WinASPECT®

Spectroanalytical Software
## Contents

### 1 WinASPECT

1.1 Described version ..........................................................5
1.2 Notes on the use of this manual ...........................................5
1.3 What is WinASPECT? ..........................................................5
1.4 Installation of WinASPECT ..................................................7
1.4.1 System requirements .......................................................7
1.4.2 Installation procedure ....................................................7
1.4.3 Installation of a SPECORD with USB port .........................8
1.4.4 Installation of additional modules .....................................8
1.5 Operation of WinASPECT ....................................................9
1.5.1 General ........................................................................9
1.5.2 Starting / exiting WinASPECT ..........................................9
1.5.3 The WinASPECT desktop .................................................10
1.5.4 General settings via Extras / Options ...............................13

### 2 Measurements with WinASPECT

2.1 General measurement functions ..........................................17
2.1.1 Displays during running measurements .............................17
2.1.2 Initialization of the device ...............................................18
2.1.3 Reference Measurement ................................................18
2.1.4 Sample measurement .....................................................19
2.1.5 Serial measurement ........................................................19
2.1.6 Online measurement .......................................................23
2.1.7 Setting, saving and loading measurement parameters ............23
2.1.8 Configuration of analytical device and result storage ..........24
2.1.9 Dark-current measurement (only on SPECORD\textsuperscript{®} Sxxx) .................................................................26
2.2 Measurement parameters / Device adjustment for scanning spectrophotometers .................................................27
2.2.1 Measurement parameters window for scanning spectrophotometers .................................................................27
2.2.2 Settings tab (Scanning SPECORD) .................................28
2.2.3 Device tab (Scanning SPECORD) .....................................30
2.2.4 Mode tab (Scanning SPECORD) ......................................32
2.2.5 Accessories tab (Scanning SPECORD) ............................36
2.2.6 Wavelength correction and standard correction on scanning spectrophotometers .........................................................36
2.3 First measurement with scanning SPECORD .........................38
2.4 Measurement parameters for SPECORD Sxxx ........................41
2.4.1 Menu functions available in SPECORD Sxxx measurement parameter box .........................................................41
2.4.2 General tab (Measurement parameters SPECORD Sxxx) ....42
2.4.3 Device tab (Measurement parameters SPECORD Sxxx) ....43
2.4.4 Mode tab (Measurement parameters SPECORD Sxxx) ....45
2.4.5 Interval tab (Measurement parameters SPECORD Sxxx) ....46
2.4.6 Accessories tab (Measurement parameters SPECORD Sxxx) ....50
2.5 First measurement with the SPECORD Sxxx ........................51

### 3 Properties and Handling of Document Windows

3.1 Properties and functions of document windows .....................53
3.1.1 Elements of the document window ...................................53
3.1.2 Display options for document windows .............................55
3.1.3 Editing document windows ..............................................59
3.1.4 Defining a section of a spectral curve ...............................64
3.1.5 Obtaining time-based data from a cyclic spectrum ...............64
3.1.6 3D-representation of a flight of spectra ............................65
## Contents

3.1.7 Multi-spectrum overlay mode .................................................. 66  
3.1.8 Signing measured data and showing signatures .......................... 66  
3.1.9 Overwriting measured data with original data ......................... 66  
3.2 Handling of document windows .............................................. 68  
3.2.1 Opening files ........................................................................ 68  
3.2.2 Printing files ........................................................................ 69  
3.2.3 Saving and closing document windows ................................. 71  
3.2.4 Exporting the contents of document windows ........................ 72  
3.2.5 Arranging document windows on the workplace ..................... 72  

### 4 Quantitative Analyses (Quant Module) ................................. 73

4.1 Calibration .................................................................................. 73  
4.1.1 Menu functions of the Calibration dialog box ......................... 74  
4.1.2 Setting up a new calibration curve ......................................... 75  
4.1.3 Printing of calibration curves and data .................................. 86  
4.2 Concentration ........................................................................... 87  
4.2.1 Menu functions of the Concentration dialog box .................... 88  
4.2.2 Selecting the parameters for concentration analysis ............... 89  
4.2.3 Concentration determination procedure ................................ 93  
4.2.4 Printing concentration measurement series ........................... 98  

### 5 Quant Routine Module .............................................................. 99

5.1 Elements of Quant Routine dialog box .................................... 100  
5.1.1 Preselection screen of Quant Routine module ....................... 100  
5.1.2 Menu commands in Quant Routine module .......................... 101  
5.2 Measurement settings in Quant Routine .................................. 102  
5.3 Selection of analytical method and input of sample table in Quant Routine .......................................................... 103  
5.3.1 General Quant Routine settings ......................................... 103  
5.3.2 Selection of analytical method for Quant Routine ................. 103  
5.3.3 Entering sample table for a Quant Routine ......................... 105  
5.4 Measurement with Quant Routine .......................................... 111  
5.5 Multi Measurement with Quant Routine ................................ 112  
5.6 Maintaining result files in Quant Routine ............................... 114  
5.6.1 Quant Routine result file display resources ......................... 114  
5.6.2 Graphical representation of results measured in Quant Routine .......... 115  
5.6.3 Saving and opening result files in Quant Routine .................. 116  
5.6.4 Printing Quant Routine results ............................................ 116  
5.7 Methods in Quant Routine ...................................................... 118  
5.8 Calibration in Quant Routine .................................................... 119  

### 6 Methods for Water Analysis .................................................... 121

6.1 Selection of a Water Analysis method ..................................... 121  
6.2 Measurement with a Water Analysis method ......................... 123  
6.3 Overview of implemented Spectroquant test kits .................... 123  

### 7 Kinetics Module ........................................................................ 129

7.1 Measuring a kinetic reaction ..................................................... 131  
7.1.1 Parameter settings for kinetic measurements on scanning spectrophotometers ................................................ 132  
7.1.2 Parameter settings for kinetic measurements on SPECORD Sxxx. 133  
7.2 Loading a file for kinetic analysis ............................................ 134  
7.3 Evaluating kinetic reactions ...................................................... 134  
7.3.1 Selecting a sample for kinetic analysis ................................. 135  
7.3.2 Defining the parameters for the kinetic analysis ................... 135  
7.4 Graphic presentation of sample data in the Kinetics module .... 136  
7.4.1 Displaying measured kinetic curves .................................... 136
Contents

7.4.2 Scaling of kinetic curve presentation ............................................. 137
7.5 Printing a kinetic analysis ................................................................. 138

8 Biochemical Analysis (Bio Module) .................................................. 139
  8.1 Measurement settings in Bio module ............................................. 141
  8.2 Measurement procedure in the Bio Method module ..................... 143

9 Formula Module ............................................................................. 145
  9.1 Measurement parameters in Formula module ............................... 146
  9.2 Entry of formula ......................................................................... 147
  9.3 Measurements in the Formula module ......................................... 150

10 Color Measurement ....................................................................... 153
  10.1 Tools in Color Measurement Dialog Window ............................. 154
  10.2 Settings for Color Measurement ..................................................... 156
  10.2.1 Measurement parameter settings for color measurement ........ 156
  10.2.2 Selection of chromaticity values and settings for sample series 156
  10.3 Sample Measurement Performed with Color Measurement Module 159
  10.4 Display of Results in Color Measurement Module ..................... 160
  10.5 Management of Result Files in Color Measurement Module .... 161

11 Film Thickness Measurement ......................................................... 163
  11.1 Tools in Film Thickness Measurement Dialog Window ................ 164
  11.2 Settings for Film Thickness Analysis ............................................. 166
  11.2.1 Settings for film thickness measurement ................................ 166
  11.2.2 Settings for sample series and material-related data .............. 166
  11.3 Sample Measurement with Film Thickness Module .................... 167
  11.4 Display of Results in Film Thickness Module .............................. 168
  11.5 Management of Result Files in Film Thickness Module ............. 169
  11.6 Creating a Material File ............................................................... 171

12 Mathematical Data Handling .......................................................... 173
  12.1 Mathematical operations with two spectra .................................. 173
  12.1.1 Addition ............................................................................... 175
  12.1.2 Subtraction .......................................................................... 175
  12.1.3 Multiplication ................................................................. 175
  12.1.4 Division ............................................................................. 176
  12.1.5 Normalization ................................................................. 176
  12.1.6 Adaptation .......................................................................... 176
  12.1.7 Link .................................................................................. 177
  12.2 Mathematical operations with a single spectrum ....................... 177
  12.2.1 Offset ............................................................................... 178
  12.2.2 Factor ............................................................................... 178
  12.2.3 Smooth ............................................................................ 178
  12.2.4 Derivative, 1\textsuperscript{st} to 4\textsuperscript{th} order .................... 179
  12.2.5 Interpolation .................................................................... 179
  12.2.6 Baseline correction ............................................................. 179
  12.2.7 Integration ......................................................................... 180
  12.2.8 Peaklist ............................................................................ 181
  12.2.9 Values of defined wavelengths ............................................ 184

