UV WINLAB SOFTWARE

User's Guide

PerkinElmer ®

precisely.

UV WinLab Software
User's Guide

Release History

Part Number	Release	Publication Date
09934426	A	September 2000

Contents

Introduction

PerkinElmer's UV WinLab is a Windows-based software application used to control your UV spectrometer and manage, process and extract information from the spectra collected.

This *User's Guide* tells you how to install UV WinLab and associated software products and explains how to use the on-screen Help files. It also includes a brief tutorial to help explain the general principles involved in using UV WinLab software to scan samples.

Conventions

The following conventions are used in this manual:

Normal text is used to provide information and instructions.

Bold text refers to text that is displayed on the screen.

UPPERCASE text, for example ENTER or ALT, refers to keys on the PC keyboard. '+' is used to show that you have to press two keys at the same time, for example, ALT+F.

NOTE: *indicates additional, significant information that is provided with some procedures.*

Installation 1

Minimum PC Requirements

The PC you install the software on must meet the following specification. To ensure successful installation of the software, please check these requirements before starting the installation:

- Intel® Pentium processor with 200 MHz or greater clock speed.

- At least 16 MB of Random Access Memory (RAM).
  64 MB is recommended.

- The capability of displaying High Color (16 bit) at 1024 x 768 SVGA.

- Hard disk with at least 200 MB free space.

- Quad speed CD-ROM drive.

- A 1.44-MegaByte floppy disk drive for 3.5-inch floppy disks.

- A keyboard and PS/2®-style mouse.

- RS-232 interface.

- One of the following operating systems (or later versions):

  Windows 95/98
  Windows NT 4.0

NOTE: *If you have a Windows NT system, it is important to note that you must be logged on at Administrator level before installing the software.*

Installing the Software

The UV WinLab CD contains an Installation Wizard to help you install the correct software on your PC.

1. Set up and connect your instrument and PC as discussed in the manual for your instrument.

2. Place your UV WinLab CD into your CD drive.

3. From the Start menu select **Run**.
   The Run dialog is displayed.
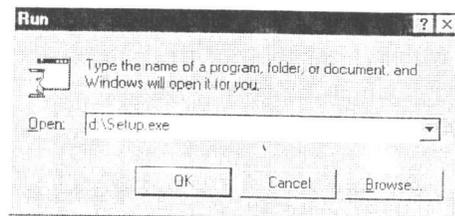
4. Enter **d:\Setup.exe** and click **OK**.
   Replace d:\ with the drive letter for your CD.
   The Setup screen is displayed.
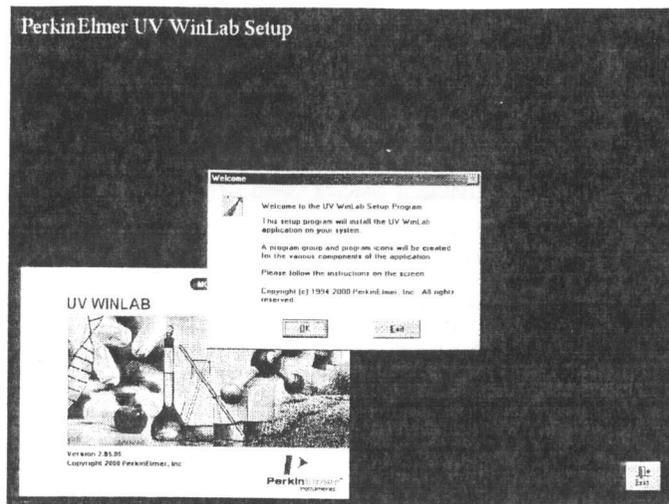
5. Click **OK**.

The Instrument configuration dialog is displayed.
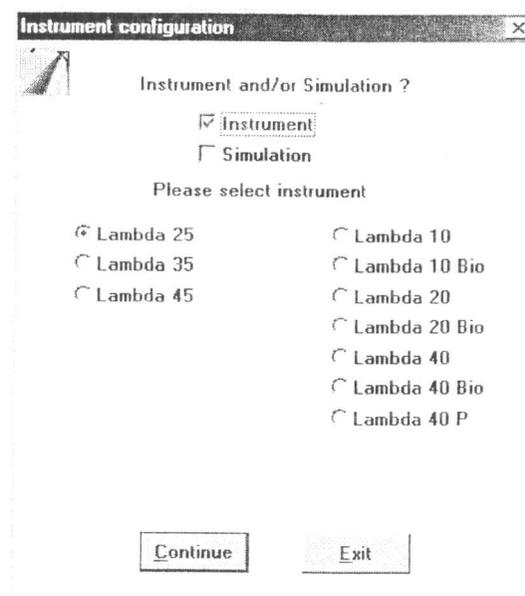
6. Select **Instrument** and the correct instrument, for example **Lambda 45**, and then click **Continue**.

   Select **Simulation** if you are not connecting your PC to an instrument.

   The Cell Changer Indexing dialog may be displayed.

Cell Changer Indexing   [×]

If your Lambda 10, 20, 40 or 40P spectrometer has an 8-cell changer installed, you can choose its mode of operation.

OPTION 1 will automatically reindex the cell changer after each cycle. This ensures that the cell changer will work reproducibly for extended length experiments (i.e. 12-hour kinetics experiments). This option does not provide for reproducible operation with reduced volume (50 uL) cuvettes.

