NIRS Vision - Instrument Calibration

Ω Metrohm

NIRS Vision - Instrument Calibration

Tutorial

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Disclaimer

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1   Introduction

This tutorial describes how a NIRS XDS Analyzer or the DS2500 Solid Analyzer is calibrated with the Vision software for the very first time in a non-regulated environment.

Information on recalibration or on calibration in a regulated environment can be found in the Vision Reference manual.

1.1   Prerequisites for this Tutorial

In order to be able to follow this tutorial, the following prerequisites must be met:

- The Vision Software must be installed on your computer. Information on how to install Vision can be found in the document **Vision installation** delivered with the software. This document can also be downloaded from the internet (*http://www.metrohm.com*), search for **8.105.8046**.
- Your computer is connected to a NIRS XDS instrument via direct cable connection.
- The instrument must be
    - Connected to the computer.
    - Switched on.
    - Running for at least 30 minutes.

1.2   Symbols and conventions

The following symbols and formatting may appear in this documentation:

*(5-**12**)*	**Cross-reference to figure legend** The first number refers to the figure number, the second to the instrument part in the figure.
1	**Instruction step** Perform the steps one after the other.
Method	**Dialog text**, **parameter** in the software
File ▶ New	Menu or menu item
[Continue]	**Button** or **key**

⚠	**WARNING**
	This symbol draws attention to a possible life-threatening hazard or risk of injury.
⚡	**WARNING**
	This symbol draws attention to a possible hazard due to electrical current.
♨	**WARNING**
	This symbol draws attention to a possible hazard due to heat or hot instrument parts.
☣	**WARNING**
	This symbol draws attention to a possible biological hazard.
❗	**CAUTION**
	This symbol draws attention to possible damage to instruments or instrument parts.
ℹ	**NOTE**
	This symbol highlights additional information and tips.

1.3   Field and parameters

In this tutorial all fields and other screen elements (parameters) are not explained. Only parameters which need to be filled or changed are listed.

Do not fill in fields or change parameters not mentioned in the following instructions. Explanations for all parameters can be found in the *Vision Reference manual*.

2 NIRS XDS RapidContent (Solid) Analyzer

For the setup and calibration of the NIRS XDS RapidContent (Solid) Analyzer you will need the following accessories:

- NIRS XDS Iris adapter (6.7425.000)
- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

2.1 Preparing the instrument

For the initial instrument diagnostics, the iris adapter must be installed.

1 If necessary, remove the sample carrier from the sample compartment.

Align the holes in the iris adapter with the pins on the sample platform, and carefully lower into place.

The pins hold the iris adapter securely in position over the sample window.

2.2 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1 Double click on .

2 In the **Login** dialog box, enter the following information:

- **User ID** NIRS
- **Password** NIRS

3 Press **[Enter]** or click on **[OK]**.

2.3 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:

- **Project ID** e. g. "rapidcontent_solids"
- Click on **[OK]**.
- When asked "Create database C:\Vision\ rapidcontent_solids?", click on **[Yes]**.

Configure Data Sources

1　In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2　In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3　Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1　Go to the **Connect to Instrument** dialog box.

2　Select **[Use Existing Data]**.

2.4　Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1　Click on **Configure ▶ Options**.

2　In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Reference Standardization**
- **Use Instrument Calibration**

3　Click on the **System Project** tab.

4　In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

2.5 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

2.5.1 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

2.5.2 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "RCA_Reflectance"
- **Reference Standardization** enabled

In the **Sampling System** box, select the following:

- **Cell: Stationary**
- **Spot Size (mm): 17.25**

Edit Data Collection Method - XDS Instrument

Method: RCA_Refelctance   ☑ Reference Standardization

Instrument
Model: XDS   Range: Full Range 400-2500nm

Sampling System
Module: Rapid Solid Module with Spot Size
Cell: Stationary
Detector: Reflectance
Spot Size (mm): 17

Sample
Scans: 32
Position
○ Reference
⦿ Sample

Reference
32
Position
⦿ Reference
○ Sample

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **RCA_Reflectance**.
- Click on **[OK]**.
  Wait for the System to stabilize.

2.5.3 Wavelength Linearization

If the instrument is connected to the software for the first time, wavelength linearization starts automatically.

1 An **Instrument Error** dialog box appears, informing that no wavelength linearization constants exist for this instrument.

- Click on **[OK]**.

2 If asked "Do you want to create Linearization Constants?", click on **[OK]**.

ℹ NOTICE

If wavelengths linearization does not start automatically, start it manually.

Click on **Instrument ► XDS Setup/Diagnostics ► Wavelength Linearization**.

Wavelength Linearization

The **Wavelength Linearization** dialog box shows the progress of the wavelength linearization process.

1 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

2 When asked "Send Linearization Constants to instrument?" again, click on **[Yes]**.

2.5.4 Reference Standardization

As soon as the wavelength linearization is complete, the following message pops up:

"Instrument is not Reference Standardized and not calibrated. Run Reference Standardization and Calibration now?"

1 Click on **[Yes]**.

2 When asked "It's time to run Reference Standardization. Do you want to run it now?", click on **[Yes]**.

> **ℹ NOTICE**
>
> If reference standardization does not start automatically, start it manually.
>
> Click on **Instrument ► XDS Setup/Diagnostics ► Create Reference Standard**.

Perform Reference Standardization

Required accessory: NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

1 In the **Instrument Configuration** dialog box, click on **[OK]**.

Reference Standardization starts.

2 When asked "Please position the Certified 80% Reflectance Reference",

- Place the Standard R80XXXXXX from the calibration set into the iris adapter. The label must be parallel to the long axis of the tray.

- Center the Reference Standard closing the iris and opening it again.
- Close the lid of the sample chamber.
- Click on **[OK]**.

3 When the **Select Standard File** dialog box opens,

- Plug the USB stick into a USB port of your computer or place the minidisk into the CD drive.
- Navigate to the content of the USB stick or the minidisk, respectively.
- Select File **RSSXXXXX.da**.
- Click on **[Open]**.

4 When asked "Ready to plot standard file…", click on **[OK]**.

5 When asked "Ready to plot correction…", click on **[OK]**.

6 When asked "Ready to plot correction and Certified 80% Reflectance Standard…", click on **[OK]**.

7 In the **Reference Standardization** dialog box, click on **[Print Report]**.

2.5.5 Instrument Calibration

Instrument Calibration starts automatically.

> **ℹ️ NOTICE**
>
> If instrument calibration does not start automatically, start it manually.
>
> Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Instrument Calibration**.

Perform Instrument Calibration

The **Instrument Calibration** dialog box shows the progress of the instrument calibration process.

1 When the **Select Standard File** dialog box opens,

- Select the file **RSSXXXXX.da**.
- Click on **[Open]**.

2 When asked "Please insert wavelength standard WSRXXXXX",

- Remove the calibration standard R80XXXXX from the iris adapter.
- Place wavelength standard WSRXXXXX into the iris adapter. The label must be parallel to the long axis of the tray.
- Center the wavelength standard closing the iris and opening it again.
- Close the lid of the sample chamber.
- Click on **[OK]**.

3 In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed, click on **[OK]**.

2.5.6 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Run Performance Test**.

2 Wait until test is completed.

3 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

4 Remove the Standard from the sample compartment.

5 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

3 NIRS XDS MasterLab Analyzer – Tablet Transmission

The NIRS XDS MasterLab Analyzer can be used in two distinct modes:

- Transmission mode for tablets
- Reflectance mode

The process of initialization is distinct for each mode. This chapter describes the setup for the Tablet Transmission Mode.

For the setup and calibration of the NIRS XDS MasterLab Analyzer in Tablet Transmission Mode you will need the following accessories:

- MasterLab transmission reference (6.7440.580)
- MasterLab transmission calibration standard (6.7450.020)

3.1 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:

- **Project ID**   e. g. "masterlab_transm"
- Click on **[OK]**.
- When asked "Create database C:\Vision\ masterlab_transm?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box.

2 Select **[Use Existing Data]**.

3.2 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Reference Standardization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.

- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

3.3 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

3.4 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "MasterLab_Transmission"
- **Reference Standardization** enabled

In the **Sampling System** box, select **Detector: Transmission**.

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

3.5   Setting up the Tray

Set Tray Settings

1 Click on **Configure ▶ Tray**.

2 Enable **Use Tray**.

3 Select **Tablet Transmission Standard**.

4 Click on **[Select]**.

The MasterLab moves the sample carrier to the appropriate position to install the reference standard.

Install the MasterLab transmission reference

1 If necessary, remove any accessory from the sample compartment.

2 Move the detector head sideways.

3 Mount the MasterLab transmission reference and lightly tighten it by hand.
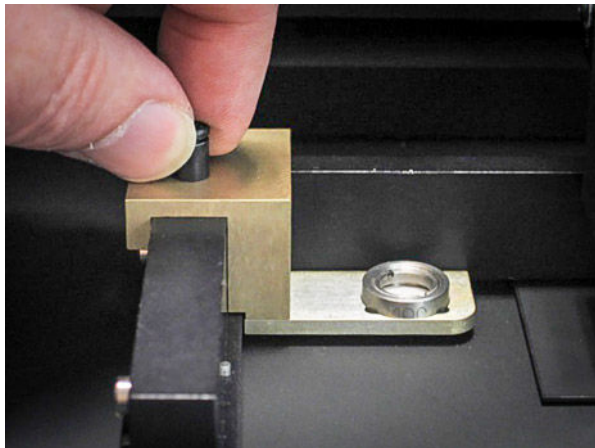
4 Place the aperture plate.