13 Validation ..................................................................................... 187
  13.1 Starting the Validation module ..................................................... 187
  13.2 Test parameters and required aids .............................................. 189
  13.2.1 Test parameters .................................................................... 189
  13.2.2 Required aids ..................................................................... 190
  13.3 Entry of validation parameters ................................................... 191
<table>
<thead>
<tr>
<th>Contents</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.3.1 Selection of validation parameters to be tested: General tab</td>
<td>191</td>
</tr>
<tr>
<td>13.3.2 Selection of limit values: Limit values tab</td>
<td>193</td>
</tr>
<tr>
<td>13.3.3 Entry of the data of the used standards</td>
<td>193</td>
</tr>
<tr>
<td>13.4 Validation procedure</td>
<td>194</td>
</tr>
<tr>
<td>13.4.1 Switching on and calibration of SPECORD</td>
<td>195</td>
</tr>
<tr>
<td>13.4.2 Running the validation tests</td>
<td>195</td>
</tr>
<tr>
<td>13.4.3 Presentation of validation results</td>
<td>197</td>
</tr>
<tr>
<td>13.5 Printing the results of validation</td>
<td>197</td>
</tr>
<tr>
<td>14 Service Check for scanning SPECORD®</td>
<td>199</td>
</tr>
<tr>
<td>14.1 Activating Service Check</td>
<td>199</td>
</tr>
<tr>
<td>14.2 Performing the diagnosis</td>
<td>200</td>
</tr>
<tr>
<td>14.3 Printing the results of diagnosis</td>
<td>201</td>
</tr>
<tr>
<td>14.4 Sending the results of diagnosis by e-mail</td>
<td>201</td>
</tr>
<tr>
<td>14.5 Lamp Check</td>
<td>202</td>
</tr>
<tr>
<td>14.6 Zeroth order</td>
<td>203</td>
</tr>
<tr>
<td>14.7 Beam position</td>
<td>203</td>
</tr>
<tr>
<td>15 User Management and Electronic Signatures</td>
<td>205</td>
</tr>
<tr>
<td>15.1 User Management</td>
<td>205</td>
</tr>
<tr>
<td>15.1.1 Hierarchy and access to functions</td>
<td>205</td>
</tr>
<tr>
<td>15.1.2 Configuration of User Management / Activating the login list</td>
<td>207</td>
</tr>
<tr>
<td>15.1.3 Passwords and login names</td>
<td>212</td>
</tr>
<tr>
<td>15.2 Electronic signature</td>
<td>213</td>
</tr>
<tr>
<td>15.2.1 Setting the signature status</td>
<td>213</td>
</tr>
<tr>
<td>15.2.2 Signing a file</td>
<td>213</td>
</tr>
<tr>
<td>15.2.3 Viewing signatures</td>
<td>214</td>
</tr>
<tr>
<td>16 Additional settings to ensure FDA conformity according to 21 CFR Part 11</td>
<td>215</td>
</tr>
<tr>
<td>16.1 Authorization settings in the operating system</td>
<td>215</td>
</tr>
<tr>
<td>16.2 Additional supporting functions of WinASPECT to achieve FDA</td>
<td>217</td>
</tr>
<tr>
<td>conformation according to 21CFR Part 11</td>
<td></td>
</tr>
<tr>
<td>17 Appendix</td>
<td>219</td>
</tr>
<tr>
<td>17.1 New Features in WinASPECT®</td>
<td>219</td>
</tr>
<tr>
<td>17.2 Statistical calculations</td>
<td>220</td>
</tr>
<tr>
<td>17.3 Determination of sample data and acquisition of reference data</td>
<td>221</td>
</tr>
<tr>
<td>18 Table of figures</td>
<td>225</td>
</tr>
<tr>
<td>19 Index</td>
<td>229</td>
</tr>
</tbody>
</table>
1 WinASPECT

1.1 Described version

The descriptions in this manual are based on the following program versions:

- WinASPECT® 2.3
- WinASPECT® Validation for SPECORD Version 2.3

For an overview of newly added or revised WinASPECT® 2.3 functionalities, you should refer to section "New Features in WinASPECT™" on page 219.

1.2 Notes on the use of this manual

To fully utilize the many options and capabilities of WinASPECT®, please carefully read the instructions given in this manual.

For easy reference and orientation, the manual uses the following symbols and methodology:

- Observe the notes marked in this way to avoid operating errors and obtain correct results.
- Denotes a step of operation.
- Denotes a step of operation that may be applied alternatively to the step of operation described in the preceding paragraph.
- Cross-reference to other sections or illustrations (italic).
- In the description of the operating steps, menu commands, dialog boxes, buttons and options, etc. are formatted in bold characters.
- Menu commands of a command sequence are separated by a slash ( / ), e.g. File / Open.
- Buttons are marked by square brackets, e.g. [Save].

1.3 What is WinASPECT?

WinASPECT® is a modularly designed Windows-based software for the control of UV-Vis spectrophotometers of Analytik Jena AG and for the display and analysis of the results obtained on these instruments.

The instruments include the scanning spectrophotometers with monochromator

SPECORD® 250  SPECORD® 205  Spekol 1300
SPECORD® 210  SPECORD® 50  Spekol 1500
SPECORD® 200  SPECORD® 40  Spekol 2000
and simultaneously measuring spectrophotometers with polychromator setup.

SPECORD® S600.  SPECORD® S300 UVVIS  SPECORD® S300VIS
WinASPECT

What is WinASPECT?

Scanning-type SPECORD®s with a monochromator will be collectively referred to as “scanning SPECORD®” and simultaneously measuring SPECORD®s as “SPECORD® Sxxx” hereafter.

WinASPECT® does not only allow you to control the basic units of the above-mentioned instruments, but also the accessories available for them. Control is performed through device specific drivers that have to be installed additionally. The device drivers fully integrate with the WinASPECT® user interface. If you use several of the above instruments, you may control all of them from one PC. For this, you need only activate the corresponding device driver in WinASPECT® and load a device-specific parameter file. The parameter files may be viewed, edited and saved under WinASPECT®.

WinASPECT® provides GLP-compliant operation (GLP = Good Laboratory Practice). Measurement results may be logged completely.

Data exchange with other Windows applications (e.g. MS Excel) is unproblematic.

The basic package of WinASPECT®, consisting of the measurement module, the file management and the quantitative analysis modules, may be extended by special modules at any time thus allowing optimum customization to your analytical needs. The following special modules are available:

- Quant Routine
- Kinetics
- Data Handling
- Bio module for the evaluation of biochemical analyses
- Water Analysis module for Spectroquant® test kits from Merck
- Validation
- Method programming
- Color measurement
- Film thickness measurement.

WinASPECT® FDA21FR Part11 - Version

The software version WinASPECT® FDA21FRPart11 has been developed to comply with FDA rules. This version additionally includes a user management module and the possibility to sign measured data.

Intended use

WinASPECT® was developed as control, measurement and analysis software for the above-mentioned instruments. The software may only be used in combination with these instruments.

The manufacturer will not accept any liability for problems or damage caused by improper and non-intended use of WinASPECT®.

WinASPECT® and the instrument to be controlled by the software may only be operated by qualified and instructed personnel. The user should be familiar with the contents of this manual and that of the analytical instrument.
1.4 Installation of WinASPECT

Caution!
Administrator-level PC rights are required for installation of WinASPECT®!

1.4.1 System requirements

The use of WinASPECT® requires that your PC meet the following minimum requirements:

- Operating system: Windows 2000 or higher
- Processor: Pentium IV
- Main memory: 256 MB
- Free hard disk space: 40 GB
- Drive: CD-ROM drive
- Screen resolution: 800 x 600

1.4.2 Installation procedure

WinASPECT® is delivered on CD-ROM. The CD-ROM additionally contains the device drivers for the SPECORD® devices listed in Section "What is WinASPECT?" p. 5. The optional modules, such as the Kinetics and Data Handling module, are delivered on 3½” floppy disk.

1. Start your PC and Windows. Should your PC already be running and other applications be open, close all running applications for the installation of WinASPECT®.

2. Insert the WinASPECT® CD-ROM in the CD-ROM drive. On most PCs, the CD-ROM will be automatically started. After a short time, the installation routine will display the following dialog box. If the WinASPECT® CD-ROM does not start automatically, start the preinstall.exe file in the root directory of the CD-ROM.

3. Click on [Install] and follow the prompts of the installation routine.

4. Choose the desired language for the installation.

5. Choose the target folder for the installation of the program files. The default folder is C:\Programs\WinASPECT.

6. In the Select Components dialog box, mark the components to be installed (WinASPECT® software and the device driver of your SPECORD®).

7. Enter the name under which you wish to start the software in the Program Manager group of the Windows Start menu. The default name is WinASPECT.

The following folders will be created for the storage of data:

- Storage of measurement results, parameters and data analyses: Documents and Settings\All Users\Documents\Analytik Jena\WinASPECT and corresponding sub-folders
- Storage of software and device internal settings: Documents and Settings\All Users\Application Data\WinASPECT
The preset folder for the storage of measurement results, parameters and data analyses ensures that all users logged in to WinASPECT® have access to the data according to their privileges.

However, you can change the preset folders when you store any data. The path for the automatic saving of measurement results can be changed in the Measurement Configuration dialog box (menu command Measurement / Measurement Configuration).

1.4.3 Installation of a SPECORD with USB port

Note
Administrator-level PC rights are required for installation of the USB driver.

1. With the SPECORD® switched off and without being connected to the PC install WinASPECT® as described in Section "Installation procedure" p. 7.
2. Afterwards, connect the SPECORD® to the PC via USB port and switch it on.
3. When you are asked for the USB driver, choose the folder Programs\WinASPECT\DriverUSB, or \DriverUSB in the folder you may have chosen for the installation.
5. Use the Measurement / Initialize device menu command for device initialization.

Note
After re-connecting the SPECORD® to another USB port, it may again be necessary to specify the folder that contains the USB driver.

1.4.4 Installation of additional modules

The software of the additional modules

- Kinetics
- Data Handling
- Bio Module for the evaluation of biochemical analyses
- Method programming.
- Validation
- Water Analysis module for Merck Spectroquant® Test Kits
- Methode Programming
- Color measurement
- film thickness measurement

is supplied on CD-ROM.

The installation routine for the software stored on CD-ROM is the same as that used for the installation of WinASPECT®.
1.5 Operation of WinASPECT

1.5.1 General

WinASPECT® is a Windows-based application whose operation corresponds to that of other Windows-based software. That’s why the Windows-typical operating functions are not described in this manual. If you should have any questions regarding these functions, consult your Windows documentation.