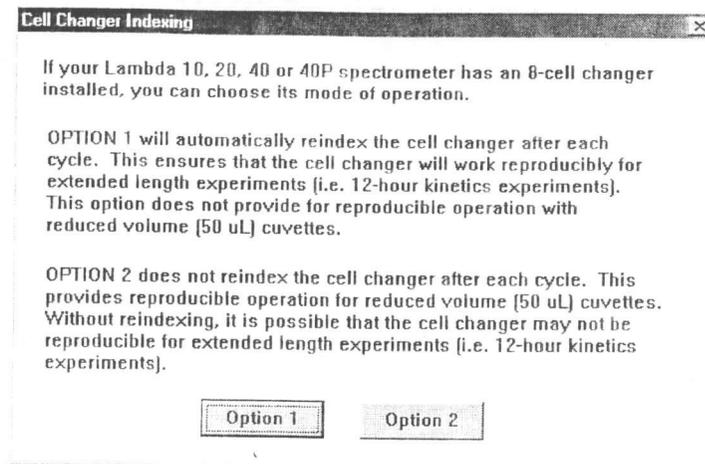OPTION 2 does not reindex the cell changer after each cycle. This provides reproducible operation for reduced volume (50 uL) cuvettes. Without reindexing, it is possible that the cell changer may not be reproducible for extended length experiments (i.e. 12-hour kinetics experiments).

          [Option 1]   [Option 2]

---

7. Click either **Option 1** or **Option 2** as required.

   The Serial Number of Instrument dialog is displayed.

Serial Number of Instrument   [×]

Serial number: [1   ]

          [OK   ]   [E xit]

---
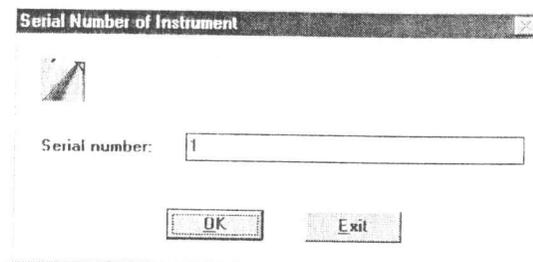
8. Enter the **Serial number** of your instrument and then click **OK**.

   The serial number of the instrument is shown to the rear of the sample area.

   The Communication port dialog is displayed.

Communication port

Which port do you want to use ?

- ⦿ COM1
- ○ COM2
- ○ COM3
- ○ COM4

[Continue]   [Exit]
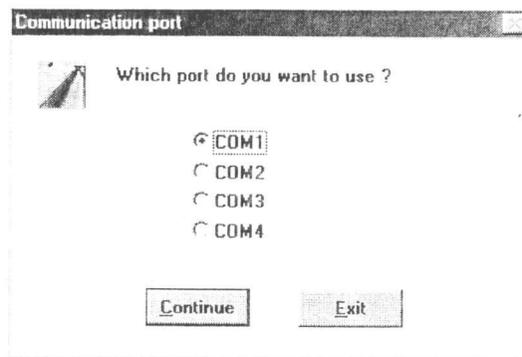
9. Select the port on your PC that the instrument is connected to, for example **COM1**, and then click **Continue**.

The Installation Aditional Modules dialog is displayed.

Installation Additional Modules

Which modules do you want to install ?

- ☐ UV-BioLab
  Method collection for DNA, protein, enzymes

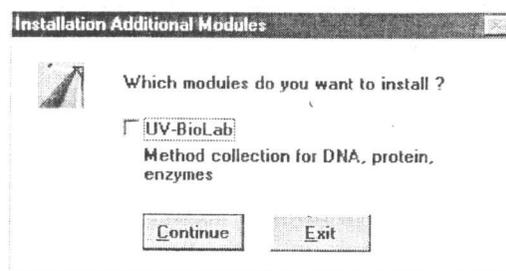[Continue]   [Exit]

10. Select whether you want to install any of the additional modules available, and then click **Continue**.

The Installation Directory dialog is displayed.

Installation Directory

The setup program will copy the UV WinLab application files under the following directory.

Application Path: C:\UVWINLAB

[OK]   [Exit]
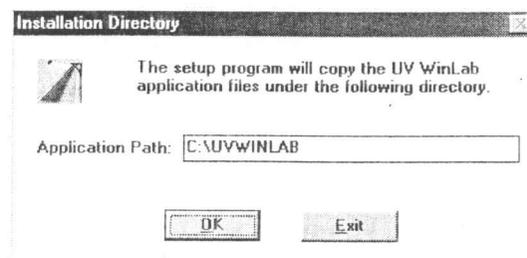
11. Enter the **Application Path** required and then click **OK**.

The UV WinLab Setup dialog is displayed.
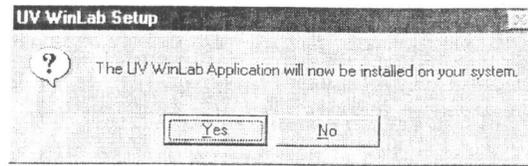
12. Click **Yes**.

The installation of the files begins.

At the end of the installation the Language support dialog is displayed.
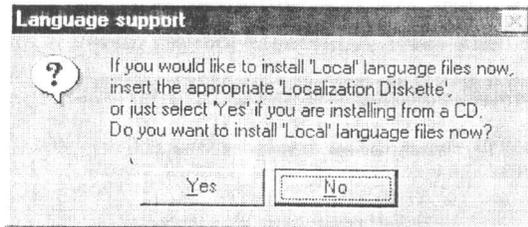
13. Follow the instructions for installing the local language files you require and then click **Yes**.

OR

Click **No**.

The Installation Complete dialog is displayed.
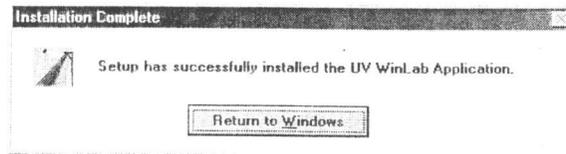
14. Click **Return to Windows**.

The installation program closes.

15. Reboot your PC by selecting **Shut Down** from the Start menu.

    Once the PC has been rebooted, the software installation is complete and you can start to use UV WinLab.
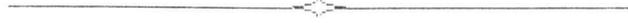
Using the Software   2

Using UV WinLab

Starting the software

1. Start the spectrometer, as detailed in the manual for your spectrometer.

2. Start the PC.

3. From the Windows Start menu, open the **PerkinElmer Applications** group under **Programs** and start UV WinLab, which will have the name of the instrument you set up during the installation procedure, for example Lambda 35.