If the sample holder is in the wrong place to place the aperture plate, move it: Click on **Configure ▶ Send Tray to Iris Position**.
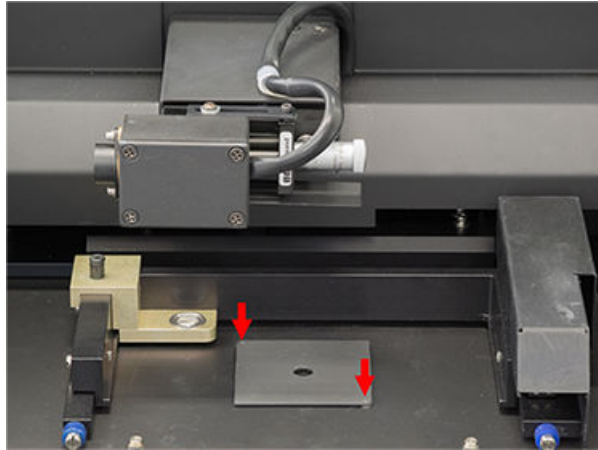
5 Flip the detector into vertical position.
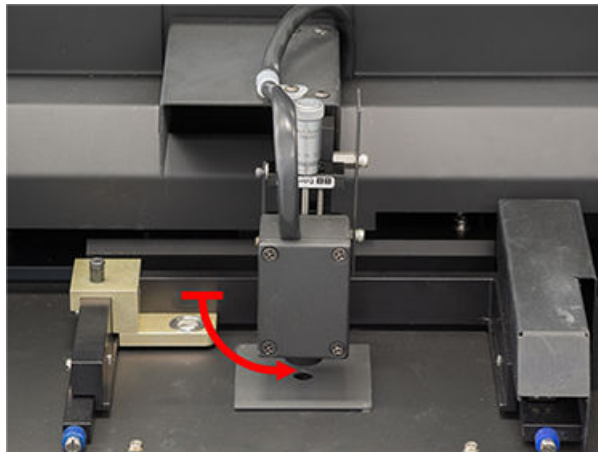
3.6 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **MasterLab_Transmission**.
- Click on **[OK]**.
  Wait for the System to stabilize.

3.6.1 Wavelength Linearization

If the instrument is connected to the software for the first time, wavelength linearization starts automatically.

1 An **Instrument Error** dialog box appears, informing that no wavelength linearization constants exist for this instrument.

Click on **[OK]**.

2 If asked "Instrument is not Reference Standardized and not Calibrated. Run Reference Standardization and Calibration now?", click on **[Yes]**.

3 If asked "It's now time to run Reference Standardization. Do you want to run it now?", click on **[Yes]**.

4 In the **Instrument Configuration** dialog box, click on **[OK]**.

5 If asked "Do you want to create Linearization Constants?", click on **[OK]**.

> **ℹ NOTICE**
>
> If wavelengths linearization does not start automatically, start it manually.
>
> Click on **Instrument ► XDS Setup/Diagnostics ► Wavelength Linearization**.

Wavelength Linearization

Follow the Progress on the status bar at the bottom right of the screen.

1 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

2 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

Wavelength Linearization

Send Linearization Constants To Instrument?

Yes   No
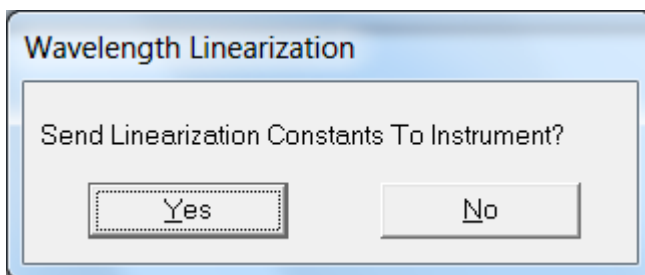
3.6.2 Reference Standardization

As soon as the wavelength linearization is complete, the following message pops up:

"Instrument is not Reference Standardized and not Calibrated. Run Reference Standardization and Calibration now?"

1 Click on **[Yes]**.

2 When asked "It's time to run Reference Standardization. Do you want to run it now?", click on **[Yes]**.

> **i**   **NOTICE**
>
> If reference standardization does not start automatically, start it manually.
>
> Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Create Reference Standard**.

Perform Reference Standardization

Required accessory: MasterLab transmission calibration standard (6.7450.020)

1 In the **Instrument Configuration** dialog box, click on **[OK]**.

Reference Standardization starts.

2 When asked "Please Insert Tablet Transmission Standard Tray", click on **[OK]**.
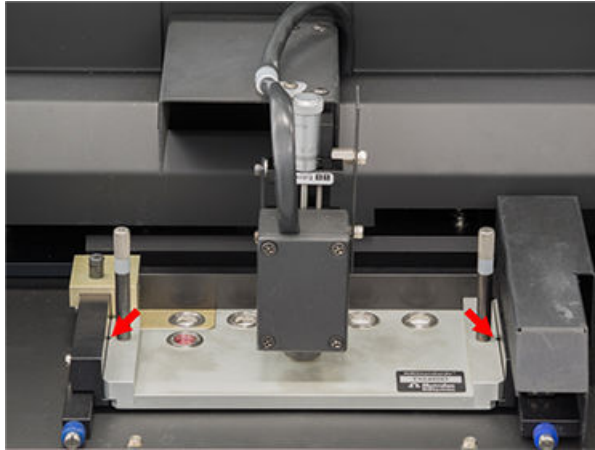
3 When the **Select Standard File** dialog box opens,

- Plug the USB stick into a USB port of your computer or place the minidisk into the CD drive.
- Navigate to the content of the USB stick or the minidisk, respectively.
- Select File **TSSXXXXX.da**.
- Click on **[Open]**.

4 When asked "Ready to plot standard file…", click on **[OK]**.

5 When asked "Ready to plot correction…", click on **[OK]**.

6 When asked "Ready to plot correction and Reflectance Standard…", click on **[OK]**.

7 In the **Reference Standardization** dialog box, click on **[Print Report]**.

3.6.3 Instrument Calibration

Instrument Calibration starts automatically.

> **NOTICE**
>
> If instrument calibration does not start automatically, start it manually.
>
> Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Instrument Calibration**.

Perform Instrument Calibration

The **Instrument Calibration** dialog box shows the progress of the instrument calibration process.
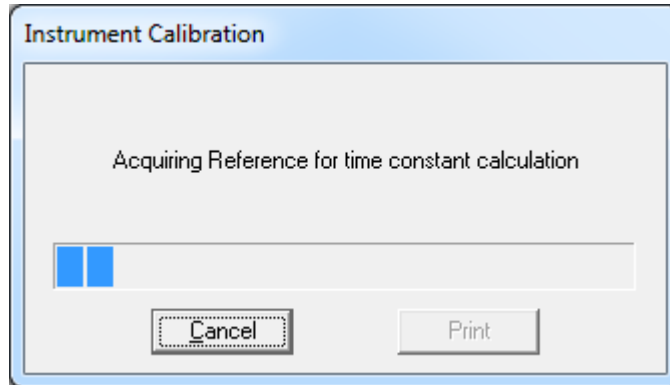
1 When the **Select Standard File** dialog box opens,

- Select the file **TSSXXXXX.da**.
- Click on **[Open]**.

2 When asked "Please insert Tablet Transmission Standard Tray", click on **[OK]**.

3 Close the sample compartment.

4 In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed, click on **[OK]**.
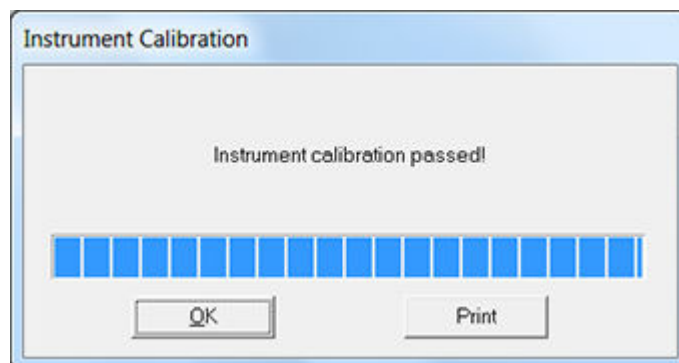
3.6.4 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Click on **Instrument ► XDS Setup/Diagnostics ► Run Pero-formance Test**.
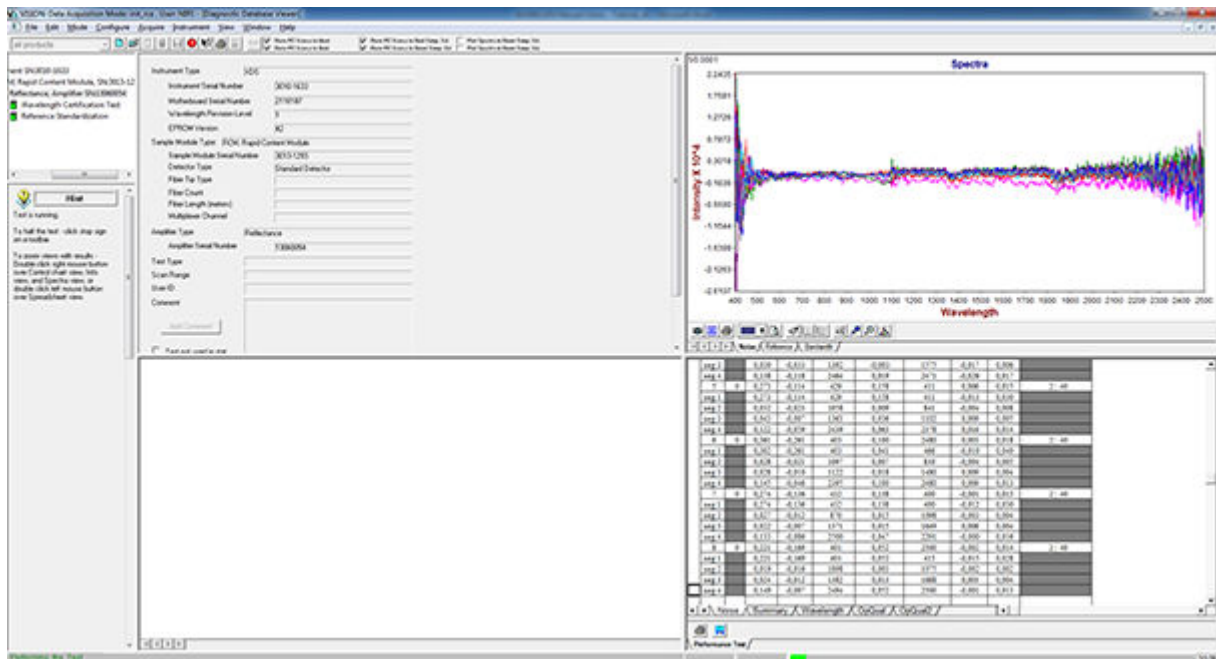
2 Wait until test is completed.