1.5.2 Starting / exiting WinASPECT

Starting of WinASPECT

- To start WinASPECT®, on the Windows desktop activate the following menu command: Start / Programs / WinASPECT / WinASPECT.

- If you have the WinASPECT® FDA21FRPart11 (program version with user management and electronic signature), the dialog box for user login will appear. In the textboxes, type your user name and your password. If the User Management should not have been configured yet, enter “admin” for both user name and password.

![User Login dialog box]

Fig. 1-1 User Login dialog box

On doing so, the WinASPECT® desktop will appear.

Exiting WinASPECT®

- Activate the menu command File / Exit.

- If at this time there are still any open document windows that you have just created or edited, the following program query will appear:
Click on [Yes], if you want to save the files.

Save the file(s) as described in Section "Saving document windows" p. 71.

Then, exit WinASPECT® by activating the menu command File / Exit once more.

### 1.5.3 The WinASPECT desktop

On starting WinASPECT® software, the WinASPECT® workplace will appear.

![Fig.1-3 WinASPECT® workplace](image)

The workplace contains the typical elements of Windows-based applications, such as:

- Title bar with the standard buttons for resizing the window and closing the application
- Menu bar
- Toolbar with buttons for quick access to frequently used program functions
- Workplace for documents to be opened (e.g. spectra)
- Status bar at the bottom of the workplace

In addition, the following elements may optionally be displayed:

- Quick-start buttons for greater operating comfort of the SPECORD®
• Continuous display of currently measured value (online measurement)
• Currently selected measurement parameters as background

1.5.3.1 Display of enlarged measurement buttons and active measurement parameters

Choose the display of these elements in the Measurement Configuration dialog box.

- Activate the following menu command: Measurement / Measurement Configuration.
- In the Show in main window field, activate the Parameters and Quick start options.

The quick-start buttons have the following functions:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Start measurement" /></td>
<td>Start command for sample measurement. Alternative menu command: Measurement / Measurement or</td>
</tr>
<tr>
<td><img src="image" alt="Reference" /></td>
<td>Start command for the reference measurement. Alternative menu command: Measurement / Reference Measurement or</td>
</tr>
<tr>
<td><img src="image" alt="Parameters" /></td>
<td>Display and adjustment of measurement parameters. Alternative menu command: Measurement / Set Parameters or</td>
</tr>
<tr>
<td><img src="image" alt="Serial measurement" /></td>
<td>Opens the Serial Measurement dialog box. Alternative menu command: Measurement / Serial Measurement.</td>
</tr>
</tbody>
</table>

**Note**

A continuously running online measurement process performed at a given wavelength can be additionally displayed via measurement buttons (→ "Online measurement" p. 23).

1.5.3.2 Menu bar and toolbar

The software will automatically adapt menu bar and toolbar to the current window contents. They will be extended by menus or buttons, if this is necessary and useful for the documents you have opened. Menus and buttons that are not accessible for the current content of the workplace appear grayed out. The type and scope of functions available under WinASPECT® also depends on the installed device driver.

- **File / Open**
  - Opens a result file.

- **Window / Close all**
  - Closes all document windows
### Operation of WinASPECT

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extras / Options</td>
<td>Opens the &quot;Options&quot; dialog box</td>
</tr>
<tr>
<td>Measurement / Measurement</td>
<td>Starts a sample measurement</td>
</tr>
<tr>
<td>Measurement / Reference</td>
<td>Starts a reference measurement.</td>
</tr>
<tr>
<td>Measurement / Set Parameters</td>
<td>Opens the measurement parameter window.</td>
</tr>
<tr>
<td>File / Save As.</td>
<td>Saves the file under a new name.</td>
</tr>
<tr>
<td>File / Print</td>
<td>Prints the current results.</td>
</tr>
<tr>
<td>Edit / Copy</td>
<td>Copies selected spectra.</td>
</tr>
<tr>
<td>Edit / Paste</td>
<td>Pastes copied spectra in a document window.</td>
</tr>
<tr>
<td>View / Scale</td>
<td>Entry of graph scales via dialog box</td>
</tr>
<tr>
<td>View / Zoom</td>
<td>Defining graph scales by means of the mouse.</td>
</tr>
<tr>
<td>View / Scale</td>
<td>Autoscaling of graphs.</td>
</tr>
<tr>
<td>View / Grid Options</td>
<td>Overlays horizontal grid lines on the graph.</td>
</tr>
<tr>
<td>View / Grid Options</td>
<td>Overlays vertical grid lines on the graph.</td>
</tr>
<tr>
<td>View / Grid Options</td>
<td>Overlays horizontal and vertical gridlines on the graph.</td>
</tr>
<tr>
<td>Edit / Select curve</td>
<td>Selecting and moving a curve from a family of curves.</td>
</tr>
<tr>
<td>Edit / Undo Curve Move</td>
<td>Undoes the curve movement.</td>
</tr>
<tr>
<td>View / Left side (Notes,</td>
<td>Displays or hides the left side of the document window.</td>
</tr>
<tr>
<td>Parameters...)</td>
<td></td>
</tr>
<tr>
<td>Edit / Header</td>
<td>Editing of header data of a file</td>
</tr>
<tr>
<td>Edit / New Textbox</td>
<td>Creates a textbox beside a curve.</td>
</tr>
</tbody>
</table>
1.5.3.3 Help

You may obtain online help on the operation of WinASPECT® via the Help menu. Besides, while working with WinASPECT®, you may press the F1 function key on your keyboard at any time. This will bring up the Help window with information on the currently active dialog box. In addition, the program will show short notes on the toolbar buttons when you move the mouse pointer onto the button.

1.5.3.4 Status bar

The status bar shows information on the current content of the document windows (e.g. absorbance/transmittance values under the mouse pointer, name of folder to which the currently open result file is saved, etc.).

1.5.4 General settings via Extras / Options

WinASPECT® provides possibilities to vary spectrum representation colors on the screen, and, hence, the color of a printout as required to match a specific user environment. You may save a selected color pattern and load it again when required for reapplication. Furthermore, you can choose between German and English as the desktop workspace, or you may compile signature patterns.

EXTRAS / OPTIONS

- Activate menu command Extras / Options or, on the toolbar, click on .

This will bring up the Options dialog box.
On the tabs, choose the desired options and then confirm your choice by a click on the [Set] button on the respective tab each.

1.5.4.1 General tab

On the General tab, choose the language of the user interface and the list separator for data export to ASCII files.

Available languages:
- German / Deutsch
- English / Englisch.

As decimal separator for the automatic export to ASCII or JCAMP files, you can choose between:
- Dot "." 
- Comma ",".

Any one of the following eight modules - if installed - can immediately be loaded, once WinASPECT® has started:
- Quant – Calibration
- Quant – Concentration
- Quant – Routine
- Quant – Formula
- Kinetic
- Bio – Method
1.5.4.2 Data Formats tab

On the **Data Formats** tab, you can define the desired number of decimal places for result presentation of measurements or calculations.

Use the arrow keys beside the quantity to be measured to increase or reduce the number of decimal places.

1.5.4.3 Colors tab

On the left, this tab shows a schematic presentation of a spectral curve. Above it, the name of the currently loaded color scheme appears. Under the spectral curve is a pull-down list box and under the list box, the color palette is displayed.

- **On the list box, select the element of spectrum presentation the color of which you want to change.**
- **On the color palette, click onto the desired color.**
  
  On the "scan" above, the selected element will instantly appear in this color.
- **When you have changed all the desired elements, click on the [Save] button. This will bring up a dialog box where you can enter a name for the selected color scheme and then save it.**
- **With [Load] you can recall a saved color scheme. This will bring up a small dialog box for choosing a saved color scheme.**
- **With [Default] restore the default color scheme.**
- **With [Set] the selected options are instantly applied to the workplace. This also applies if you have not saved the modified color scheme.**

**Note**

To make individualized settings for spectrum colors in a graphical view chart, use the *Edit / Spectrum Properties* menu command of the display menu (→ Section "Sample names, colors and marks for graphic presentation" p. 55).

1.5.4.4 Signature tab

The results of measurements and calculations can be encrypted and signed to comply with FDA requirements. On this tab, you can enter possible signatures (→ Section "Electronic signature" p. 213).

1.5.4.5 Quant tab

On this tab, you can define a value for the coefficient of determination, **R2 adjust** (→ Section "Statistical calculations" p. 220), to be applied to recorded calibration curves. Concentration determination can be based only on calibration curves meeting the criterion defined here.
1.5.4.6 Kinetics tab

On this tab, you can choose the default unit of time for result presentation: Minutes or Seconds.

However, you can change this setting in the Kinetics module individually for every result presentation using the menu command View /Display in minutes (seconds).

1.5.4.7 Fixed Scaling tab

On the Fixed Scaling tab, you can preset the scaling of curve presentation.

If these options have been activated, curves will always be displayed in the selected units and limits of ordinate and abscissa both during measurements in WinASPECT® and after loading (*.dat files only). However, later re-scaling is possible at any time.

If these options have been deactivated, the result curves will appear with autoscaled limits when displayed the first time.
2 Measurements with WinASPECT

WinASPECT® serves as control and analysis software for both the scanning
SPECORD® 40     SPECORD® 250
SPECORD® 50     SPECORD® 210
SPECORD® 205     SPECORD® 200
and the simultaneously measuring spectrophotometers
SPECORD® S600     SPECORD® S300 UVVIS     SPECORD® S300 VIS

Because of the different design of these two types of spectrophotometers, the entry of
measurement parameters is different, too.

In the first section, “General measurement functions”, those commands are described
that are identical for both device types, such as the start of sample or reference meas-
urements and device initialization.

The section "Measurement parameters / Device adjustment for scanning spectropho-
tometers" p. 27 describes the entry of measurement parameters and the software-
assisted device adjustment for this device type. For quickly getting started with the
measurements using scanning SPECORD® models, read section "First measurement
with scanning SPECORD" p. 38.