   The UV WinLab software starts and the Methods window is displayed.

   The main areas of the UV WinLab application window are:

Title bar

Menu bar

Toolbar

Workspace

Active window (in this case the Method Editor)

Tabs

Minimized windows

Live display

Status line

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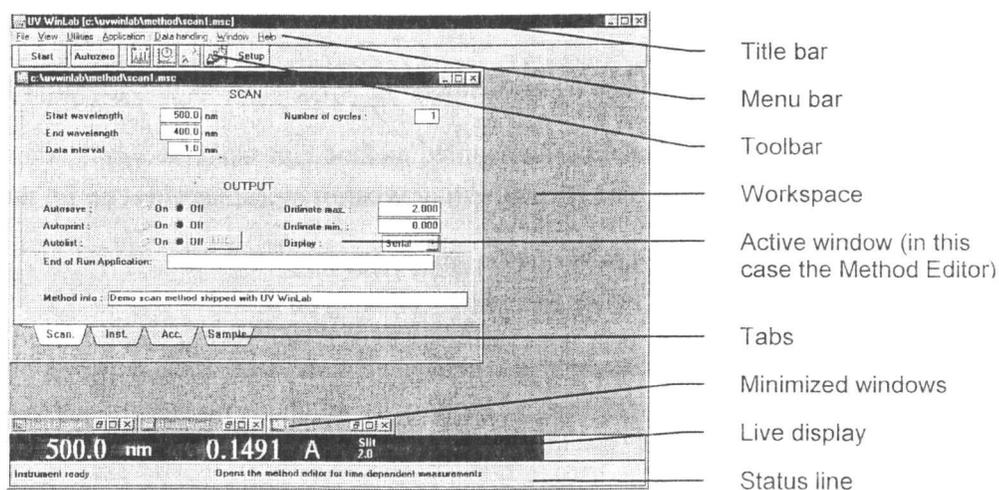
Working with Methods

Methods are a collection of those parameters necessary for a particular analysis using the spectrometer and are stored as method files. You can process large numbers of samples efficiently using methods.

UV WinLab offers four types of method:

- **Scan** – for scanning spectra

- **Time Drive** – for ordinate value measurements over time, for example for kinetics measurements

- **Wave Prog** – for ordinate value measurement at different wavelengths, and for calculating differences and ratios at these ordinate values

- **Conc** – for concentration measurements from calibration curves

To create a new method:

1. Select the required method type from the Application menu.
   The Method Editor window is displayed set up for the required type of method.

2. Set the various parameters.
   Select each tab by clicking on it.

3. When all the parameters have been set as required, click **Setup**.
   The new parameters are set on the instrument and the **Start** button changes to green to show that the instrument is ready to perform an analysis.

NOTE: *You must remember to save your method when it is complete so it can be used at another time. If you built a method by editing a previous method you must use the* **Save As** *command on the File menu when saving the new method or you will overwrite the old method.*

Data Calculations

The Arithmetic module is used for spectral manipulation, data conversion and comparison, and data reduction. One Graph Window displays the original, unaltered spectrum whilst a second window displays the spectral or tabular results of the calculations.

➢   Select **Arithmetic** from the Data Handling menu.

The Arithmetic module is displayed.

The applications available are listed below.

Menu Item	Application
Area	To calculate the area beneath the spectral curve.
Arithmetic Spectrum	To perform mathematical operations on spectral data, e.g. add two spectra or multiply a spectrum by a factor.
Arithmetic Value	To perform mathematical operations on spectral data, e.g. Ratio, Difference or multiply an ordinate value with a factor.
Average and Standard Deviation Spectrum	To calculate the average and standard deviation from spectra.
Average and Standard Deviation Value	To calculate average, standard deviation, and rms at a specified wavelength range.
Build Spectra	Build a spectrum via input values.
Calculate Height	To calculate the total height and the height to a specified base.
Convert X	To convert the abscissa unit.
Convert Y	To convert the ordinate unit.

Menu Item	Application
Derivative	To calculate the first, second, third or fourth derivative of a spectral curve.
Interpolate	To change the data interval and to copy part of a spectral curve.
Merge	To merge two spectral curves.
Normalize	To normalize spectral curves to a given ordinate value.
Reflection Correction	To correct a reflectance spectrum for dark and white values.
Selection	To display ordinate values at defined abscissa values.
Slope	To calculate the slope and the standard deviation of a spectral curve within a selected abscissa range. For Time Drive curves, also use to calculate the enzyme activity.
Smooth	To smooth spectral data.
Film Thickness	To calculate the film thickness of single layers.

Further Information

New users should work through the simple tutorial given in the *Getting Started* chapter of this manual, to familiarize themselves with the general operations of UV WinLab.

For further information on using UV WinLab or the Arithmetic module, refer to the on-screen help system, started by selecting **Contents** from the Help menu. See also *Using On-screen Help* on page 27.

Using UV KinLab

What is UV KinLab?

UV KinLab is a separate software application, installed at the same time as UV WinLab, which is used for kinetic analyses.

With UV KinLab the following tasks can be performed:

- Record the TimeDrive data of an enzyme or other kinetic reaction.

- Calculate the enzyme factor from the data gathered.

- Evaluate previously collected data or repeat an evaluation after changing the parameters (post-run kinetics).

- Export data for use in a spreadsheet program.

Starting the software

➤ From the Windows Start menu, select **UV KinLab** from the **PerkinElmer Applications** group under **Programs**.
  The UV KinLab software starts.

  OR

 From UV WinLab, select **KinLab** from the Application menu.
  The UV KinLab software starts and UV WinLab remains open so that you can easily switch between the two applications.

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Working with Methods

Analysis in UV KinLab is performed using methods. A method is a set of parameters for the designated task, for example running an enzymatic analysis or evaluating previously collected data.

Methods are created, modified, saved and started from the Method Editor window.

