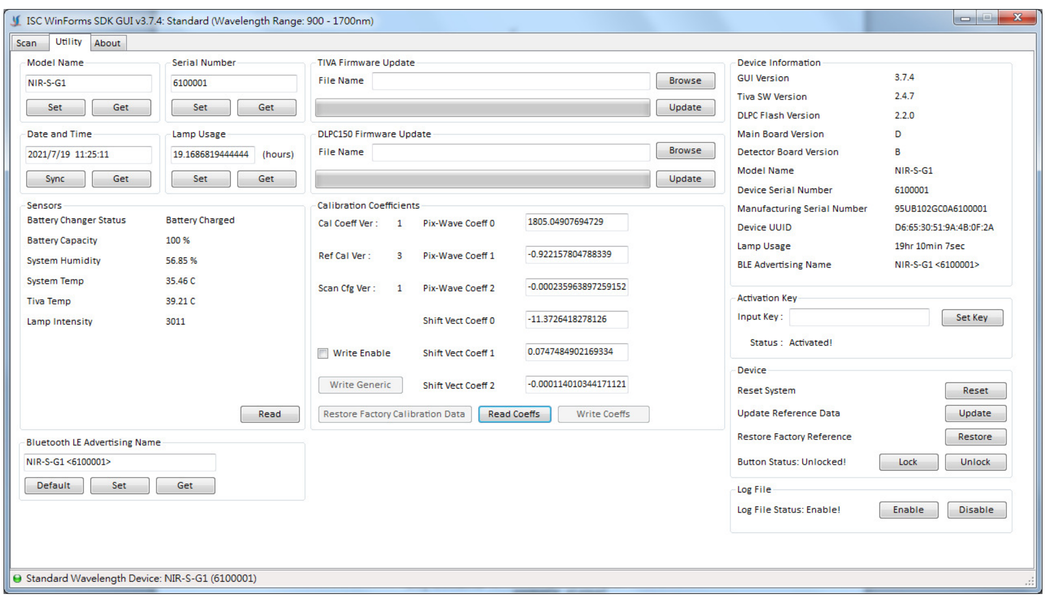


Figure 2.8 Utility Screen

2.2.5 CSV File

The CSV (Comma Separated Values) file can be imported into a spreadsheet application. The CSV file contains the following information:

- Scan Config Information: Scan Config Name, Scan Config Type, Num Section, Section Config Type, Start Wavelength (nm), End Wavelength (nm), Pattern

Width (nm), Exposure (ms), Digital Resolution, Num Repeats, PGA Gain, System Temp (C), Humidity (%), Lamp Intensity, Data Date-Time, Total Measurement Time in sec.

- General Information: Model Name, Serial Number, GUI Version, TIVA Version, DLPC Version, UUID, Main Board Version, Detector Board Version.
- Scan Data: Wavelength (nm), Absorbance (AU), Reference Signal, Sample Signal.
- Reference Scan Information: Scan Config Name, Scan Config Type, Num Section, Section Config Type, Start Wavelength (nm), End Wavelength (nm), Pattern Width (nm), Exposure (ms), Digital Resolution, Num Repeats, PGA Gain, System Temp (C), Humidity (%), Lamp Intensity, Data Date-Time.
- Calibration Coefficients: Shift Vector Coefficients, Pixel to Wavelength Coefficients, Versions (Cal/Ref/Cfg).
- Lamp Usage: Total Time (HH:MM:SS).
- Device Status.
- Error Status: Error Status, Error Code, Error Details.

	A	B	C	D	E	F	G	H	I	J	K
1	***Scan Config Information***							***Reference Scan Information***			
2	Scan Config Name:	Column 1						Scan Config Name:	Local New Reference		
3	Scan Config Type:	Slew	Num Section:	1				Scan Config Type:	Slew	Num Section:	1
4	Section Config Type:	Column						Section Config Type:	Column		
5	Start Wavelength (nm):	900						Start Wavelength (nm):	900		
6	End Wavelength (nm):	1700						End Wavelength (nm):	1700		
7	Pattern Width (nm):	7.03						Pattern Width (nm):	7.03		
8	Exposure (ms):	0.635						Exposure (ms):	0.635		
9	Digital Resolution:	228						Digital Resolution:	228		
10	Num Repeats:	30						Num Repeats:	30		
11	PGA Gain:	64						PGA Gain:	64		
12	System Temp (C):	34.34						System Temp (C):	34.06		
13	Humidity (%):	59.9						Humidity (%):	60.13		
14	Lamp Intensity:	3008						Lamp Intensity:	3006		
15	Data Date-Time:	2021/07/19T11:08:42						Data Date-Time:	2021/07/19T11:08:29		
16	Total Measurement Time in sec:	8.9298929									
17											
18	***General Information***							***Calibration Coefficients***			
19	Model Name:	NIR-S-G1						Shift Vector Coefficients:	-11.37264183	0.07474849	-0.00011401
20	Serial Number:	6100001	(95UB102GC0A6100001)					Pixel to Wavelength Coefficients:	1805.049077	-0.922157805	-0.000235964
21	GUI Version:	3.7.4						Versions (Cal/Ref/Cfg):	1	3	1
22	TIVA Version:	2.4.7						***Lamp Usage ***			
23	DLPC Version:	2.2.0						Total Time(hh:mm:ss):	19hr 10min 7sec		
24	UUID:	D6:65:30:51:9A:4B:0F:2A						***Device/Error Status***			
25	Main Board Version:	D						Device Status:	0x00000001		
26	Detector Board Version:	B						Error status:	0x00000000	Error Code:	0x00000000000000000000000000000000
27										Error Details:	Not found
28	***Scan Data***										
29	Wavelength (nm)	Absorbance (AU)	Reference Signal (unitless)	Sample Signal (unitless)							
30	901.3281822	0.000383547	78164	78095							
31	905.2414401	0.000553966	87861	87749							
32	909.1504507	0.00091793	95672	95470							
33	913.055214	0.000813765	103632	103438							
34	916.9557299	-0.000315001	113013	113095							
35	920.8519985	0.000626507	124866	124686							
36	926.0404162	0.00051264	144952	144781							
37	929.9267743	0.000162701	162857	162796							
38	933.808885	0.000824889	182338	181992							
39	937.6867484	-0.000531324	200953	201199							
40	941.5603644	0.00047761	218354	218114							
41	945.4297331	0.000306605	233799	233634							
42	949.2948544	0.000674464	248098	247713							
43	953.1557283	0.000180726	261987	261878							
44	957.012355	9.77E-05	275717	275655							
45	960.8647342	0.000285357	289262	289072							
46	964.7128662	0.000233867	302775	302612							
47	969.8371017	0.000245151	320739	320558							

Figure 2.9 CSV File Content

2.3 Obtaining High-Quality Spectrum Data

High-quality spectra can be collected with correct configuration and operation. We will introduce how to set the scan configuration to obtain a stable, reliable spectrum in detail.

2.3.1 Reference Signal

To calculate the absorbance of a sample, you need a reference signal.

$$Absorbance = log_{10} \frac{reference\ signal}{sample\ signal}$$

There are two options for reference signal: Built-in or New/Previous.

- Built-in: The "built-in" reference signal is stored in the internal memory of the device. The "built-in" reference signal of the diffuse reflective module is obtained by scanning the Spectralon® diffuse reflectance standard (SRS-99). The scan configuration of the "built-in" reference signal is as follows.

Reference Select	Built-in
Section Config Type:	Column
Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	7.03
Exposure (ms)	0.635
Digital Resolution:	228
Num Repeats	30
PGA Gain	64

- New/Previous: The "previous" reference signal is obtained by performing a "new" reference scan. You can place a high diffuse reflectance material (SRS-99 or NIR-RM-1/2) on the scan window of the diffuse reflective module and perform a "new" reference scan. The "new" scan data will be stored in the computer and become a "previous" reference signal. The scan configuration of the "new/previous" reference signal can be edited and saved in the scan configuration dialog box. For example, you can perform a "new" reference scan with a different pattern width and digital resolution, as shown below.

Reference Select	New / Previous
Section Config Type:	Column
Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	10.54
Exposure (ms)	0.635
Digital Resolution:	160
Num Repeats	30
PGA Gain	64

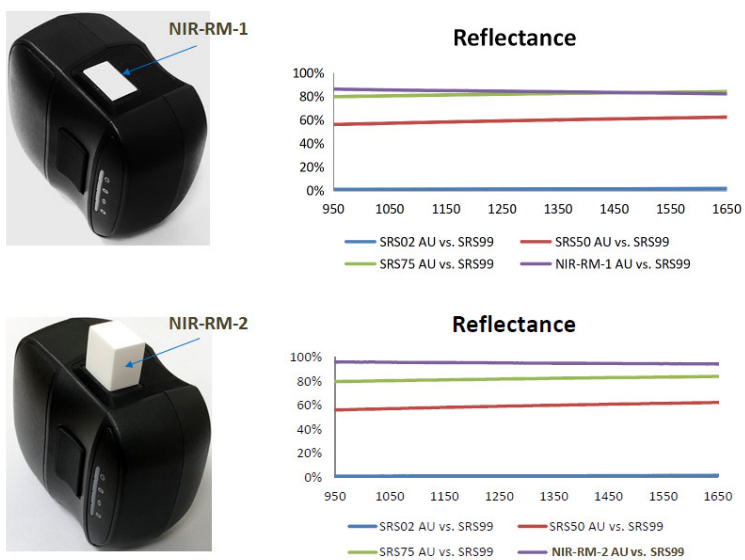


Figure 2.10 Reference Materials

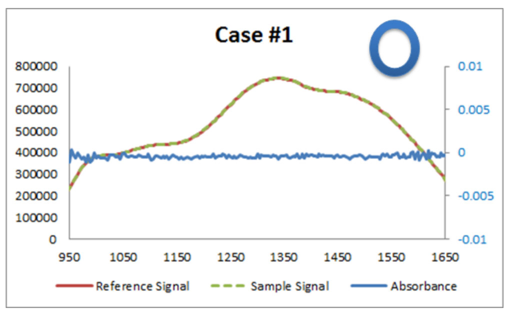
After performing the reference scan, you can scan the sample to obtain the absorbance data of the sample. If the scan configuration of the sample signal is different from the scan configuration of the reference signal, the reference signal may not perfectly match the sample signal in terms of wavelength point and signal intensity. It may be necessary to interpolate or scale the reference signal to accommodate different pattern widths and digital resolutions of the sample signal. Please refer to the following three different situations. To simplify the discussion, we scan SRS-99 to obtain the reference signal and the sample signal, so the absorbance should theoretically be zero.

Case #1: The “built-in” reference signal is selected. The sample signal is scanned by using the same pattern width and digital resolution as the “built-in” reference signal. As a result, the absorbance is flat and very close to zero.

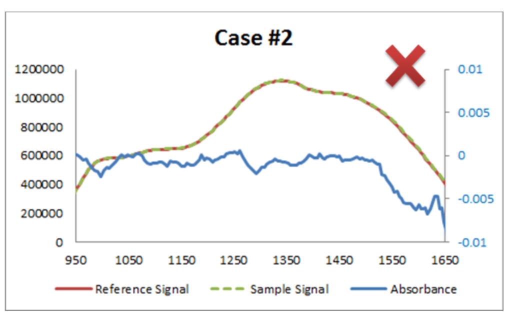
Case #2: The “built-in” reference signal is selected. The sample signal is scanned by using different pattern width and digital resolution. As a result, the “built-in” reference signal is interpolated and scaled to match the settings of sample signal and the absorbance is not flat.

Case #3: It is similar to case #1, but the “built-in” reference signal is replaced by the “new/previous” reference signal. Both the reference signal and the sample signal are scanned with the same pattern width and digital resolution. Therefore, the absorbance is flat and very close to zero.

Case #1	Sample signal	Reference signal
Section Config Type:	Column	Column
Start Wavelength (nm)	900	900
End Wavelength (nm)	1700	1700
Pattern Width (nm)	7.03	7.03
Exposure (ms)	0.635	0.635
Digital Resolution:	228	228
Num Repeats	6	30
PGA Gain	64	64



Case #2	Sample signal	Reference signal
Section Config Type:	Column	Column
Start Wavelength (nm)	900	900
End Wavelength (nm)	1700	1700
Pattern Width (nm)	10.54	7.03
Exposure (ms)	0.635	0.635
Digital Resolution:	160	228
Num Repeats	6	30
PGA Gain	64	64



Case #3	Sample signal	Reference signal
Section Config Type:	Column	Column
Start Wavelength (nm)	900	900
End Wavelength (nm)	1700	1700
Pattern Width (nm)	10.54	10.54
Exposure (ms)	0.635	0.635
Digital Resolution:	160	160
Num Repeats	6	6
PGA Gain	64	64

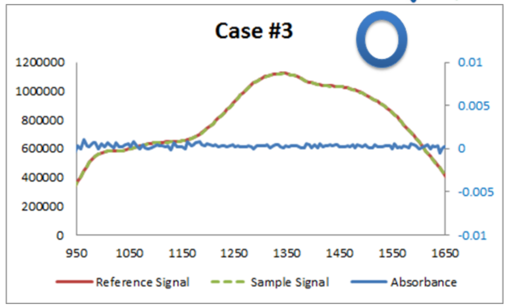


Figure 2.11 Cases with Matched or Unmatched Scan Configuration

The “built-in” reference signal is suitable for user doing a scan when there is no reference sample available in hand. In order to match with the “built-in” reference signal, please choose same scan configuration to minimize the absorbance variation. You can choose any scan configuration which perfectly matches your sample conditions. Please periodically perform a “new” reference scan and then you can select the “previous” reference signal to match your current scan configuration, and then the absorbance variation will be minimized.

Unless you can use SRS-99 to scan the reference signal, do not replace the "built-in" reference signal. The built-in reference signal can be replaced by the following procedure. However, we do not recommend that you change this reference signal unless you have reliable reference materials on hand and are very familiar with the purpose of the built-in reference signal.

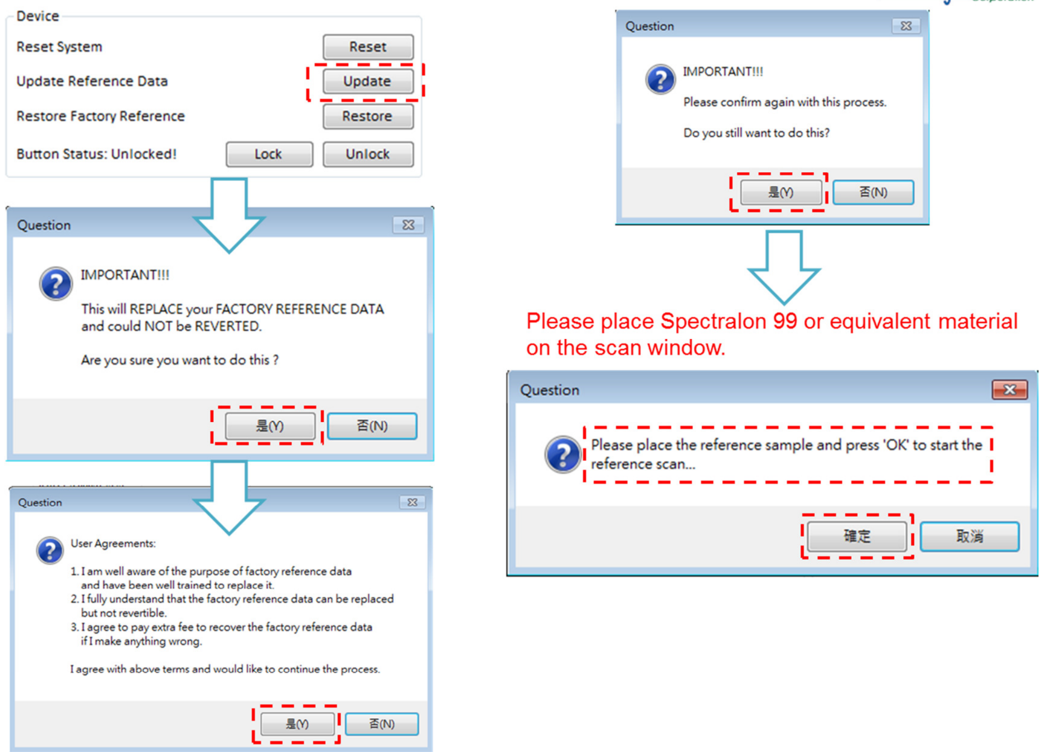


Figure 2.12 Updating Built-in Reference Data for Diffuse Reflective Modules

2.3.2 Black Level

ISC NIRScan uses a digital micromirror device (DMD) as the wavelength selector. The DMD's micromirror array is programmed to reflect light into or away from the single-element photodetector. Because the DMD micromirror works in dynamic mode, the stray light phenomenon of ISC NIRScan is different from the traditional design, so the black level measurement (dark scan) is performed in a completely different way. ISC NIRScan performs periodic black level measurement which is handled by software automatically. By inserting a periodic pattern of all turned off pixels in the sample scan, the black level will calculated and compensated automatically. You only need to perform a reference scan before the sample scan. No dark scan is required before the sample scan.

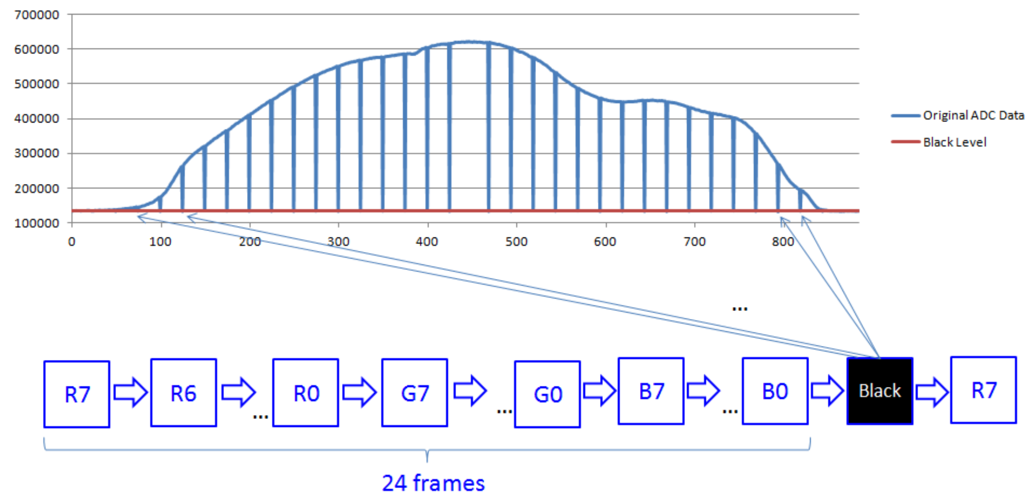


Figure 2.13 Black Level Measured with Black DMD Pattern

When measuring the black level, the light source and input signal are not blocked, and all DMD mirrors are set to OFF state. As a result, the black level contains all noise information. Therefore, the sample signal is equal to the raw data minus the black level (Sample signal = raw data –black level).

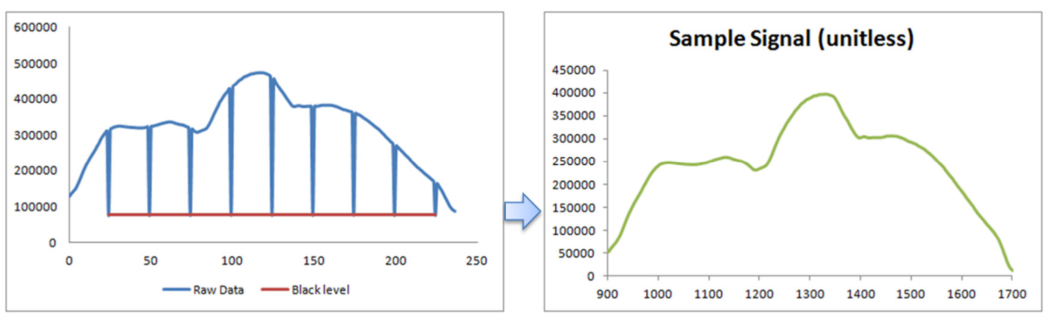


Figure 2.14 Sample Signal=Raw Data - Black Level

Please note that when the measurement is performed under low light conditions or the sample is a strong NIR absorber, the raw data of the measurement may be very weak and interfered. The calculated sample signal (=raw data-black level) may become negative. As a result, the absorbance data (AU= $\log_{10}$ (reference signal/sample signal)) will become NaN (Not a Number) because the operand of the absorb calculation must be a positive number. When AU is NaN, the software will replace NaN with 0 in order to display AU in the GUI.

For example, when measuring water in transmission mode, the absorbance level will reach saturation when the path length is up to 5mm. If the path length is increased to 10mm, the raw signal become very weak and interfered, and the sample signal may become negative after 1450nm.

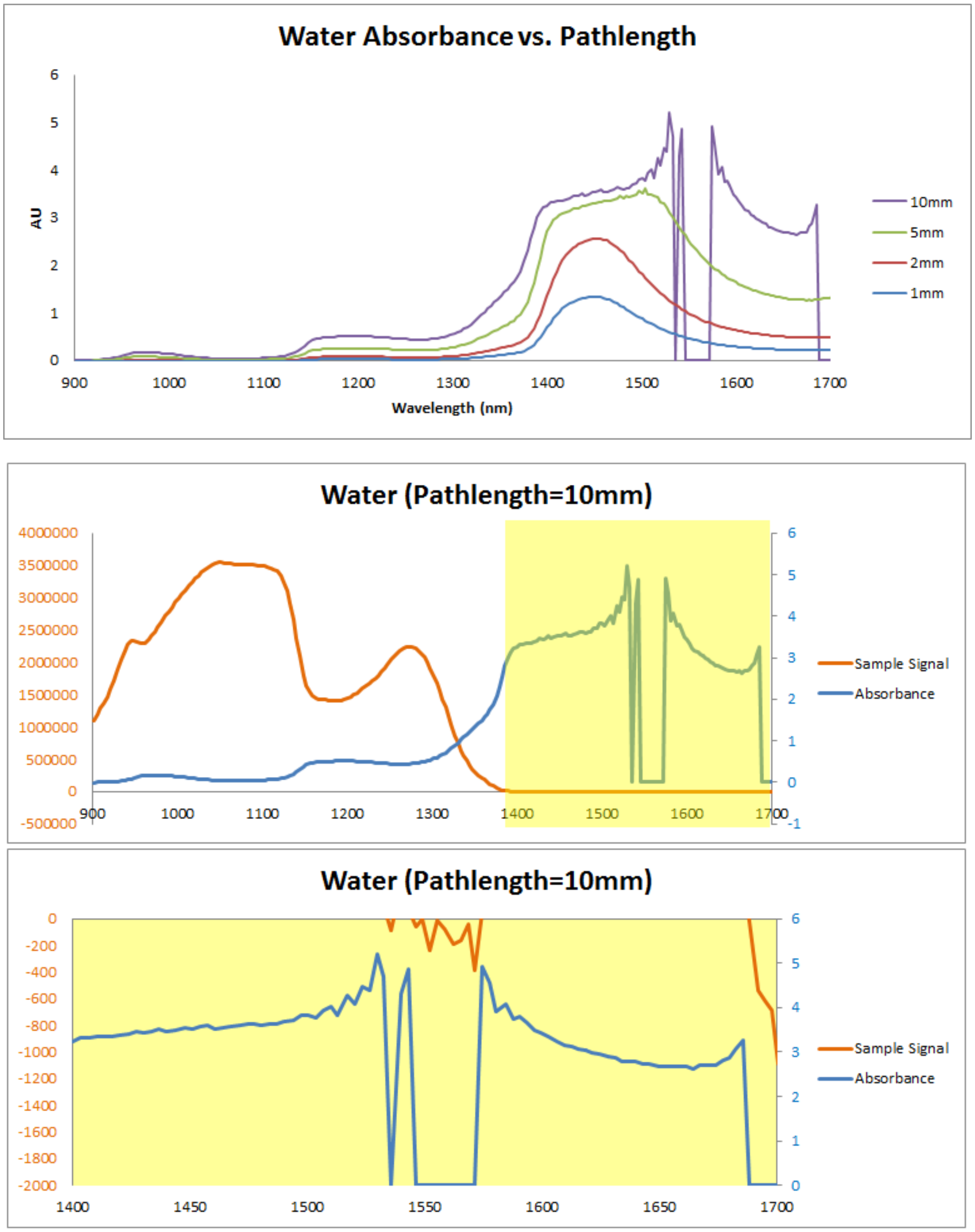


Figure 2.15 Water Measured at Different Path Length

2.3.3 PGA Gain Control

The NIRScan device uses a single-element InGaAs detector to receive light of different wavelengths reflected by the DMD. InGaAs detector generates a small amount of current when a photo impacts the P-N junction of the semiconductor. The NIRScan device uses a transimpedance amplifier to convert the photodiode current into a voltage and then digitize the voltage with ADC. The ADC has a Programmable Gain Amplifier (PGA), which increases the dynamic range by amplifying low-amplitude signals before they are fed to the 24-bit ADC. There are two options for PGA setting: “Auto” or “Fixed”. To evaluate a new sample, please choose “Auto” first. The software will set a proper PGA value to optimize the dynamic range automatically. If you are familiar with the device and sample conditions, you can try to assign an appropriate value to the PGA. The options for the PGA values are 1, 2, 4, 8, 16, 32 and 64.

The PGA value set by you cannot be greater than the PGA value obtained in "Auto" PGA mode, otherwise the signal will become saturation. For example, if the auto PGA value is 16, you cannot set the PGA value to 32.

If one PGA value (for example, 64) is used to scan the reference signal, but another PGA value (for example, 16) is used to scan the sample signal, the reference signal will be scaled down (x 1/4) to match the PGA value of the sampled signal. However, the actual reference signal at PGA 16 is not equal to quarter of the reference signal at PGA 64, this will induce absorbance error. To make an accurate measurement, the reference signal and the sample signal need the same PGA value.

The relationship between PGA settings and ADC readings is studied as follows. The ADC input is supplied with a constant voltage source. By changing the PGA setting and reading the ADC data, a linear relationship between the actual ADC reading and

PGA setting can be calculated. The ADC input is connected to a voltage source, the PGA is set to 64, and the input voltage is increased to make the ADC reading close to the maximum value. After that, fix the input voltage but reduce the PGA value to obtain different ADC readings. The ADC reading increases as the PGA value increases. The relationship between ADC reading and PGA value is basically linear. However, the increase in ADC readings is lower than the increase in PGA values. When PGA is larger, the deviation will be more obvious.

By comparing the PGA and ADC reading, the linear regression result of PGA setting vs. ADC reading ratio is very close to each other but not equal to multiple. When PGA is larger, the deviation will be more obvious.

PGA setting	ADC reading (K)	ADC reading ratio	ADC reading ratio vs. PGA setting
1	146	1	100.00%
2	291	1.993150685	99.66%
4	578	3.95890411	98.97%
8	1140	7.808219178	97.60%
16	2222	15.21917808	95.12%
32	4241	29.04794521	90.77%
64	8388	57.45205479	89.77%

PGA setting in ADC is not an ideal case.