The entry of measurement parameters for the SPECORD® Sxxx simultaneous spectro-
photometer is described in section "Measurement parameters for SPECORD S" p. 41.
For information on how to measure a survey spectrum, read section "First measurement
with the SPECORD " p. 51.

2.1 General measurement functions

2.1.1 Displays during running measurements

During any type of measurement involving a scanning-type spectrophotometer or any
type of kinetic measurement job performed on a SPECORD® Sxxx, the screen will
display the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Stop]</td>
<td>Stops the measurement.</td>
</tr>
<tr>
<td>![View]</td>
<td>Minimizes the dialog box. The dialog box contains the buttons [Stop] and [View] and, in kinetic measurements, additionally the [Pause] button. A progress bar keeps you informed of the measurement process. To display the dialog box in standard size again, click once more on [View]. Accessible only in time-based measurements (kinetics). A click on this button interrupts the measurement allowing you to open the sample compartment and add, for instance, a starting reagent to the sample. By a click on the now displayed [Continue] button, the measurement is continued.</td>
</tr>
<tr>
<td>![Pause]</td>
<td></td>
</tr>
</tbody>
</table>

WinASPECT® Issue 05/2008 17
Measurements with WinASPECT
General measurement functions

2.1.2 Initialization of the device

When the device is initialized, the connection between PC and SPECORD® is being established. The software checks the spectrometer connected and the loaded parameter file.

In the spectrometer, the spectral lamps are ignited depending on the options selected in the parameter file.

When you use a scanning spectrometer, the monochromator will be driven to a defined start position.

- Activate the menu command Measurement / Initialize Device.

On the screen, the message "Initializing" appears. Afterwards, the device is ready for taking measurements.

If an error occurs in initialization, the system will display an error message.

**Note**

Before fastening the transport lock on scanning SPECORD® models, the device must be initialized to move the monochromator into the correct position.

If in the general measurement settings (Measurement / Measurement Configuration) you activated the Parameters and Quick start options in the field Display in main window, the currently active measurement parameters will be displayed in the background of the workspace, and the dialog box with quick-start measurement buttons inserted.

**Automatic device initialization as part of program start**

Device initialization can be set to run in an automatic background routine as part of a program start procedure.

As a necessary precondition for automated background initialization, the Automatic initialization while launch WinASPECT® option in Measurement / Measurement Configuration must be active.

For powering on, you should observe this order of working steps:

1. Turn SPECORD® on.
2. Trigger WinASPECT®.

2.1.3 Reference Measurement

Reference measurements are intensity measurements (I_{Reference}) taken at the same wavelength or in the same spectral region as in the following sample measurement.

- Start the reference measurement by activating the menu command Measurement / Reference Measurement or by a click on on the toolbar of WinASPECT®.

The program starts recording the correction values. On the screen, a dialog box appears allowing you to follow the process of correction data measurement.

The reference data are stored and taken into account in the calculation of the measured values of your samples. To this end, when using scanning double-beam spectrophotometers, you must have activated the Correction – Reference option in the measurement parameters (→ Section "Settings tab (Scanning SPECORD) " p. 28).
Measurements with WinASPECT

General measurement functions

The thus found reference values are valid only as long as you use the same parameters for your measurements and WinASPECT® remains activated. When you changed the measurement parameters or restarted WinASPECT®, you must run a new reference measurement.

2.1.4 Sample measurement

Before you can take a sample measurement, you must run a reference measurement, or you must have selected the Correction – Standard option (possible only with double-beam scanning spectrophotometers) in the measurement parameter record.

Sample measurements are intensity measurements of the light transmitting the sample \( I_{\text{sample}} \). This intensity is normalized to the reference measurement resulting in the transmission spectrum

\[
T(\lambda) = \frac{I_{\text{sample}}(\lambda)}{I_{\text{Reference}}(\lambda)} \quad \text{or the absorption spectrum}
\]

\[
A(\lambda) = -\lg T(\lambda), \quad \text{respectively.}
\]

Start the sample measurement by activating the menu command Measurement / Measurement or by a click on on the toolbar of WinASPECT®.

The software starts the measurement with the measurement parameters stored in the active parameter file.

On the screen, a dialog box appears allowing you to follow the measurement process.

On completion of the measurement(s), you can view the result files saved under the name specified and edit them.

2.1.5 Serial measurement

The Serial Measurement function facilitates running routine measurements. Based on a predefined measurement program and a corresponding reference measurement, you need only start the individual measurements by the click of a button. The results of the measurements will be stored altogether to a cyclic result file.

Activate the menu command Measurement / Serial Measurement.

This will bring up the Serial Measurement dialog box.
Measurements with WinASPECT

General measurement functions

Fig.2-1 Serial Measurement dialog box

The serial measurement box includes its own menu bar and three card tabs:

- **Measure settings** – shows currently valid measurement parameter settings.
- **Notes** – shows measurement-related note entries.
- **Table** – displays the analytical results of serial measurement.

**Menu functions of the Serial Measurement dialog box**

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>New</td>
<td>Starts a new serial measurement.</td>
</tr>
<tr>
<td>Open</td>
<td>Opens a saved serial measurement.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves the serial measurement under the same name.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the serial measurement under a new name.</td>
</tr>
<tr>
<td>Sign documents</td>
<td>Signs the serial measurement.</td>
</tr>
<tr>
<td>View Signatures</td>
<td>Displays the signatures of the open serial measurements.</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Displays the Audit Trail of the open serial measurement.</td>
</tr>
<tr>
<td>Print</td>
<td>Prints a serial measurement.</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>The results can be printed optionally as table, graph, along with the</td>
</tr>
<tr>
<td></td>
<td>measurement parameters and/or Audit Trail data.</td>
</tr>
<tr>
<td>Close</td>
<td>Copies the results of the serial measurement to the clipboard</td>
</tr>
<tr>
<td></td>
<td>thus making them accessible to other Windows applications.</td>
</tr>
<tr>
<td></td>
<td>Quits the serial measurement and exits the dialog box.</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT

General measurement functions

<table>
<thead>
<tr>
<th>Measurement parameters</th>
<th>Sets measurement parameters.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setup</td>
<td>Sets parameters for serial measurement (e.g. number of samples, sample names, etc.).</td>
</tr>
<tr>
<td>Start!</td>
<td>Starts the sample measurement.</td>
</tr>
<tr>
<td>Reference</td>
<td>Starts the reference measurement.</td>
</tr>
<tr>
<td>Help</td>
<td>Displays online help for serial measurements.</td>
</tr>
<tr>
<td>Close</td>
<td>Quits the serial measurement and exits the dialog box.</td>
</tr>
<tr>
<td>To document</td>
<td>Transfers serial measurement results into a WinASPECT® document window.</td>
</tr>
</tbody>
</table>

Taking serial measurements

The serial measurement is taken with the currently active measurement parameters. These parameters are displayed in the left part of the dialog box.

- Using the menu command **Edit / Measurement Parameters**, you can open the measurement parameters window and load a saved parameter file or select new parameters.

To open the dialog box for the configuration of the serial measurement, activate the menu command **Edit / Setup**. In this dialog box, choose the following settings:

![Serial measurement settings](image)

Fig.2-2 Serial measurement settings
Measurements with WinASPECT

General measurement functions

<table>
<thead>
<tr>
<th>General tab</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
<td>Optional entry of a comment on the measurement.</td>
</tr>
<tr>
<td>Operator</td>
<td>Optional entry of the operator’s name. With the FDA conforming version of WinASPECT®, the logged in user will be entered here automatically.</td>
</tr>
<tr>
<td>Notes</td>
<td>For optional input of a note relating to serial measurement. A note will be saved together with the actual data and can be printed out.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Samples tab</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of measurements</td>
<td>Number of measurements of the current measurement series.</td>
</tr>
<tr>
<td>Automatic sample names</td>
<td>Sample names are generated automatically. No entry of individual sample names before the measurement.</td>
</tr>
<tr>
<td>Table of sample names</td>
<td>Entry of individual sample names. A sample table appears that corresponds to the entered number of samples. You can either enter sample names directly in the table or import them from ASCII files.</td>
</tr>
<tr>
<td>[Import]</td>
<td>Import of sample names from an ASCII file. A click on this button brings up the standard Open dialog box for choosing the desired file. In the import process, one line of the ASCII file corresponds to one sample name.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Extras tab</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result calculation after measurement with</td>
<td>The results of the sample measurement can optionally be multiplied by a Factor, divided by a Divisor or added to a Summand. Enter the value to be used for the calculation in the textbox.</td>
</tr>
<tr>
<td>Automatically save as...</td>
<td>Saves the measurement series under a defined name. A click on the [Choose] button brings up the standard Save File As... window. Choose a name and confirm your choice with [Save].</td>
</tr>
</tbody>
</table>

- If you need a current reference measurement, run this measurement by activating menu command Reference Measurement.
- Start the sample measurement using the Start! menu command.
  The first measurement is being taken. Follow the prompts displayed by the application:
  You will be prompted to insert the next sample. With [OK] you can start the measurement of the next sample. Proceed analogously until the last sample of the series has been measured. At the end of the measurement series, the results appear in the document window.
- The measurement series is concluded with the measurement of the last sample. You can append further series with the same settings by a click on Start!. In this case, sample names are assigned automatically first (Sample 1, Sample 2, etc.).
- You can edit the sample names later. To this end, double-click on the sample name to be edited, and enter the new name. Afterwards, save the file with the new sample names.
To start a new serial measurement with new settings, activate the File / New menu command.

The results of a serial measurement session can also be directly transferred to a WinASPECT® document window for further processing with the help of a To Document command.

2.1.6 Online measurement

With online measurement in active state, the value measured for a specified wavelength will be continuously updated and displayed. Please note that this reading cannot be saved nor can it be printed out.