➢ To open the Method Editor, select **Open Method** from the File menu.
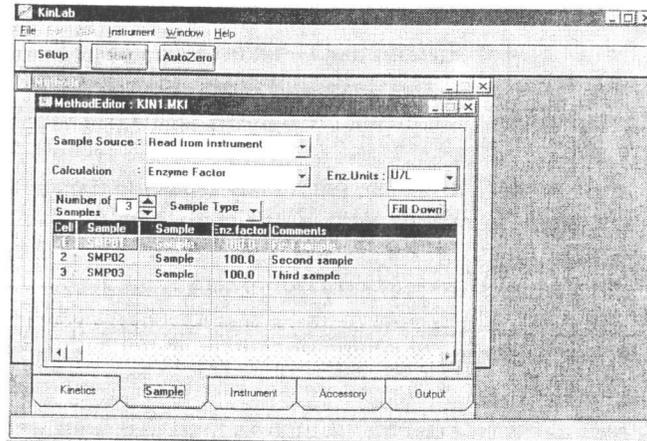
Online Recording

UV KinLab enables you to record the TimeDrive curves of an enzyme analysis online and to evaluate the data at completion of the run. To do this, set up a method for online recording in the Method Editor:

1. Select **Open Method** from the File menu.

   A file selector is displayed.

2. Select a method.

   It is best to select a previous online recording method as this will be used to create the new method.

   The Method Editor is displayed.

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3. On the Sample tab select **Read from Instrument** as the **Sample Source**.

4. Enter the remaining parameters as required on each tab of the Method Editor.

5. Click **AutoZero** to autozero the instrument.

   The **Start** button changes its color to green.

   If the instrument parameters are already the same as those specified in the method, the Start button is displayed in green already and you do not have to set up the instrument.

6. Click **Start**.

   Online recording of data is started and the TimeDrive curves are shown in the TimeDrive window.

   At the end of the run, the data is saved to disk, and then data evaluation starts.

Postrun Kinetics

UV KinLab enables evaluation of previously recorded data and the ability to repeat the evaluation of online measurement. To do this, you set up a method for Postrun Kinetics in the Method Editor:

1. Select **Open Method** from the File menu.

   A file selector is displayed.

2. Select a method.

   It is best to select a previous Postrun Kinetics method as this will be used to create the new method.

   The Method Editor is displayed.

3. On the Sample tab select **Read from File** as the **Sample Source**.

4. Click .

   A file selector is displayed

5. Select the files to be evaluated.

6. Enter the required parameters on each tab of the Method Editor.

7. Click **Start Evaluation**.

   The evaluation of the data is started.

   The procedure of data evaluation depends on the selected evaluation mode, as discussed below.

Data Evaluation

UV KinLab calculates the enzyme factor from the time drive curves. The software offers you different evaluation modes for the selection of the data range. The evaluation mode is selected on the Kinetics tab of the Method Editor. The evaluation can be repeated with different options as many times as required.

The following evaluation modes are available:

Total Range Mode

The results are calculated from the complete data range of the curves.

Fixed Range Mode

The results are calculated from a fixed data range. The data range is entered numerically on the Kinetics page and is the same for all curves.

Automatic Mode

The software searches automatically for the linear range of the curves and uses this range for data calculation.

The linear range is detected using the following algorithm:

1. From the original curve, the differences from data point to data point are calculated.

   These differences should be constant if the curve is exactly linear.

2. Next, a window the size of 10% of the data points is moved over the differences to identify the region with best linearity.

   The linearity is weighted by the slope in the window (often the baseline shows good linearity, but the baseline is obviously not what should be looked for).

3. When the region with best linearity is identified, the window is moved to both sides up to the point where the linearity is worse by a certain factor or the start/end of the curve is reached. The start and end point where the linearity decreases define the linear range for the evaluation.

Interactive Mode

Interactive selection of the evaluation range. The interactive evaluation is performed in the Evaluation window. For online recording, the interactive mode is started at completion of data recording.

The data range for evaluation can be selected on the screen and check the results immediately after calculation. If necessary, you can repeat the evaluation with different parameters.

The data range can be selected manually (**Manual**) or, UV KinLab can search for the linear range automatically (**Automatic**). Data can be processed in **Batch** mode (all selected curves are processed in a batch) or in **Single** mode (the selected curves are processed consecutively).

UV KinLab can process up to 50 curves, but only 16 curves can be displayed simultaneously in the evaluation window. During batch evaluation, the graph is cleared after the first 16 curves. At completion of evaluation, the first 16 curves are displayed again. To see all curves, process the data in single mode. The curves will be displayed consecutively.

Further Information

For further information on using UV KinLab, refer to the on-screen help system, started by selecting **Contents** from the Help menu. See also *Using On-screen Help* on page 27.

Using Report Builder

Report Builder is a separate application that helps turn data into a single page report.
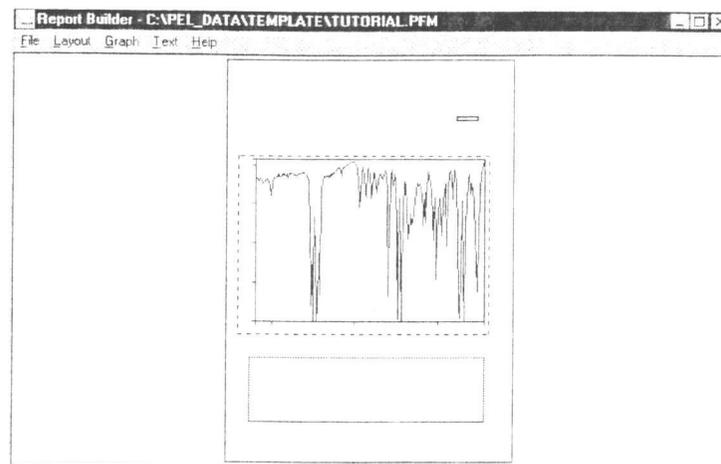
The report can contain System, Status and Instrument information related to the spectrum as well as text you enter yourself, and templates can be set up to always lay out the information in the same way.