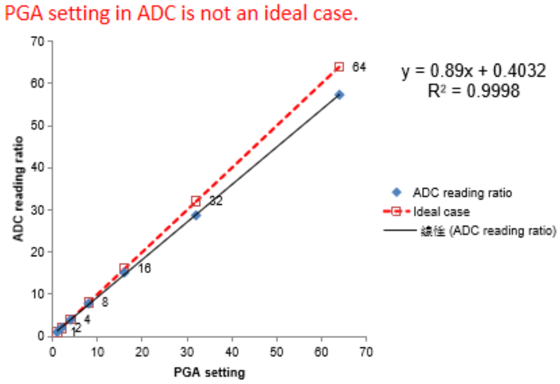


Figure 2.16 ADC Readings vs. PGA Settings

As mentioned above, the ADC reading ratio does not follow the ratio of the PGA value. For example, the ADC reading at PGA32 is not twice the ADC reading at PGA16. If you assume that the ADC reading of PGA32 is exactly twice the ADC reading of PGA16, you will see the problem of inconsistent absorbance.

The figure below shows a further comparison of the two different scanning procedures. Procedure #A will rescan the reference signal for each smaller PGA. Procedure #B will scale down the reference signal according to the PGA ratio to match the smaller PGA. As a result, procedure #A will ensure the consistency of absorbance under different PGA settings. Procedure #B will have consistent reference signal ratios but inconsistent absorbance results.

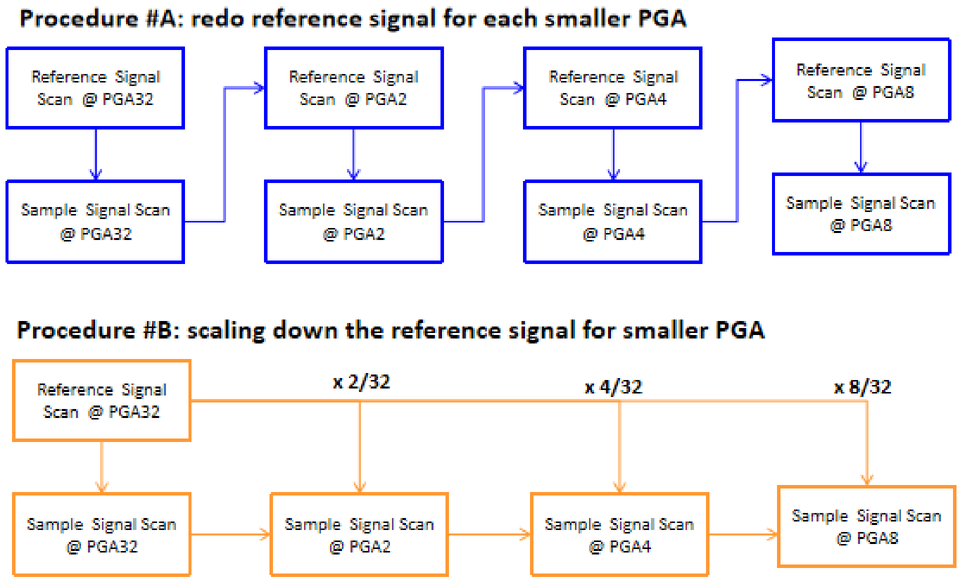


Figure 2.17 Different Scanning Procedures

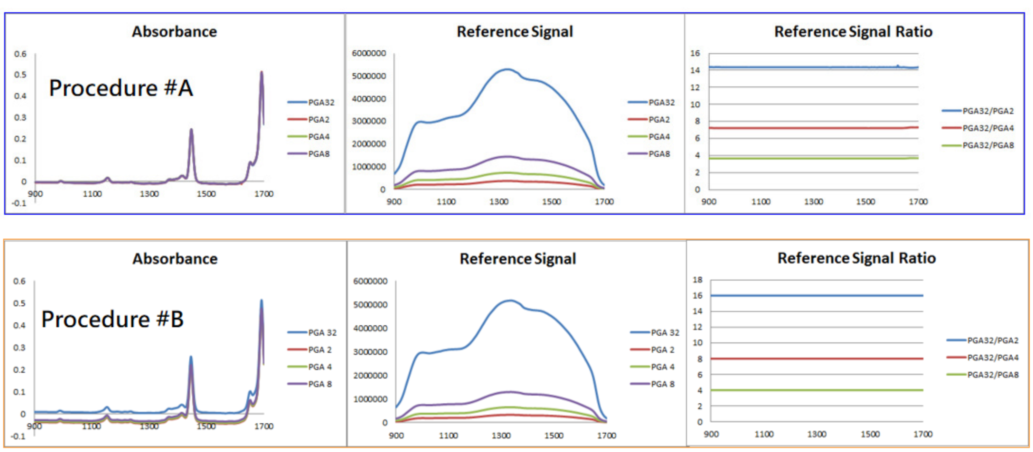
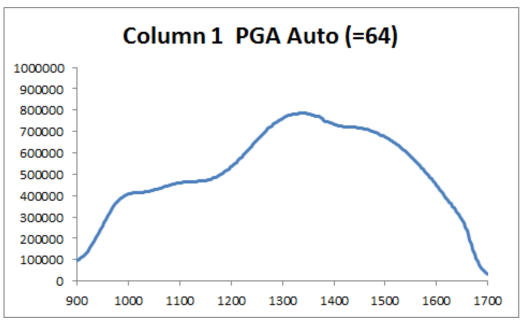


Figure 2.18 Absorbance of Different Scanning Procedure

The following is an example of comparing PGA settings for different scan types. By scanning SRS-99 with NIR-S-G1, the Auto PGA of "Column 1" is 64, but the Auto PGA of "Hadamard 1" is 16. In the Hadamard scan, the DMD pattern is wider, so the InGaAs detector will capture higher optical energy. The PGA value in the Hadamard scan must be reduced to avoid saturation of the ADC reading.

Scan Config Name	Column 1	Hadamard 1
Scan Type	Column	Hadamard
Start Wavelength (nm)	900	900
End Wavelength (nm)	1700	1700
Pattern Width (nm)	7.03	7.03
Exposure (ms)	0.635	0.635
Digital Resolution	228	228
Num Repeats	6	6
PGA Gain	64 (Auto)	16 (Auto)



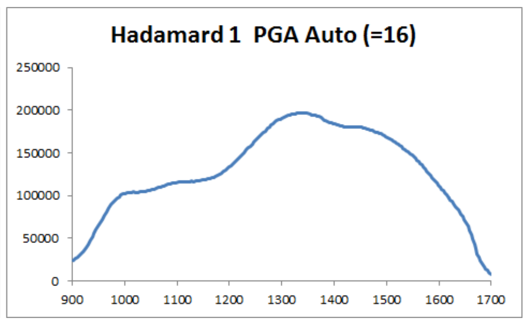


Figure 2.19 Auto PGA vs. Scan Type

Below is an example that demonstrates the side effects of fixed PGA. PGA gain affects the signal intensity obviously, a larger PGA gain will increase signal intensity, but the specified PGA gain can't be set more than auto PGA gain. To evaluate a new sample, please tick "auto" first. After you are experienced with your device and sample condition, you can try to fix the PGA gain. The PGA gain can be fixed at 1, 2, 4, 8, 16, 32 or 64. In case (a), by using NIR-S-G1 to scan SRS-99 with "Hadamard 1", the Auto PGA function selects 16 as the appropriate PGA gain. In case (b), the PGA gain is reduced and fixed to 8, and there is no problem. In case (c), the PGA gain is increased and fixed to 32, which will cause signal saturation at multiple wavelength points. In case (d), the PGA gain is further increased to 64, which is very large and will cause signal saturation at all wavelength points.

Scan Configuration	(a)	(b)	(c)	(d)
Scan Config Name	Hadamard 1	Hadamard 1	Hadamard 1	Hadamard 1
Scan Type	Hadamard	Hadamard	Hadamard	Hadamard
Start Wavelength (nm)	900	900	900	900
End Wavelength (nm)	1700	1700	1700	1700
Pattern Width (nm)	7.03	7.03	7.03	7.03
Exposure (ms)	0.635	0.635	0.635	0.635
Digital Resolution	228	228	228	228
Num Repeats	6	6	6	6
PGA Gain	16 (Auto)	8 (Fixed)	32 (Fixed)	64 (Fixed)

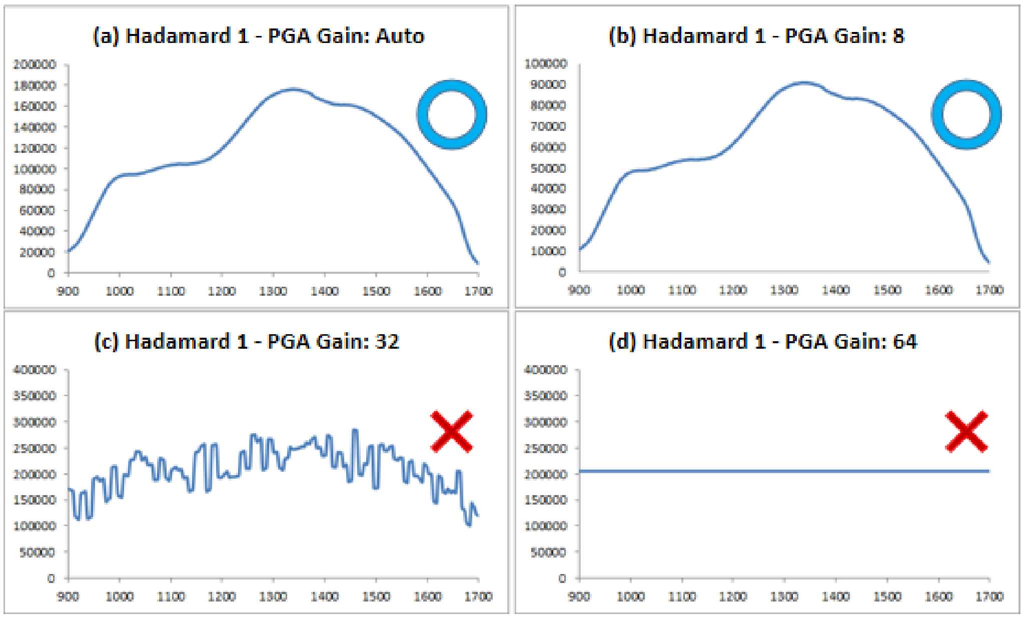


Figure 2.20 Side Effect of Fixed PGA

As mentioned above, the scan configuration and PGA gain will affect the measurement results. Please pay attention to setting a proper PGA. When collecting a batch of spectral data, please set the same PGA gain. If you change the PGA gain, make sure to scan the new reference signal.

2.3.4 Pattern Width and Digital Resolution

Besides light source intensity, pattern width can be increased to enhance signal level. You can increase pattern width to the maximum width which still produces good enough spectrum resolution. For example, a plastic sample is scanned with different pattern width settings as follows. The AU still looks fine when pattern width is not increased too much.

Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	7.02 / 10.53 / 12.87 / 16.38
Digital Resolution	128
Num Repeats	6

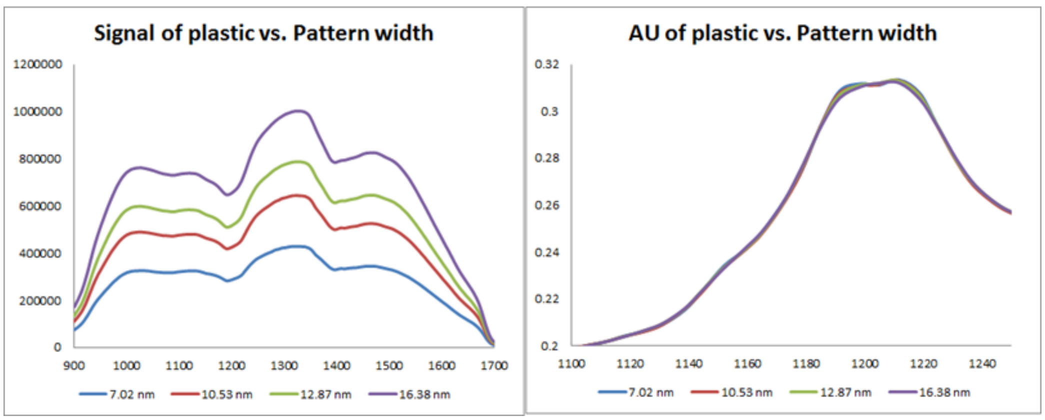


Figure 2.21 Signal and AU vs. Pattern Width

If the pattern width increases too much, the spectral resolution will become unacceptable.

Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	10.53 / 31.59 / 60.84
Digital Resolution	128
Num Repeats	6

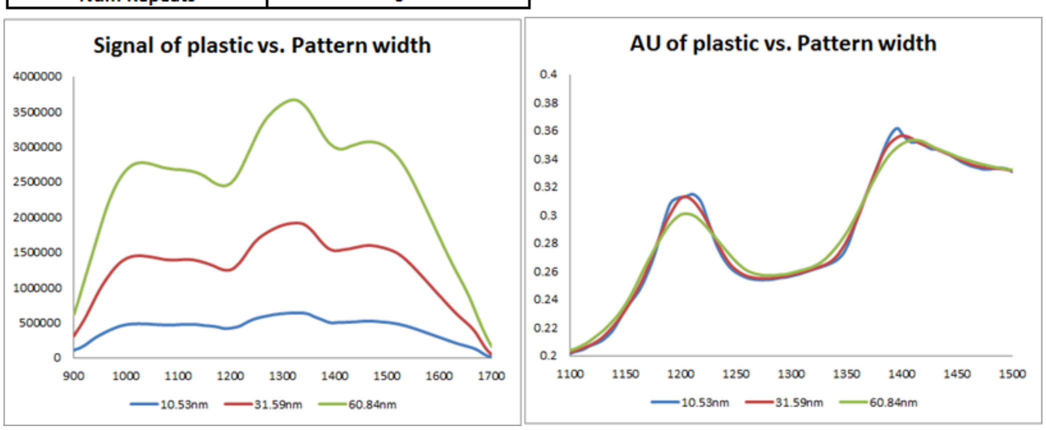
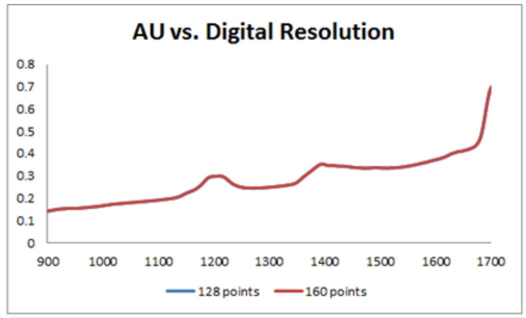


Figure 2.22 Signal and AU vs. Pattern Width

Digital resolution (=number of sampling points) can be increased to improve spectral resolution. Digital resolution can also be reduced to save scanning time if resolution is still good enough. For example, 128pts and 160pts don't make much difference in the following case.

Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	10.53
Digital Resolution	128 / 160
Num Repeats	6



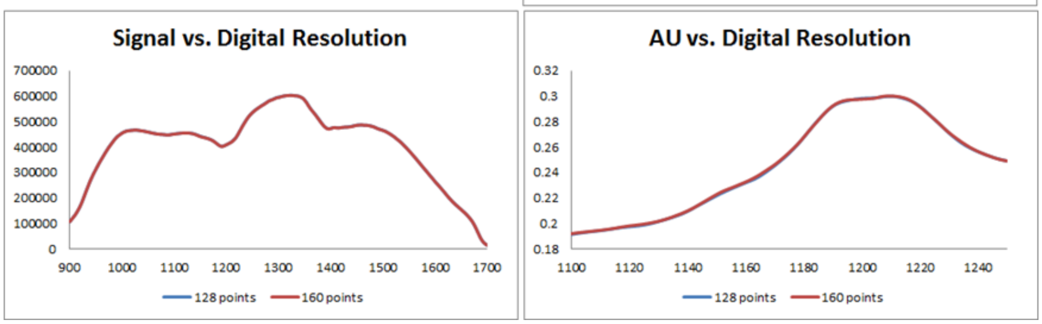
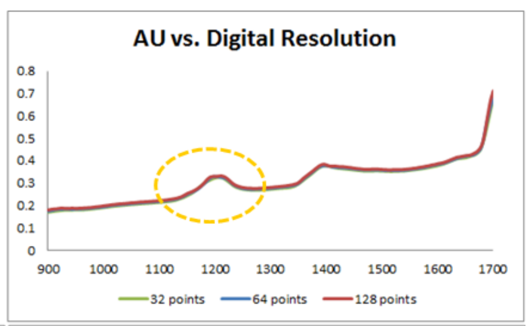


Figure 2.23 Signal and AU vs. Digital Resolution

By reducing the digital resolution to 64pt or even 32pt, the absorbance distortion will be observed and unacceptable.

Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	10.53
Digital Resolution	32 / 64 / 128
Num Repeats	6



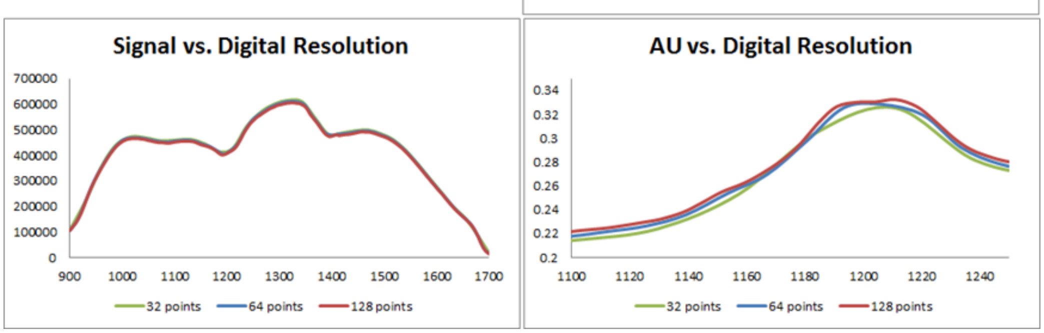


Figure 2.24 Signal and AU vs. Digital Resolution

2.3.5 Exposure Time

InGaAs photodiodes generate a small amount of current when a photon impacts the P-N junction of the semiconductor. The following architectures amplify and digitize the small current of the photodiode:

- Transimpedance amplifier through discrete components or an integrated photodiode and amplifier. This architecture converts the photodiode current into a voltage and then digitizes the voltage with an ADC. The voltage is typically oversampled by the ADC to average out the noise.
- Charge integration through discrete components or a charge digitizing ADC. This architecture utilizes capacitors for charge accumulation and then converts this charge into a digital value. The converted digital value is dependent on the integration time.

The NIRScan device uses a transimpedance amplifier to convert the photodiode current into a voltage. During each DMD pattern display time (the so-called exposure time), the ADC samples the voltage multiple times. Therefore, increasing the exposure time will increase the number of samples to be averaged, but will not increase the voltage level at the ADC input.

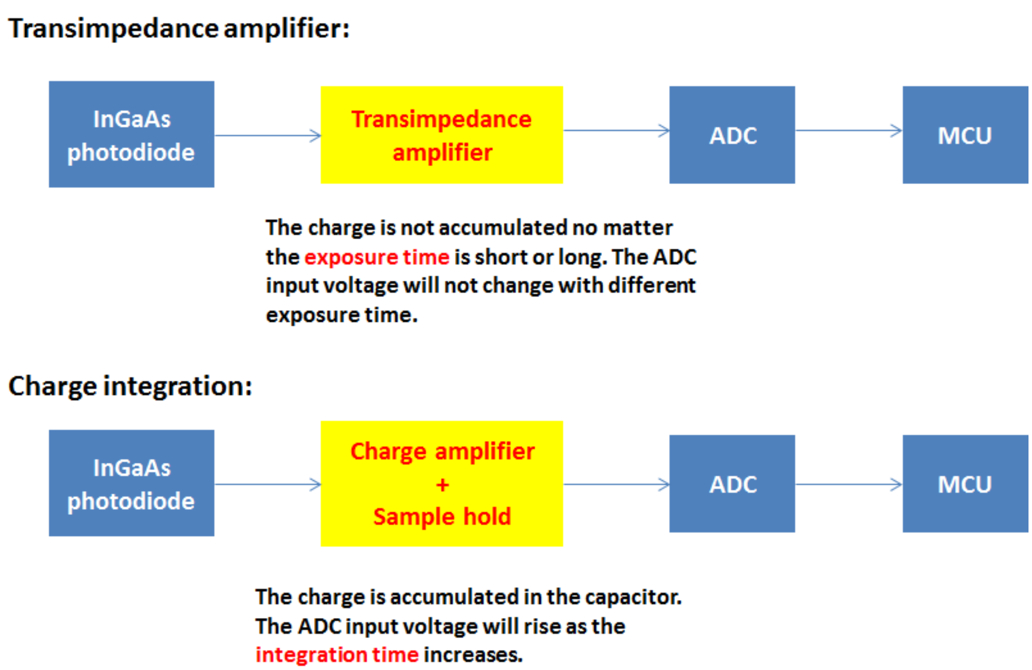


Figure 2.25 Transimpedance Amplifier vs. Charge Integration

The effective sample scans will increase with the exposure time. For each exposure, we count the effective sample scan only after the sample signal is stable. Whether you choose a short or long exposure time, the stable time is basically the same. Under the same total measurement time, multiple scans of short exposure time will waste multiple stable time, while a single long exposure time will only spend a single stable time, which is why long exposure time generates more effective sample scans and then improve SNR. When the exposure time increases from 0.635 ms to 5.08 ms, the SNR will increase by 2.8 times (=SQRT (5.08/0.635)).

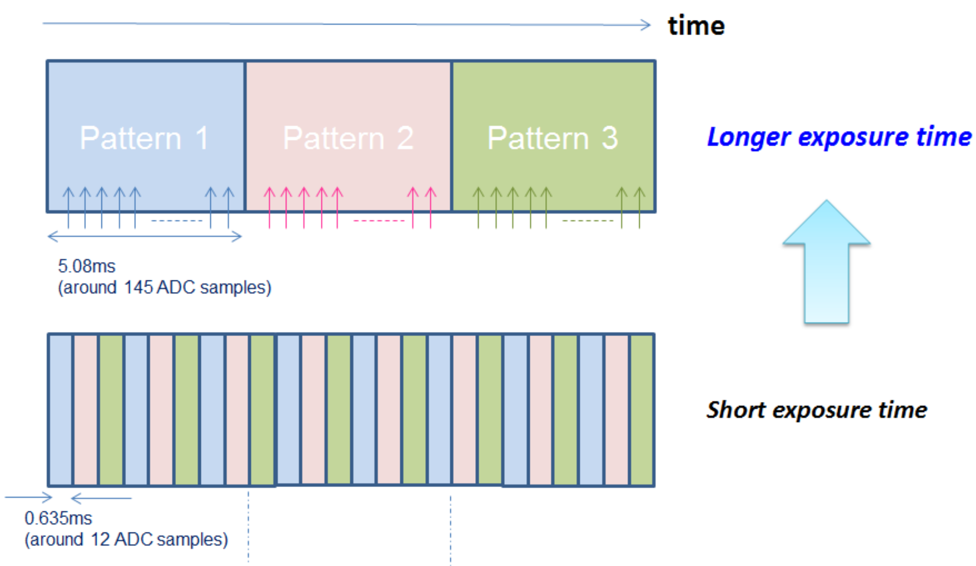


Figure 2.26 Short Exposure Time vs. Long Exposure Time

In theory, Hadamard mode should still also benefit from increased exposure time. However, it may be less noticeable if the SNR is already high. Depending on the Hadamard scan configuration, it will likely increase the SNR by 2x-7x. Increasing the exposure time will increase the SNR relative to the square root of the exposure time. The difference between 0.635ms pattern exposure time Column scan and 0.635ms pattern exposure time Hadamard scan may be similar to the difference between 0.635ms exposure time Column scan and 5.08ms exposure time Column scan. This function may be cooperated with slew scan to enhance the spectra quality.

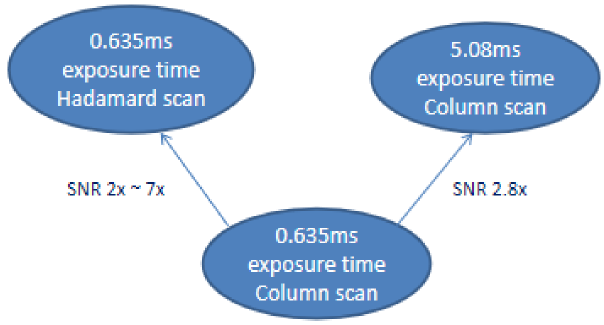
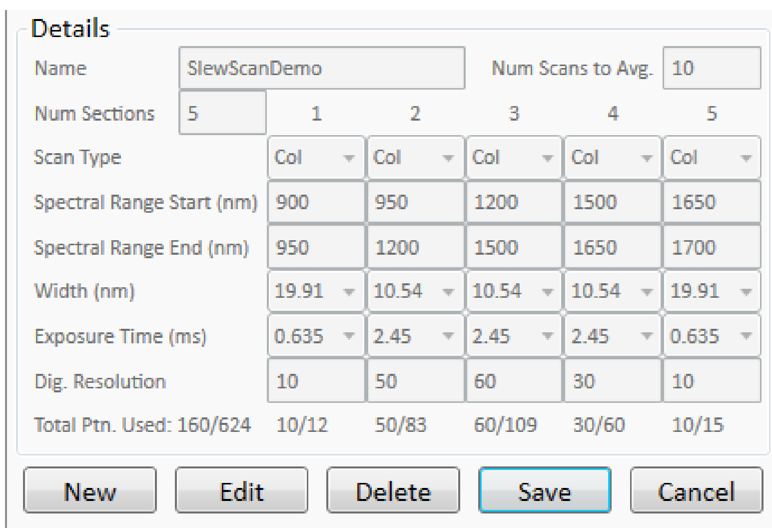


Figure 2.27 The Impact of Scan Mode and Exposure Time on SNR

2.3.6 Slew Scan

Compared with traditional linear array spectrometers, DLP-based spectrometers can be configured to scan samples using the so-called slew scanning method. The slew scan configuration can consist of multiple sections. Each section has its own scanning type, wavelength range, pattern width, exposure time and digital resolution. A demonstration of slew scan is shown below.



Details

Name: SlewScanDemo   Num Scans to Avg.: 10

Num Sections: 5	1	2	3	4	5
Scan Type	Col	Col	Col	Col	Col
Spectral Range Start (nm)	900	950	1200	1500	1650
Spectral Range End (nm)	950	1200	1500	1650	1700
Width (nm)	19.91	10.54	10.54	10.54	19.91
Exposure Time (ms)	0.635	2.45	2.45	2.45	0.635
Dig. Resolution	10	50	60	30	10
Total Ptn. Used: 160/624	10/12	50/83	60/109	30/60	10/15

New Edit Delete Save Cancel

Figure 2.28 Slew Scan Configurations

For example, the slew scan configuration consists of five sections. Sections 1 & 5 have larger pattern width to boost signal intensity. Sections 2~4 have smaller pattern width but with longer exposure time to improve signal quality. As shown below, the reference signal and sample signal are not continuous curves, but AU is continuous.