3 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

4 Eject the USB stick or minidisk and remove it from the computer.

5 Remove the MasterLab transmission calibration standard from the sample compartment.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

4 NIRS XDS MasterLab Analyzer – Reflectance

The NIRS XDS MasterLab Analyzer can be used in two distinct modes:

- Transmission mode for tablets
- Reflectance mode

The process of initialization is distinct for each mode. This chapter describes the setup for the Reflectance mode.

For the setup and calibration of the NIRS XDS MasterLab Analyzer in Reflectance mode you will need the following accessories:

- NIRS XDS Iris adapter (6.7425.000)
- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

If you intend to use the NIRS XDS MasterLab with a vial tray, follow the calibration procedure described in chapter 5.5.4 *(see chapter 3.6.3, page 21)*.

4.1 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1 Double click on .

2 In the **Login** dialog box, enter the following information:
- **User ID**   NIRS
- **Password**   NIRS

3 Press **[Enter]** or click on **[OK]**.

4.2   Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:

- **Project ID**   e. g. "masterlab_reflec"
- Click on **[OK]**.

2 When asked "Create database C:\Vision\masterlab_reflec?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box, select **[Use Existing Data]**.

4.3 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Reference Standardization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

4.4 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

4.5 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

4.5.1 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "MasterLab_Reflectance"
- **Reference Standardization**   enabled
  In the **Sampling System** box, select the following:
- **Detector: Reflectance**
- **Cell: Stationary**

Edit Data Collection Method - XDS Instrument

Method: MasterLab_Reflectance   ☑ Reference Standardization

Instrument

Model: XDS   Range: Full Range 400-2500nm

Sampling System

Module: MasterLab

Cell: Stationary

Detector: Reflectance

Spot Size (mm): 17.25

Sample

Scans: 32

Position
- ○ Reference
- ● Sample

Reference

32

Position
- ● Reference
- ○ Sample

OK
Cancel
Test Param
Mux Table

3 Click on **[OK]**.

4.6 Setting up the Tray

Required accessory:

- NIRS XDS Iris adapter (6.7425.000)
- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

Set Tray Settings

1 Click on **Configure ▶ Tray**.
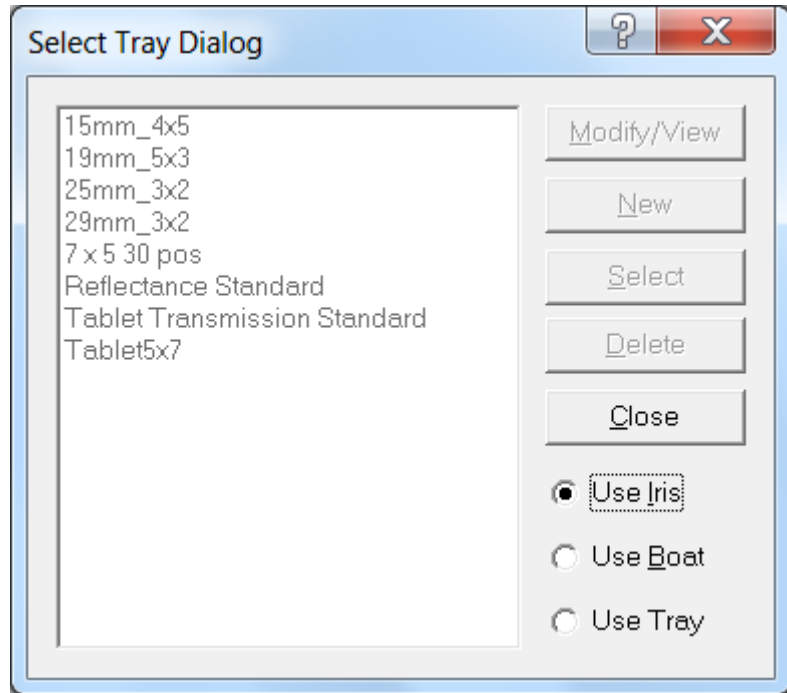
2 Enable **Use Iris**.

3 The MasterLab moves the sample carrier to the appropriate position to install the iris adapter.

Mount the iris adapter

This procedure describes reference standardization with the iris adapter.

1 If necessary, remove all items from the sample compartment.

2 Place the iris adapter. Align the holes in the iris adapter with the pins on the sample platform, and carefully lower into place.
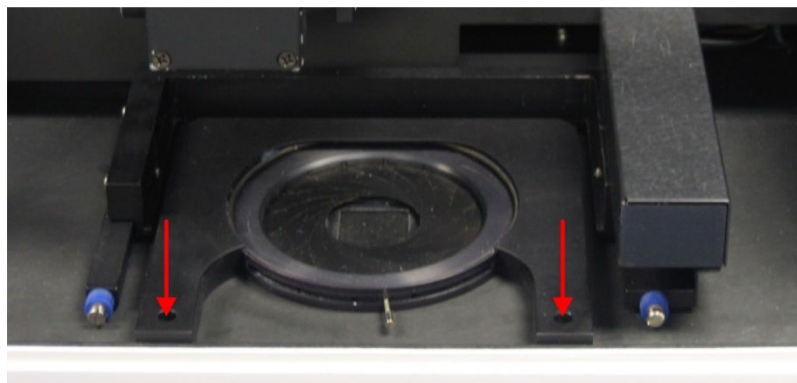
The pins hold the iris adapter securely in position over the sample window.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **MasterLab_Reflectance**.
- Click on **[OK]**.
  Wait for the System to stabilize.

4.7 Wavelength Linearization

If the instrument is connected to the software for the first time, wavelength linearization starts automatically.

Wavelength Linearization

The **Wavelength Linearization** dialog box shows the progress of the wavelength linearization process.
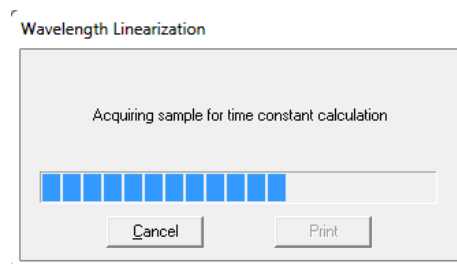
1 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

2 When asked "Send Linearization Constants to instrument?" again, click on **[Yes]**.

> **ℹ NOTICE**
>
> If wavelengths linearization does not start automatically, start it manually.
>
> Click on **Instrument ► SDX Setup/Diagnostics ► Wavelength Linearization**.

4.8   Reference Standardization

The required accessory for reference standardization depends on the type of samples you want to measure.

The following table gives an overview of the sample types and their respective accessories.

Detector position	Reflectance				
Sample type	Tablet in Tray	Vial in Tray	Coarse Granular Sample Cell (6.7402.040)	Sample Cup (6.7402.030)	Single Vial
Aperture	Installed	Removed	Removed	Removed	Removed
Iris adapter	Removed	Removed	Removed	Installed	Installed
Calibration Standard	NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)				

The following instructions refer to the reference standardization with the iris adapter.

Perform Reference Standardization

1 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Create Reference Standard**.

2 In the **Instrument Configuration** dialog box,

- Click on **[OK]**.

Reference Standardization starts.

3 When asked "Please position the Certified 80% Reflectance Reference",

- Place the Standard R80XXXXXX from the calibration set into the iris adapter. The label must be parallel to the long axis of the tray.

- Center the Reference Standard closing the iris and opening it again.
- Close the lid of the sample chamber.
- Click on **[OK]**.

4 When the **Select Standard File** dialog box opens,

- Plug the USB stick into a USB port of your computer or place the minidisk into the CD drive.
- Navigate to the content of the USB stick or the minidisk, respectively.
- Select File **RSSXXXXX.da**.
- Click on **[Open]**.

5 When asked "Ready to plot standard file…", click on **[OK]**.

6 When asked "Ready to plot correction…", click on **[OK]**.

7 When asked "Ready to plot correction and Certified 80% Reflectance Standard…", click on **[OK]**.

8 In the **Reference Standardization** dialog box, click on **[Print Report]**.

4.9 Instrument Calibration

Instrument Calibration starts automatically.

ℹ NOTICE

If instrument calibration does not start automatically, start it manually.

Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Instrument Calibration**.

Perform Instrument Calibration

The **Instrument Calibration** dialog box shows the progress of the instrument calibration process.

1. When the **Select Standard File** dialog box opens,

   - Select the file **RSSXXXXX.da**.
   - Click on **[Open]**.