Creating a Report

1. Select **Report Builder** from the Application menu.
   Report Builder opens with a blank report.

2. In UV WinLab, select the data to be sent to Report Builder.

3. Select **Copy to Report Builder** from the View menu in UV WinLab.
   The selected data is sent to Report Builder.

For further information on using Report Builder, refer to the on-screen help system, started by selecting **Contents and Index** from the Help menu. See also *Using On-screen Help* on page 27.

Using On-screen Help

The on-screen help system for UV WinLab has been designed to be the main reference when using the software.

➢ To start the help for UV WinLab at the main window, select **Contents** from the Help menu.
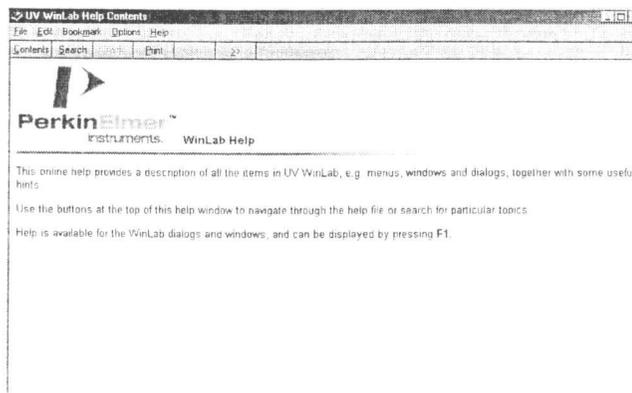
NOTE: *UV WinLab, UV KinLab, the Arithmetic module and Report Builder each have their own separate help files. To get help with each of these applications, start the application and then start the help file from the Help menu within that application.*

➢ To display the table of contents for the help file, click **Contents**.

NOTE: *Under Windows NT 4, instead of the Contents button, you need to click* **Help Topics**, *(which is only visible under Windows NT 4). The Table of Contents displayed will look slightly different to the one shown above.*

➢ To start the help file at the page most relevant for the current dialog of the software, select **Help active window** from the Help menu.

OR

Press F1 on the keyboard.
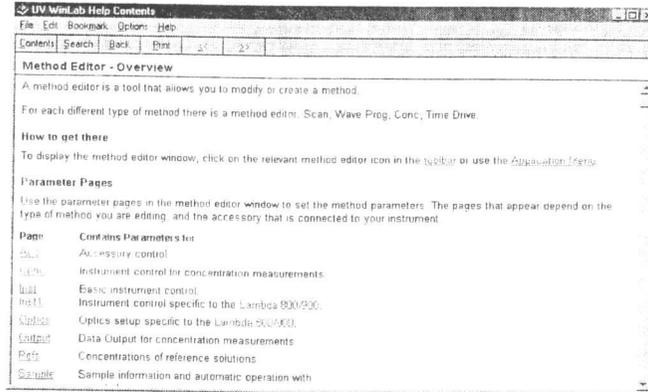
Getting Started 3

Setting up the Tutorial

The following is a simple tutorial that introduces the basic principles of operating the UV WinLab software to scan a spectrum of acetone.

The tutorial will take about 30 minutes and requires the following:

- Deionized water

- Acetone

- A 500 ml volumetric flask

- A 5 ml pipette

- 2 quartz cells

Setting up

The following procedure details how to get the instrument and software up and running:

1. Make sure that the beam path through the sample compartment of the instrument is clear.

   The reference and sample cell holders must be empty, or any accessory must be properly installed, otherwise the instrument will not initialize correctly.

2. Switch on the instrument and leave it for approximately 10 minutes to allow the lamp to warm up and stabilize.

3. Switch on the PC.

4. From the Windows Start menu, open the **PerkinElmer Applications** group under **Programs** and start UV WinLab, which will have the name of the instrument set up during the installation procedure.

   The UV WinLab software starts and the Methods window is displayed.

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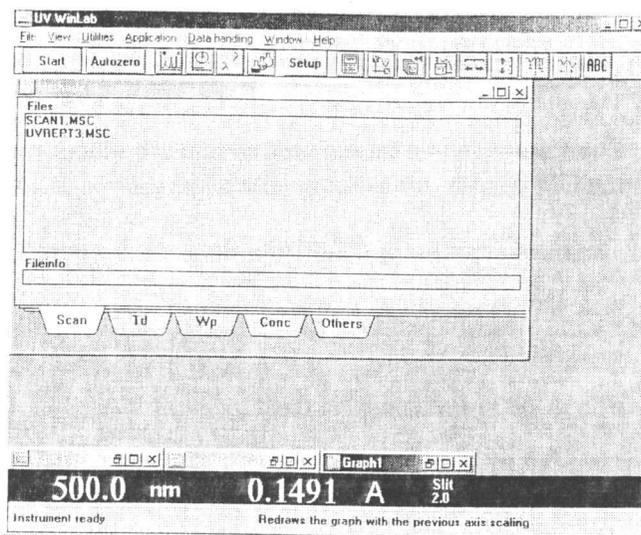
Sample Preparation

1. Pipette 5 ml of acetone into the 500 ml volumetric flask.

2. Fill the flask to the 500 ml mark with deionized water.

NOTE: *This solution will be used in a later tutorial, so ensure the flask is well stoppered to prevent evaporation of the acetone.*

Creating the Method

When UV WinLab was started, the Methods window was displayed. This window has four tabs at the bottom which relate to the four different types of method available:

- **Scan** – methods for scanning spectra

- **Td** – methods for time-dependent (Time Drive) measurements

- **Wp** – methods for running wavelength programs

- **Conc** – methods for concentration measurements

- **Others** – other methods, for example, UV KinLab methods
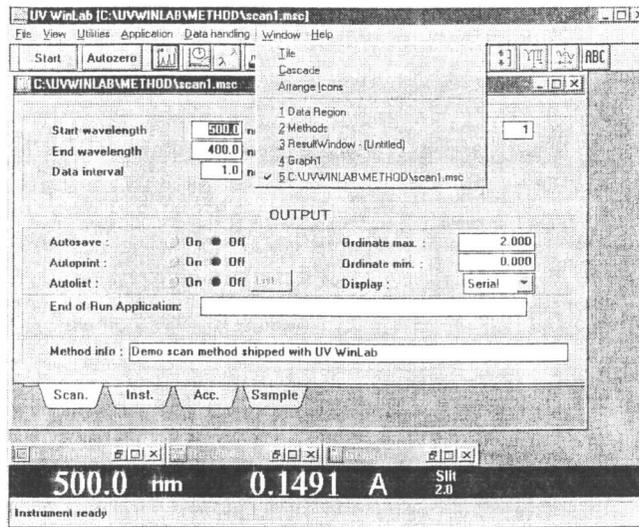
1. Click ▥.

   The Method Editor window is displayed, with the first Scan method from the Methods window loaded.
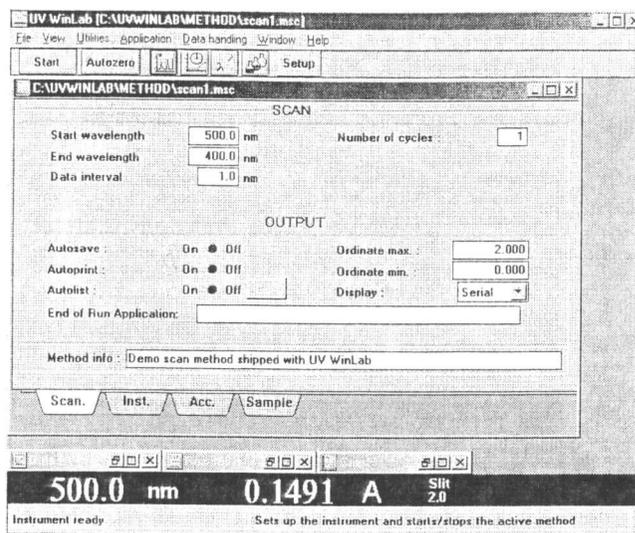
   Beneath the Method Editor window are minimized windows for **Data Region**, **ResultWindow** and **Graph1**.

   - **Data Region** is the temporary memory where data is stored as long as the UV WinLab software is running.

   - **ResultWindow** is where the numerical results of the current method or command are displayed.

   - **Graph1** is where the graphical results of the current method or command are displayed.

2. Display the Window menu.

This menu contains a list of the available windows, which also enables you to switch between the windows.

3. Close the menu by clicking somewhere else on the window.

4. Enter details on the Scan tab of the Method Editor window so that it looks like the picture below:
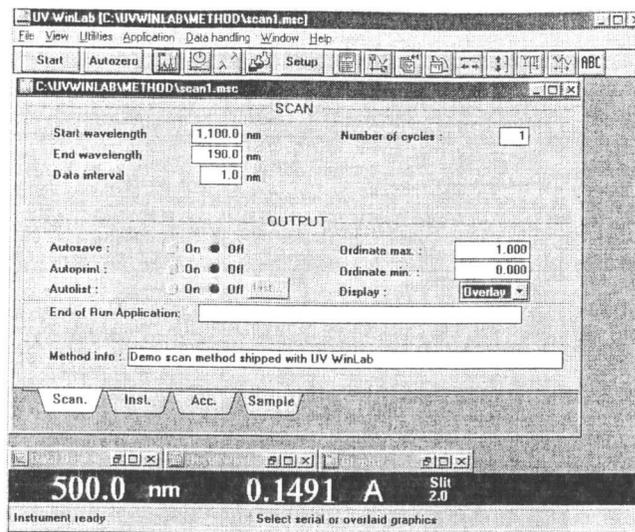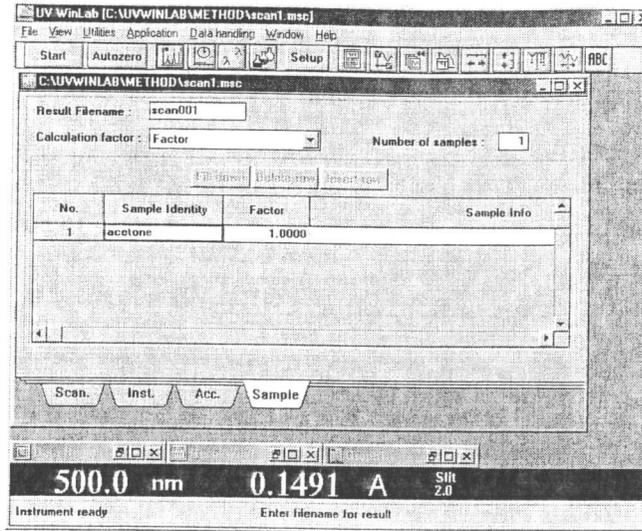
5. Select the Inst tab by clicking on it.