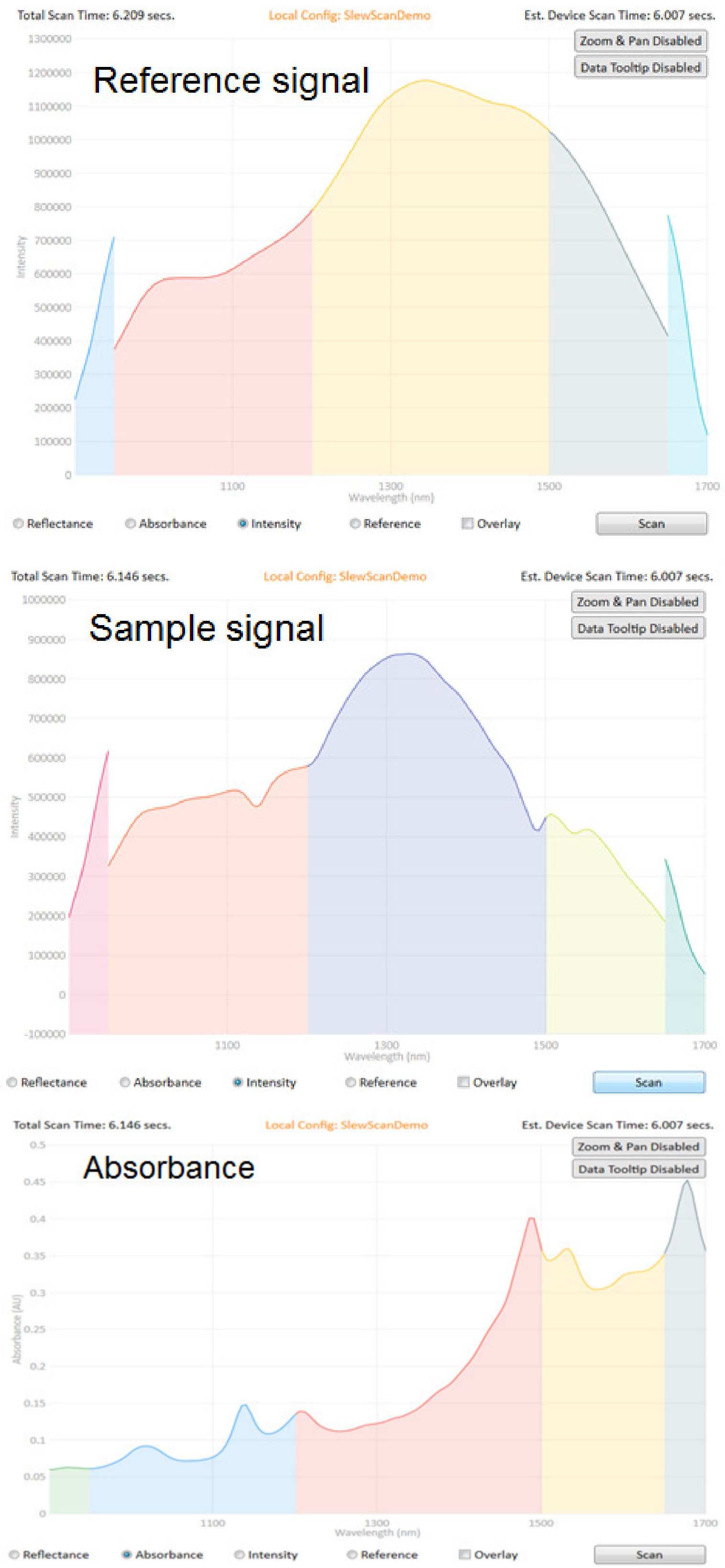


Figure 2.29 Slew Scan Results

The following figure shows the typical photosensitivity of an uncooled InGaAs detector within the standard wavelength range. When the wavelength is greater than 1650nm, the photosensitivity will change with temperature. Therefore, when the temperature changes, the absorbance data at 1650-1700nm will be unstable. On the other hand, when the wavelength is less than 950nm, the photosensitivity is low. As mentioned above, the DLP-based spectrometer is configurable, so you can consider setting the wavelength range to 950nm to 1650nm.

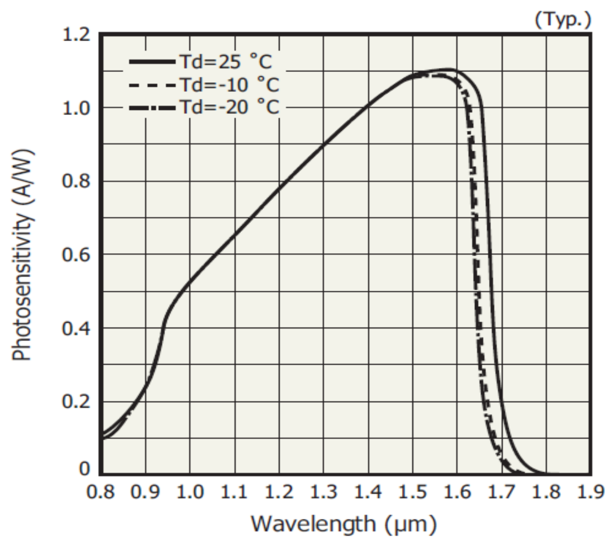


Figure 2.30 Photosensitivity of InGaAs Detector

2.3.7 Operating Point

The operating point is a specific point within the operating characteristics of the spectrometer. The operating point of the spectrometer is closely related to the state of the tungsten filament lamp. The lamp has just been cold-started or has been warmed up represents two different operating points. The following is an experiment to demonstrate the changes of AU at different operating points. Perform 200 scans continuously, set a 5s delay before the next scan, and start from the cold start, the total time is about 46 minutes. Spectrum intensities of the initial reference scan and 200 sample scans are shown below: R stands for the initial reference signal (cold start), S1 stands for the 1st sample signal, S2 for the 2nd sample signal, and S200 stands for the 200th sample signal. The spectrum change is observed as follows.

Scan Config Name	Hadamard 1
Scan Type	Hadamard
Start Wavelength (nm)	900
End Wavelength (nm)	1700
Pattern Width (nm)	9.37
Exposure (ms)	0.635
Digital Resolution	170
Num Repeats	30
PGA Gain	16

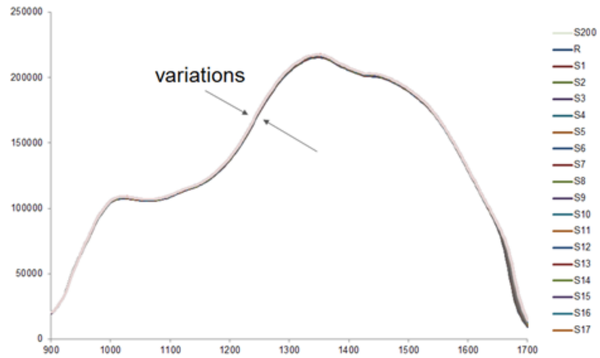


Figure 2.31 Spectral Changes in Cold Start

By using the initial reference signal R as the reference signal and Sn (n=1 to 200) as sample signal to calculate AU, the 1st AU and the 200th AU are shown below. The 200th AU not only has level shift but also has spectrum distortion.

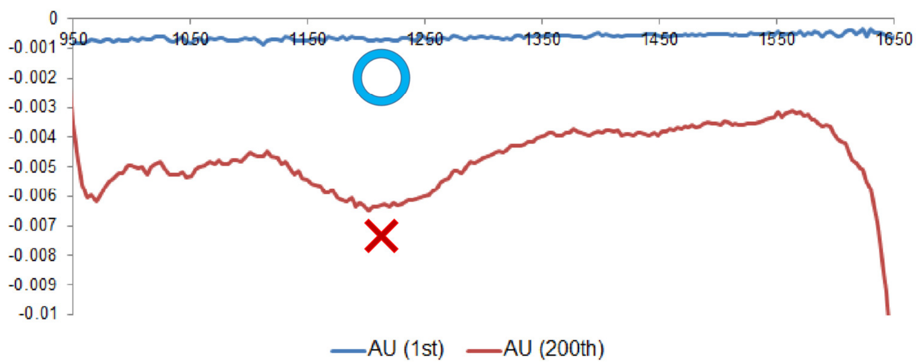


Figure 2.32 AU (1st) vs. AU (200th)

The spectrum intensity at 1300nm during 200 scans is shown below.

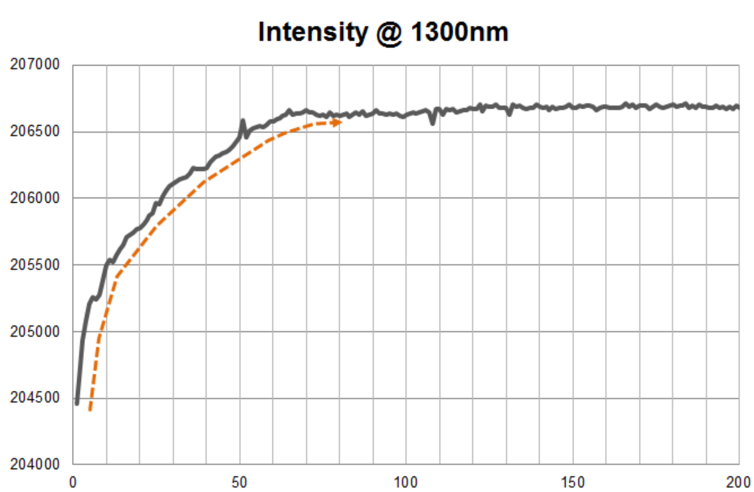


Figure 2.33 Spectral Intensity at 1300nm of 200 Scans

Obviously, it is not proper to take R (reference signal at cold-start) as the reference signal for calculating the AU for all the following 200 sample signals because the spectrum intensity will change rapidly from cold-start. By using R (reference signal at cold start) as the reference signal, the calculated AU is affected by the warm-up process obviously. AU (S10 vs. R) shows the following nonlinear behavior.

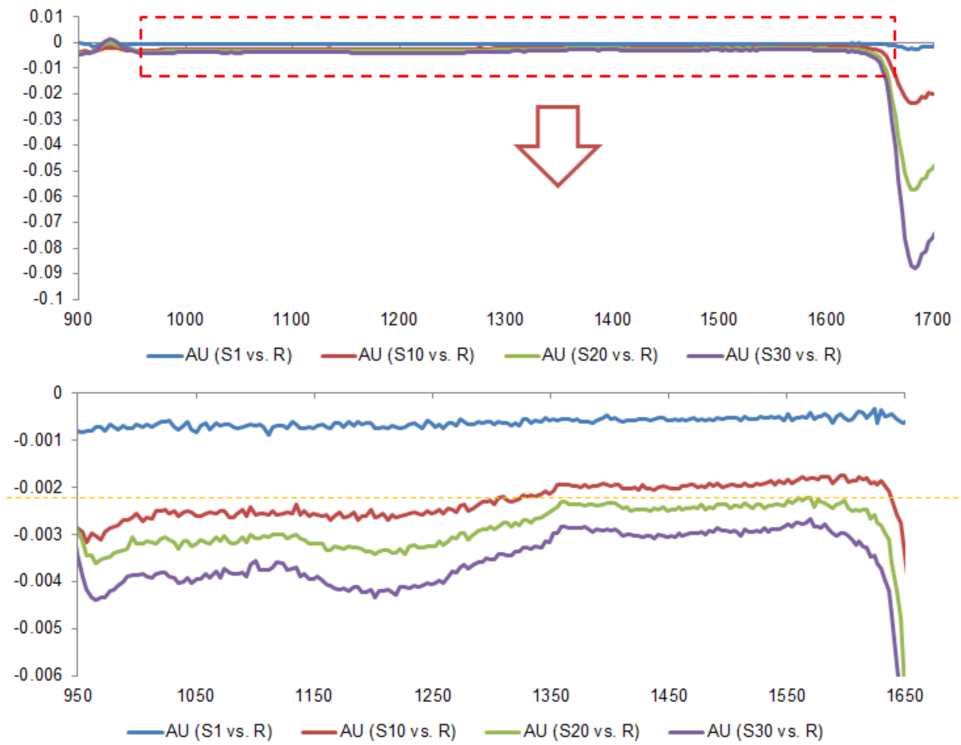


Figure 2.34 AU Changes in Cold Start

If S100 is used as a new reference signal, the result will be much better. By using S100 as reference signal, the AU deviations are within 0.0005 for the following 100 scans.

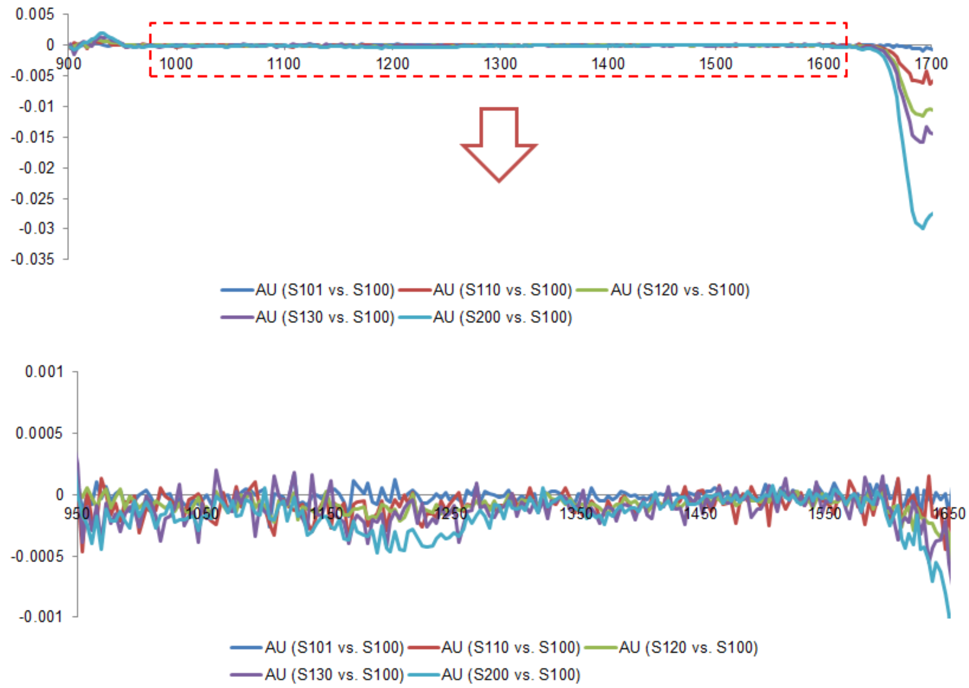


Figure 2.35 AU Changes after Warm Up

As above, if both reference and sample scans are taken after sufficient warm-up time, the calculated AU will be much stable. If device is operated randomly among different operating points, then a frequent reference scan is required to get stable AU.

As shown below, a lamp warm-up option has been added to the WinForms GUI. The default warm-up time is 3 minutes. Sufficient warm-up time can stabilize the lamp output and set a proper operating point for the spectrometer.

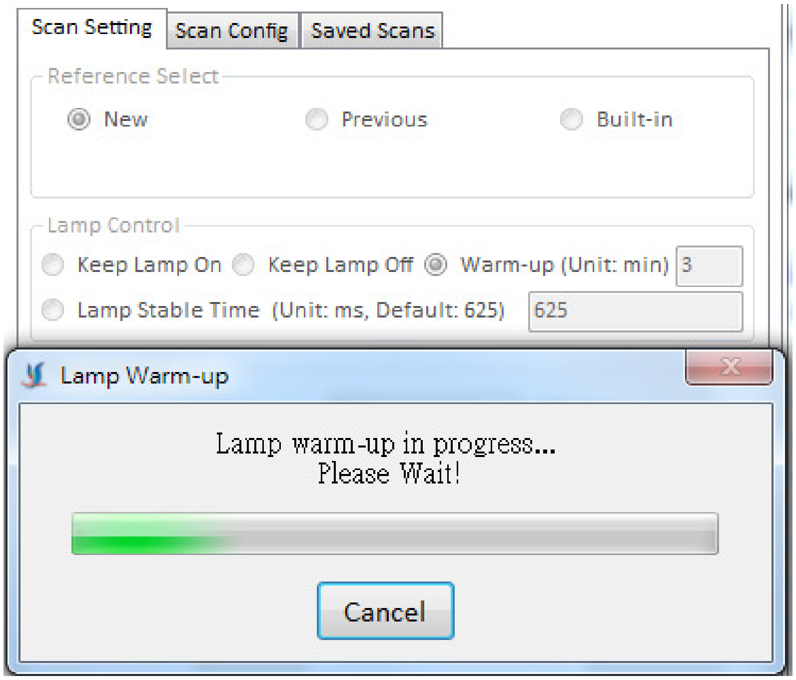


Figure 2.36 Lamp Warm-up Option

Chapter 3 Spectrometer Operation and Calibration

In this chapter, we will introduce the operation of the spectrometer in different measurement modes.

3.1 Diffuse Reflectance Mode

3.1.1 Diffuse Reflective Illumination Module

NIR-M-R2, NIR-S-G1 and NIR-S-RT1 are designed for diffuse reflective measurement in the standard wavelength range. The diffuse reflective illumination module operates by illuminating the sample under test at an angle so that specular reflections are not collected, while gathering and focusing diffuse reflections to the slit. Each lens-end lamp produces a beam of light at 40 degree angles that intersect past the sapphire window at about 0.75mm. There is about +/-0.25mm tolerance to the beam intersection due to the mechanical tolerances of the chassis, the variations of lens-end from lamp to lamp, the variations of lamp shape, and the placement of the lamps. The lens-end lamps focus the light beam at about 3 mm away from the lamps and create a spot size that covers the sapphire sample window. The collection lens gathers light from a 2.5 mm diameter region at the sample window. The size of the collection region was matched to the nominal illumination spot size created by the lens-end lamps. This requires that the sample be placed directly against the sapphire window, where the two angled light source paths intersect the collection vision cone of the lens. If the sample is shifted farther away from the window, the sample may not receive enough illumination for the system to perform an accurate scan. For best performance, place sample against sapphire window during a scan.

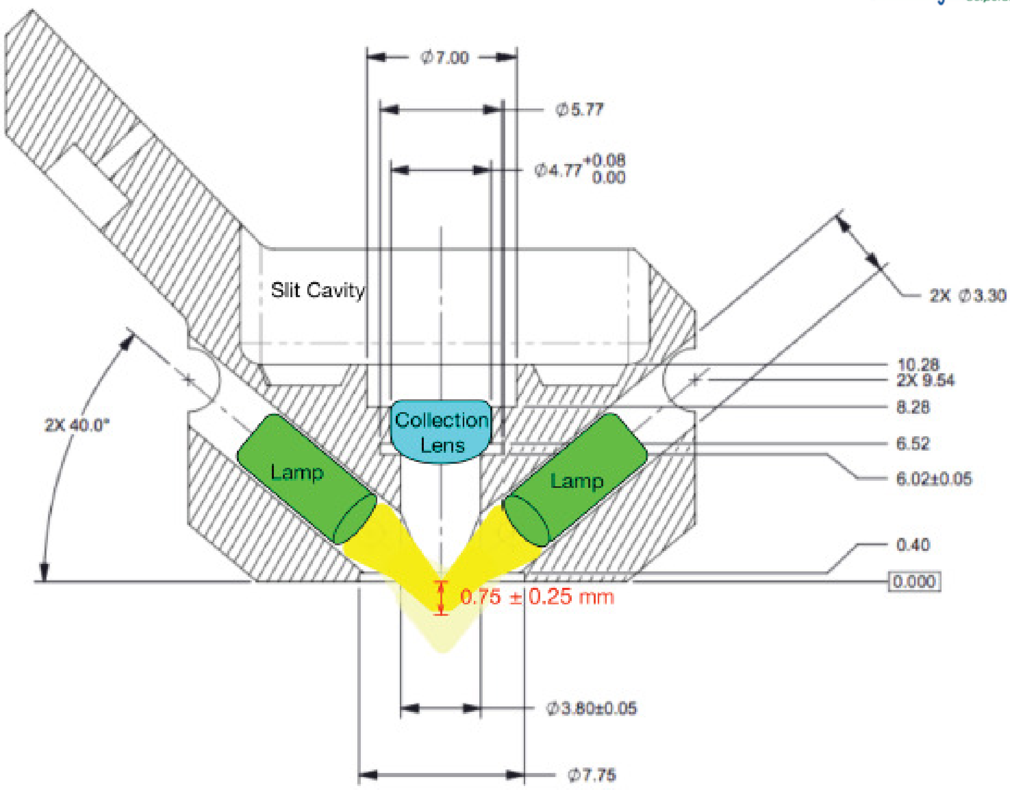


Figure 3.1 Diffuse Reflective Sampling Module

3.1.2 Diffuse Reflective Measurement

Users can easily find opaque plastic bottle caps and use them to learn NIR spectrum measurement in diffuse reflectance mode. For instance, Coke's plastic bottle caps are made of high-density polyethylene (HDPE) resin.

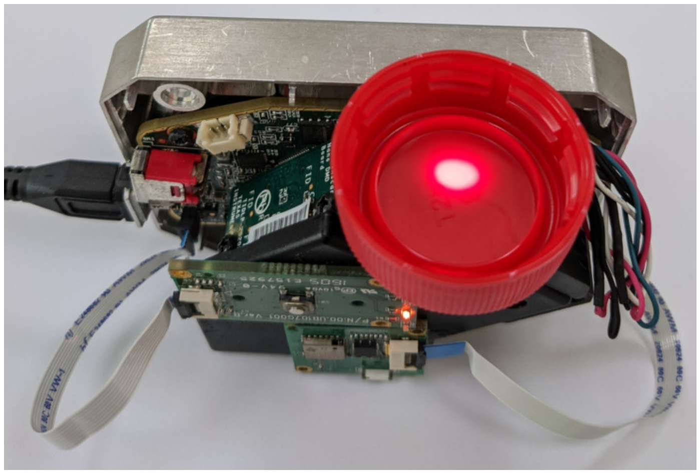


Figure 3.2 Diffuse Reflective Measurement of Plastic Bottle Cap (HDPE)

1. Please connect the NIRScan device to the PC. After launching the WinForms GUI, please check "Warm-up" to start the lamp warm-up process for at least 3 minutes.

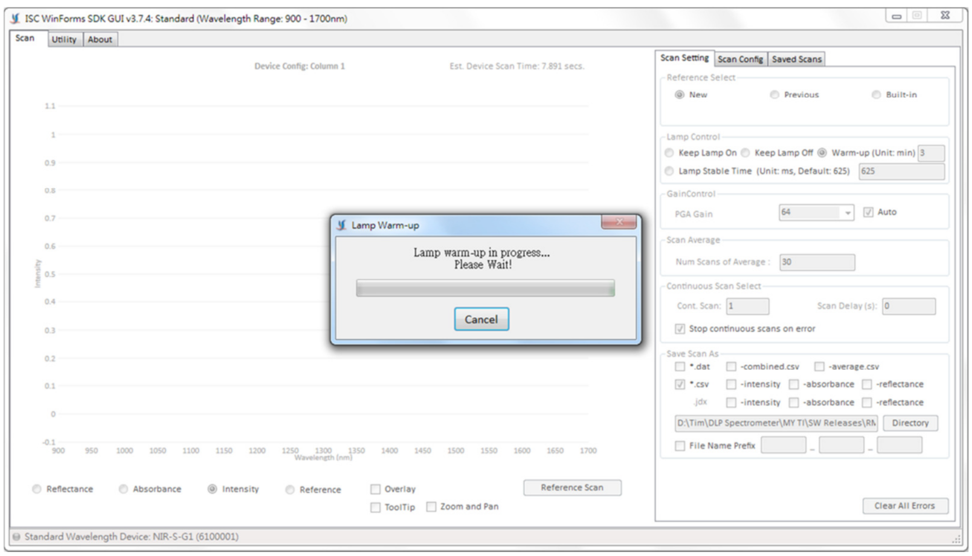


Figure 3.3 Warm-up for 3 Minutes

2. Select "Column 1" as the scan configuration. Place the reference material (SRS-99 or NIR-RM-1/2) on the scan window. Select "New" from "Reference Select" menu. Then, click "Reference Scan" to execute “New” reference scan. The reference signal will be displayed as follows:

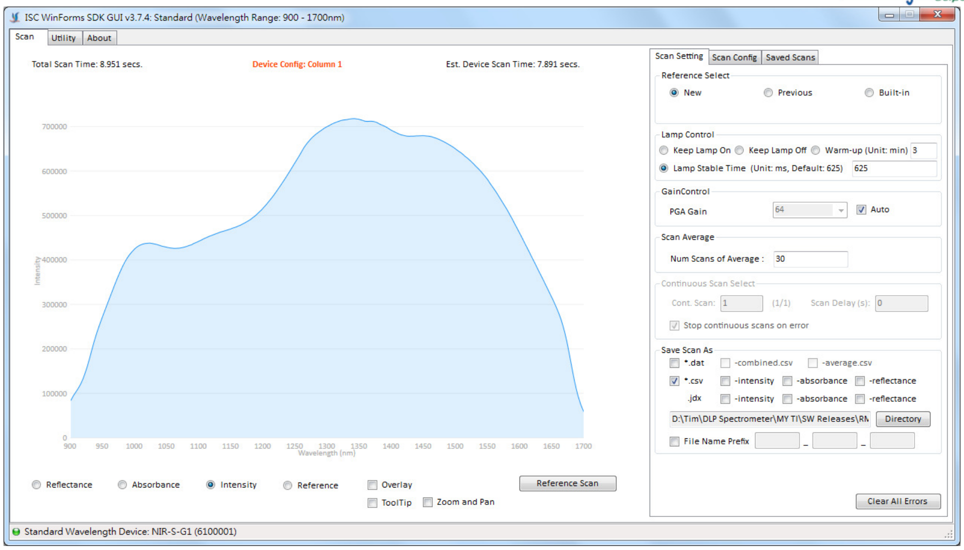


Figure 3.4 New Reference Scan

3. Place the plastic cap made of HDPE on the scan window, select "Previous" from "Reference Select" menu and click "Scan" to execute sample scan. The absorbance of the plastic cap will be displayed as follows:

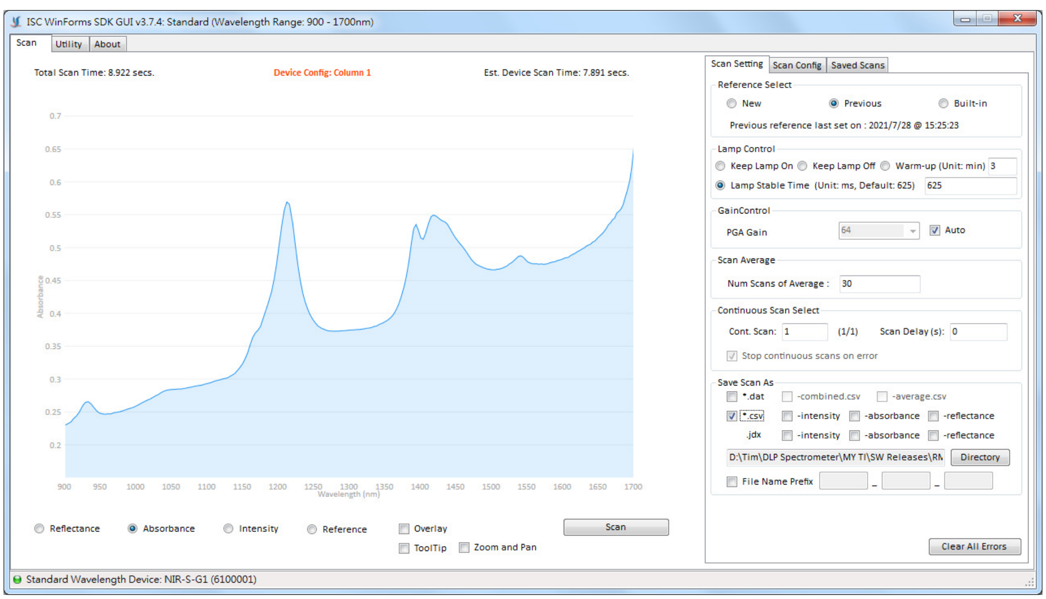


Figure 3.5 Sample Scan and HDPE Absorbance

4. Now, you can find the saved CSV file in the default directory (C:\Users\User Name\Documents\InnoSpectra\ Scan Results\). Then you can see and plot the spectral data as shown below.