2. When asked "Please insert wavelength standard WSRXXXXX",

   - Remove the calibration standard R80XXXXX from the iris adapter.
   - Place wavelength standard WSRXXXXX into the iris adapter. The label must be parallel to the long axis of the tray.
   - Center the wavelength standard closing the iris and opening it again.
   - Close the lid of the sample chamber.
   - Click on **[OK]**.

3. In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed. Click on **[OK]**.

4 Remove the wavelength standard from the sample compartment.

5 Remove the USB stick or minidisk from the CD drive.

4.10 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Run Performance Test**.
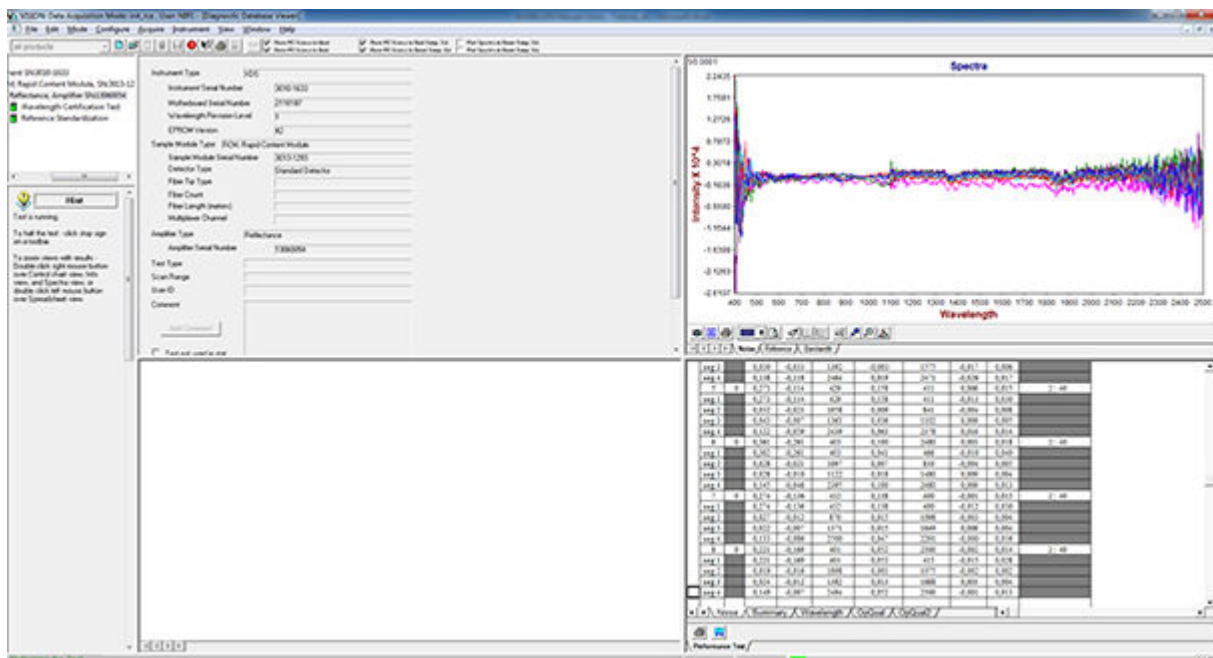
2 Wait until test is completed.

3 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

4 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

5 NIRS XDS MultiVial Analyzer

For the setup and calibration of the NIRS XDS MultiVial Analyzer you will need the following accessories:

- NIRS XDS tray for reflection standard (6.7410.000)
- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

If you intend to use the NIRS XDS MultiVial Analyzer with a tablet tray, see *(see chapter 4.10, page 34)* for the calibration procedure.

5.1 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1

Double click on .

2 In the **Login** dialog box, enter the following information:

- **User ID** NIRS
- **Password** NIRS

3 Press **[Enter]** or click on **[OK]**.

5.2 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:

- **Project ID**   e. g. "multivial"
- Click on **[OK]**.
- When asked "Create database C:\Vision\ multivial?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box, select **[Use Existing Data]**.

5.3 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Reference Standardization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

5.4 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

5.4.1 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

5.4.2   Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "MultiVial_Reference"
- **Reference Standardization**   enabled

In the **Sampling System** box, select the following:

- **Cell: Stationary**
- **Spot Size (mm): 17,25**

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **MultiVial_Reference**.
- Click on **[OK]**.

Wait for the System to stabilize.

2 An **Instrument Error dialog** box appears, informing that no wavelength linearization constants exist for this instrument. Click on **[OK]**.

3 If asked "Do you want to create Linearization Constants?", click on **[No]**.

5.5 Preparing the Instrument

The required accessory for the calibration of the instrument depends on the type of samples you want to measure and on the software you use for routine analysis.

To perform the routine analysis with **Vision Air**, set up the tray for the NIRS XDS MultiVial Analyzer in the same manner as for the NIRS XDS MasterLab Analyzer in Reflectance mode *(see chapter 4.6, page 28)*.

To perform the routine analysis with **Vision**, set up the tray as described in this chapter.

The following table gives an overview of the sample types and their respective accessories.

Detector position	Reflectance	
Sample type	Vial in Tray	Single Vial

Tray for the reflection standard (6.7410.000)	Installed	Removed
Iris adapter (6.7425.000)	Removed	Installed
Calibration Standard	NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)	

The following instructions refer to the calibration with the tray for the reflection standard.

5.5.1 Setting up the Tray

Required accessory:

- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)
- NIRS XDS tray for reflection standard (6.7410.000)

Set Tray Settings

1 Click on **Configure ▶ Tray**.
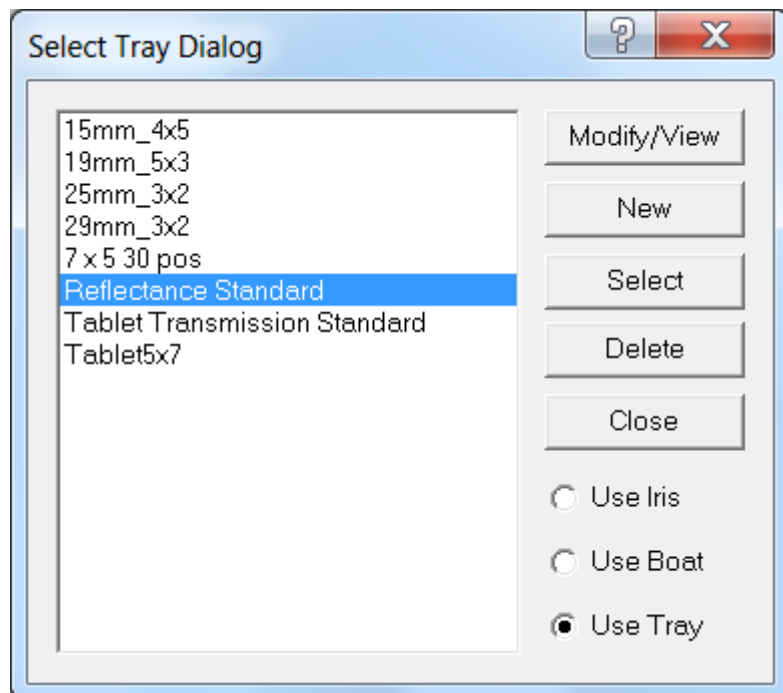
2 Enable **Use Tray**.

3 Select **Reflectance Standard**.

The MultiVial moves the sample carrier to the appropriate position to install the tray for the reflection standard.

Mount the tray for the reflection standard

This procedure describes reference standardization with the tray for the reflection standard.

1 If necessary, remove all items from the sample compartment.

2 Place the tray for the reflection standard.

5.5.2 Wavelength Linearization

If the instrument is connected to the software for the first time, wavelength linearization starts automatically.

1 An **Instrument Error dialog** box appears, informing that no wavelength linearization constants exist for this instrument. Click on **[OK]**.

2 If asked "Do you want to create Linearization Constants?", click on **[Yes]**.

Wavelength Linearization

The **Wavelength Linearization** dialog box shows the progress of the wavelength linearization process.

1 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

2 When asked "Send Linearization Constants to instrument?" again, click on **[Yes]**.

5.5.3 Reference Standardization

Perform Reference Standardization

Required accessory: NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

1 Click on **Instrument ► XDS Setup/Diagnostics ► Create Reference Standard**.

2 In the **Instrument Configuration** dialog box, click on **[OK]**.

Reference Standardization starts.

3 When asked "Please position the Certified 80% Reflectance Reference",

- Place the Standard "R80XXXXXX" from the calibration set into the tray for the reflection standard. The label must be parallel to the long axis of the tray.

- Close the lid of the sample chamber.
- Click on **[OK]**.

4 When the **Select Standard File** dialog box opens,

- Plug the USB-Stick into a USB socket of your computer.
- Navigate to the content of the USB-Stick.
- Select File **RSSXXXXXX.da**.
- Click on **[Open]**.

5 When asked "Ready to plot standard file…", click on **[OK]**.

6 When asked "Ready to plot correction…", click on **[OK]**.

7 When asked "Ready to plot correction and Certified 80% Reflectance Standard…", click on **[OK]**.

8 In the **Reference Standardization** dialog box, click on **[Print Report]**.

5.5.4 Instrument Calibration

Perform Instrument Calibration

1 Click on **Instrument ▸ XDS Setup/Diagnostics ▸ Instrument Calibration**.

The **Instrument Calibration** dialog box shows the progress of the instrument calibration process.
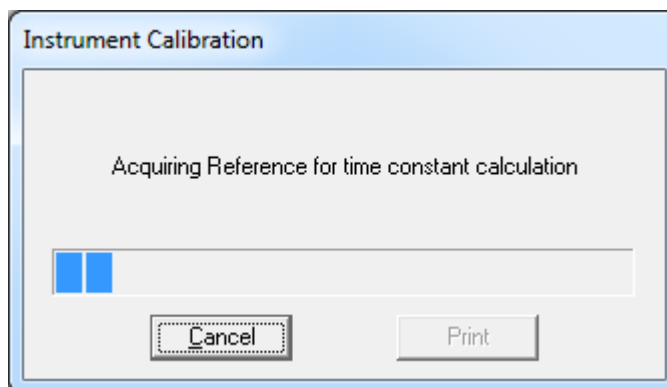
2 When the **Select Standard File** dialog box opens,

- Select the file **RSSXXXXX.da**.
- Click on **[Open]**.