To have the measured value displayed in online mode, you must turn on the Online measurement option in Measurement / Measurement Configuration.

Scanning SPECORD®'s

Where operation involves a scanning SPECORD®, the value which is measured for a wavelength currently set in the monochromator will always be displayed.

- Open the measurement parameters box. Then select the Wavelengths option and set a desired wavelength of analysis on the Mode register tab.
- Launch a reference measurement sequence.
  As part of reference measurement, the monochromator moves to the position for the wavelength to be analyzed and stops, once it has arrived there.
- Position your samples in the measuring beampath and take the measured reading in the Online field of your desktop workspace.

SPECORD® Sxxx

Where operation involves a simultaneously measuring SPECORD® Sxxx, you can set a desired wavelength directly in the measurement parameters box. To do this, proceed as follows:

- Open the measurement parameters box. Then type a desired value in the Online wavelength entry field of the Mode register tab.
- Trigger a reference measurement sequence.
- Position your samples in the beampath and take the measured reading from the Online field of your desktop workspace.

2.1.7 Setting, saving and loading measurement parameters

2.1.7.1 Setting device-specific parameters

The adjustable measurement parameters are device-specific and depend on the installed device driver.

The available setting options are described in Sections "Measurement parameters / Device adjustment for scanning spectrophotometers", p. 27 and "Measurement parameters for SPECORD S", p. 41.
Measurements with WinASPECT

2.1.7.2 Loading device-specific parameters

You can also load stored measurement parameters and use them for the following measurements.

- Activate the menu command **Measurement / Open Parameter File**.

This will bring up the standard dialog box for opening files. Parameter files have the extension ".par" and are saved to the folder \\WinASPECT\para by default.

- Choose the parameter file you want to use for the measurement and confirm your choice with **OK**.

The measurement parameters saved to the parameter file are being activated and will be applied then to all following measurements.

2.1.7.3 Viewing the current parameters

You can recall the active measurement parameters for viewing without editing being possible. When using the version WinASPECT® FDA21FRPart11, this function allows users with Level 4 privileges to view the currently active parameters.

- Activate the menu command **Measurement / View current parameters**.

This will bring up the Parameters dialog box listing the currently used measurement parameter settings.

2.1.8 Configuration of analytical device and result storage

In addition to the measurement parameters and the type of correction to be used, you must choose options regarding the following items:

- Storage of results
- Automatic export of results
- Automatically launched programs
- Used spectrometer
- Additional displays and buttons for the measurement.

- Activate the menu command **Measurement / Measurement Configuration**.

This will bring up the **Measurement Configuration** dialog box.
Measurements with WinASPECT

General measurement functions

This dialog box provides the following options:

<table>
<thead>
<tr>
<th>List box / check box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Choose device</strong></td>
<td>Select the SPECORD® used.</td>
</tr>
<tr>
<td>List box</td>
<td>If activated, displays the results after the measurement on the screen in a separate document window.</td>
</tr>
<tr>
<td><strong>Show results after measurement</strong></td>
<td>You should always activate this option unless you have activated the “Save results automatically”. If you fail to do so, the results of the measurement will get lost!</td>
</tr>
<tr>
<td><strong>Automatic initialization while launch WinASPECT</strong></td>
<td>Device initialization will begin immediately after the program has started. Please note that powering on must follow a prescribed order: turn power to the SPECORD® on at first, then launch WinASPECT®.</td>
</tr>
<tr>
<td><strong>Online-measurement</strong></td>
<td>Performs continuous measurement at a given wavelength and display measured value on the desktop workspace.</td>
</tr>
<tr>
<td><strong>Save results</strong></td>
<td>On-line measured values will not be saved, nor can they be printed out.</td>
</tr>
<tr>
<td><strong>Save results automatically</strong></td>
<td>Automatic storage of measurement results.</td>
</tr>
<tr>
<td></td>
<td>For that, in the Path textbox, enter the complete path or open the dialog box for opening files by a click on .</td>
</tr>
<tr>
<td></td>
<td>For the assignment of file names, the measurements are numbered consecutively. The software will automatically append the number to the entered file name.</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT

General measurement functions

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Export results to file</td>
<td>Automatic export of the results to an ASCII or JCAMP file. The files are named as described above with the corresponding extension &quot;<em>.csv&quot; or &quot;</em>.dx&quot;. This option is accessible only, if you activated the automatic result saving function.</td>
</tr>
<tr>
<td>Start after measurement</td>
<td>Starts another application after the measurement, e.g. MS Excel. In the corresponding textbox, type the path to the .exe-file of the application to be launched, or choose this file after a click on ![file icon] in the thus opened dialog box. This option is accessible only, if you activated the option for automatic export of results.</td>
</tr>
<tr>
<td>Launch application automatically</td>
<td></td>
</tr>
<tr>
<td>Show in main window parameters</td>
<td>With this option being activated, the current measurement parameters are displayed on the background of the main window. With this option being activated, additionally the three function buttons [Start Measurement], [Reference] and [Parameters] are displayed in the top right corner of the main window. With these buttons, you can start sample or reference measurements or activate the dialog box for setting the measurement parameters.</td>
</tr>
<tr>
<td>Quick start</td>
<td></td>
</tr>
</tbody>
</table>

- After you selected the desired options, exit the dialog box with [OK]. The selected settings remain stored until the next activation of this dialog box.

2.1.9 Dark-current measurement (only on SPECORD® Sxxx)

Dark-current measurements serve to determine the dark current on the diode array. You can select automatic dark-current correction in the measurement parameters. However, for very fast kinetic reactions, it may be more useful to run a separate dark-current measurement.

- Start the dark-current measurement by activating menu command Measurement / Dark Measurement.
2.2 Measurement parameters / Device adjustment for scanning spectrophotometers

2.2.1 Measurement parameters window for scanning spectrophotometers

In the measurement parameters window, choose the settings required for the measurement. You can save the settings to a parameter file. This allows you to create parameter files for different analytical tasks and recall them at any time for a measurement.

Open the measurement parameters dialog box by activating menu command Measurement / Set Parameters.

![Measurement parameters window for scanning spectrophotometers](image)

The dialog box contains a toolbar with labeled buttons as well as four tabs (Settings, Device, Mode, Accessories) for the selection of measurement parameters.

**Toolbar functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="OK icon" /></td>
<td>Confirms the selected parameters for the following measurement(s) and closes the device driver dialog box. The measurement parameters thus become the &quot;current&quot; measurement parameters.</td>
</tr>
<tr>
<td><img src="image" alt="Cancel icon" /></td>
<td>Rejects any previous changes of measurement parameters and closes the device driver dialog box. The changes will not be activated for the following measurement(s).</td>
</tr>
<tr>
<td><img src="image" alt="Open icon" /></td>
<td>Opens a saved measurement parameter file. The <strong>Open standard</strong> dialog box appears. The default path for measurement parameter files is <em>C:\WinASPECT\para</em>.</td>
</tr>
<tr>
<td><img src="image" alt="Save icon" /></td>
<td>Saves the current settings of measurement parameters to the currently active file.</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
Measurement parameters / Device adjustment for scanning spectrophotometers

### 2.2.2 Settings tab (Scanning SPECORD)

![Settings tab](image)

**Title**

Entries in this textbox are optional. In this textbox, enter e.g. a designation for the type of measurement to be taken with this parameter file.

**Cycle Mode**

Here, choose single or cyclic repeat measurements.

The results of cyclic repeat measurements are stored together in cycle files.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Runs a single measurement (normal measuring mode).</td>
</tr>
<tr>
<td>Manual</td>
<td>Runs repeat measurements of a sample.</td>
</tr>
<tr>
<td>Manual</td>
<td>The individual sample measurements are started “manually”.</td>
</tr>
</tbody>
</table>
After every measurement, a dialog box appears allowing you to start another sample measurement or terminate the measurement series.
In this mode, you need not define in advance the number of measurements to be taken in the cycle.

**Automatic**
Runs automatic repeat measurements of a sample.
In the **Number** textbox, type the number of repeat measurements to be run.

**Time controlled**
Time controlled repeat measurements for reaction kinetics.
In the **Number** textbox, type the number of repeat measurements to be run.
In the **Interval time** textbox, enter the desired time interval between successive measurement starts within a measurement series in seconds.
Consider that for the actual measurement a certain time is needed. If the interval time turns out to be too short during the measurement, the program switches over to the Automatic mode and the measurement will then be executed as fast as possible.

---

**Display**
In this field, select the desired ordinate unit and the ordinate range in which the results shall be displayed while the measurement is running.

- Choose the desired option:
  - Transmission
  - Absorbance
  - Energy
  - Reflectance (only if a corresponding accessory is used)

- In the Min and Max textboxes, enter the desired lower and upper limits of the display range.

---

**Note**
The time controlled cycle mode is suitable for kinetic measurements over a spectral range or at several discrete wavelengths. For time-dependent measurements at a single wavelength only, the **Time Scan** mode selectable on the **Mode** tab is more comfortable and better suitable (→Section "Measuring mode: Time Scan" p. 34).

---

**Correction**
In this field, you can choose the type of baseline correction (reference measurement):

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>No</strong></td>
<td>No baseline correction is carried out.</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
Measurement parameters / Device adjustment for scanning spectrophotometers

**Standard**
Not available for SPECORD® 30 and SPECORD® 40.
Standard correction data is used as baseline. This type of correction is suitable only for quick survey measurements.

It is not necessary to run a reference measurement before the sample measurement. On double-beam devices, the samples are to be placed in the sample beam and the reference in the reference beam. On the SPECORD® 50, measurement versus air is possible only due to the device-internal reference beam.

The standard correction is run with defined measurement parameters and empty sample compartment. Because of the differences in the measurement parameters used for standard correction and the following sample measurement and the difference in time between standard correction and sample measurement, this type of correction is less accurate than the Reference correction option!