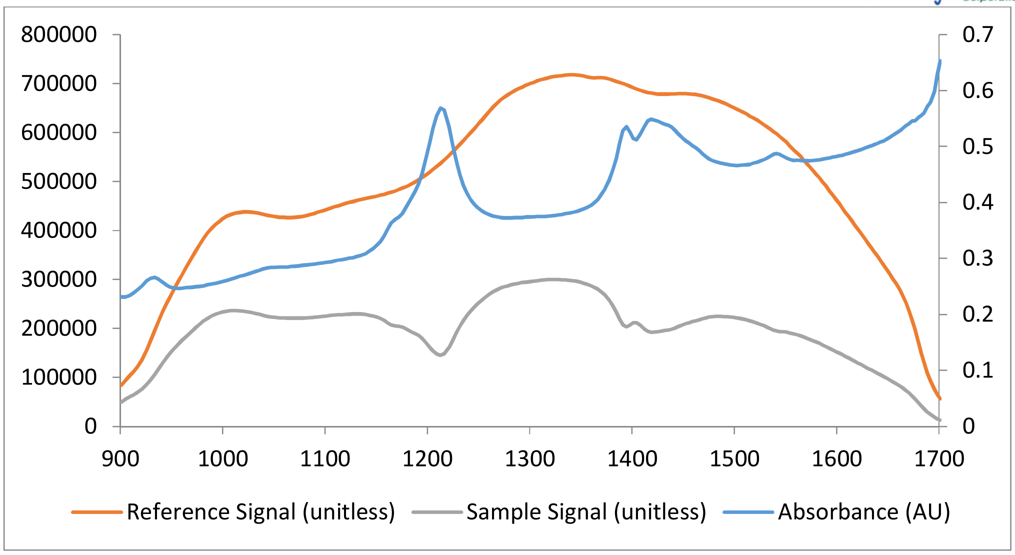


Figure 3.6 Spectral Data Saved in CSV File

3.2 Transmission Mode

3.2.1 Transmissive Illumination Module

NIR-M-T1 and NIR-M-T11 are designed for transmissive measurement. NIR-M-T1 supports a standard wavelength range from 900nm to 1700nm, while NIR-M-T11 supports an extended wavelength range from 1350nm to 2150nm. The working principle of the transmissive illumination module is to illuminate the sample under test through a collimating lens, and at the same time gather and focus the transmission light to the slit. NIR-M-T1 and NIR-M-T11 are designed with a sample holder to support cuvettes or vials with an optical path length of up to 10 mm. The sample holder is designed with two screw holes, and the sample position can be fixed by ball plunger screws. For vials or short path cuvettes, you can load them into an adapter first, and then put them into the sample holder. The Z-dimension (beam height) of NIR-M-T1 is 4.75mm, while the Z-dimension of NIR-M-T11 is 15mm. Both modules use only one tungsten filament lamp that consumes only 0.7W for illumination.

Please refer to the figure below to load enough samples into the cuvettes or vials for measurement. It is recommended that the sample height is 5mm higher than the Z-dimension value.

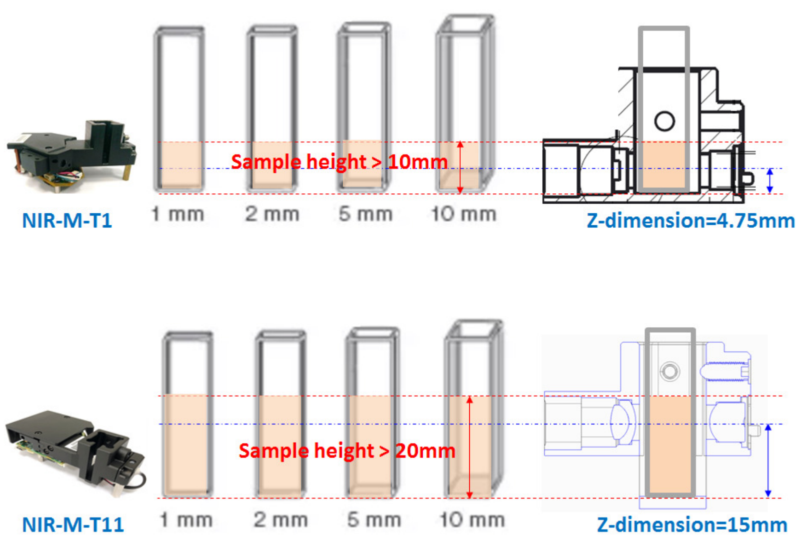


Figure 3.7 Z-dimension and Sample Height

Please refer to the figure below to align the standard 10mm cuvette with the optical axis. Please adjust the ball plunger screws until the ball end contacts the cuvette and starts to compress, do not over tighten the ball plunger screws.

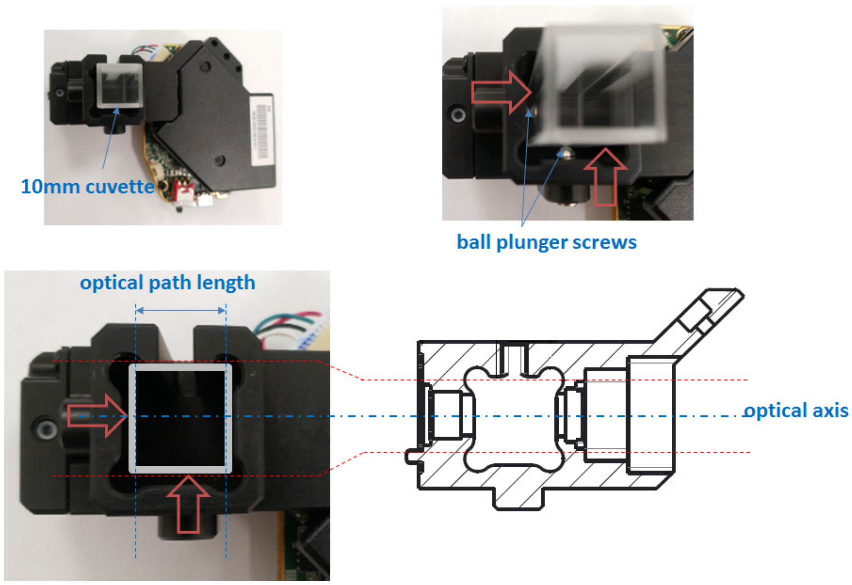


Figure 3.8 Alignment of Standard Cuvette

Please refer to the figure below for the alignment of sample vials and short path length cuvettes. Please contact ISC to obtain the CAD file of the adapter.

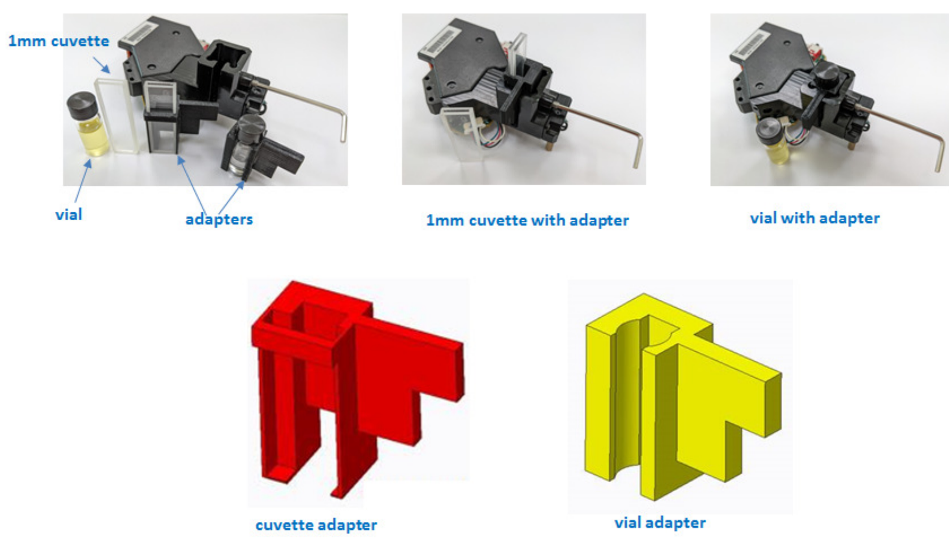


Figure 3.9 Alignment of Sample Vial and Short Path Length Cuvette

3.2.3 Transmissive Measurement

NIR-M-T1 and NIR-M-T11 can be used not only to measure liquid samples, but also to measure transparent solid materials, such as water, wine, edible oil, milk, syrup, gasoline, plastic sheets, filters, sunscreen window films, etc. Note, please use glass or quartz cuvette instead of plastic cuvette for liquid measurement. Please also choose a cuvette with a proper path length to avoid absorbance saturation.

Here is an example of plastic measurement and identification by means of NIR-M-T1. We will show you the measurement of PET and PMMA plates (thickness = 3mm).

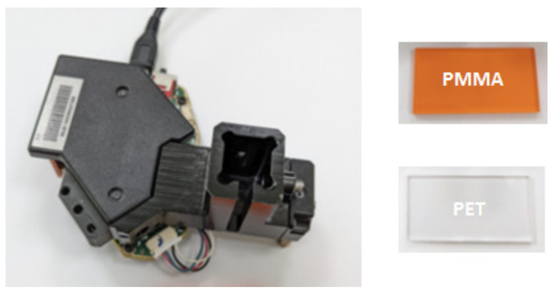


Figure 3.10 NIR-M-T1 and Plastic Plates

1. Connect the NIRScan device to the PC. After launching the WinForms GUI, check "Warm-up" to start the lamp warm-up process for at least 3 minutes. After that, select "Column 1" as the scan configuration. Scan air to get the new reference signal as follows:

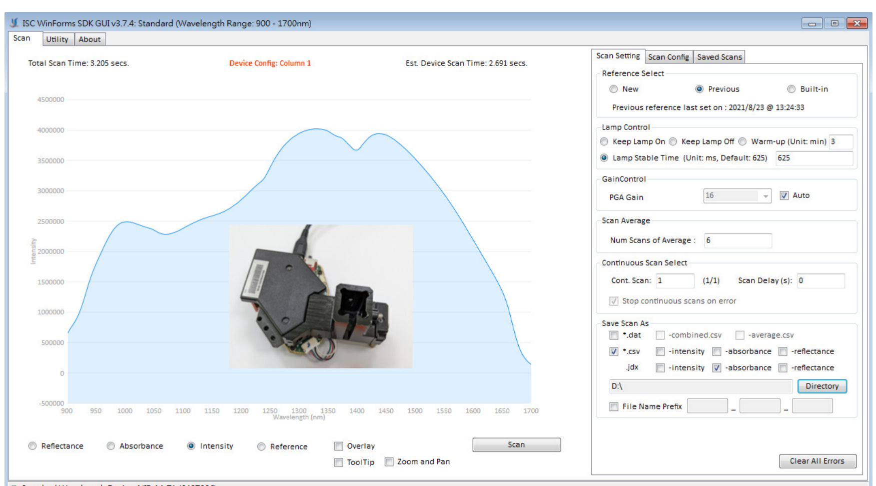


Figure 3.11 New Reference Scan

2. Insert the plastic plate into the sample holder and measure the sample signal. The absorbance data of the two samples are shown below.

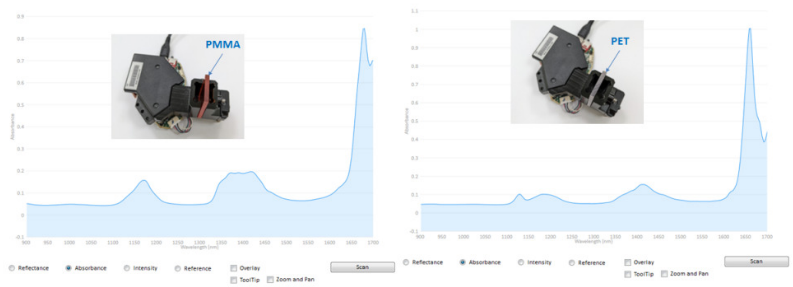


Figure 3.12 Sample Scan

3. By comparing the absorbance data, it is easy to identify different plastic plates.

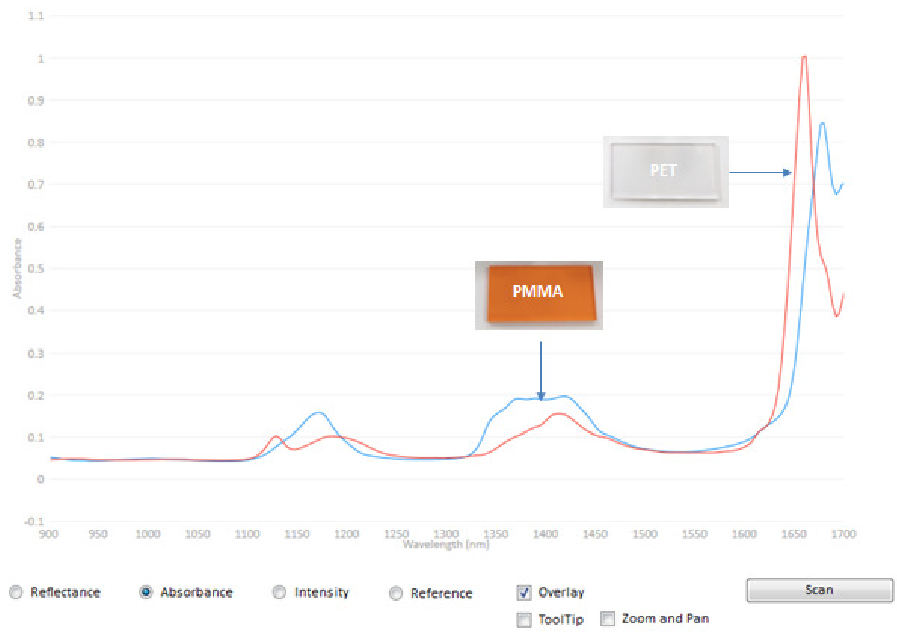


Figure 3.13 Comparison of Absorbance of PET and PMMA

The following is an example of the absorbance of 75% ethanol measured using different path lengths. Obviously, the 10mm path length is too long for this application because the absorbance data is already saturated.

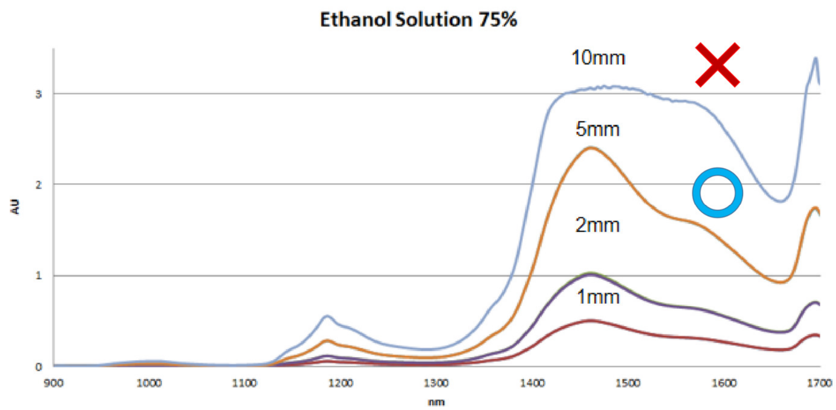


Figure 3.14 The Absorbance of 75% Ethanol Solution

The following is an example of the absorbance of water measured using different path lengths. Obviously, the 5mm path length is too long for this application because the absorbance data is already saturated.

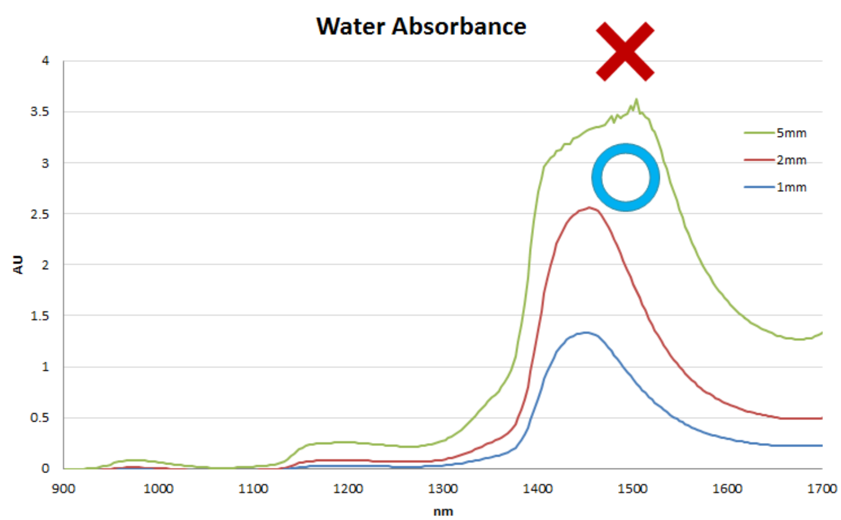


Figure 3.15 The Absorbance of Water

Soy milk and dairy milk are generally opaque, white or off-white in color, and are strong scattering materials. If you plan to measure milk in transmissive mode, you need to apply a very short path length. Here is an example of the absorbance of soy milk measured using 100um path length.

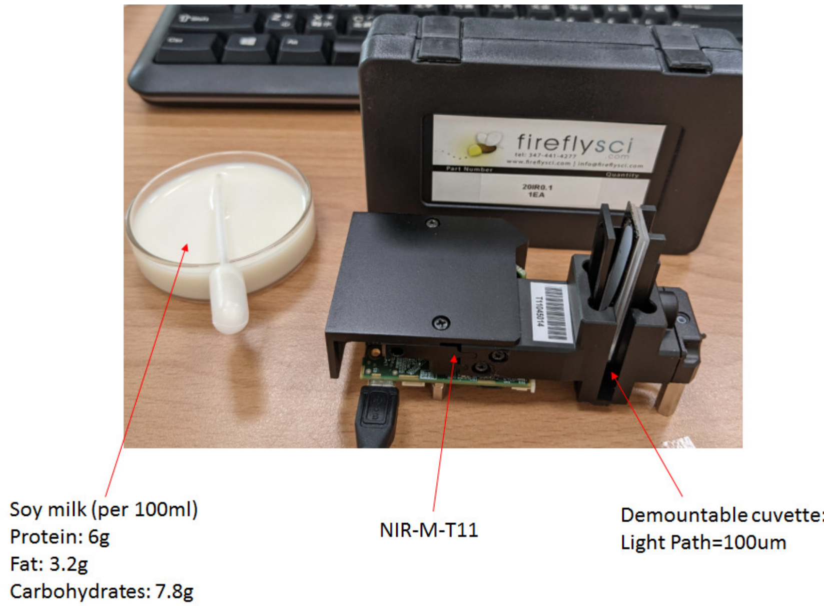
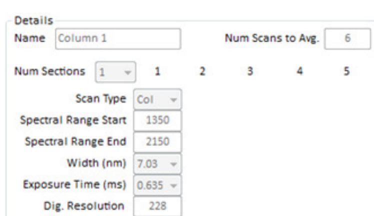


Figure 3.16 Use 100um Cuvette to Measure Soy Milk in Transmissive Mode

The following is the scanning configuration and scanning results of soy milk in transmissive mode.



- Scan Config: Column 1 has been good enough to maintain spectral quality.
- Reference Signal: Empty cuvette (air).

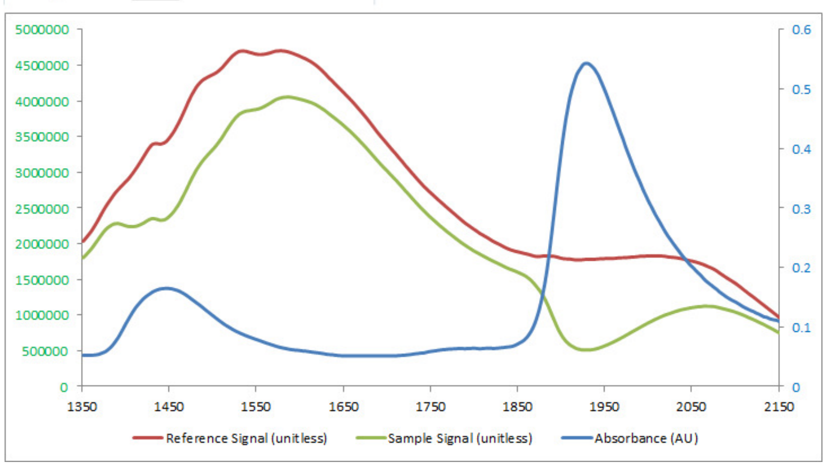


Figure 3.17 Scan Configuration and Absorbance of Soy Milk

With NIR-M-T1 and NIR-M-T11, we do not suggest using the Hadamard mode because it is very possible to cause reference signal saturation even when PGA=1 (without ND filter). Once signal is saturated, the absorbance calculation will never be correct.

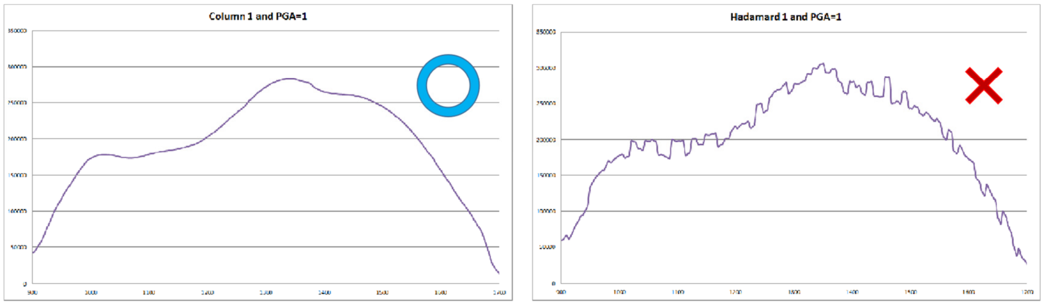


Figure 3.18 Column Mode vs. Hadamard Mode

3.3 Fiber Input

3.3.1 Fiber Input Module

NIR-M-F1 and NIR-M-F11 are designed with SMA905 connectors, which can couple light to the entrance slit of the spectrometer through an optical fiber. NIR-M-F1 supports a standard wavelength range from 900nm to 1700nm, while NIR-M-F11 supports an extended wavelength range from 1350nm to 2150nm. The dimensions and tolerances of SMA905 connector are designed according to IEC 61754-22: 2005. The length of the optical fiber ferrule should not exceed 9.812mm to prevent it from hitting the slit plate. The SMA905 connector is designed with a V-shaped notch and a key slot, which can be used to align the fiber bundle with the entrance slit of the spectrometer.

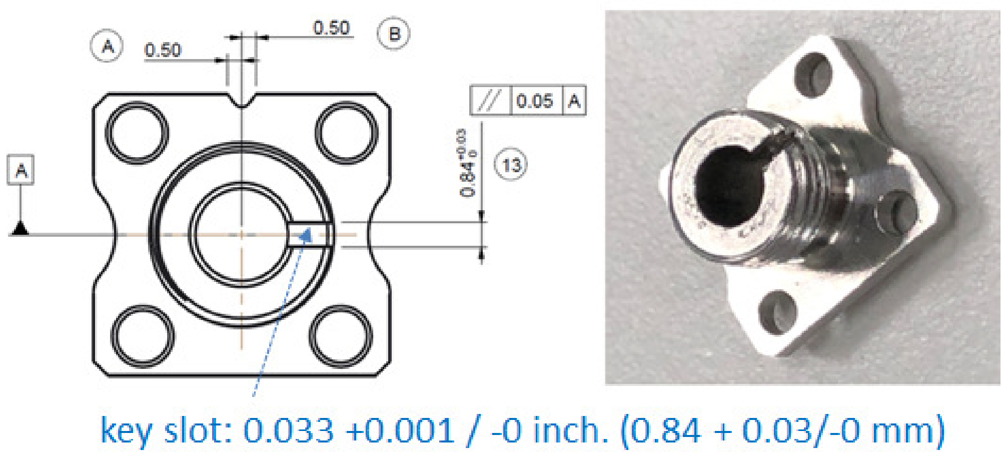


Figure 3.19 SMA905 Connector with V-shaped Notch and Key Slot

NIRScan spectrometers have taller entrance slits than array detector systems because the DMD is taller than the array detector. This allows for increased signal throughput, but can make fiber coupling more complex. Standard optical fibers can be utilized, but will only illuminate a small section of the entrance slit. In order to take advantage of the DLP-based spectrometer's large etendue, a round-to-linear fiber bundle should be used. These optical fibers have multiple cores arranged in a circular pattern at one end, and a linear configuration at the opposite end. The round end can be utilized at the sample as in typical spectroscopy illumination modules, while the linear end can be more effectively coupled to the slit.