3 When asked "Please insert wavelength standard WSRXXXXX",

- Remove the calibration standard R80XXXXX from the tray for the reflection standard.
- Place wavelength standard WSRXXXXX into the tray for the reflection standard. The label must be parallel to the long axis of the tray.
- Close the lid of the sample chamber.
- Click on **[OK]**.

4 In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed, click on **[OK]**.

5.5.5 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Run Performance Test**.
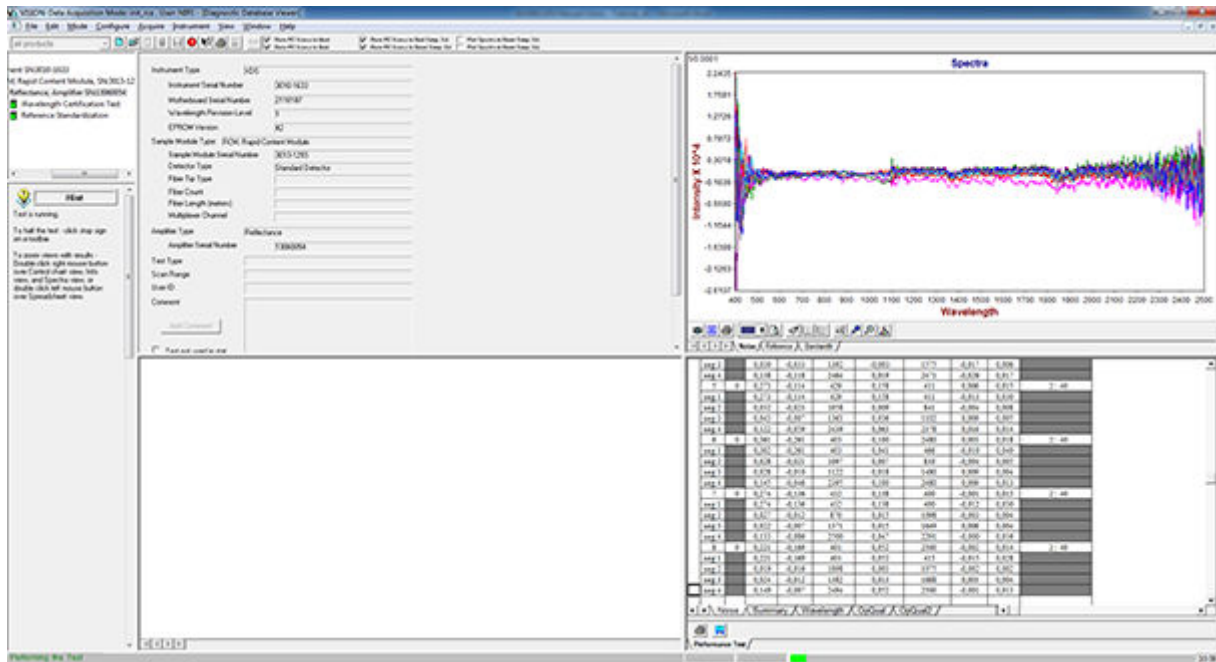
2 Wait until test is completed.

3 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

4 Remove the Standard from the sample compartment.

5 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

6 NIRS XDS RapidLiquid Analyzer

For the setup and calibration of the NIRS XDS RapidContent Analyzer you will need the following accessories:

- NIRS transmission wavelength calibration standard (6.7450.130)

6.1 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1

Double click on .

2 In the **Login** dialog box, enter the following information:

- **User ID**   NIRS
- **Password**   NIRS

3 Press **[Enter]** or click on **[OK]**.

6.2 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:

- **Project ID**   e. g. "rapidliquid"

- Click on **[OK]**.
- When asked "Create database C:\Vision\ rapidliquid?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box, select **[Use Existing Data]**.

6.3 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Blank Correction**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

6.4 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

6.5 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

6.5.1 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "RapidLiquid_transmission"
- **Blank correction**   enabled

In the **Sampling System** box, select the following:

- **Detector: Transmission**

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **RapidLiquid_transmission**.
- Click on **[OK]**.

Wait for the System to stabilize.

6.5.2 Wavelength Linearization

If the instrument is connected to the software for the first time, wavelength linearization starts automatically.

1 An **Instrument Error** dialog box appears, informing that no wavelength linearization constants exist for this instrument. Click on **[OK]**.

2 If asked "Do you want to create Linearization Constants?", click on **[Yes]**.

3 In the **Instrument Configuration** dialog box, click on **[OK]**.

> **ℹ** **NOTICE**
>
> If wavelengths linearization does not start automatically, start it manually.
>
> Click on **Instrument ▸ XDS Setup/Diagnostics ▸ Wavelength Linearization**.

#### Perform Wavelength Linearization

Follow the progress on the status bar at the bottom right of the screen.

1 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

2 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

6.5.3 Blank Correction

Perform Blank Correction

1 As soon as the wavelength linearization is complete, the following message pops up:

"Instrument is not blank corrected and not Calibrated. Run Blank Correction and Calibration now?", click on **[Yes]**.

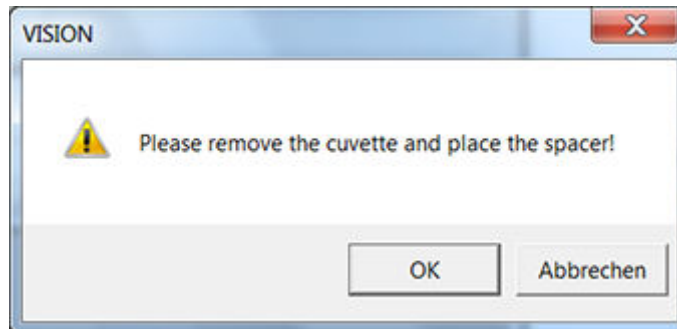**2** If the following message pops up:
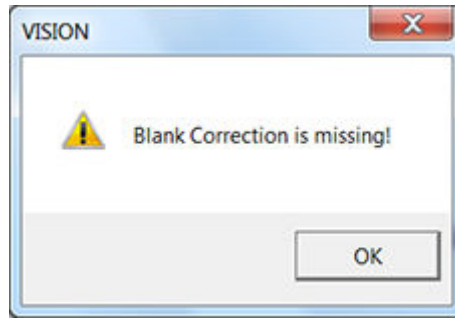
- Click on **[OK]**.

3 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Create Blank Correction**.
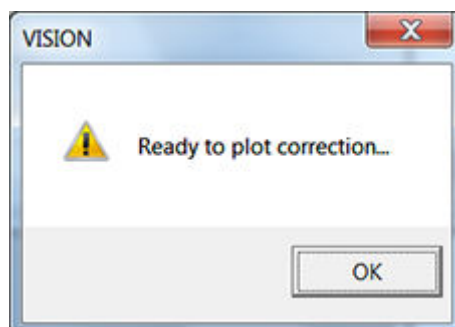
4 In the **Instrument Configuration** dialog box, click on **[OK]**.

5 When asked:

- Place the spacer for the cuvette.
- Click on **[OK]**.

6 When asked:

- Click on **[OK]**.

7 In the **Blank Correction** dialog box indicating that Blank Correction has passed, click on **[Print Report]**.

6.5.4 Instrument Calibration
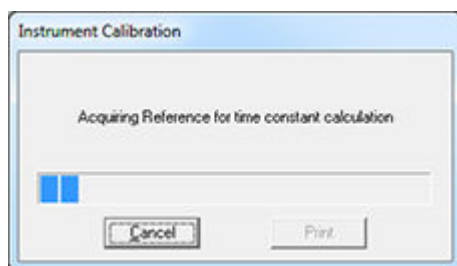
Instrument Calibration starts automatically.

> **ℹ NOTICE**
>
> If instrument calibration does not start automatically, start it manually.
>
> Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Instrument Calibration**.

Perform Instrument Calibration

The **Instrument Calibration** dialog box shows the progress of the instrument calibration process.

1 When the **Select Standard File** dialog box opens,

- Insert the USB-stick into the USB-socket on your PC.
- Navigate to the content of the USB-Stick.
- Select the file **TSS3WXXX.da**.
- Click on **[Open]**.

2 When asked "Please insert wavelength standard WST3WXXX",

- Remove any accessory from the sample compartment.
- Insert the wavelength standard WST3WXXX.
- Click on **[OK]**.