6. Make sure that the details entered are the same as shown below:
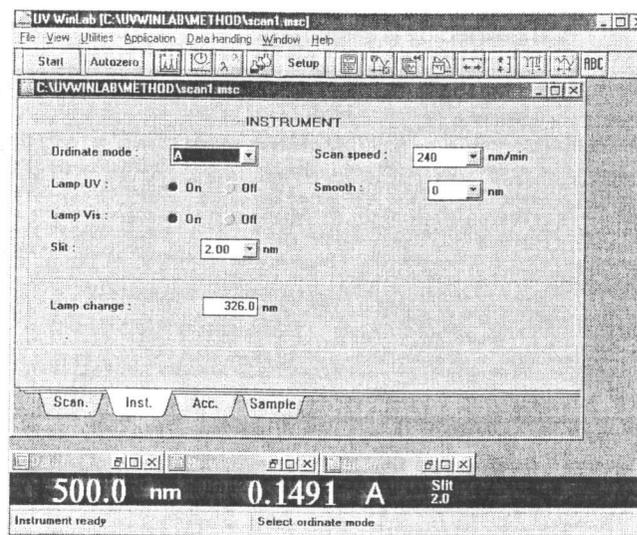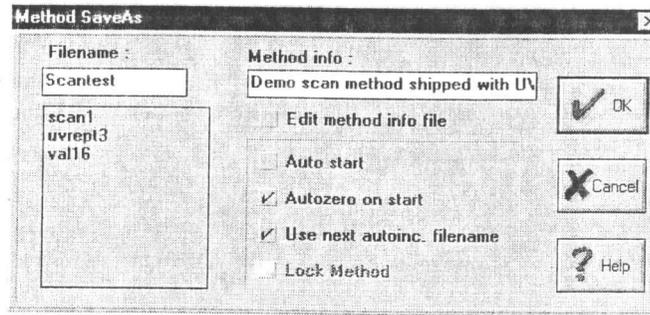

7. Select the Sample tab by clicking on it.

8. Change the **Sample Identity** of the first sample to **acetone**, as shown below:

The method is now complete, but must be saved.

9. Select **Save As** from the File menu.

A file selector is displayed.

10. Enter **Scantest** as the **Filename**.

11. Select **Autozero on start.**

Whenever a method is started, the instrument will autozero (perform background correction) before the measurement is made.

12. Select **Use next autoinc. filename**.

    Future samples will be automatically saved with the filename plus three digits that are automatically updated for each sample.

Using the Method

1. Place a quartz cell containing deionized water in the reference cell holder and close the cover.

   The deionized water is a reference solution for the sample as it is the solvent used to dilute the sample.

2. Click **Start**.

   The instrument autozeros and a blank sample is requested.

3. Place the other quartz cell, again containing just deionized water, in the sample cell holder and close the cover.

   This is the blank solution, that is a solution without any of the chemical you want to analyze.

4. Click **OK**.

   The background correction is performed (which takes a while) and then the sample is requested.
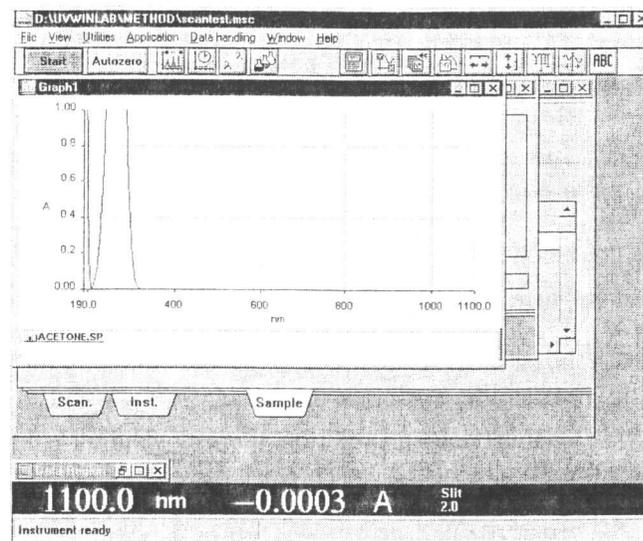
5. Empty the sample cell and re-fill it with the acetone solution made earlier.

6. Place the sample cell back in the holder and close the cover.

7. Click **OK**.

    The analysis is performed. During the analysis the current readings are shown on the live display near the bottom of the UV WinLab window.

   When the scan is complete the spectrum is displayed in the Graph1 window.

    As can be seen, acetone absorbs only in a small wavelength band and absorbs so strongly that the Ordinate max that was set on the Scan tab is too low.

8. Click .

    This is the same as the **Expand Ordinate** command on the View menu.
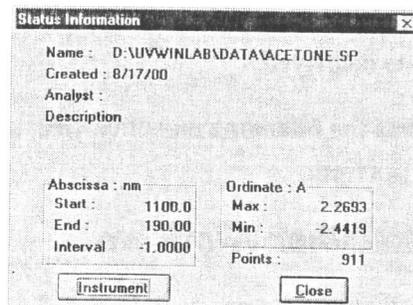
    The graph is redisplayed with a larger ordinate axis so the top of the peak can be seen.
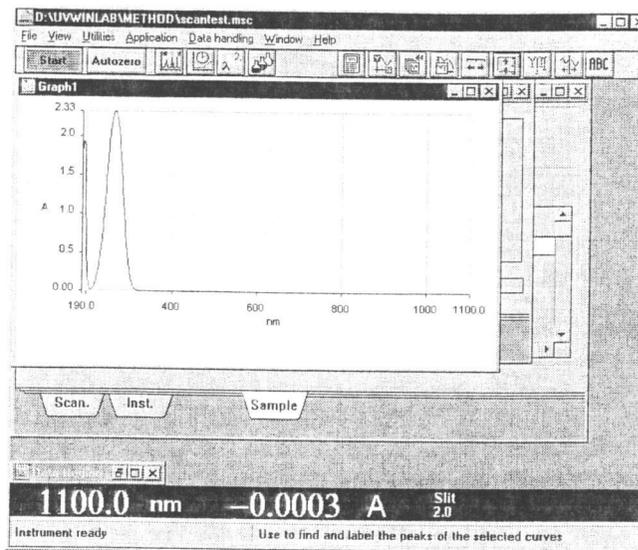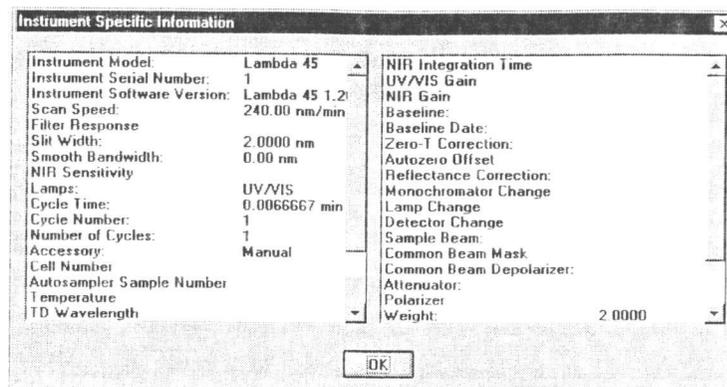
Viewing Status Information

1. Click ⊥⊥, next to the name of the spectrum.

   The status information for the spectrum is displayed in a new window.