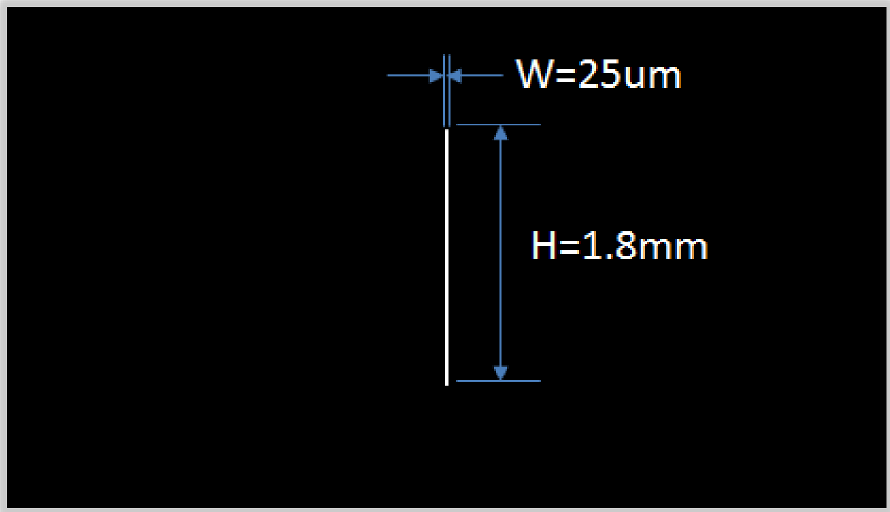


Figure 3.20 Entrance Slit

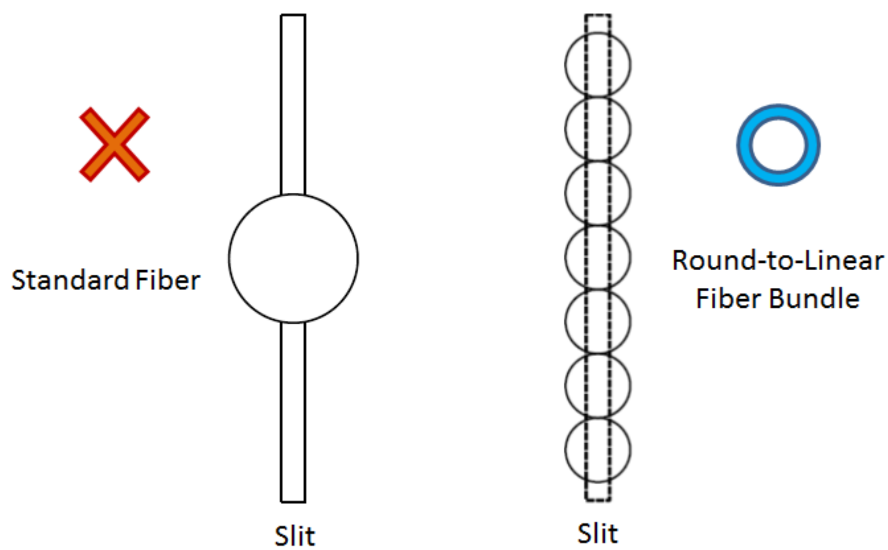


Figure 3.21 Slit Fill Factor with Standard Fiber and Round-to-Linear Fiber Bundle

It is recommended to use Thorlabs' round-to-linear fiber bundle or equivalent fibers. For alternative fiber options, please select 0.22 NA step-index multimode fibers and low hydroxyl ion (OH) cores for NIR applications.

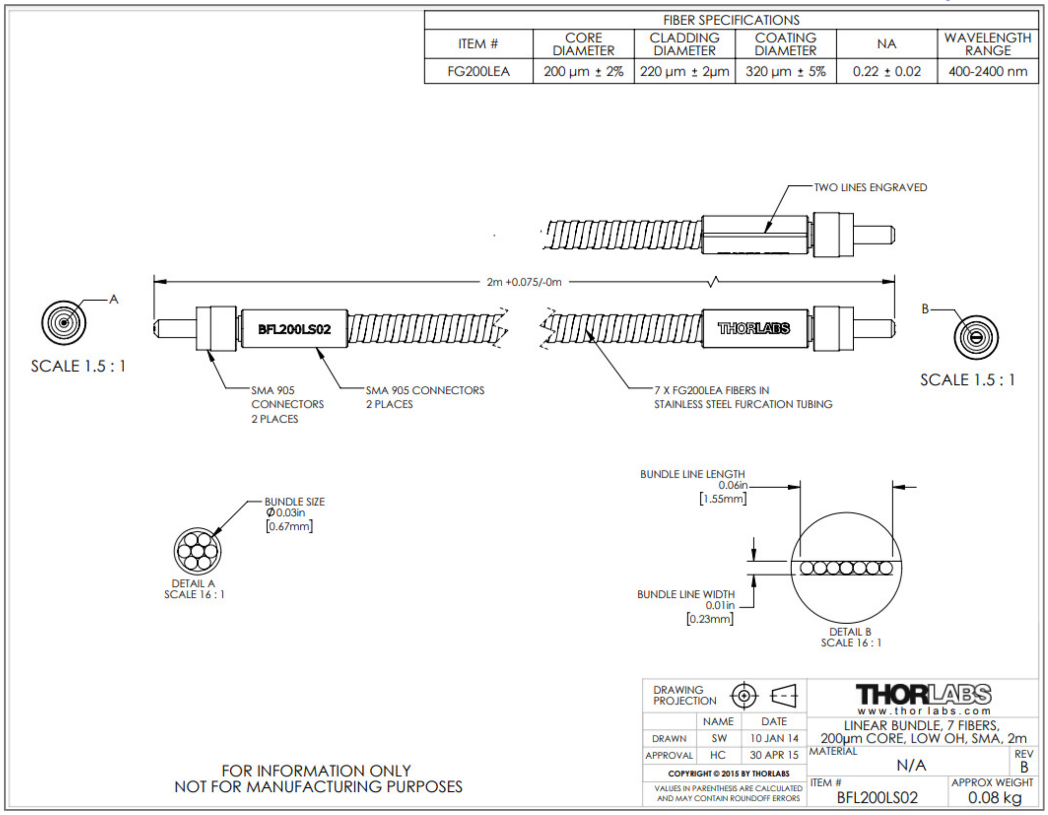


Figure 3.22 Round-to-Linear Fiber Bundle

When using a round-to-linear fiber bundle, please ensure the engraved mark of the fiber bundle is aligned with the V-shape notch of the SMA905 connector.

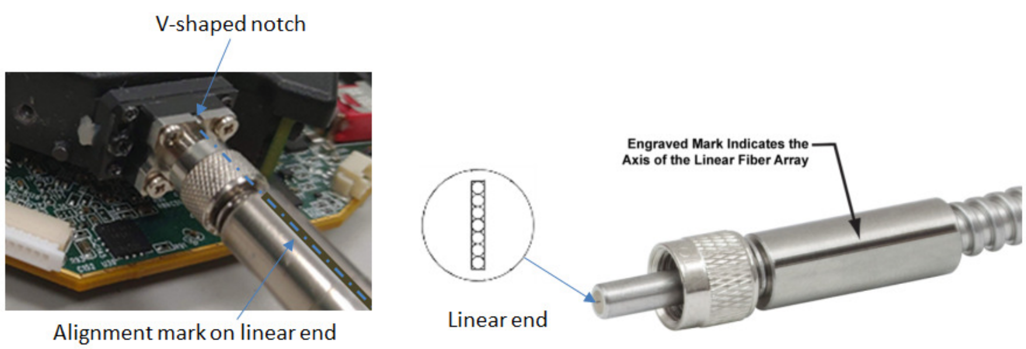


Figure 3.23 Alignment of Linear End Bundle

In addition, a key can be added to the linear end of the fiber bundle to further assist in the alignment of the fiber bundle with the entrance slit, as shown below.

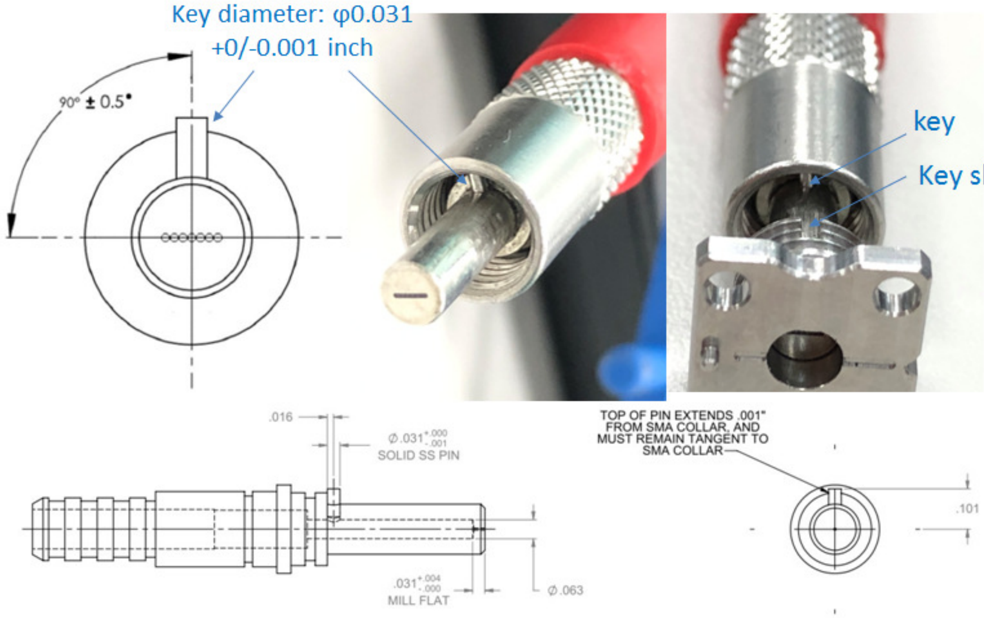


Figure 3.24 Linear End Bundle with Key

3.3.1 Fiber Input Measurement

Here is a typical setup of transmissive measurement by using the fiber input module.

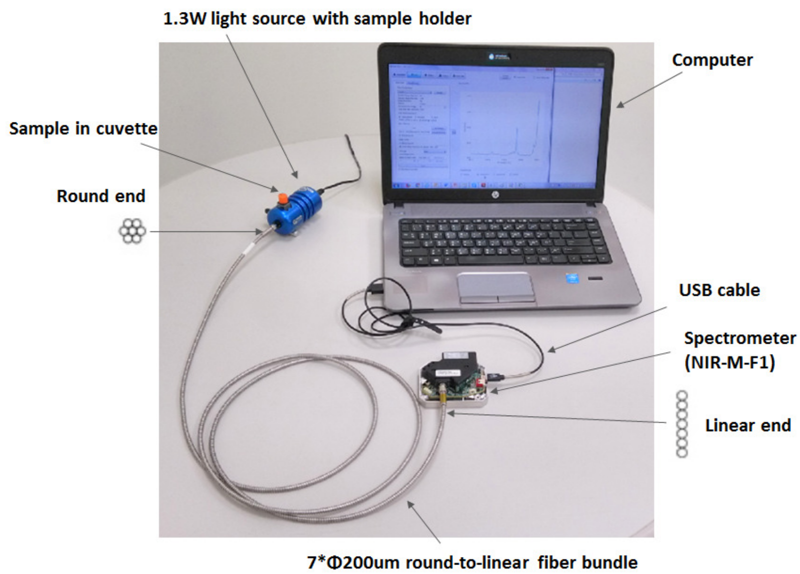
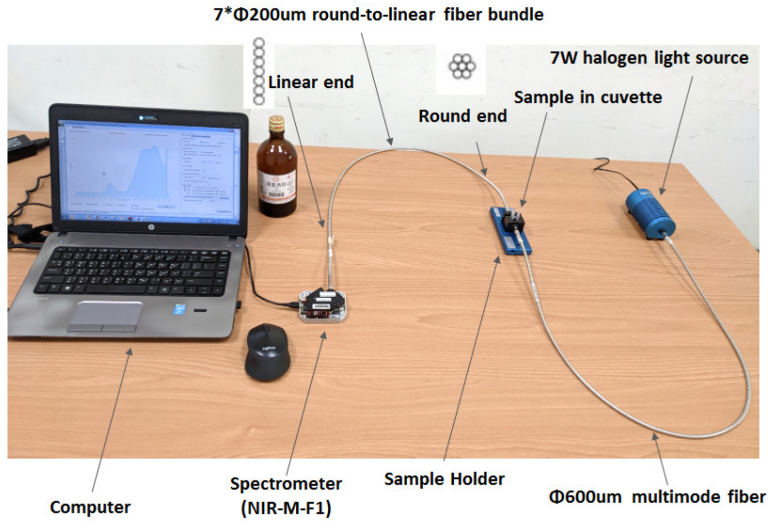


Figure 3.25 Transmissive Measurement with Fiber Input Module

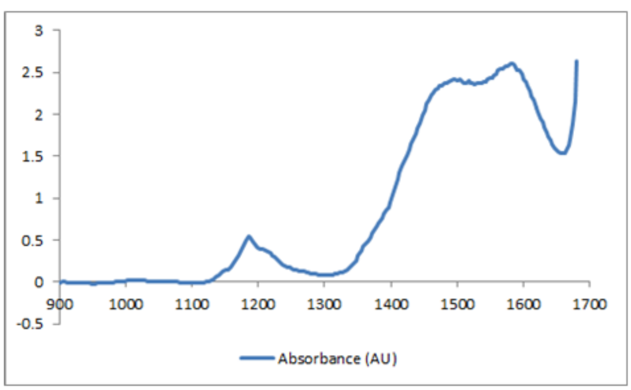
Here is another typical transmissive measurement setup with separate light source and sample holder. By using the recommended scan configuration to scan the reference signal (empty cuvette) and the sample signal (95% alcohol loaded in glass cuvette), the absorbance of 95% alcohol is displayed as follows.



(a) Measurement Setup

Scan Config Name:	Column 1
Scan Config Type:	Slew
Section Config Type:	Column
Start Wavelength (nm):	900
End Wavelength (nm):	1700
Pattern Width (nm):	7.03
Exposure (ms):	0.635
Digital Resolution:	228
Num Repeats:	30

(b) Scan Configuration



(c) Absorbance of 95% Alcohol Loaded in 10mm Cuvette

Figure 3.26 Transmissive Measurement with Fiber Input Module

Here is a typical setup of diffuse reflective measurement by using the fiber input module.

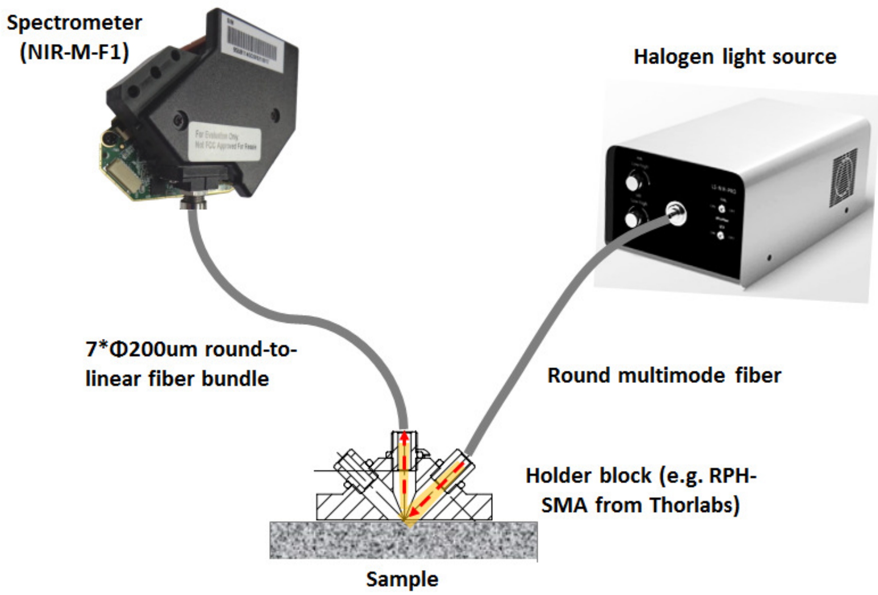
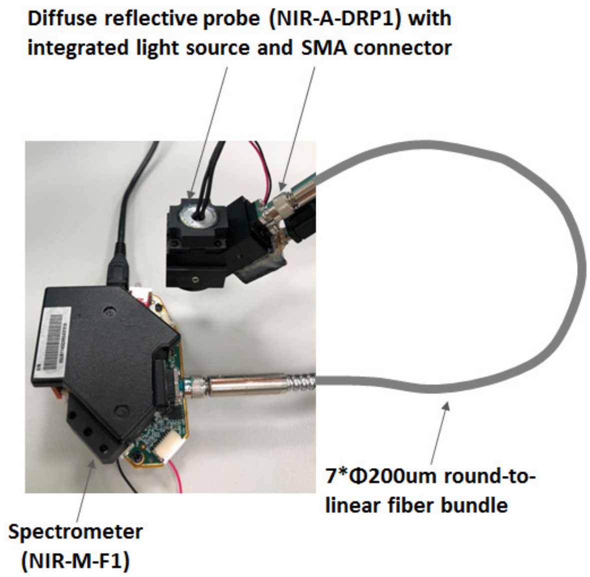
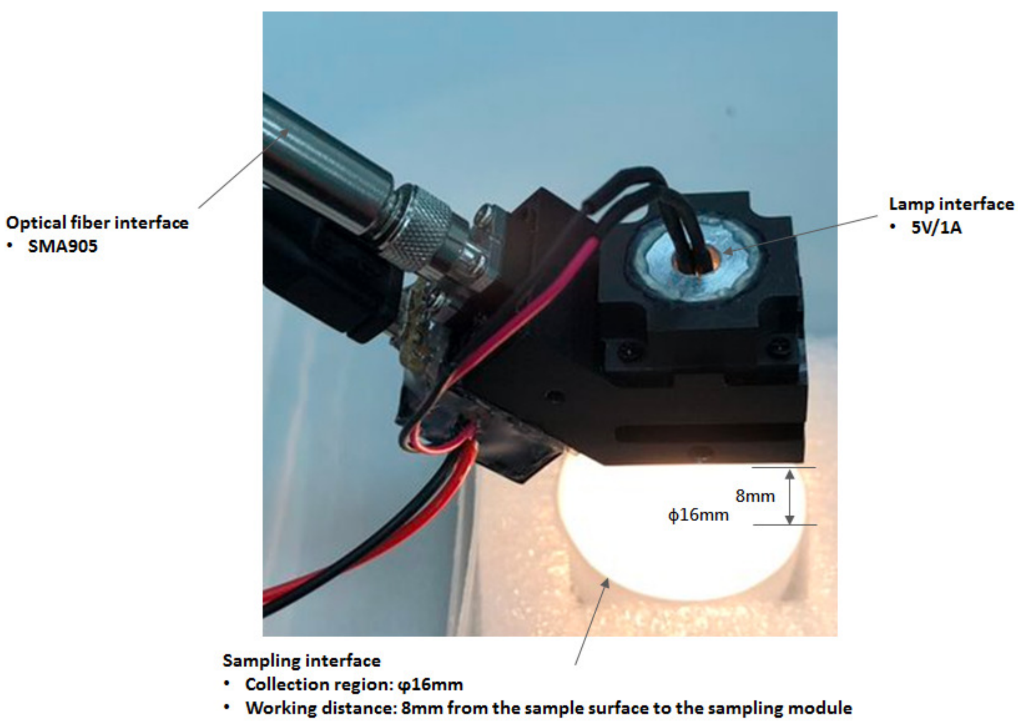


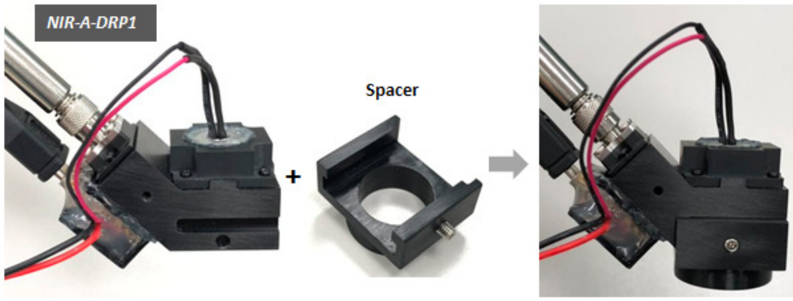
Figure 3.27 Diffuse Reflective Measurement with Fiber Input Module

Here is another setup of diffuse reflective measurement by using the diffuse reflective probe. The diffuse reflection probe (NIR-A-DPR1) integrates a collimated light source, a collecting lens and an SMA905 connector. When using optical fiber input spectrometer, NIR-A-DRP1 greatly simplifies the diffuse reflective measurement setup. NIR-A-DRP1 supports both contact and non-contact measurement. By using the recommended scan configuration to scan the reference signal (SRS-99 or equivalent) and the sample signal (plastic bottle cap), the absorbance of plastic bottle cap (HDPE) is displayed as follows.



(a) Diffuse Reflective Measurement with NIR-A-DRP1



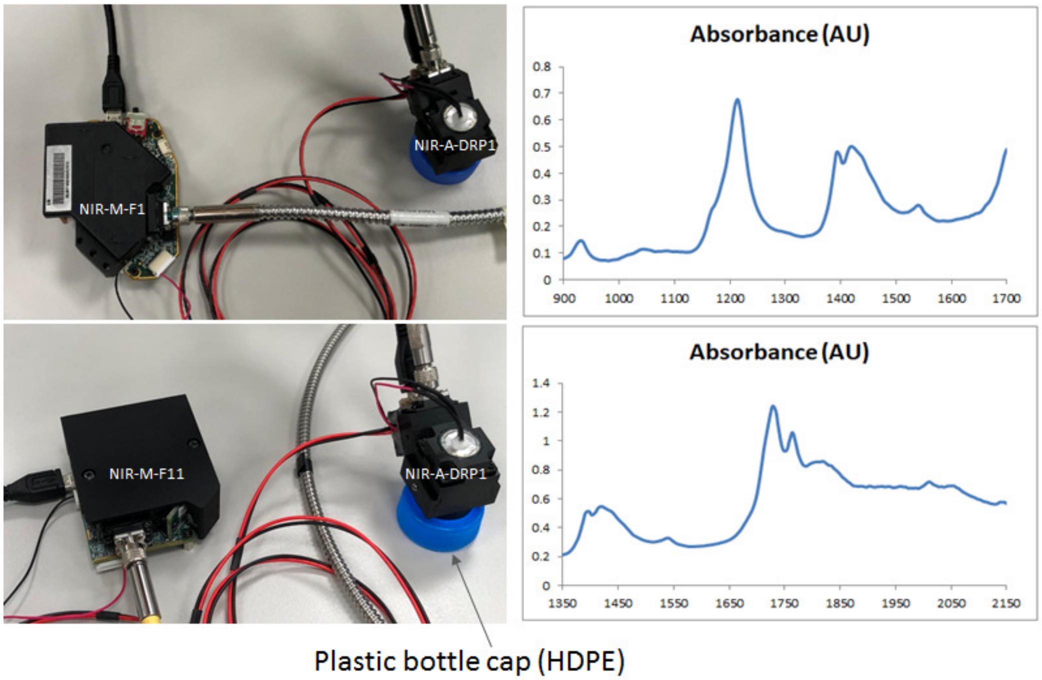


- **Illumination Module: one 5W tungsten filament lamp with reflector, constant current (CC) driver board with lamp on-off control interface will be provided separately.**
- **Sampling Module: Diffuse reflective sampling module**
- **Collection Region: Typ. 16mm in diameter**
- **Working Distance: Typ. 8mm from the sample surface to the sampling module**
- **Fiber Connector: SMA905**
- **Power Supply: DC 5V/1A**
- **Dimensions: 44.5 mm * 35 mm * 27 mm (include spacer)**
- **Weight: 40 g (include spacer)**
- **Operating Temperature: 0 ~ 40 ℃, RH Max. 85%**

(b) Brief Introduction of NIR-A-DRP1

Fiber Input Module:	NIR-M-F1	NIR-M-F11
Section Config Type:	Hadamard	Hadamard
Start Wavelength (nm):	900	1350
End Wavelength (nm):	1700	2150
Pattern Width (nm):	10.54	10.54
Exposure (ms):	1.27	1.27
Digital Resolution:	160	160
Num Repeats:	6	12

(c) Scan Configuration



(d) Plastic Bottle Cap (HDPE) Measurement Results

Figure 3.28 Fiber Input Module with Diffuse Reflective Probe

Here is the setup for transflective measurement. This setup includes a Y-shaped fiber bundle and a tip for the transmission dip probe.

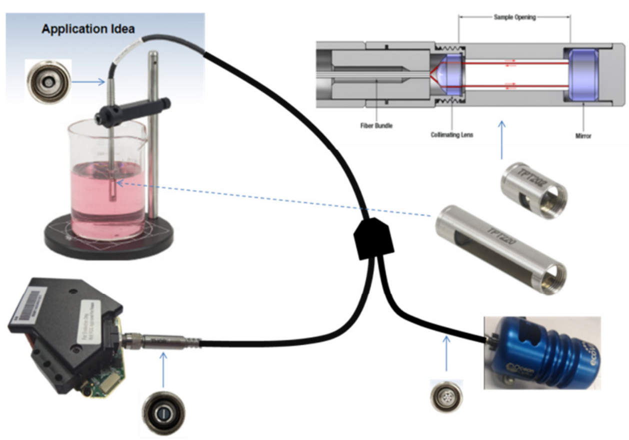


Figure 3.29 Transflective Measurement with Dip Probe

3.4 Spectrometer Calibration

By using DMD as the wavelength selector, the wavelength of the spectrum is a mapping of DMD pixels. The mapping between each pixel and wavelength is determined by the pixel-to-wavelength coefficients (a, b, and c). The corresponding wavelength of each pixel is calculated from $\lambda = a*P^2 + b*P + c$, where λ is a wavelength and P is the DMD pixel position. It is recommended that the user checks the wavelength accuracy regularly. Once any offset is found between the expected and observed peak wavelength points, the user can consider re-calibrating the spectrometer. In order to check the wavelength accuracy and re-calibrate the NIRScan devices, users have to prepare standard reference material and test sample. For diffuse reflective module and spectrometer, users are advised to prepare **SRS-99** (Labsphere) and **SRM2036** (NIST). For transmissive module and spectrometer, users are advised to prepare **RM-NIR** (Starna Scientific). For fiber input module and spectrometer, it depends on your application to prepare standard reference material and test sample for wavelength accuracy check and wavelength calibration.