3 In the **Instrument Calibration** dialog box indicating that Instrument Calibration bandwidth correction has passed, click on **[OK]**.
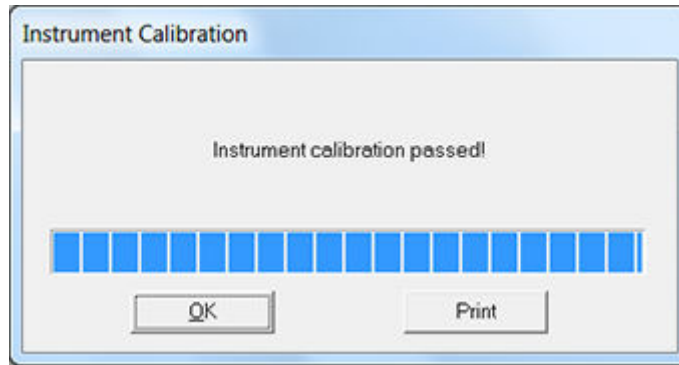
6.5.5 Performance Test

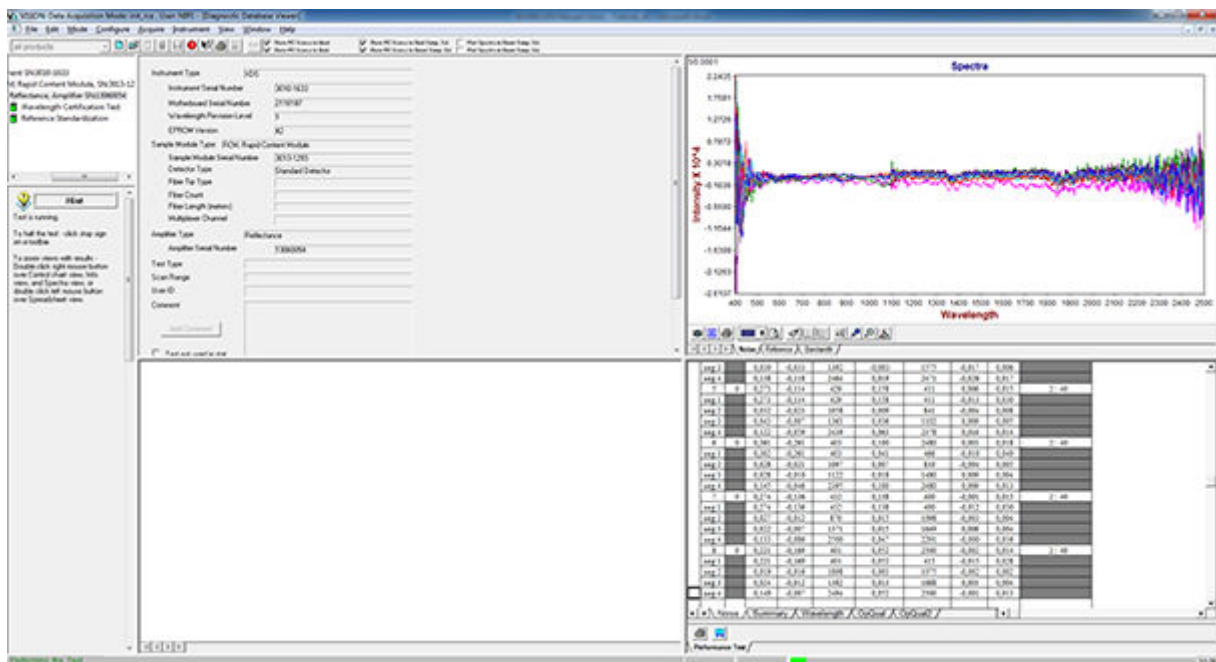Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Click on **Instrument ► XDS Setup/Diagnostics ► Run Performance Test**.

2 Wait until test is completed.

3 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

4 Eject the USB stick or minidisk and remove it from the computer.

5 Remove the Wavelength Standard from the sample compartment.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

7 NIRS XDS Interactance OptiProbe and SmartProbe Analyzers

Both the Interactance OptiProbe Analyzer and the SmartProbe Analyzer can be used in two modes:

- Interactance Reflectance (for powders)
- Interactance Immersion (for liquids)

For the calibration you will need two standard boxes:

- NIRS reflection standard, set 2 pcs (6.7450.000) or NIRS reflection standard, set 7 pcs (6.7450.010)
- Certified NIRS 99% reflection standard for laboratory sensors (6.7450.030)

The following calibration procedures apply to both instruments when used in the reflectance mode.

7.1 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1

Double click on .

2 In the **Login** dialog box, enter the following information:

- **User ID** NIRS
- **Password** NIRS

3 Press **[Enter]** or click on **[OK]**.

7.2   Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1   Click on **File ▶ Project ▶ New**.

2   When asked to close the open project, click on **[OK]**.

Define Project information

1   In the **Create New Project** dialog box enter the following information:

- **Project ID**   e. g. "optiprobe interactance"
- Click on **[OK]**.
- When asked "Create database C:\Vision\ optiprobe interactance?", click on **[Yes]**.

Configure Data Sources

1   In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2   In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3   Back in the **Configure Data Sources** window, click on **[OK]**.

| **Connect to the instrument** |

1 In the **Connect to Instrument** dialog box, select **[Use Existing Data]**.

7.3 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

| **Open the Edit Options dialog box** |

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Reference Standardization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

7.4 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

7.4.1 Connecting the instrument

| **Connect the instrument** |

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

7.4.2 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box, click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "OptiProbe_Interactance"
- **Reference Standardization**   enabled

In the **Sampling System** box, select the following:

- **Tip Type: Interactance Reflectance Probe**
- **Fiber Length:** e.g. **Less than 3 Meters**

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **OptiProbe_Interactance**.
- Click on **[OK]**.

Wait for the System to stabilize.

2 An **Instrument Error** dialog box appears, informing that no wave-length linearization constants exist for this instrument. Click on **[OK]**.

3 If asked "Do you want to create Linearization Constants?", click on **[Yes]**.

7.4.3   Wavelength Linearization

Make sure that the reflectance probe is used.

Perform Wavelength Linearization

1 When asked to "Position Reference", place the Probe into the upper slot marked with "REF". Click on **[OK]**.

2 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

3 When asked "Send Linearization Constants to instrument?" again, click on **[Yes]**.

7.4.4 Reference Standardization

As soon as the wavelength linearization is complete, the following message pops up:

"Instrument is not Reference Standardized and not Calibrated. Run Reference Standardization and Calibration now?"

1 Click on **[Yes]**.

2 When asked "It's time to run Reference Standardization. Do you want to run it now?", click on **[Yes]**.

> **NOTICE**
>
> If reference standardization does not start automatically, start it manually.
>
> Click on **Instrument ► XDS Setup/Diagnostics ► Create Reference Standard**.

Perform Reference Standardization

Required accessory: "Certified NIRS 99% reflection standard for laboratory sensors" (6.7450.030) standard box

1 In the **Instrument Configuration** dialog box, click on **[OK]**.

2 When asked to "Position Reference", place the Probe into the upper slot marked with "REF". Click on **[OK]**.

3 When asked:
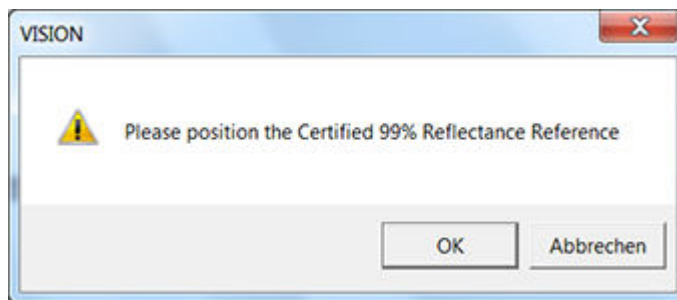
- Place the reflection standard onto the tip of the probe. Click on **[OK]**.

4 When asked "Rotate Sample 90°",

- Rotate the reflection standard by 90°.
- Click on **[OK]**.

5 You will be asked to rotate the standard two more times.

- Rotate the reflection standard by 90°.
- Click on **[OK]**.

6 When the **Select Standard File** dialog box opens,

- Plug the USB stick into a USB port of your computer or place the minidisk into the CD drive.
- Navigate to the content of the USB stick or the minidisk, respectively.
- Select File **RSSXXXXX.da**.
- Click on **[Open]**.

7 When asked "Ready to plot standard file…", click on **[OK]**.

8 When asked "Ready to plot correction…", click on **[OK]**.

9 When asked "Ready to plot correction and Certified 99% Reflectance Standard…", click on **[OK]**.

10 In the **Reference Standardization** dialog box, click on **[Print Report]**.

7.4.5 Instrument Calibration

Instrument Calibration starts automatically.

> **i** **NOTICE**
>
> If instrument calibration does not start automatically, start it manually.
>
> Click on **Instrument ► XDS Setup/Diagnostics ► Instrument Calibration**.
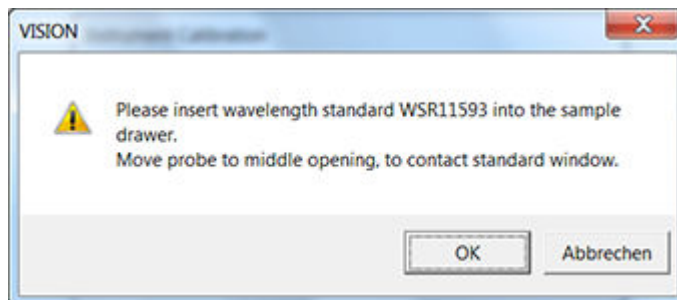
Perform Instrument Calibration

Required accessory: NIRS reflection standard, set of 2 (6.7450.000)

1 When asked to "Position Reference", place the Probe into the upper slot marked with "REF". Click on **[OK]**.

2 When the **Select Standard File** dialog box opens,

- Plug the USB-Stick of the NIRS reflection standard, set of 2 (6.7450.000) into a USB socket of your computer.
- Navigate to the content of the USB-Stick.
- Select File **RSSXXXXX.da**.
- Click on **[OK]**.
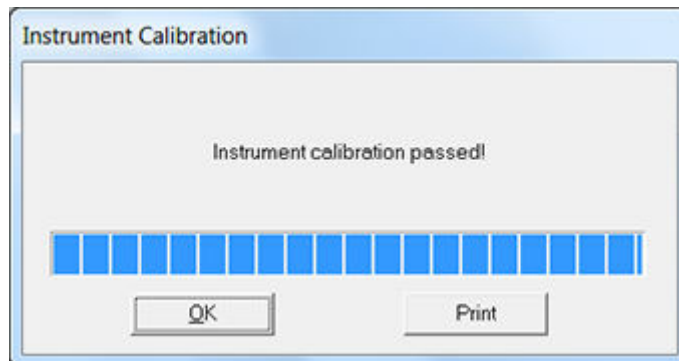
3 When this message appears:

- Place the wavelength standard from the NIRS reflection standard, set of 2 (6.7450.000) with its light side upwards into the drawer.