\((\rightarrow\text{Section "Measurement of Standard baseline correction data" p. 36})\)

**Reference**
A reference is measured before the sample.

This registration of reference data is performed using the same measurement parameters as in the following sample measurement. In most cases, distilled water or the solvent of the sample is used as reference.

\((\rightarrow\text{Section "Reference Measurement" p. 18})\)

**Special**
Uses the data of a saved file as reference data.

The reference file must meet the following requirements:

- The file must have been created with the Correction – None option selected in the parameter file. Any references used must have been placed in the sample beam while the reference beam remains free.

- For every measured value, a correction value must be available.

  Thus, the correction data file may have been created with a data point interval smaller than that used in the later sample measurement. Conversely, however, the correction data file must not have a data point interval greater than that of sample measurement.

- Accessory units partly masking the beam path must already be in place when you measure the reference data.

- In the textbox, type the complete path and file name or click on the [Open] button and choose the file in the standard dialog box for opening files.

2.2.3 **Device tab (Scanning SPECORD)**

On this tab, choose slit width (spectral resolution), the interface for PC connection and the lamp-change wavelength.
Fig. 2-6 Measurement parameters – Scanning SPECORD® - Device tab

**COM Port**

From this list box, choose the COM or USB port of the PC to which the SPECORD® has been connected.

**Slit (adjustable only for SPECORD 200 / 210 / 250)**

Choose the spectral slit width (optical resolution) to be used for the measurement:

<table>
<thead>
<tr>
<th>SPECORD® 200</th>
<th>SPECORD® 210</th>
<th>SPECORD® 250</th>
</tr>
</thead>
<tbody>
<tr>
<td>1; 2; 4 nm</td>
<td>0.5; 1; 2; 4 nm</td>
<td>0.5; 1; 2; 4 nm</td>
</tr>
</tbody>
</table>

**Lamp change (not available for SPECORD 30)**

From this list box, select the lamp to be used for sample measurement or the wavelength, at which the lamp shall be changed.

<table>
<thead>
<tr>
<th>List option / Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>D2E</strong></td>
<td>Uses only the deuterium lamp for the measurement (reduced stray light in measurements in UV region).</td>
</tr>
<tr>
<td><strong>Halogen</strong></td>
<td>Uses only the halogen lamp for the measurement (measurements in VIS region).</td>
</tr>
<tr>
<td><strong>Wavelength</strong></td>
<td>Select the wavelength, at which the system shall switch from deuterium lamp to halogen lamp. The wavelength is selectable in 10 nm intervals between 300 nm and 450 nm. To obtain a good energy distribution throughout the complete spectrum, lamp change at 320 nm is optimal. For DNA/RNA measurements at 320 nm, you should select the lamp change at 400 nm.</td>
</tr>
<tr>
<td><strong>D2E automatically</strong></td>
<td>If this option is activated, the deuterium lamp is ignited already when the device is initialized. Otherwise, the deuterium lamp will be switched on only at the start of a measurement requiring the use of the deuterium lamp. It will remain switched off in measurements in the visible wavelength region.</td>
</tr>
<tr>
<td><strong>HL automatically</strong></td>
<td>The halogen lamp is switched on already at device initialization. Otherwise, the halogen lamp is switched on only at the start of a</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
Measurement parameters / Device adjustment for scanning spectrophotometers

Measurements requiring the halogen lamp.

Note
The SPECORD® 30 only employs a halogen lamp. Therefore, the lamp change options are not accessible in the corresponding device driver.

Simulation mode
With the Simulation mode being active, the software functions can be tested without the SPECORD® connected.

2.2.4 Mode tab (Scanning SPECORD)
On this tab, choose the desired measuring mode. The Meas. mode list box provides the following options:

- Scan Mode
- Step Mode
- Time Scan
- Wavelengths

Depending on the selected measurement mode the appearance of the bottom part of the Mode tab changes and shows only those options (textboxes, list boxes and buttons) that are necessary for this mode.

2.2.4.1 Measuring mode: Scan Mode
In Scan Mode, the grating drive is continuously moving on during the measurement. Spectral measurements are faster in this mode than in "Measuring mode: Step Mode" p. 33.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range [nm]</td>
<td>Wavelength range of the scan. Setting range for SPECORD® 40, 50, 200, 205, 210: 190 nm ... 1100 nm</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT

Measurement parameters / Device adjustment for scanning spectrophotometers

Setting range for SPECORD® 30:
300 nm ... 1100 nm

**Delta lambda [nm]**
Data point interval (step size) in the selected spectral range.
Setting range: 0.1 ... 10 nm

**Speed [nm/s]**
Scanning speed to be used in scanning the spectrum.
Setting range: 0.5 ... 100.0 nm/s

**Integration time [s]**
Display of integration time (measuring time for one measuring point).
The integration time is the quotient of Delta lambda and Speed.
The minimum value possible is 0.02 s. All other values must be an integer multiple of 0.02 s.

---

**Note**
If you selected a combination of Delta lambda and Speed selected that is not useful or possible, the system will display a corresponding message in the field beside the parameters.

---

### 2.2.4.2 Measuring mode: Step Mode

This mode is recommended for analyses requiring high accuracy. In this mode, the spectrophotometer moves to the data points at the selected data point interval. With the grating drive stopped, the system measures the data in reference and sample beam. When the measurement is finished, the grating drive moves to the next data point. This procedure is repeated until all data points of the selected wavelength range have been measured.

Due to the measurements being taken with the grating drive stopped, high wavelength accuracy is obtained in scanning the spectrum. Therefore, this mode is particularly suitable for scanning very narrow peaks and for running absorbance measurements that require high accuracy.

![Step Mode](image)

**Fig.2-8 Mode tab – Activated Step Mode**

<table>
<thead>
<tr>
<th><strong>Parameter</strong></th>
<th><strong>Description</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Range [nm]</strong></td>
<td>Wavelength range for the scan.</td>
</tr>
<tr>
<td></td>
<td>Setting range for SPECORD® 40, 50, 200, 205, 210: 190 nm ... 1100 nm</td>
</tr>
<tr>
<td></td>
<td>Setting range for SPECORD® 30: 300 nm ... 1100 nm</td>
</tr>
</tbody>
</table>
**Measurements with WinASPECT**

Measurement parameters / Device adjustment for scanning spectrophotometers

**Delta lambda [nm]**  
Data point interval (step size) in the selected spectral region.  
Setting range: 0.2 ... 20 s

**Integration time**  
Time for measuring a data point.  
Setting range: 0.04 ... 10.0 s

### 2.2.4.3 Measuring mode: Time Scan

In this mode, you may measure a sample repeatedly at a fixed, preselected wavelength.

![Time Scan](Figure 2-9 Mode tab – Activated Time Scan)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
</table>
| **Wavelength [nm]** | Wavelength to be used.  
Setting range for SPECORD® 40, 50, 200, 205,210  
190 nm ... 1100 nm  
Setting range for SPECORD® 30  
300 nm ... 1100 nm |
| **Wait time [s]** | The wait time is the delay between the release of the measurement and the first actual measurement.  
This time can be used as reaction time after the addition of the starting reagent for a kinetic measurement. |
| **Integration time [s]** | Time for measuring a data point.  
Setting range: 0.04 ... 50.0 s |
| **Measuring time** | The total measuring time can be subdivided into maximally four partial periods. For every partial period, you can define the measuring times and the integration times individually.  
The measuring time is the time used for one partial period. It can be specified in seconds or minutes (to be selected from the corresponding list box). |
| **Data points [s]** | List boxes for selection of temporal "data point interval". This parameter indicates the time after which the next measurement is started.  
Setting range: 0.2 ... 50.0 s  
You can also left-click on the boxes and enter any desired time via the keyboard. |
In kinetic measurements, after activation of menu command **Measurement / Measurement** or a click on , first the system will make the necessary device settings (driving to measurement wavelength, checking the reference, etc.). The actual measurement or wait time (see above) begins only after you confirmed the program query "**Start time cycle? [OK]**". Thus, there is sufficient time left for preparing the sample, such as the addition of a starting reagent.

---

**Note**

When you select the **Time Scan** mode, a cycle mode (automatic, time controlled) previously selected on the **Settings** tab will be deactivated.

---

### 2.2.4.4 Measuring mode: Wavelengths

This measuring mode allows the measurement at up to ten preselected wavelengths.

<table>
<thead>
<tr>
<th>Buttons / textbox</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Add]</td>
<td>Adding a wavelength to the list. By a click on the [Add] button, a textbox appears for the entry of another wavelength. When you confirm the entry with the ENTER key, the wavelength is added to the list.</td>
</tr>
<tr>
<td>[Edit]</td>
<td>Editing a wavelength selected on the list. By a click on the [Edit] button, a textbox appears allowing you to edit the selected wavelength. When you confirm the action with the ENTER key, the wavelength on the list will be corrected accordingly.</td>
</tr>
<tr>
<td>[Remove]</td>
<td>Deleting a selected wavelength from the list. On activation of the [Remove] button, the wavelength will be instantly deleted from the list.</td>
</tr>
<tr>
<td>Integration time [s]</td>
<td>Time used for measuring a data point. Setting range: 0.04 ... 50.0 s</td>
</tr>
</tbody>
</table>

---

**Note**

The system accepts wavelengths with one decimal. If you enter wavelengths with more than one decimal, the software will round the wavelength up or down to one decimal.
2.2.5 Accessories tab (Scanning SPECORD)

On this tab, you can choose the accessory to be used for the measurement from the corresponding list box. For a detailed description, read the user’s manuals of the accessories. The measurement parameter options are also explained in online help.