2. Click **Instrument**.

   The instrument parameters are displayed.

Instrument Specific Information

Instrument Model:	Lambda 45	NIR Integration Time	
Instrument Serial Number:	1	UV/VIS Gain	
Instrument Software Version:	Lambda 45 1.2	NIR Gain	
Scan Speed:	240.00 nm/min	Baseline:	
Filter Response		Baseline Date:	
Slit Width:	2.0000 nm	Zero-T Correction:	
Smooth Bandwidth:	0.00 nm	Autozero Offset	
NIR Sensitivity		Reflectance Correction:	
Lamps:	UV/VIS	Monochromator Change	
Cycle Time:	0.0066667 min	Lamp Change	
Cycle Number:	1	Detector Change	
Number of Cycles:	1	Sample Beam:	
Accessory:	Manual	Common Beam Mask	
Cell Number		Common Beam Depolarizer:	
Autosampler Sample Number		Attenuator:	
Temperature		Polarizer	
TD Wavelength		Weight:	2.0000

OK

3. Click **OK**.

   The Instrument window closes.

4. Click **Close**.

   The Status Information window closes.

5. Select **Print** from the File menu.
   Graph1 is printed.

6. Select **Save** from the File menu.
   A file selector is displayed.

7. Enter **acetone** as the **Filename** and click **OK**.
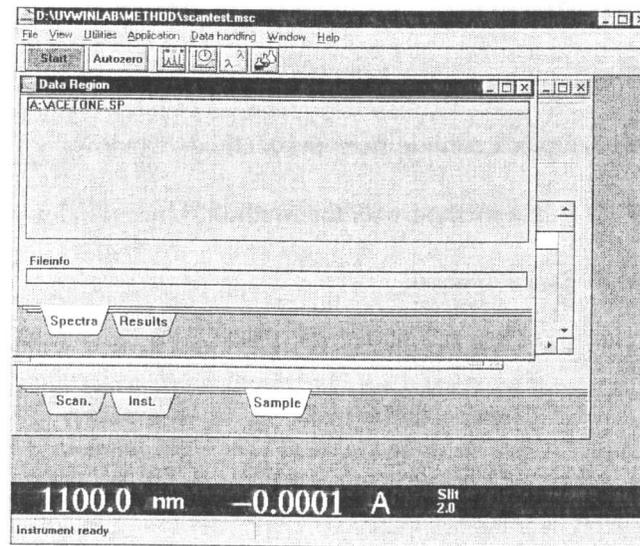   The spectrum is saved.

Looking at the Other Windows

1. Select **ResultWindow** from the Window menu.
   The results window is displayed, with details about the acetone spectrum.
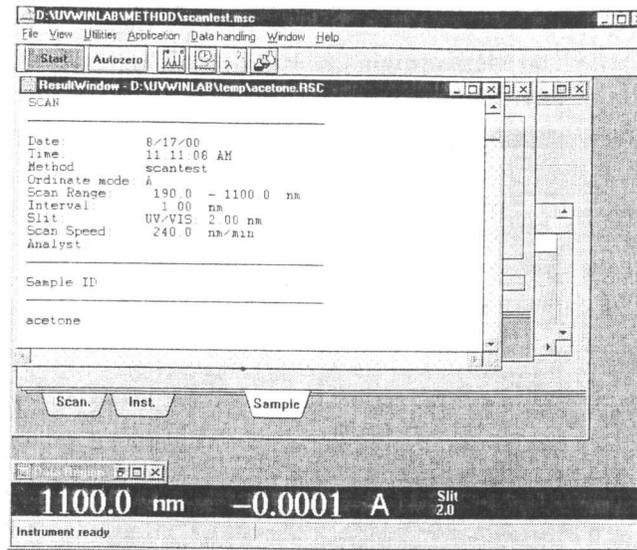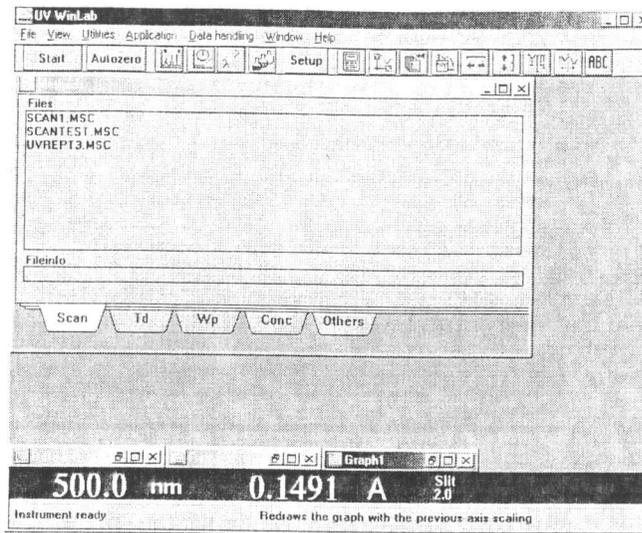
2. Select **Data Region** from the Window menu.

   The Data Region window shows the spectra (Spectra tab) and results files (Results tab) currently held in the temporary memory.

3. Select **Methods** from the Window menu.

The Methods window is displayed and now contains a new Scan method, **Scantest**.

Summary

You have now completed the tutorial, where you learned how to:

- Open a method from the Methods window.

- Edit a method with the Method Editor window.

- Run a method.

- View the Graph, Results and Data Region windows.