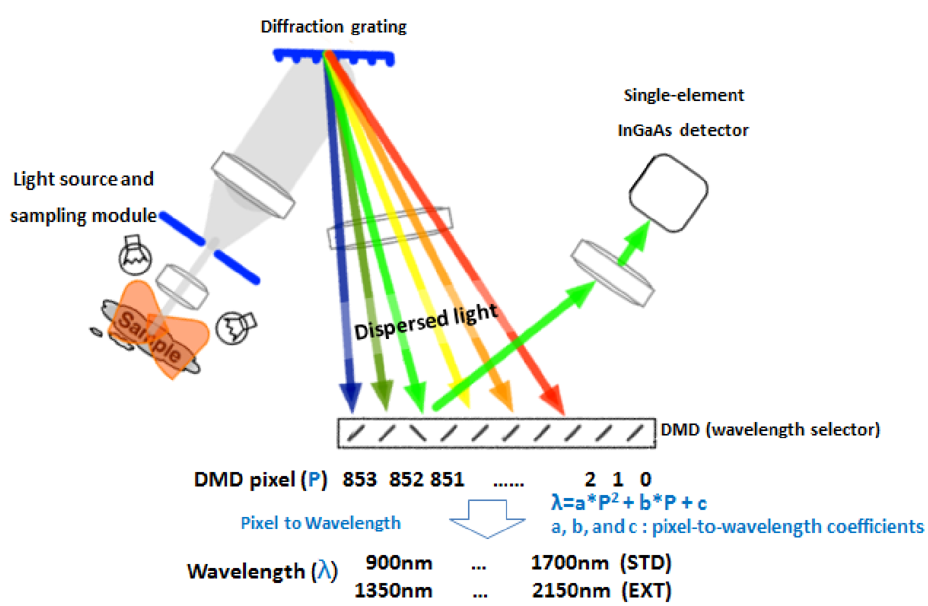


Figure 3.30 Pixel-to-Wavelength Mapping

3.4.1 Diffuse Reflectance Mode

For **NIR-M-R2**, **NIR-S-G1** and **NIR-S-RT1**, please warm up the device first and use the following scan configuration to perform scan test. Please scan **SRS-99** to get the reference signal, scan **SRM2036** to get the sample signal, and then you will get the absorbance data of SRM2036 to check the wavelength accuracy.

Section Config Type:	Column
Start Wavelength:	900
End Wavelength:	1700
Pattern Width:	7.03
Exposure:	0.635
Digital Resolution:	228
Num Repeats:	30

SRM2036 from NIST

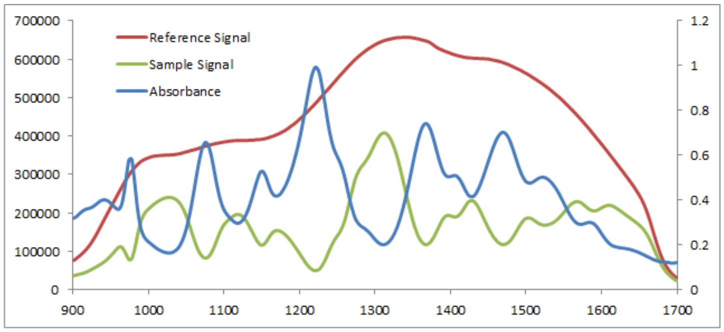


Figure 3.31 Scanning of Standard Reference Material and Test Sample

For example, there is one spectrometer found with wavelength offset as follows:

Expected (SRM2036 AU)	Observed	Offset
975.900	977.356	1.456
1075.800	1077.025	1.225
1222.100	1223.280	1.180
1367.300	1368.811	1.511
1469.500	1471.405	1.905

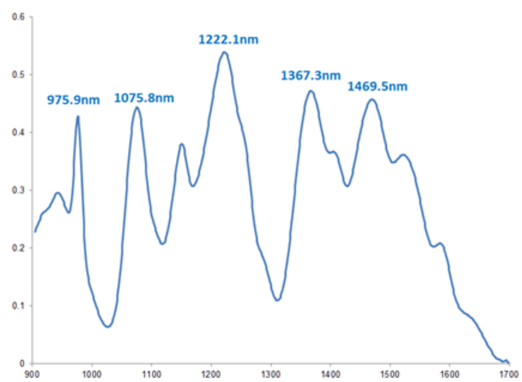


Figure 3.32 Observed Peak Position and Offset

Note: The Lagrange polynomial can be used to find the peak position of NIR absorbance. Three data points near the peak position are used to form a quadratic Lagrange polynomial. The vertex (maximum point) of the quadratic Lagrange polynomial is the peak position we want to find.

Linear regression can be applied to come out a transfer function between the expected wavelength points and the observed wavelength points as below. The linear regression has a perfect fit between two vectors. You can use Excel to calculate the slope and intercept of a linear transfer function as follows:

- **Slope** (Expected wavelength list, Observed wavelength list)
- **Intercept** (Expected wavelength list, Observed wavelength list)

Expected (SRM2036 AU)	Observed
975.900	977.356
1075.800	1077.025
1222.100	1223.280
1367.300	1368.811
1469.500	1471.405

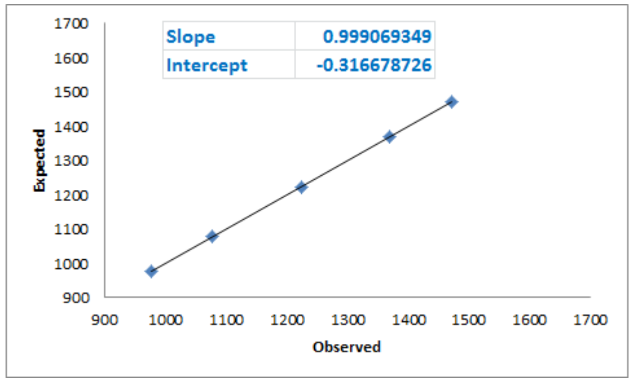


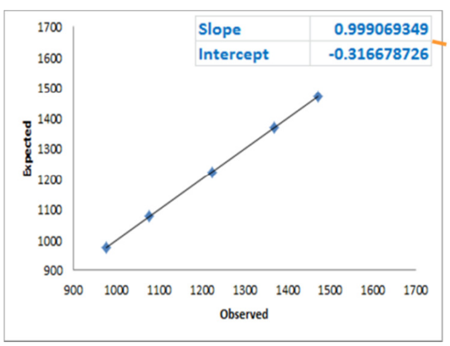
Figure 3.33 Linear Regression of Expected and Observed Wavelength Points

New calibration coefficients are calculated as below:

a3= a2 * a1

b3= a2 * b1

C3= a2 * c1 + b2



Original		Expected vs. Observed		New Coefficients	
a1	-0.00023527	a2	0.999069349	a3	-0.000235051
b1	-0.917665	b2	-0.316678726	b3	-0.916810974
c1	1829.12			c3	1827.10105

Figure 3.34 Calculate New Calibration Coefficients

Use the WinForms GUI to update the calibration coefficients:

Original		Expected vs. Observed		New Coefficients	
a1	-0.00023527	a2	0.999069349	a3	-0.000235051
b1	-0.917665	b2	-0.316678726	b3	-0.916810974
c1	1829.12			c3	1827.10105

WinForms GUI / Utility:

Steps:

1. **Read Coefficients**
2. **Write enable**
3. **Input new coefficients**
4. **Write Coefficients**

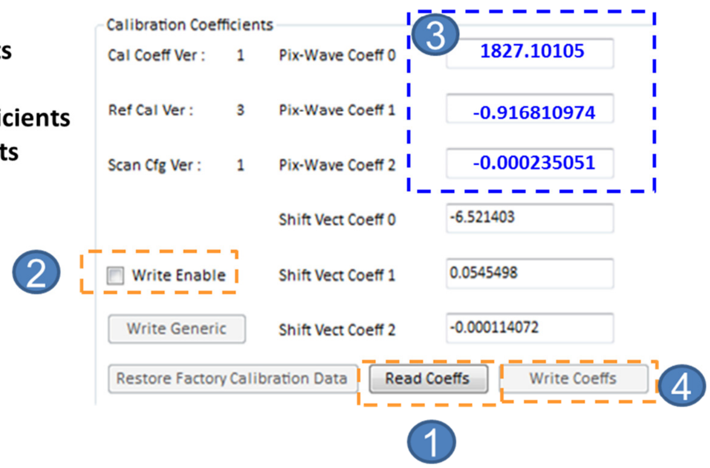


Figure 3.35 Update Calibration Coefficients

After updating the calibration coefficients, please also update the built-in reference data as below:

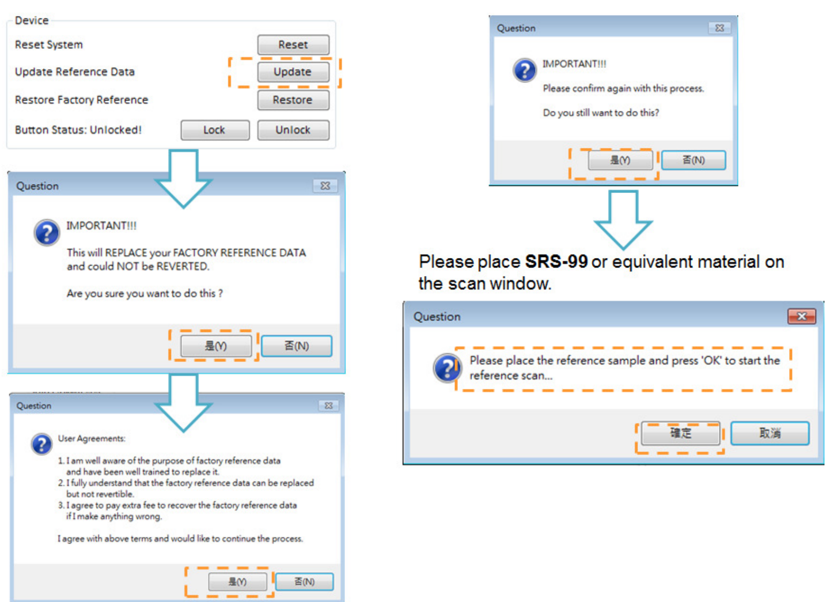


Figure 3.36 Update Built-in Reference Data

3.4.2 Transmission Mode

For **NIR-M-T1** and **NIR-S-T1**, please warm up the device first and use the following scan configuration to perform scan test. Please scan **air** to get the reference signal, scan **RM-NIR** to get the sample signal, and then you will get the absorbance data of RM-NIR to check the wavelength accuracy.

Section Config Type:	Column
Start Wavelength:	900
End Wavelength:	1700
Pattern Width:	7.03
Exposure:	0.635
Digital Resolution:	228
Num Repeats:	30

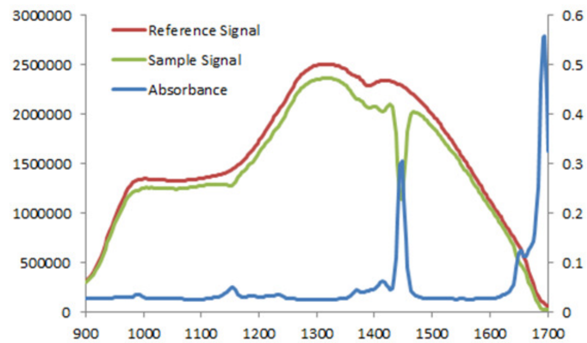


Figure 3.37 Scanning of Standard Reference Material and Test Sample

For example, there is one spectrometer found with wavelength offset as follows:

Expected (RM-NIR AU)	Observed	Offset
990.7	990.8799477	0.179947726
1446.6	1447.630782	1.030781616
1693.1	1693.063432	-0.036568474

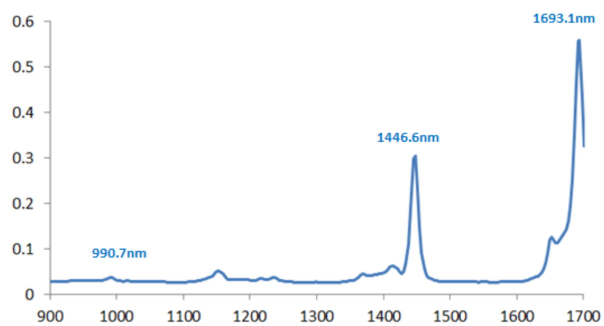


Figure 3.38 Observed Peak Position and Offset

Note: The Lagrange polynomial can be used to find the peak position of NIR absorbance. Three data points near the peak position are used to form a quadratic Lagrange polynomial. The vertex (maximum point) of the quadratic Lagrange polynomial is the peak position we want to find.

Linear regression can be applied to come out a transfer function between the expected wavelength points and the observed wavelength points as below. The linear regression has a perfect fit between two vectors. You can use Excel to calculate the slope and intercept of a linear transfer function as follows:

- **Slope** (Expected wavelength list, Observed wavelength list)
- **Intercept** (Expected wavelength list, Observed wavelength list)

Expected (RM-NIR AU)	Observed
990.7	990.8799477
1446.6	1447.630782
1693.1	1693.063432

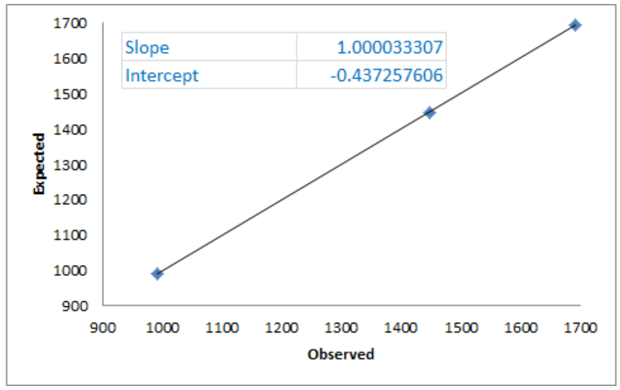


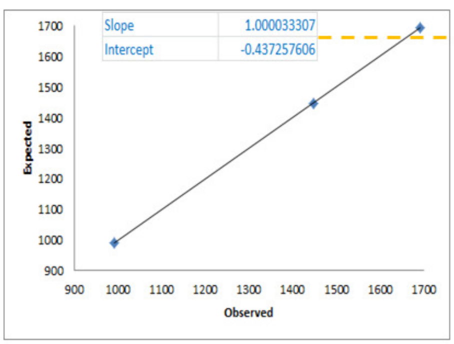
Figure 3.39 Linear Regression of Expected and Observed Wavelength Points

New calibration coefficients are calculated as below:

a3= a2 * a1

b3= a2 * b1

C3= a2 * c1 + b2



Original Coefficients		Expected vs. Observed		New Coefficients	
a1	-0.000243109	a2	1.000033307	a3	-0.000243117
b1	-0.924906715	b2	-0.437257606	b3	-0.924937521
c1	1744.949722			c3	1744.570584

Calculate new calibration coefficients

Figure 3.40 Calculate New Calibration Coefficients

Use the WinForms GUI to update the calibration coefficients:

Original Coefficients		Expected vs. Observed		New Coefficients	
a1	-0.000243109	a2	1.000033307	a3	-0.000243117
b1	-0.924906715	b2	-0.437257606	b3	-0.924937521
c1	1744.949722			c3	1744.570584

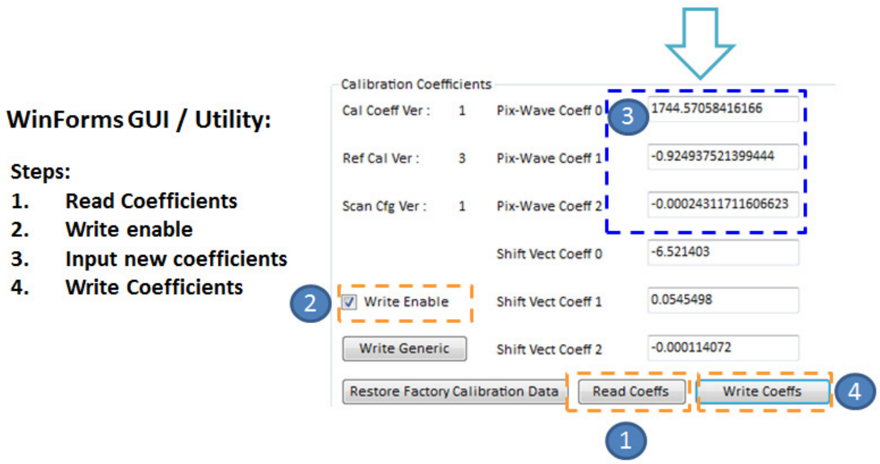


Figure 3.41 Update Calibration Coefficients

After updating the calibration coefficients, please also update the built-in reference data as below:

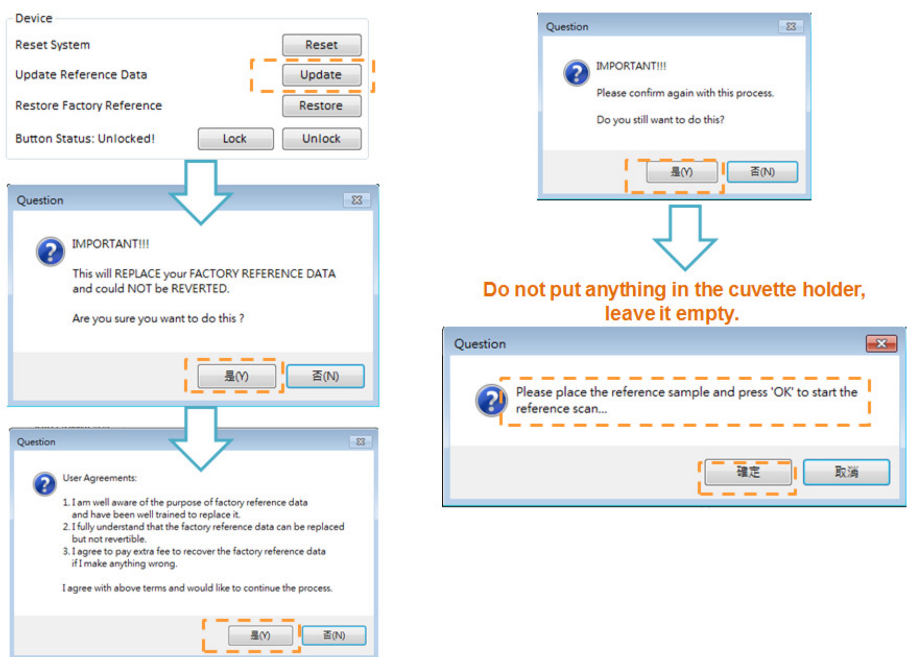


Figure 3.42 Update Built-in Reference Data

For **NIR-M-T11**, please warm up the device first and use the following scan configuration to perform scan test. Please scan **air** to get the reference signal, scan **RM-NIR** to get the sample signal, and then you will get the absorbance data of RM-NIR to check the wavelength accuracy.

Section Config Type:	Column
Start Wavelength (nm):	1350
End Wavelength (nm):	2150
Pattern Width (nm):	7.03
Exposure (ms):	0.635
Digital Resolution:	228
Num Repeats:	30

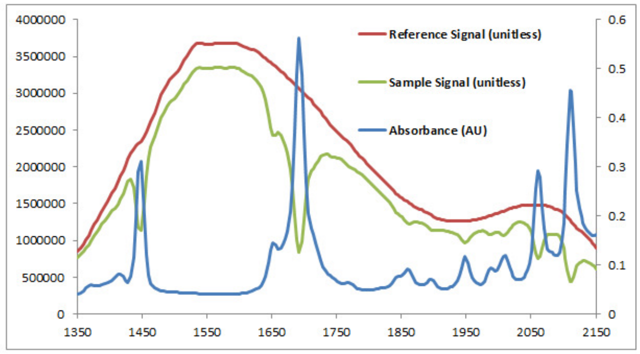


Figure 3.43 Scanning of Standard Reference Material and Test Sample

For example, there is one spectrometer found with wavelength offset as follows:

Expected (RM-NIR AU)	Observed	Offset
1446.6	1446.78219	0.18219
1693.1	1692.80041	-0.29959
2111	2110.94638	--0.05362

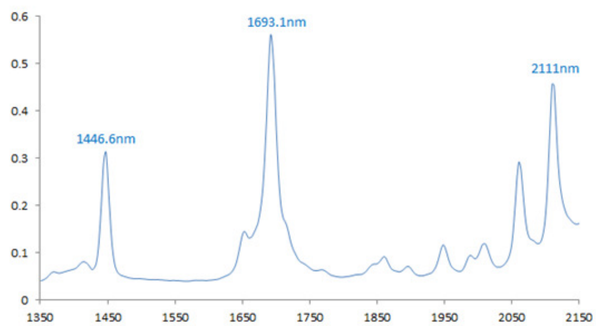


Figure 3.44 Observed Peak Position and Offset

Note: The Lagrange polynomial can be used to find the peak position of NIR absorbance. Three data points near the peak position are used to form a quadratic Lagrange polynomial. The vertex (maximum point) of the quadratic Lagrange polynomial is the peak position we want to find.

Linear regression can be applied to come out a transfer function between the expected wavelength points and the observed wavelength points as below. The linear regression has a perfect fit between two vectors. You can use Excel to calculate the slope and intercept of a linear transfer function as follows:

- **Slope** (Expected wavelength list, Observed wavelength list)
- **Intercept** (Expected wavelength list, Observed wavelength list)

Expected (RM-NIR AU)	Observed
1446.6	1446.78219
1693.1	1692.80041
2111	2110.94638

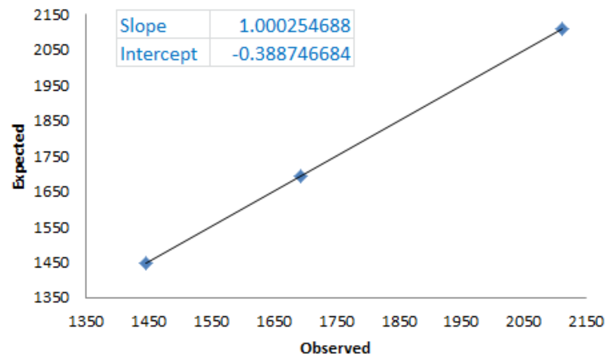


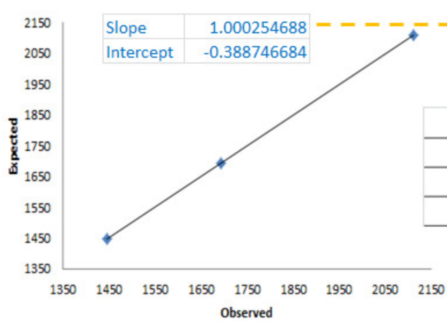
Figure 3.45 Linear Regression of Expected and Observed Wavelength Points

New calibration coefficients are calculated as below:

a3= a2 * a1

b3= a2 * b1

C3= a2 * c1 + b2



Original Coefficients		Expected vs. Observed		New Coefficients	
a1	-0.0002481	a2	1.0002547	a3	-0.0002482
b1	-0.8725199	b2	-0.3887467	b3	-0.8727421
c1	2224.93			c3	2225.1079

Figure 3.46 Calculate New Calibration Coefficients

Use the WinForms GUI to update the calibration coefficients:

Original Coefficients		Expected vs. Observed		New Coefficients	
a1	-0.0002481	a2	1.0002547	a3	-0.0002482
b1	-0.8725199	b2	-0.3887467	b3	-0.8727421
c1	2224.93			c3	2225.1079

WinForms GUI / Utility:

Steps:

1. **Read Coefficients**
2. **Write enable**
3. **Input new coefficients**
4. **Write Coefficients**

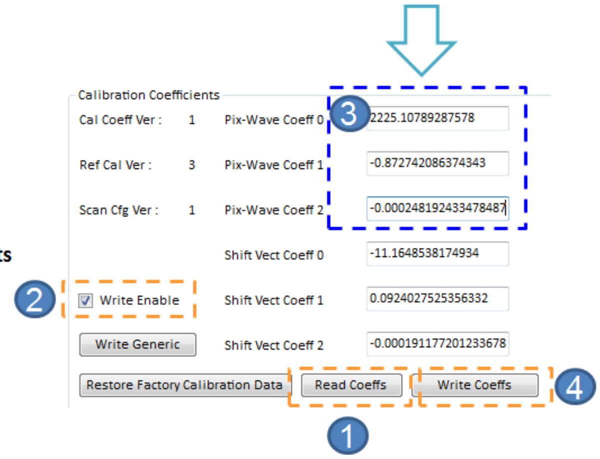


Figure 3.47 Update Calibration Coefficients

After updating the calibration coefficients, please also update the built-in reference data as below:

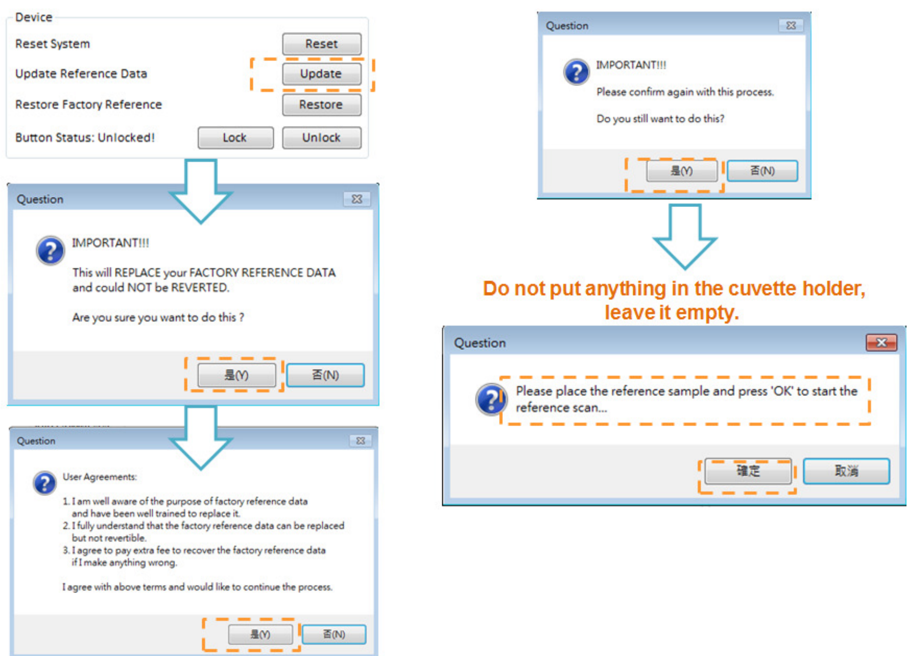


Figure 3.48 Update Built-in Reference Data

3.5 Consistency of NIR Absorbance

The consistency of the NIR absorbance is demonstrated by checking the photometric reproducibility, spectral resolution and wavelength accuracy. Here we take the diffuse reflective module NIR-M-R2 as an example to review the consistency of NIR absorbance. We collect system test data from more than 500 NIR-M-R2 modules. The standard reference materials and scan configuration for system testing are shown below.