- Place the Probe into the middle slot marked with "STD".

- Click on **[OK]**.
- In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed, click on **[OK]**.
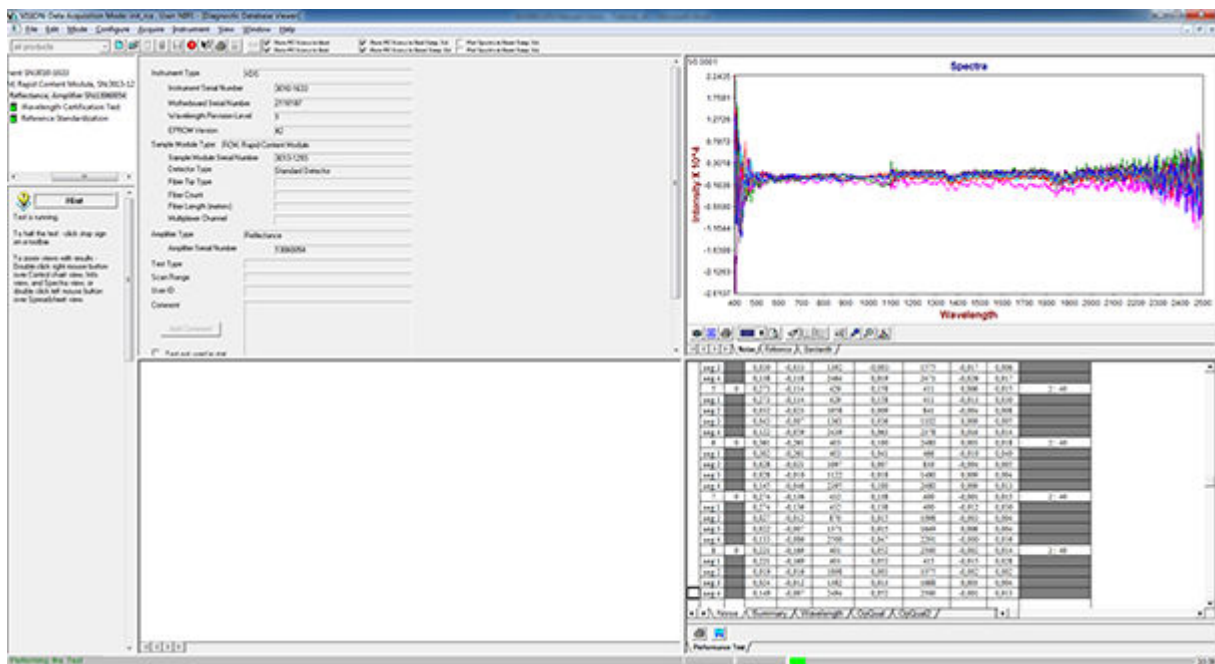
7.4.6 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Place the probe into the upper slot marked with "REF".

2 Click on **Instrument ▶ XDS Setup/Diagnostics ▶ Run Performance Test**.

3 Wait until test is completed.

4 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

5 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

8 NIRS XDS OptiProbe Transmission

For the setup and calibration of the NIRS XDS OptiProbe Analyzer in transmission mode you will need the following accessories:

- NIRS transmission wavelength calibration standard (6.7450.040)

8.1 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1

Double click on .

2 In the **Login** dialog box, enter the following information:
- **User ID** NIRS
- **Password** NIRS

3 Press **[Enter]** or click on **[OK]**.

8.2 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open:

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:
- **Project ID** e. g. "optiprobe _transm"

- Click on **[OK]**.
- When asked "Create database C:\Vision\ optiprobe _transm?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS XDS-series Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box, select **[Use Existing Data]**.

8.3   Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Use Auto-Linearization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use XDS System**.
- Click on **[OK]**.

8.4 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

8.4.1 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Select Data Collection Method** dialog box appears.

8.4.2 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "OptiProbe_transmission"
- **Reference Standardization**   enabled

In the **Sampling System** box, select the following:

- **Tip Type: Transmission Pair**
- **Fiber Length:** e.g. **Less than 3 Meters**

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **OptiProbe_transmission**.
- Click on **[OK]**.
  Wait for the System to stabilize.

2 An **Instrument Error** dialog box appears, informing that no wavelength linearization constants exist for this instrument. Click on **[OK]**.

3 If asked "Do you want to create Linearization Constants?", click on **[Yes]**.
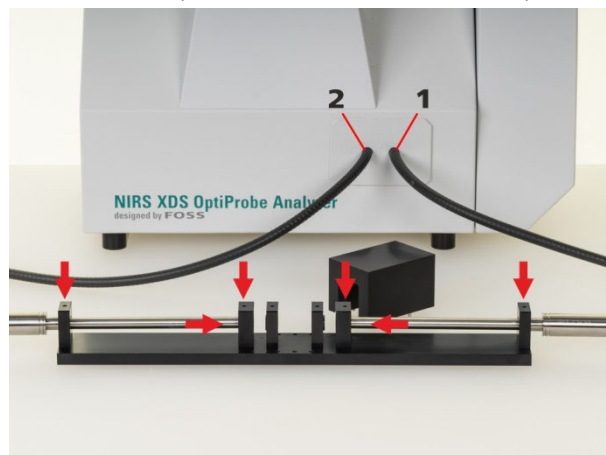
8.4.3   Wavelength Linearization

Required accessory:

- NIRS transmission pair calibration fixture (6.7430.030)

Perform Wavelength Linearization

1 When asked to "Position Reference",

- Place the two probes into the transmission pair calibration fixture.

- Cover the center area with the rectangular cover provided.
- Click on **[OK]**.

2 When asked "Send Linearization Constants to instrument?", click on **[Yes]**.

3 When asked "Send Linearization Constants to instrument?" again, click on **[Yes]**.

8.4.4 Instrument Calibration

Instrument Calibration starts automatically.

> **ℹ NOTICE**
>
> If instrument calibration does not start automatically, start it manually.
>
> Click on **Instrument ▸ XDS Setup/Diagnostics ▸ Instrument Calibration**.
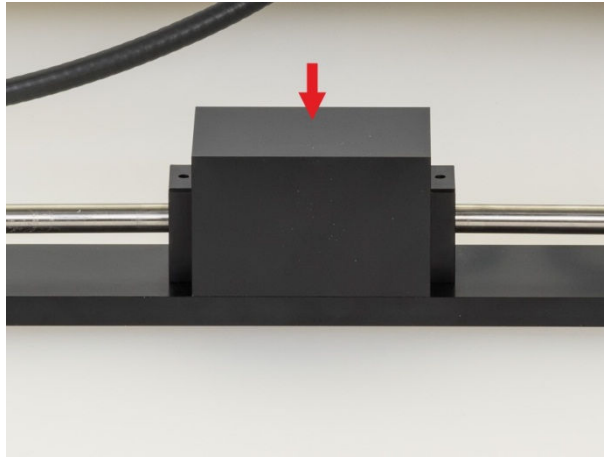
Perform Instrument Calibration

1 When asked "Instrument is not Calibrated. Run Calibration now?", click on **[Yes]**.

2 When asked to "Position Reference", click on **[OK]**.

3 When the **Select Standard File** dialog box opens,

- Plug the USB-Stick of the NIRS transmission wavelength calibration standard (6.7450.040) into a USB socket of your computer, or place the minidisk into the CD drive, respectively.
- Navigate to the content of the USB stick or the minidisk.
- Select File **TSS3WXXX.da**.
- Click on **[Open]**.

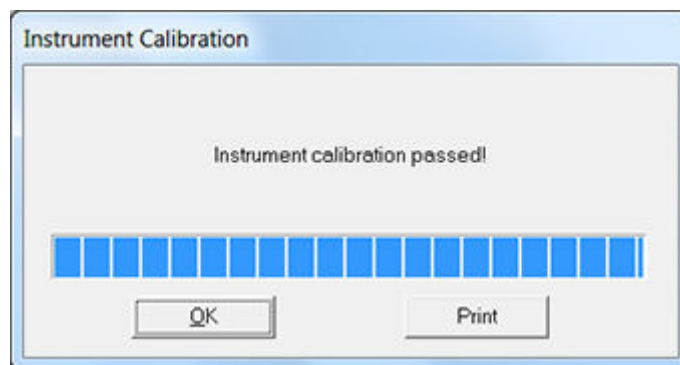**4** When the following message appears:
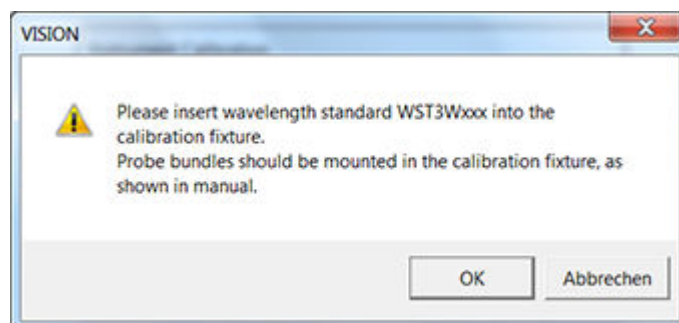
- Place the wavelength standard into the transmission pair calibration fixture.
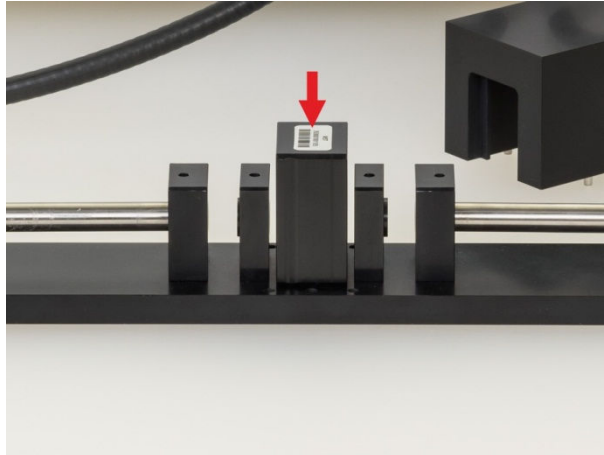
- Place the cover.