2.2.6 Wavelength correction and standard correction on scanning spectrophotometers

2.2.6.1 Wavelength Correction

The **Wavelength Correction** function allows the correction of variations of the adjustment of wavelength accuracy of the spectrophotometer without the need for mechanical manipulations inside the instrument. Such variations may be caused by transportation of the instrument or major temperature differences.

On the completion of the wavelength correction, the system automatically determines the gain stages for the individual lamps and filter regions and carries out a standard correction (only with double-beam instruments).

The wavelength correction procedure depends on the device type used. Therefore, it is accessible only after initialization of the device.

---

**Note**

Do not start wavelength correction unless the device has warmed up for about two hours after switch-on of the deuterium lamp.

---

**MEASUREMENT / WAVELENGTH CORRECTION**

- Remove any accessory or samples from the beam paths of the SPECORD®. The beam paths must be completely free.
- Start the wavelength correction by activating menu command **Measurement / Wavelength Correction**.

The wavelength correction is being started. The wavelength correction is automatically followed by standard correction and the check of the gain stages of diode detectors for the individual spectral and filter ranges.

- On completion of the wavelength correction procedure, exit WinASPECT® and re-start the program.
- Again, initialize the device.

That way, the new adjustment parameters are transferred to the SPECORD®.

2.2.6.2 Measurement of Standard baseline correction data

*(not available on SPECORD® 40)*

In place of a reference measurement run before the sample measurement, the Standard correction option can be used as reference for **survey measurements**.

This baseline correction is available for double-beam spectrophotometers and the SPECORD® 50 with internal reference channel. It is not accessible for the SPECORD® 30 and the SPECORD® 40.
The Standard correction data are measured with device-externally defined measurement parameters and stored permanently. It will be valid until you re-run the Standard correction.

The use of the Standard baseline correction offers advantages in terms of time, as in this case the sample measurement is not preceded by a reference measurement. However, this type of baseline correction is less accurate than the Reference correction option because of the possible difference in measurement parameters used for correction data measurement and sample measurement. Therefore, the Reference correction option should always be preferred.

We recommend you to use the Standard correction option only for quick survey measurements where high accuracy of results does not matter.

- Remove any accessory or samples from the beam paths of the SPECORD®. The beam paths must be completely free.
- Activate the menu command Measurement / Standard Correction.

The program starts recording the standard correction values. On the screen, a dialog box appears allowing you to follow the course of standard correction.

The Standard baseline will be used as reference, if you have activated the Correction - Standard option.
2.3 First measurement with scanning SPECORD

In this section, a survey spectrum of a sample is measured as an example for a first "acquaintance" with the operation of the SPECORD®. Beginning with the switch on of the device (preparation for measurement) through the entry of measurement parameters to the reference and sample measurement, all steps are explained in succession.

Which preparations are necessary for a measurement?

If you installed the system, you have already done the following actions:

- SPECORD® and PC have been interconnected by the serial interface cable.
- Both units have been connected to a power outlet and switched on.
- On the PC, WinASPECT® has been loaded.
- You have initialized the SPECORD® and performed a wavelength calibration.

If you have not done these steps yet, make these steps up now. To initialize the device, activate the menu command Measurement / Initialize Device. For the wavelength correction, use the menu command Measurement / Wavelength Correction.

### Note

Before starting the wavelength correction, make sure the SPECORD® and the deuterium lamp have been switched on for two hours already so that the system is thermally stable. The lamps are started when the device is initialized.

If your SPECORD® has not been switched on for two hours already, perform the wavelength correction anyhow, as the existing adjustment will be good enough for our first survey measurement. However, repeat the wavelength correction after two hours to achieve optimum alignment for subsequent "real" sample measurements.

How to set the measurement parameters?

The possibilities of measurement parameter selection are very extensive with the SPECORD® because of the various operating modes, accessories and correction modes available. For a more detailed description of the individual options, refer to the Section "Measurement parameters / Device adjustment for scanning spectrophotometers" p. 27.

- Activate menu command Measurement / Set Parameters and, in the appearing SPECORDxxx -... dialog box choose the following settings and options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Setting / Entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Settings tab</td>
<td></td>
</tr>
<tr>
<td>Title</td>
<td>Enter a title of the measurement (optional), e.g. survey measurement</td>
</tr>
<tr>
<td>Cycle Mode</td>
<td>None</td>
</tr>
<tr>
<td>Display</td>
<td>Absorbance</td>
</tr>
<tr>
<td>Min.</td>
<td>0</td>
</tr>
<tr>
<td>Max.</td>
<td>4</td>
</tr>
<tr>
<td>Correction</td>
<td>Reference</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
First measurement with scanning SPECORD

<table>
<thead>
<tr>
<th>Device tab</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Lamp change at</td>
<td>320°</td>
</tr>
<tr>
<td>D2E automatically</td>
<td>Activated (check mark)</td>
</tr>
<tr>
<td>COM Port</td>
<td>COM port of your PC to which the SPECORD® has been connected.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mode tab</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Meas. mode</td>
<td>Scan Mode</td>
</tr>
<tr>
<td>Range [nm]</td>
<td>190.0 – 1100.0</td>
</tr>
<tr>
<td>Delta lambda [nm]</td>
<td>2.0</td>
</tr>
<tr>
<td>Speed [nm/s]</td>
<td>20.0</td>
</tr>
<tr>
<td>Integration time [s]</td>
<td>0.10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Accessories</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Accessory</td>
<td>none</td>
</tr>
</tbody>
</table>

Then, save the selected measurement parameters:

- Click on the [Save as...] button to open the Save standard dialog box.
  The default path for parameter files is \WinASPECT\para.
- Enter "Survey" as file name and confirm the entry with [Save].
- Exit the SPECORDxxx device driver dialog box with [OK].

On doing so, the parameter file just created will be automatically activated and is available for the measurements to follow.

**How to run a reference measurement?**

- Place the reference cell in the sample beam path of the spectrophotometer. On double-beam spectrophotometers, this is the front beam.

---

![Sample compartment with sample beam path](image)

Fig.2-11 Sample compartment with sample beam path
Measurements with WinASPECT
First measurement with scanning SPECORD

- Activate the menu command Measurement / Reference or click on on the toolbar.

The reference measurement is immediately being started.

How to start the sample measurement?

- Place the sample cell in the sample beam path.

- Activate the menu command Measurement / Measurement or click on on the toolbar.

The sample measurement is immediately being started. The results of the measurement appear in a separate document window. You can learn more about the properties of document windows in Section "Properties and functions of document windows" p. 53.
2.4 Measurement parameters for SPECORD Sxxx

This section with related sub-sections describes settings that are valid for:

- SPECORD® S600
- SPECORD® S300 UVVIS
- SPECORD® S300 UV.

In the measurement parameters window, choose the settings required for the measurement. You can save the settings to a parameter file. This allows you to create parameter files for different analytical tasks and recall them at any time for a measurement.

Open the measurement parameters dialog box by activating menu command Measurement / Set Parameters.

2.4.1 Menu functions available in SPECORD Sxxx measurement parameter box

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Checkmark]</td>
<td>Confirms the selected parameters for the following measurement(s) and closes the device driver dialog box. The measurement parameters thus become the &quot;current&quot; measurement parameters.</td>
</tr>
<tr>
<td>![Close]</td>
<td>Rejects any previous changes of measurement parameters and closes the device driver dialog box. The changes will not be activated for the following measurement(s).</td>
</tr>
<tr>
<td>![File Open]</td>
<td>Click this button to open a saved measurement parameter file. This will bring up the Windows standard dialog for opening files. Default path for measurement parameter files: \WinASPECT\para\</td>
</tr>
<tr>
<td>![File Save]</td>
<td>Saves the current settings of measurement parameters to the currently active file.</td>
</tr>
<tr>
<td>![File Save As]</td>
<td>Saves the current settings of measurements parameters to a new file. This will bring up the Windows standard dialog box for saving files, where you can choose a new name.</td>
</tr>
<tr>
<td>![Help]</td>
<td>Opens the Online Help on measurement parameter settings.</td>
</tr>
<tr>
<td>![Page Layout]</td>
<td>Opens the dialog box for setting the page layout. (→ Section &quot;Printing files&quot; p. 69)</td>
</tr>
<tr>
<td>![Printer Setup]</td>
<td>Opens the dialog box for selecting printer-specific options.</td>
</tr>
<tr>
<td>![Preview]</td>
<td>Opens a dialog box with a preview of the printout.</td>
</tr>
<tr>
<td>![Print]</td>
<td>Starts the printout of measurement parameters.</td>
</tr>
</tbody>
</table>
2.4.2 General tab (Measurement parameters SPECORD Sxxx)

**Title**

In this textbox, enter e.g. a designation for the type of measurement to be taken with this parameter file. Entries in this textbox are optional.

**Operator**

Optional entry of the operator's name. With the FDA conforming version of WinASPECT®, the logged in user will be entered here automatically.

**Display during measurement**

In the **Display during measurement** field, select the desired ordinate unit and the ordinate range in which the results shall be displayed while the measurement is running:

- Transmittance
- Absorbance
- Reflectance
- Energy

Display of results during the measurement:

**No**

No spectra/measured values will be displayed during the measurement. Instead of this, the following message will be flashing: „Measurement in progress, please wait...“.

**User defined**

Spectra/measured values will be displayed within the abscissa and ordinate limits specified. Enter the limits in the accessible textboxes.

**Auto scale**

Scale limits are matched to the obtained results during the measurement.
2.4.3 Device tab (Measurement parameters SPECORD Sxxx)

Basics

The integration time is the time required to read out the photodiode array. Hence, the minimum integration time is the shortest time possible to read out the photodiode array. The shorter the integration time, the less time is left for the photodiodes to capture the light intensity of the sample beam. Consequently, the signal size is reduced and the signal-to-noise ratio correspondingly worse. By contrast, a too long integration time will result in an intensity exceeding the level that the photodiode can capture. The photodiodes are overdriven and the found transmittance or absorbance data are wrong. For this reason, it is advisable to use the Monitor function in order to determine the optimum integration time.