- **Reference signal: measure the SRS-99 (Labsphere)**
- **Sample signal: measure the SRM2036 (NIST)**
- **Scan Configuration:**

Section Config Type:	**Column**
Start Wavelength:	**900**
End Wavelength:	**1700**
Pattern Width:	**7.03**
Exposure:	**0.635**
Digital Resolution:	**228**
Num Repeats:	**30**
PGA Gain:	**64**

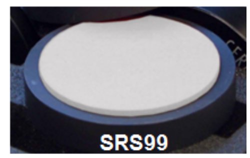
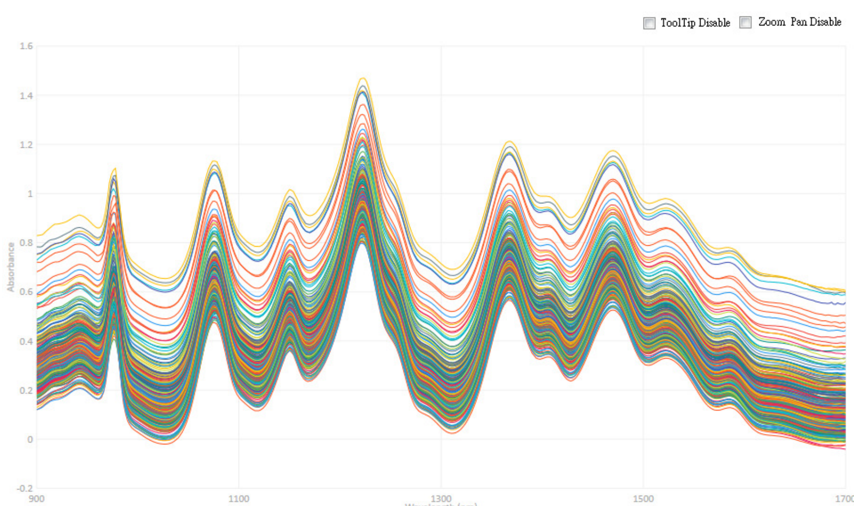
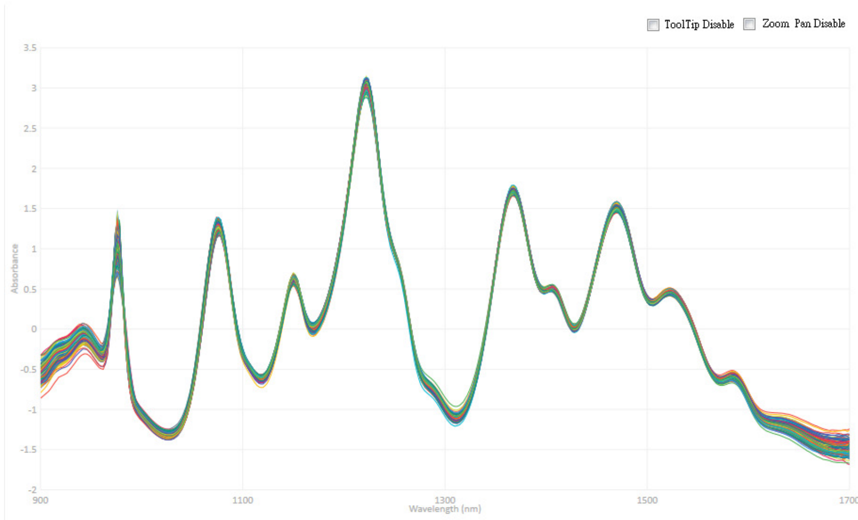


Figure 3.49 Standard Reference Materials and Scan Configuration for System Testing

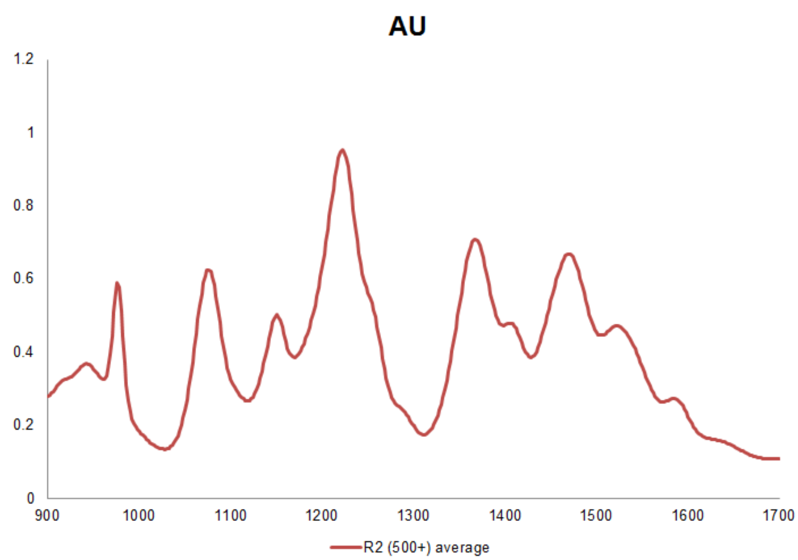
The SRM2036 AU data measured from more than 500 NIR-M-R2 modules are shown below.



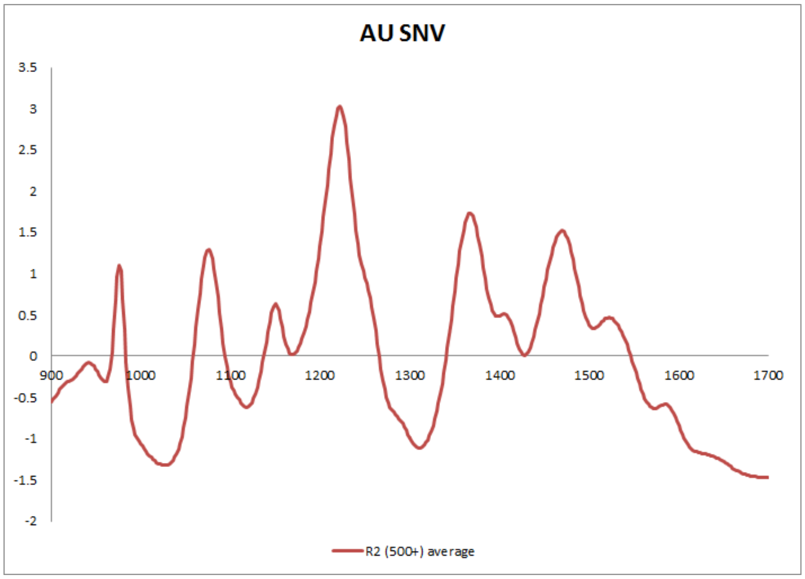
(a) AU Data



(b) AU after SNV



(c) AU average



(d) AU Average and SNV

Figure 3.50 SRM2036 AU Measured by NIR-M-R2

The SRM2036 AU measured by FOSS6500 is shown below for comparison.

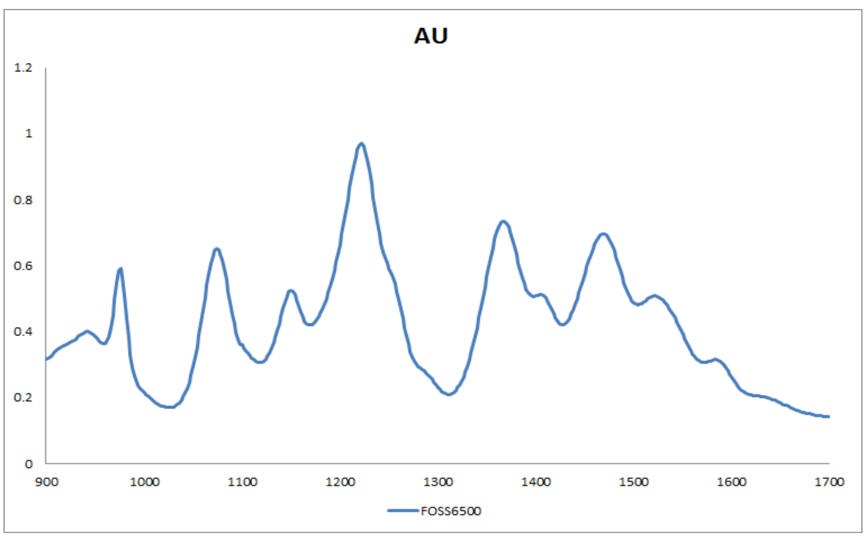


Figure 3.51 SRM2036 AU Measured by FOSS6500

The SRM2036 AU measured by NIR-M-R2 is compared with the data measured by FOSS6500 as shown below. They are very close to each other.

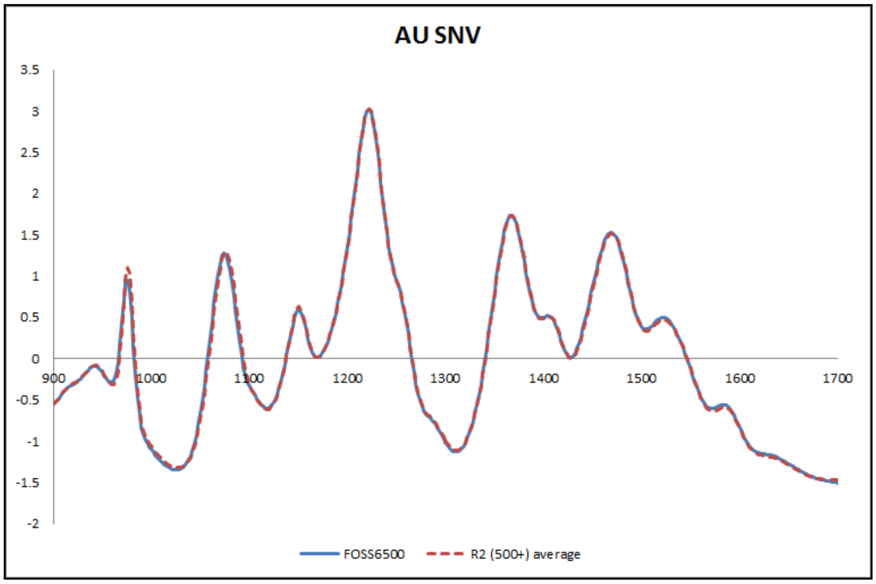


Figure 3.52 NIR-M-R2 Exhibits Good Photometric Reproducibility

The following is a comparison of the spectral resolution with reference to the data measured by MicroNIR. Obviously, the spectral resolution of NIR-M-R2 is as good as the data shown in the SRM2036 specification. However, the spectral resolution of MicroNIR is worse than the data shown in the SRM2036 specification.

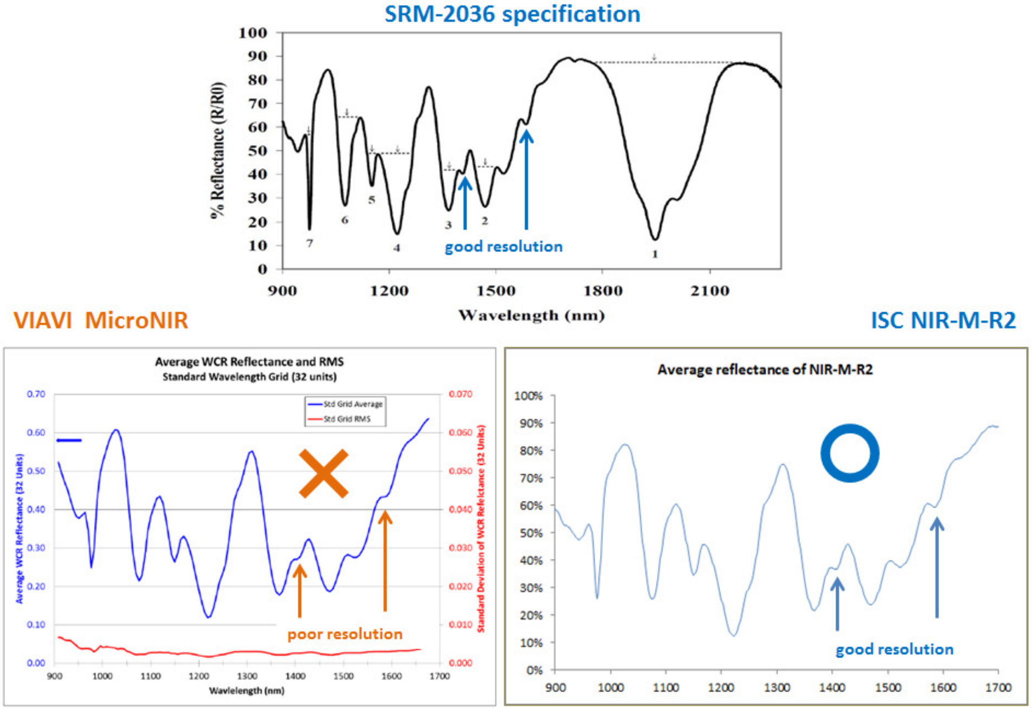


Figure 3.53 NIR-M-R2 Exhibits Good Spectral Resolution

By referring to the certified band position of SRM2036, each NIR-M-R2 module maintains a wavelength accuracy of +/-1nm with an optical resolution of 10nm.

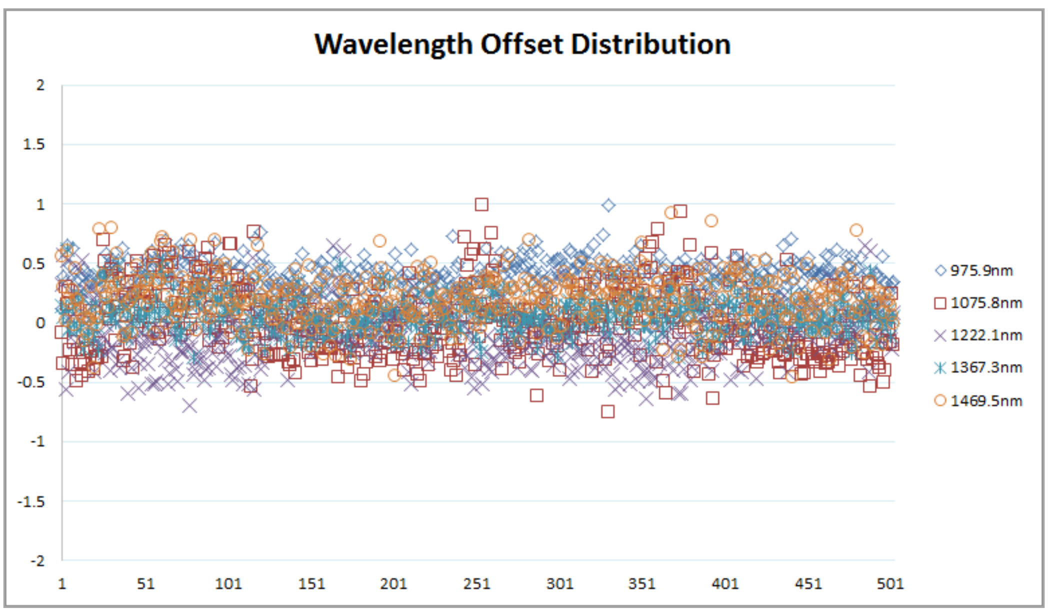
Table 2. Certified Band Locations[b,c], Air Wavelength

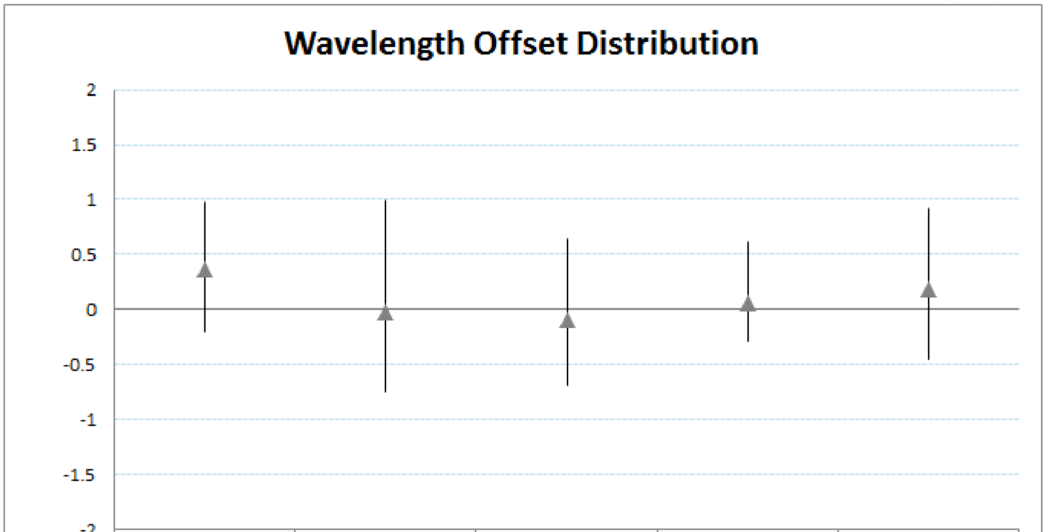
Band	3 nm SSW ± U_{95} (nm)	Standard Error of Mean[c] (nm)	5 nm SSW ± U_{95} (nm)	Standard Error of Mean[c] (nm)	10 nm SSW ± U_{95} (nm)	Standard Error of Mean[c] (nm)
7	976.0 ± 0.3	(0.02)	976.0 ± 0.2	(0.01)	975.9 ± 0.6	(0.01)
6	1075.7 ± 0.2	(0.01)	1075.7 ± 0.9	(0.01)	1075.8 ± 2.2	(0.03)
5	1151.4 ± 0.1	(0.01)	1151.2 ± 1.0	(0.01)	1151.0 ± 3.4	(0.01)
4	1222.1 ± 0.4	(0.02)	1222.1 ± 0.3	(0.02)	1222.1 ± 0.9	(0.03)
3	1367.1 ± 0.4	(0.01)	1367.2 ± 0.5	(0.01)	1367.3 ± 0.2	(0.02)
2	1469.6 ± 0.4	(0.02)	1469.6 ± 1.7	(0.02)	1469.5 ± 3.7	(0.03)
1[d]	1945.7 ± 0.3	(0.04)	1945.8 ± 0.7	(0.02)	1945.6 ± 1.5	(0.01)

[a] Band locations determined using a centroid method with a band fraction of 0.1; see Figure 1 for band identification.
[b] Uncertainties represent U_{95}, the expanded uncertainty calculation using a T statistic where n = 3, T = 4.3, in accordance with reference 12. The 95 % confidence interval of the air-wavelength bands of SRM 2036 is determined by the uncertainty of the calibration of the reference instruments with SRM 2065.
[c] The number in parentheses is the standard error of the mean centroid band location.
[d] See Information Values section for additional information pertaining to Band 1 centroid location.

Figure 3.54 Certified Band Locations of SRM2036

Here is the wavelength offset distribution from more than 500 NIR-M-R2 modules.





	975.9nm	1075.8nm	1222.1nm	1367.3nm	1469.5nm
Max	0.983336	0.988573	0.65091	0.610561	0.922258
Min	-0.202774	-0.7506	-0.696391	-0.288058	-0.454315
▲ Mean	0.366005738	-0.017780247	-0.095459555	0.065825012	0.189785879

Figure 3.55 NIR-M-R2 Wavelength Offset Distribution

Chapter 4 Spectrum Analysis and Application

4.1 Data Preprocessing

By using DMD as the wavelength selector, the wavelength of the spectrum is a mapping of DMD pixels. The mapping between each pixel and wavelength is determined by the pixel-to-wavelength coefficients (a, b, and c). The corresponding wavelength of each pixel is calculated from $\lambda = a*P^2 + b*P + c$, where λ is a wavelength and P is the DMD pixel position.

When performing a scan, the software will first determine the start pixel and the end pixel. Then according to the digital resolution setting (equivalent to the number of sampling points), the software will assign the middle pixel position for each scanning pattern. After completing a scan, the wavelength of each middle pixel is calculated by $\lambda = a*P^2 + b*P + c$. Each spectrometer has its specific pixel-to-wavelength coefficients, so you will not be able to see two spectrometers generate spectral data with the same wavelength point. For example, there are two devices with different coefficients as follows:

Device	Pixel-to-Wavelength Coefficients		
	a	b	c
#1	-0.000239298	-0.919962291	1778.580967
#2	-0.000243134	-0.915248692	1787.415668

Figure 4.1 Devices with Different Coefficients

Apply the same scan configuration to both devices to scan the same material. For example, start wavelength=900 nm, end wavelength=1700nm, pattern width=7.03nm, and digital resolution=228. The software will calculate start pixel and end pixel, and then calculate the middle position of each scan pattern as follows. Device #1 starts with pixel 790.5 (901.81554nm), and device #2 starts with pixel 798.5 (901.56655nm). Device #1 ends with pixel 82.5 (1701.055353nm), and device #2 ends with pixel 92.5 (1700.674845nm).

Device #1			Device #2		
DMD pixel	Wavelength	Absorbance	DMD pixel	Wavelength	Absorbance
790.5	901.81554	0.224794	798.5	901.56655	0.22138
787.5	905.708266	0.232175	795.5	905.474964	0.231596
784.5	909.596684	0.245492	792.5	909.379003	0.24565
781.5	913.480795	0.259135	789.5	913.278665	0.258412
778.5	917.360598	0.266282	786.5	917.17395	0.265871
775.5	921.236094	0.269959	783.5	921.064859	0.269994
772.5	925.107283	0.273843	780.5	924.951392	0.274457
769.5	928.974164	0.281498	776.5	930.126628	0.288476
765.5	934.123305	0.296326	773.5	934.002949	0.300204
762.5	937.980136	0.306333	770.5	937.874893	0.310624
	.			.	
	.			.	
	.			.	
120.5	1664.250839	0.053256	129.5	1664.813538	0.069266
116.5	1668.157543	0.048699	126.5	1667.746011	0.065344
113.5	1671.082545	0.044957	123.5	1670.674108	0.062005
110.5	1674.003241	0.041965	120.5	1673.597828	0.05733
107.5	1676.919629	0.037606	117.5	1676.517173	0.056222
104.5	1679.831709	0.034546	113.5	1680.402823	0.0525
101.5	1682.739483	0.032343	110.5	1683.311956	0.049599
98.5	1685.642949	0.032504	107.5	1686.216712	0.050973
95.5	1688.542107	0.028426	104.5	1689.117091	0.049983
91.5	1692.400951	0.025595	101.5	1692.013095	0.051087
88.5	1695.29006	0.024631	98.5	1694.904721	0.047496
85.5	1698.17486	0.024875	95.5	1697.791972	0.049891
82.5	1701.055353	0.026545	92.5	1700.674845	0.04342

Figure 4.2 DMD Pixel vs. Wavelength

The figure below shows that the sampling points of different devices have different distributions. In addition, the step lengths of the sampling points are not equally spaced.

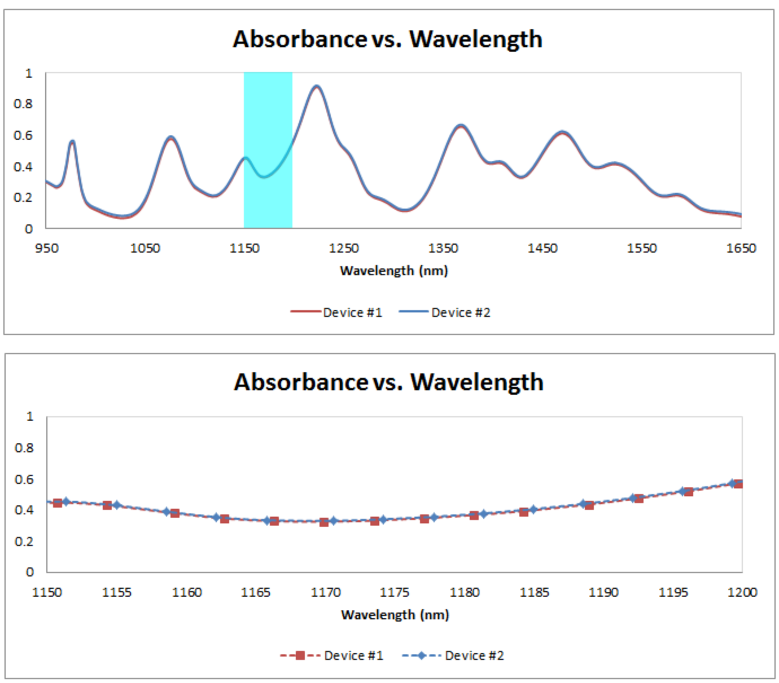


Figure 4.3 Absorbance vs. Wavelength Point

Before importing absorbance data from different devices into the same application, it is important to resample and interpolate different datasets to a common wavelength location vector. As shown below, the absorbance data from devices #1 and #2 are resampled and interpolated in a uniform wavelength space.

Wavelength	Device #1 Absorbance	Device #2 Absorbance
950	0.296034	0.301419
952	0.288592	0.294427
954	0.280868	0.287115
956	0.273425	0.279977
958	0.266677	0.27386
960	0.261763	0.26998
962	0.260839	0.270064
964	0.267741	0.277903
966	0.28798	0.299363
.		
.		
.		
1628	0.09542	0.107619
1630	0.094578	0.106753
1632	0.093435	0.105809
1628	0.09542	0.107619
1630	0.094578	0.106753
1632	0.093435	0.105809
1634	0.092073	0.104933
1636	0.09065	0.103871
1638	0.08885	0.102471
1640	0.086697	0.100803
1642	0.084429	0.099106
1644	0.082139	0.097262
1646	0.079766	0.095085
1648	0.077008	0.092514
1650	0.073867	0.089731

Figure 4.4 Re-sampled Absorbance Data

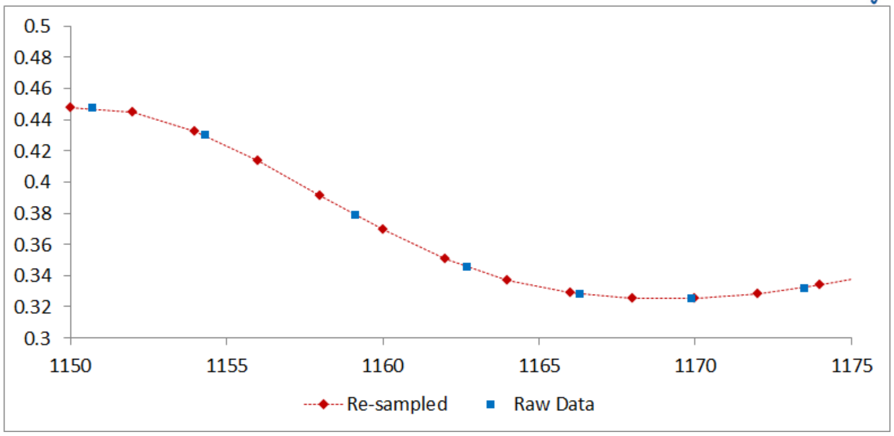


Figure 4.5 Re-sampled Data vs. Raw Data

An appropriate interpolation method is important to NIR analysis. We recommend using piecewise cubic spline interpolation instead of linear interpolation. As shown below, by using the piecewise cubic spline interpolation, re-sampled data and raw data have a better fit.