- Click on **[OK]**.
- In the **Instrument Calibration** dialog box indicating that Instrument Calibration has passed.
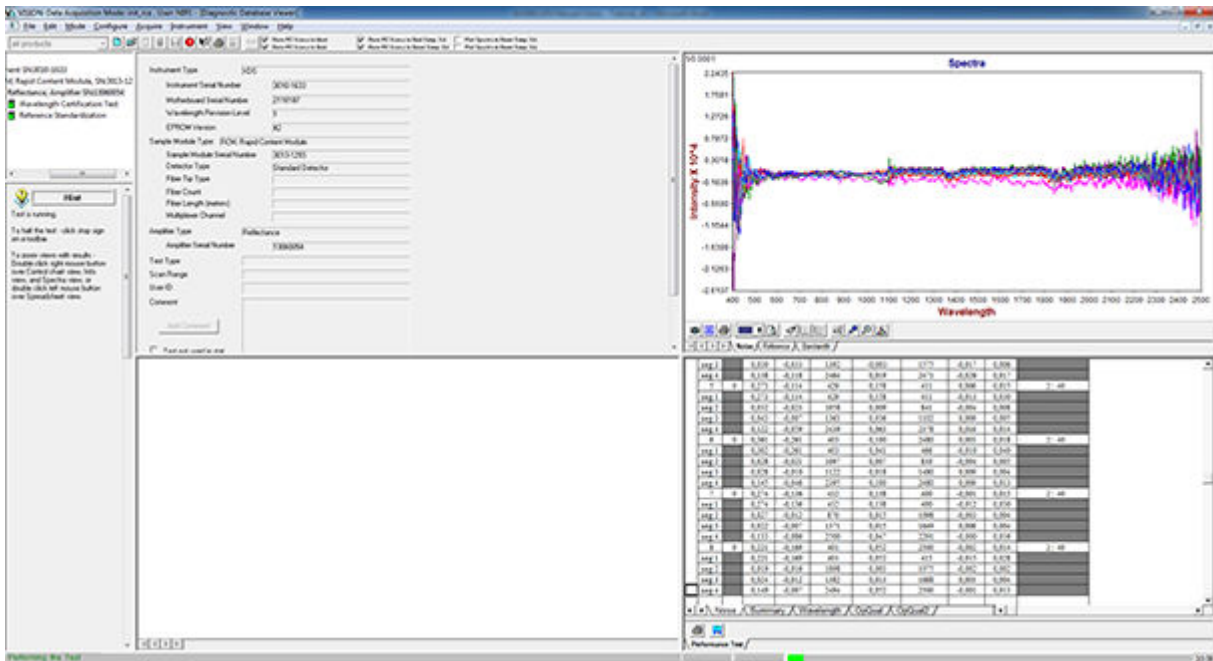

- Click on **[OK]**.

8.4.5 Performance Test

Performance Test is a comprehensive test of instrumental performance, and is the final assurance that the instrument is ready to run samples.

Perform Performance Test

1 Remove the Standard from the sample compartment.

2 Click on **Instrument ► XDS Setup/Diagnostics ► Run Performance Test**.

3 Wait until test is completed.

4 When the **Performance Test** dialog box informs that the Performance Test has passed, click on **[OK]**.

5 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.

9 DS2500 Solid Analyzer

For the setup and calibration of the DS2500 Solid Analyzer you will need the following accessories:

- DS2500 holder for sample cup (6.7430.040)
- NIRS reflection standard set, 2 pcs (6.7450.000) or NIRS reflection standard set, 7 pcs (6.7450.010)

9.1 Preparing the instrument

For the initial instrument diagnostics, the sample cup holder must be installed.

1 Place the DS2500 holder for sample cup.

The metal pin on the sample cup holder must go into the indentation on the sampling window.

9.2 Starting Vision

Once the software is installed, a Vision Icon can be found on the desktop of your computer.

1

Double click on .

2 In the **Login** dialog box, enter the following information:
  - **User ID** NIRS
  - **Password** NIRS

3 Press **[Enter]** or click on **[OK]**.

9.3 Setting-up a Project

In Vision, a project must be setup, before any data (instrument diagnostics or spectral data) can be collected.

If this is your initial entry to Vision the **Create New Project** dialog box is automatically opened. If the **Create New Project** dialog box is not open

Open the Create New Project dialog box

1 Click on **File ▶ Project ▶ New**.

2 When asked to close the open project, click on **[OK]**.

Define Project information

1 In the **Create New Project** dialog box enter the following information:
  - **Project ID**   e. g. "ds2500"
  - Click on **[OK]**.
  - When asked "Create database C:\Vision\ ds2500?", click on **[Yes]**.

Configure Data Sources

1 In the **Configure Data Sources** dialog box,

- In the **Instrument** section, select **Metrohm NIRS DS2500 Instrument Driver**.
- Click on **[Configure]**.

2 In the **NIRSystem XDS-series Instrument Configuration** window,

- Select the IP Address of your instrument.
- Click on **[OK]**.

3 Back in the **Configure Data Sources** window, click on **[OK]**.

Connect to the instrument

1 In the **Connect to Instrument** dialog box.

2 Select **[Use Existing Data]**.

9.4 Defining Project Options and System Options

Project Options apply only to the current (open) Project. System Options apply to all future Projects.

Open the Edit Options dialog box

1 Click on **Configure ▶ Options**.

2 In the **Project Options** tab enable the following options:

- **Instrument must stabilize before data acquisition**
- **Run performance test**
- **Reference Standardization**
- **Use Instrument Calibration**

3 Click on the **System Project** tab.

4 In the **System Options** tab,

- Enable the same options as in the **Project Options** tab.
- In the **System Type** section enable **Use DS/System II**.
- Click on **[OK]**.

9.5 Setting up the Data Collection Method – DCM

Each project must have at least one Data Collection Method (DCM). A Data Collection Method (DCM) defines all instrument specifications (instrument model, module and amplifier type, number of scans) and selected performance test parameters (like pass/fail limits).

9.5.1 Connecting the instrument

Connect the instrument

1 Click on **Acquire ▶ Connect**.

The **Instrument SelfTest** dialog box appears.

2 Wait until the self-test of the instrument is finished.

The **Select Data Collection Method** dialog box appears.

9.5.2 Creating a Data Collection Method

Create Data Collection Method

1 In the **Select Data Collection Method** dialog box click on **[New]**.

2 In the **Edit Data Collection Method** dialog box enter a name for the DCM.

We recommend the following structure for DCM naming: "name of instrument"_"detector type". For example:

- **Method:** e.g. "DS2500_Reflectance"
- **Reference Standardization**   enabled

In the **Sampling System** box, select the following:

- **Cell: Stationary**

Edit Data Collection Method - DS2500 Instrument

Method: DS2500_Reflectance   ☑ Reference Standardization

Instrument

Model: DS2500   Range: Full Range 400-2500nm

Sampling System

Select   Reflectance

Cell: Stationary

Detector: Reflectance

Sample

Scans: 32

Reference

Scans: 32

OK

Cancel

Test Param

3 Click on **[OK]**.

The **Select Data Collection Method** dialog box reappears.

Select Data Collection Method

1 In the **Select Data Collection Method** dialog box,

- Click on **DS2500_Reflectance**.
- Click on **[OK]**.

2 In the **Instrument Configuration** dialog box, click on **[OK]**.

3 Wait for the sampling System to stabilize.

9.5.3 Performance Test

As soon as the instrument is stable, vision starts the Performance Test automatically.

If the lid of the instrument is open, you will be asked to close the lid.

1 Wait for the performance test to finish.

2 In the **Performance Test** dialog box, click on **[Print Report]**.

9.5.4 Instrument Calibration

1 Click on **Instrument ▶ Instrument Calibration**.

2 When the **Select Standard File** dialog box opens,

- Plug the USB stick into a USB port of your computer or place the minidisk into the CD drive.
- Navigate to the content of the USB stick or the minidisk, respectively.
- Select File **RSSXXXXX.da**.
- Click on **[Open]**.

3 When asked to place the wavelength standard,

- Place the Wavelength standard WSRXXXXX into the opening of the holder. The label of the wavelength standard must be visible.

- Close the lid.
- Click on **[OK]**.

- Wait.

4 When asked to "Please position R80 standard, and close the lid",

- Remove the wavelength standard.
- Position the 80% reference **R80XXXXX**.
  The label of the reference standard must be visible.
- Close the lid.
- Click on **[OK]**.
- Wait.

5 When the **Instrument calibration passed** message appears, click on **[OK]**.

6 Remove the Standard from the sample compartment.

7 Eject the USB stick or minidisk and remove it from the computer.

The calibration of the instrument is now complete. The instrument is ready to measure samples.