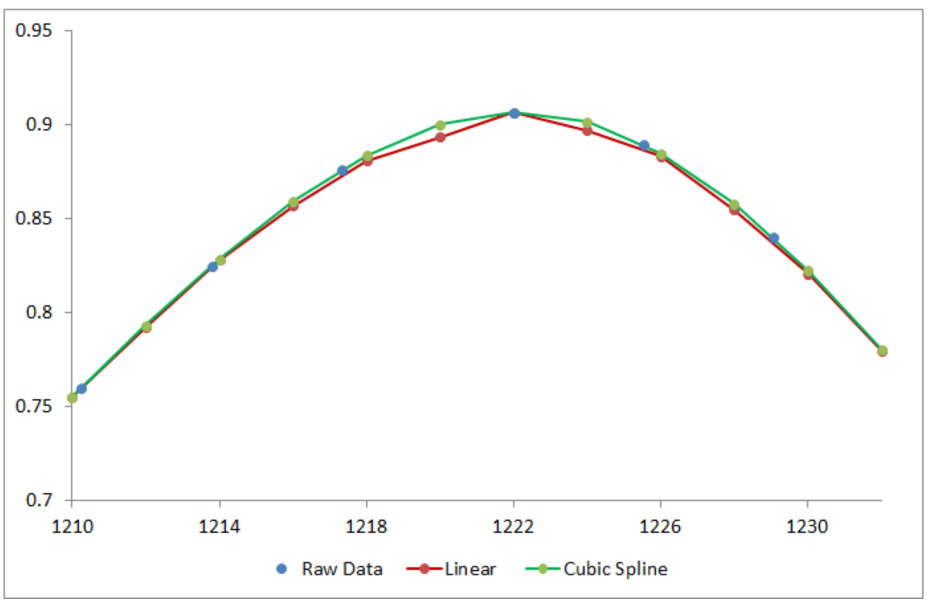


Figure 4.6 Linear Interpolation vs. Cubic Spline Interpolation

A smoothing algorithm like Savitzky-Golay is also commonly applied after the interpolation process. Once all the datasets are interpolated to a common wavelength vector, comparison between multiple units will become more straightforward.

After interpolation and smoothing, derivatives are commonly applied to correct the baseline effect, provide a better understanding of the data, and emphasize small spectral variations not evident in the raw data. The first derivative is usually applied to correct the baseline effect in the spectrum, while the second derivative is effective to remove both baseline offset and slope in the spectrum. The second derivative can also help resolve nearby peaks and sharpen spectral features. Another important feature of the second derivative is that the intensities of the original curves can be seen in the second derivatives in order of intensity. This is a very useful feature for quantitative method such as regression analysis.

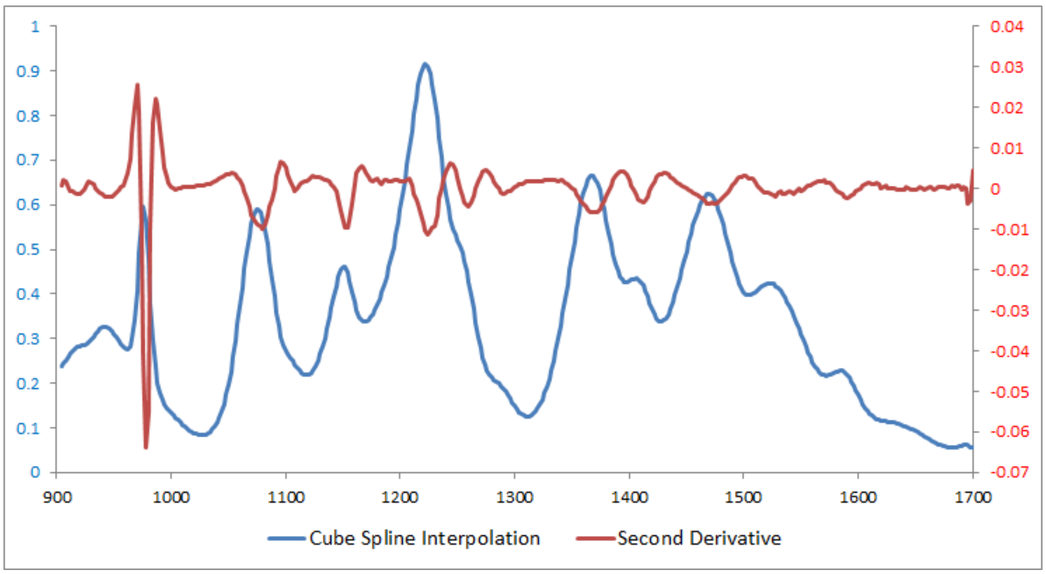


Figure 4.7 Second Derivative

However, by simply calculating derivatives between adjacent data points, there is a potential noise enhancement problem. Both Savitzky-Golay and Gap-Segment are alternative methods by using information from a localized segment of the spectrum to calculate the derivative at a particular wavelength to avoid the problem of noise enhancement.

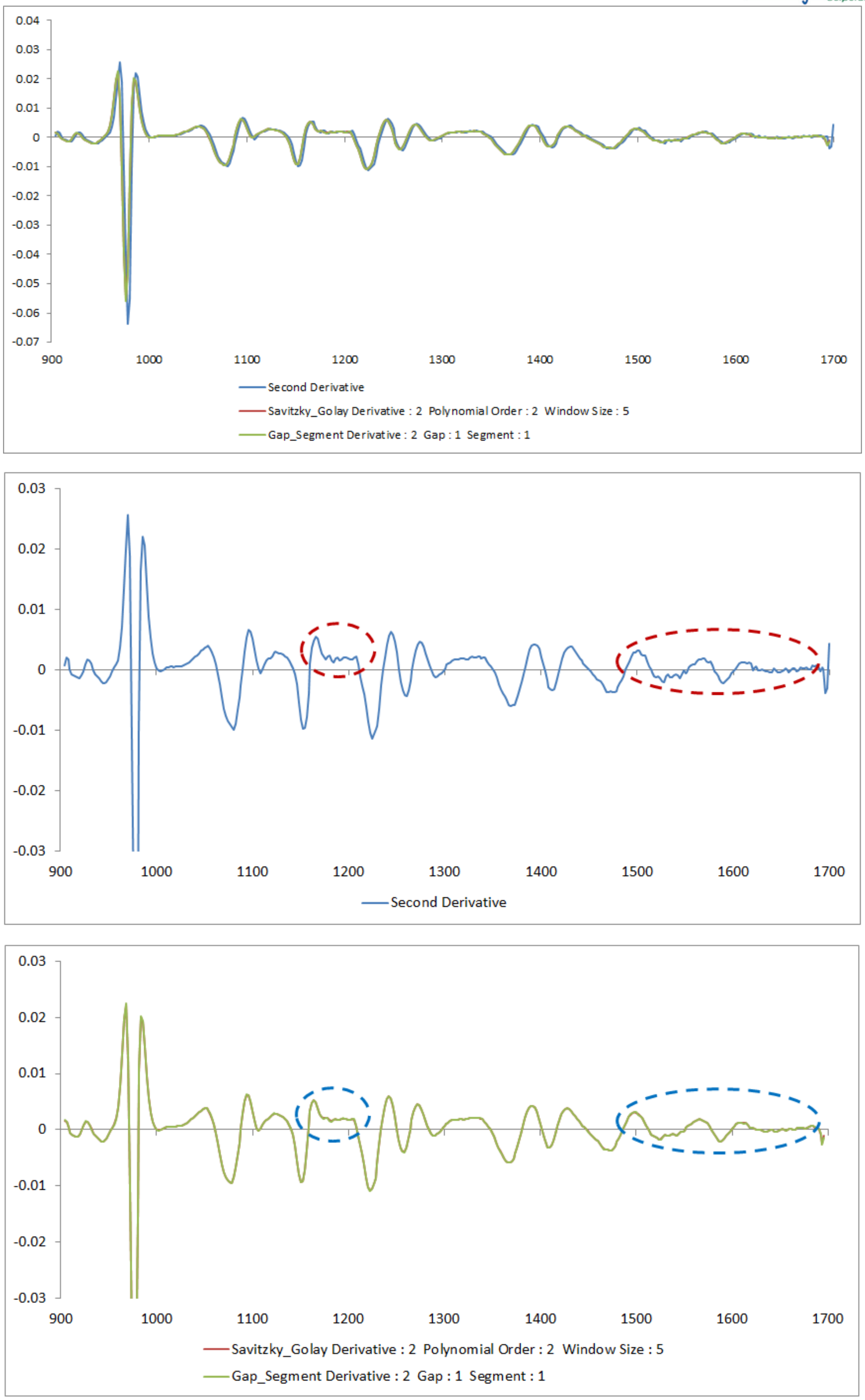


Figure 4.8 Savitzky-Golay and Gap-Segment Avoid Noise Enhancement

4.2 Qualitative Analysis

NIR spectroscopy can be applied to different types of qualitative analysis, including authentication, classification, identification, etc. Identification and classification of plastic resins is a typical application of qualitative analysis by using NIR spectroscopy. For identification and separation among resins, a linear discriminant analysis (LDA) method is proposed that is capable to distinguish among polyethylene terephthalate (PET), high density polyethylene (HDPE), polyvinyl chloride (PVC), low density polyethylene (LDPE), polypropylene (PP), polystyrene (PS), polymethyl methacrylate (PMMA), polycarbonates (PC) and polylactic acid (PLA).

First, the NIR absorption spectrum of plastic resin needs to be resampled and interpolated to a common wavelength location vector.

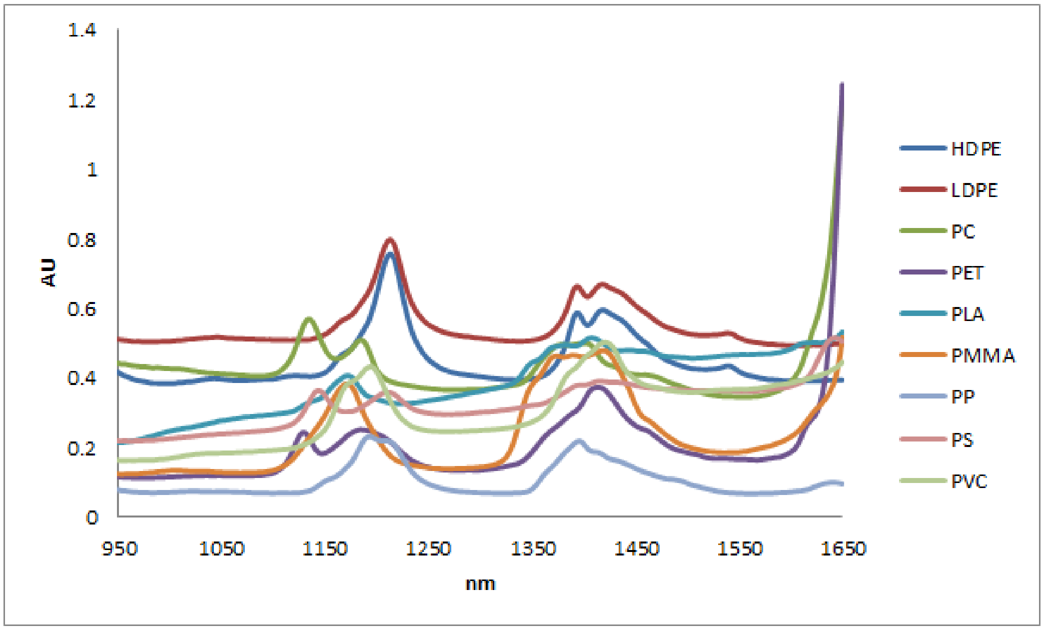


Figure 4.9 NIR Absorption Spectrum of Plastic Resin

Secondly, Savitzky-Golay derivative is applied to correct the baseline effect, provide a better understanding of the data, and emphasize small spectral variations.

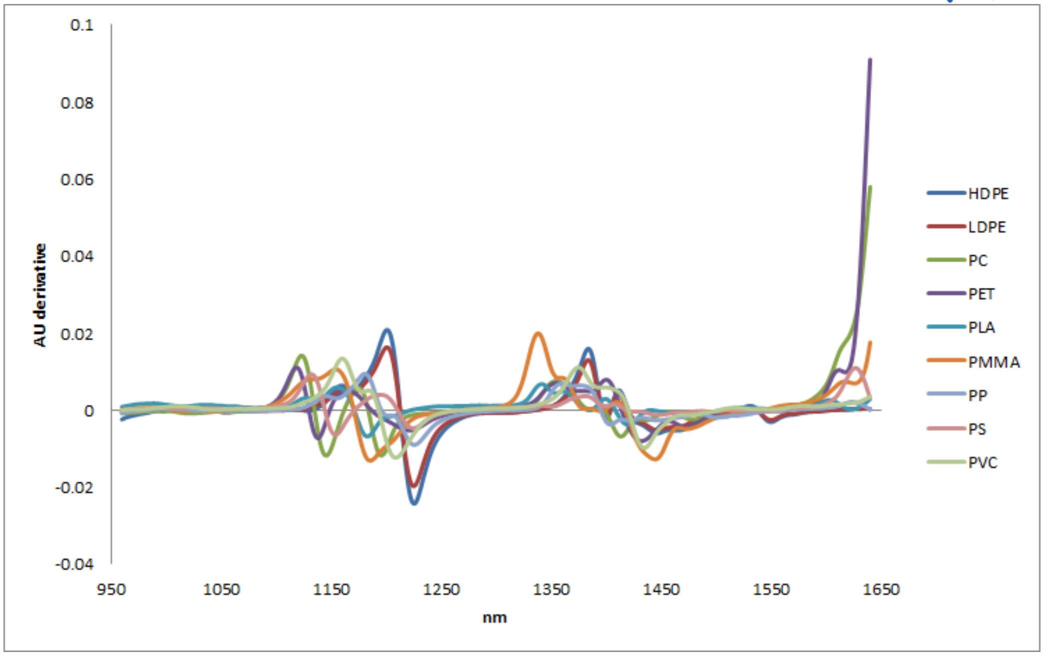


Figure 4.10 Savitzky-Golay Derivatives of NIR Absorption Spectrum

Third, use principal component analysis (PCA) to project the multi-dimensional spectral data set into a low-dimensional space to remove the relevant components in the spectral data set. Finally, linear discriminant analysis (LDA) is applied to the low-dimensional spectral data to distinguish plastic resins.

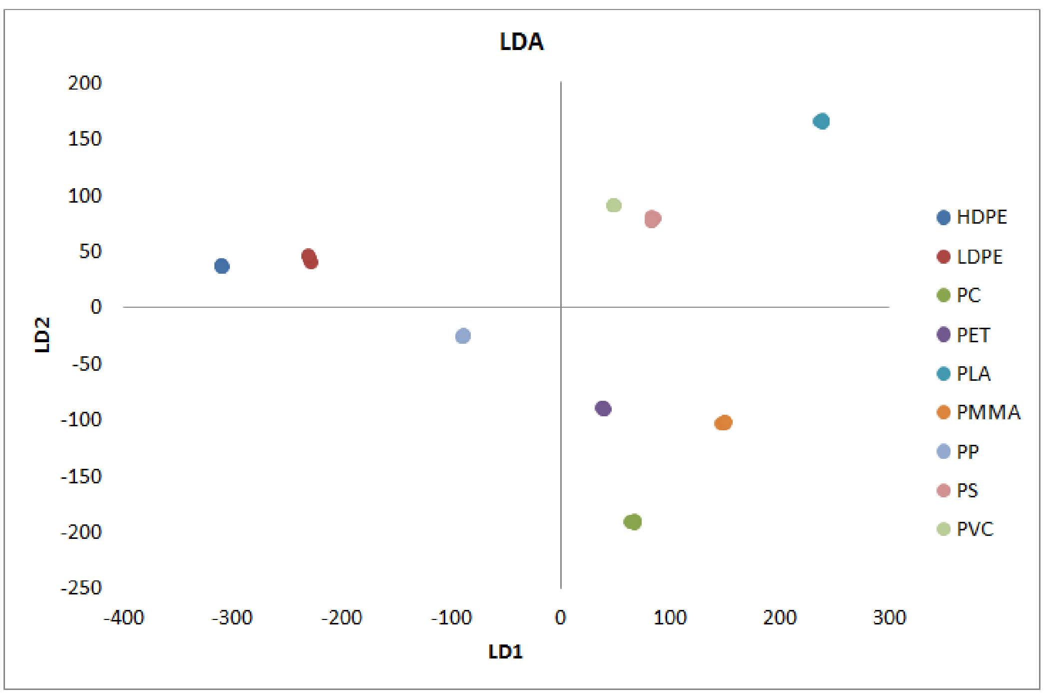


Figure 4.11 Linear Discriminant Analysis of Plastic Resin

4.3 Quantitative Analysis

Near infrared spectroscopy (NIRS) has been widely applied in both qualitative and quantitative analysis. For example, NIRS can be used for quantitative determinations of drug concentration, moisture and other important applications. For another example, NIRS can be used in agricultural operations to determine crop parameters such as water content, sugar content, and other indicators of ripeness.

The following is an example of quantitative analysis using near-infrared spectroscopy to determine the sugar content of apples.

First, the spectra of apples are resampled and interpolated to a common wavelength location vector.

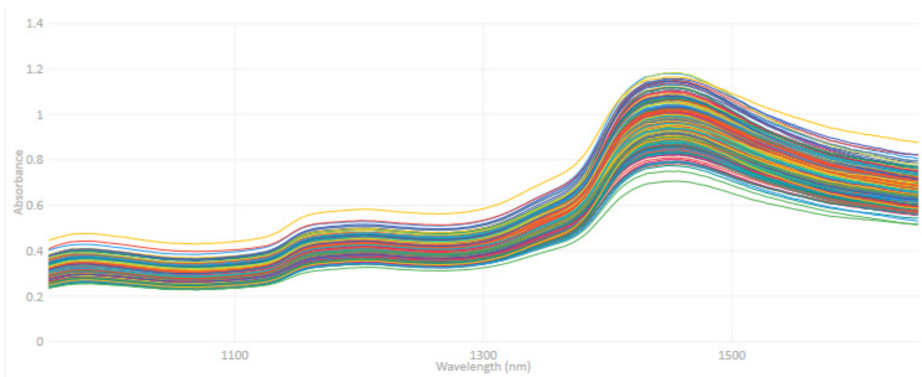


Figure 4.12 NIR Absorption Spectrum of Apple

Secondly, Savitzky-Golay derivative is applied to correct the baseline effect, provide a better understanding of the data, and emphasize small spectral variations.

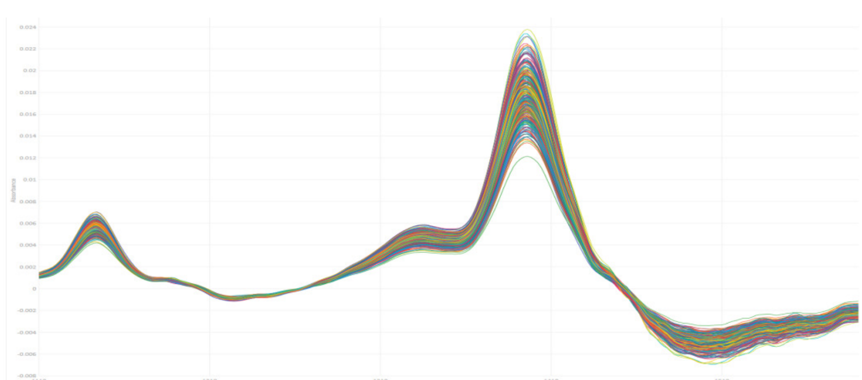


Figure 4.13 Savitzky-Golay Derivatives of NIR Absorption Spectrum

Finally, partial least squares (PLS) regression is applied to generate a calibration model for predicting Apple's Brix.

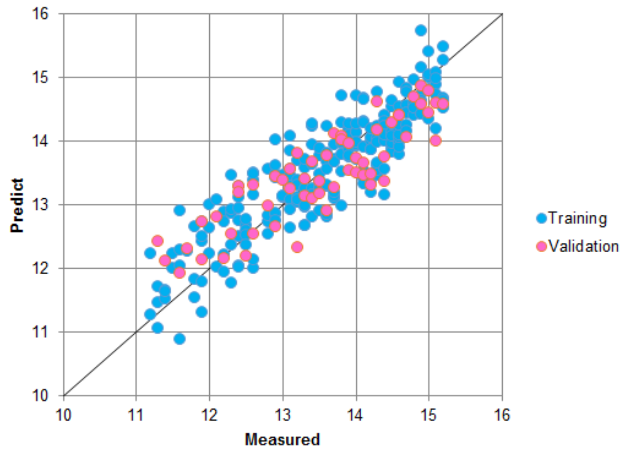


Figure 4.14 Training and Validation of Calibration Model

Appendix A

Frequently Asked Questions

A.1 Data on GitHub

1. ISC_NIRScan_Win_Winform_GUI
   https://github.com/InnoSpectra/ISC_NIRScan_Win_Winform_GUI

DFU_Driver	1. Upload user manual v1.1.
ISC-Win-WinForm-GUI-SDK	v3.7.4
packages	v3.7.4
DLP_Spectrum_Library_SLA.rtf	Upload extra license file
ISC NIRScan User Manual_EN_V1.1.pdf	1. Upload user manual v1.1.
ISC NIRScan Winform SDK GUI User's ...	v3.7.4
ISC-Win-WinForm-GUI-SDK.sln	v3.6.8
README.md	Update README.md

2. ISC_NIRScan_Android
   https://github.com/InnoSpectra/ISC_NIRScan_Android

MPChartLib	V2.10.0 Release
app	Release v2.15.5
gradle/wrapper	Release v.2.11.1
DLP_Spectrum_Library_SLA.rtf	Add license information of TI's DLP Spectrum Library
ISC-AndroidSDK-API-Introduction_V5....	Release v2.15.5
ISC-NIRScan-Android User's Guide_2...	Update user guide.
README.md	Update README.md
build.gradle	Release v.2.11.1
gradle.properties	first commit
gradlew	first commit
settings.gradle	first commit

3. ISC_NIRScan_iOS
https://github.com/InnoSpectra/ISC_NIRScan_iOS

Bolts.framework	V3.5.1 release
Charts.framework	v3.9.1
ISC NIRScan.xcodeproj	v3.9.1
ISC NIRScan	v3.9.1
NIRScanSDK.framework	v3.9.1
Parse.framework	V3.5.1 release
DLP_Spectrum_Library_SLA.rtf	V3.0.0 release
ISC NIRScan.entitlements	v3.7.1 release
ISC iOS API User Guide.pdf	Upload ISC iOS API User Guide.
README.md	Update README.md

4. ISC_NIRScan_UART_GUI-Qt

https://github.com/InnoSpectra/ISC_NIRScan_UART_GUI-Qt

ISC-NIRScan-Library	1. Synchronize the system time to device.
DLP_Spectrum_Library_SLA.rtf	v1.0.1 release
ISC_Logo.png	v1.0.1 release
ISC_NIRScan_UART_GUI-Qt.pro	v1.2.0 release
Led_Gray.png	v1.0.1 release
Led_Green.png	v1.0.1 release
NIRscanNano.ico	v1.0.1 release
NIRscanNano.rc	v1.0.1 release
README.md	Update README.md
UARTDefs.h	v1.0.1 release
isc_nirscan_uart.qrc	v1.0.1 release
main.cpp	v1.0.1 release
mainwindow.cpp	Create scan configuration interface.
mainwindow.h	Create scan configuration interface.
mainwindow.ui	Create scan configuration interface.
serialport.cpp	Create scan configuration interface.
serialport.h	Pack dlp spectrum library into isc spectrum library.

5. ISC_NIRScan_Tiva_FW_STD

https://github.com/InnoSpectra/ISC_NIRScan_Tiva_FW_STD

DLP_Spectrum_Library_SLA.rtf	Add files via upload
ISC-NIRScan-Tiva-v2.0.22.bin	Add files via upload
ISC-NIRScan-Tiva-v2.1.0.67.bin	Add files via upload
ISC-NIRScan-Tiva-v2.3.2.bin	v2.3.2 Release
ISC-NIRScan-Tiva-v2.4.4.bin	V2.4.4 Release
ISC-NIRScan-Tiva-v2.4.6.bin	v2.4.6 release.
ISC-NIRScan-Tiva-v2.4.7.bin	v2.4.7 release.
README.md	v2.4.7 release.

6. ISC_NIRScan_Tiva_FW_EXT
   https://github.com/InnoSpectra/ISC_NIRScan_Tiva_FW_EXT

DLP_Spectrum_Library_SLA.rtf	initial release
ISC-NIRScan-Tiva-Release-v3.3.1.bin	initial release
ISC-NIRScan-Tiva-Release-v3.3.4.bin	initial release
README.md	initial release

7. ISC_DLPSpectrumLibrary
   https://github.com/InnoSpectra/ISC_DLPSpectrumLibrary

TI_DLPSpectrumLibrary_2.0.3_Source	Add TI's DLP Spectrum Library V2.0.3 Source Files
bin	Release binaries and headers for Spectrum Library V2.0.3, V2.0.3.3 & ...
include	Release binaries and headers for Spectrum Library V2.0.3, V2.0.3.3 & ...
DLP_Spectrum_Library_SLA.rtf	Release binaries and headers for Spectrum Library V2.0.3, V2.0.3.3 & ...
README.md	Release binaries and headers for Spectrum Library V2.0.3, V2.0.3.3 & ...

A.2 MTBF Test Report

MTBF Test Report

Model	NIR-S-G1
Quantity	2
Time	4147 hrs
Date	Feb. 7, 2020 to Jul. 28, 2020
Temperature/Humidity	32±3℃/90%
MTBF&90%	65000 hrs(7.42 yrs)

1. MTBF Formula

$$MTBF = \frac{2T \times Af_1 \times Af_2}{\chi^2(\alpha \times 2_{\gamma+2})}$$

2. Parameter Description

T	Accumulative test time
Af_1	Temperature acceleration factor = 1.429 @ 32℃
Af_2	Scan acceleration factor = 12.672 (number of continuous scan in 24 hrs/averaged scan number in daily usage=6336/500=12.672)
χ^2	Sign of Chi-Square
α	1- C (Confidence level)
γ	Accumulative failure number

3. Parameter value

Reliability	90%
T	8294 hrs
Af_1	1.429
Af_2	12.672
$\chi^2(\alpha*2_{\gamma+2})$	4.605

4. Calculation results

MTBF&90%=2*8294*1.429*12.672/4.605=65229 > 65000 hrs(7.42 yrs)

Test Dept.	DMT	**Test Engineer**	Steven	**Approved by**	Patrick

A.3 Reliability Test Items

1	Thermal Shock (Non-Operating)	Lower stress level: -40°C Higher stress level: 70°C Dwell time at each level: 20 min. Ramp rate: 20°C/min. Number of cycles: 100 cycles
2	Thermal Cycling Test (Operation)	Lower Temp. stress level: -10°C Higher Temp. stress level: 50°C Humidity: 20%~90%RH Ramp rate at 1°C/min. Dwell time at each level: 6 hours , Number of cycles: 12
3	Storage (Packing)	-20℃ ~ 60℃, 20%~90%RH, 96 Hrs
4	Vibration Test	a. Non-Operating(non-packing): Random vibration 0.0082G^2/Hz, 10 ~ 500Hz, 2Grms, 1hr/axis
		b. Non-Operating (Packing) : Sinusoidal vibration sin-wave, 1.5G, zero to peak, 10~500~10Hz, 1.0 oct/min. 60min/axis
		c. Non-Operating(Packing) : Random vibration 0.025G^2/Hz, 10~500Hz, 3.5Grms, 1hr/axis
5	Drop Test	a. w/ Packing b. Single carton : 97 cm , 6 faces 1 corner, 3 edges, 1pulse / direct. Steel plate
6	Mechanical Shock Test (non-packing)	Half-sine wave, 100G, 2ms, 1 pulse/face, 6faces (non-operating)