On the Device tab, choose the integration time, lamp switching options and the PC interface.

<table>
<thead>
<tr>
<th>Integration time (ms)</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accumulation</td>
<td>5</td>
</tr>
<tr>
<td>Safe current comp.</td>
<td></td>
</tr>
<tr>
<td>Shutter always open</td>
<td></td>
</tr>
</tbody>
</table>

Lamp switching:
- Lamp selection:
  - D2E+HL
- D2E lamp automatically switched on

Interface:
- USB
- CD-ROM

Simulation mode:
- Active

Fig.2-13 Measurement parameters for SPECORD® S600 – Device tab

Integration time and accumulation

Integration time
Adjust the integration time using the arrow keys. The minimum integration time possible is 2 ms. Using the Monitor mode, you can automatically search for the integration time for the given wavelength region.

Accumulation
Number of repetitions of the individual measurement. The measured values of the selected spectral regions are averaged from the total number of individual measurements and the obtained result displayed. The accumulation of individual measurements serves to improve the signal-to-noise ratio.

[Monitor]
Switches to the real-time display of the current energy curve. The display is needed to find the appropriate integration time.
Measurements with WinASPECT

Measurement parameters for SPECORDP PSxxx

Dark current correction
If this option has been activated, a dark current measurement will be carried out before every reference or sample measurement. This option should always be activated unless the measurement is very time-critical, such as fast kinetic reactions in milliseconds range.

If you have not activated continuous dark current correction, this correction must be run before starting the sample measurement by activating menu command Measurement / Dark Measurement.

Shutter always open
If activated, the shutter remains open during the measurement. This option can be activated for very fast kinetic reactions.

Note
The measuring time is calculated from: Integration time x Accumulation.

Lamp switching

Lamp selection
Select the lamp combination to be used for the measurement:

- D2E Deuterium lamp for the UV region
- D2E +HL Deuterium lamp and halogen lamp together
- HL Halogen lamp only for the visible region

D2E-lamp automatically switched on
If this option has been activated, the deuterium lamp will be switched on at the next device initialization. This function will be activated the next time the device is initialized.

Interface
From this list box, choose the PC interface to which the SPECORD® Sxxx has been connected:

USB or COM.

2.4.3.1 Selecting the integration time in Monitor mode

- Switch to the Monitor mode by a click on the [Monitor] button (Device tab).
Measurements with WinASPECT
Measurement parameters for SPECORDP PSxxx

2.4.4 Mode tab (Measurement parameters SPECORD Sxxx)

On the Mode tab, choose the wavelength region or adjust the parameters for kinetic measurements at fixed wavelengths.

- You can adjust the integration time manually with the slider button.
- Click on [Autom.] to start the automatic control of the measured signal for the set wavelength region. During automatic control, the measured signal is controlled to about 95% of the maximum value. With that, the signal-to-noise ratio has been optimized for this measurement. During the automatic control process, the [Autom.] button changes its label to [Stop] allowing you to stop the control process. After the optimum integration time has been found, the label of this button changes to [Autom.] again.
- Confirm the found integration time with [OK]. On doing so, the SPECORD® S600 Monitor display is closed.

Fig.2-14 Monitor display of the current intensity curve of the measured signal I(M)

Fig.2-15 Measurement parameters for SPECORD® S600 – Mode tab
Measurements with WinASPECT
Measurement parameters for SPECORDP PSxxx

<table>
<thead>
<tr>
<th>Spectrum</th>
<th>Measures the complete spectrum between the selected limits.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed wavelengths</td>
<td>Registers the measured values at the selected wavelengths.</td>
</tr>
<tr>
<td></td>
<td>Choose the desired wavelength from the Wavelength list box.</td>
</tr>
<tr>
<td></td>
<td>Then, click on the [+ ] button beside the Choice list. The</td>
</tr>
<tr>
<td></td>
<td>wavelength will be added to the Choice list.</td>
</tr>
<tr>
<td></td>
<td>To remove a wavelength from the list, click on the wavelength</td>
</tr>
<tr>
<td></td>
<td>on the Choice list and afterwards on the [– ] button.</td>
</tr>
<tr>
<td>Two wavelengths</td>
<td>Registers measured values M1 and M2 at the two wavelengths</td>
</tr>
<tr>
<td>and difference</td>
<td>selected and forms their difference M1 – M2.</td>
</tr>
<tr>
<td>Time scan</td>
<td>Runs kinetic measurements at fixed wavelengths.</td>
</tr>
<tr>
<td></td>
<td><strong>In this mode, the time t is plotted on the abscissa.</strong></td>
</tr>
<tr>
<td></td>
<td>Choose the desired wavelength from the Wavelength list box.</td>
</tr>
<tr>
<td></td>
<td>Then, click on the [+ ] button beside the Choice list. The</td>
</tr>
<tr>
<td></td>
<td>wavelength will be added to the Choice list.</td>
</tr>
<tr>
<td></td>
<td>To remove a wavelength from the list, click on the wavelength on</td>
</tr>
<tr>
<td></td>
<td>the Choice list and afterwards on the [– ] button.</td>
</tr>
<tr>
<td></td>
<td>Measurements can be taken with equidistant (→see Section</td>
</tr>
<tr>
<td></td>
<td>&quot;Kinetic measurements with constant measuring intervals&quot;,</td>
</tr>
<tr>
<td></td>
<td>p. 47) or non-equidistant time intervals (→Section &quot;Kinetic measurements with variable measuring intervals&quot;, p. 48).</td>
</tr>
<tr>
<td></td>
<td>On selection of the Time Scan mode, the Interval tab will be</td>
</tr>
<tr>
<td></td>
<td>come inaccessible.</td>
</tr>
</tbody>
</table>

2.4.5 Interval tab (Measurement parameters SPECORD Sxxx)

On this tab, choose the options for repeat measurements. Interval measurements are saved to a common file. The measured values /spectra may later be evaluated also individually.

In interval measurements, also time-controlled ones, always the wavelength λ is plotted as abscissa in result presentation. In user-defined display mode, spectra can be displayed overlaid (→see Section "General tab", p. 42).

**Note**

The time-controlled interval measurement is suitable for kinetic measurements over a defined spectral region.

For time-controlled measurements at fixed wavelengths, choose the Time Scan option on the Mode tab. In this case, the time t will be displayed on the abscissa.
Measurements with WinASPECT

Measurement parameters for SPECORDP PSxxx

Fig.2-16  S600 measurement parameters – Interval tab

<table>
<thead>
<tr>
<th>General</th>
<th>Device</th>
<th>Mode</th>
<th>Interval</th>
<th>Accessories</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Manual</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Automatic</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time controlled</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Start request</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Manual**  
Every repeat measurement is started manually after confirmation of the query „Start next cycle?“.  
The number of repeat measurements need not be defined in advance. The measurement series will be finished, if you do not confirm the query.

**Automatic**  
A pre-selected number of measurements will be repeated without any intermediate program query after the initial measurement start.  
Define the number of automatically repeated measurements in the **Number** list box becoming accessible on activation of this option.

**Time controlled**  
This option is meant for kinetic measurements of spectra or fixed wavelengths.  

**In this measuring mode, the wavelength \( \lambda \) is plotted on the abscissa.**

The setting options for kinetic measurements are described in the Sections "Kinetic measurements with constant measuring intervals", p. 47 and "Kinetic measurements with variable measuring intervals", p. 48.

**Start request**  
With this option activated, the measurement will be started only after confirmation of the program query "Start measurement?".

### 2.4.5.1 Kinetic measurements with constant measuring intervals (Measurement parameters SPECORD Sxxx)

For this type of interval measurement, you can define up to four partial sections with different measuring intervals. To every partial section, you can assign a defined number of repeat measurements and the corresponding interval between successive measurements.

- Choose either the **Time Scan** option on the **Mode** tab (for measurements at fixed wavelengths)  
  or  
  the **Time controlled** option on the **Interval** tab (for measurements over a spectral region).

- Activate the **Equidistant Intervals** option.
Measurements with WinASPECT

Measurement parameters for SPECORDP PSxxx

2.4.5.2 Kinetic measurements with variable measuring intervals (Measurement parameters SPECORD Sxxx)

With this type of interval measurement, the intervals between the measurements are determined by a mathematical term. That way, the intervals can be varied dynamically during the measurement.

Rules for formatting mathematical formulas:

- General operators +,-,*,/.
- Multiplication/division comes before addition/subtraction.
- Unlimited bracketing is not allowed.
- The following functions can be used:

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIN(…)</td>
<td>Sine</td>
</tr>
<tr>
<td>COS(…)</td>
<td>Cosine</td>
</tr>
<tr>
<td>TAN(…)</td>
<td>Tangent</td>
</tr>
<tr>
<td>COT(…)</td>
<td>Cotangent</td>
</tr>
<tr>
<td>ARCSIN(…)</td>
<td>Arc sine</td>
</tr>
<tr>
<td>ARCCOS(…)</td>
<td>Arc cosine</td>
</tr>
<tr>
<td>ARCTAN(…)</td>
<td>Arc tangent</td>
</tr>
<tr>
<td>POW(…….)</td>
<td>Power: x to the power of y</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
Measurement parameters for SPECORDP PSxxx

| SQRT(...)  | Square root |
| MOD(......) | Residual value calculation |
| DIV(...)   | Division by integers |
| ROUND(...) | Rounding function |
| ROUND(......) | Rounding function with specification of decimals |
| TRUNC(...) | Returns integer portion of a DoubleValue |
| LN(...)    | Natural logarithm |
| LOGN(...)  | Logarithm to base N |

In the formulas, (...) stands for any mathematical term. X denotes the current index, which is counted up (number of time intervals).

Example:
Time intervals=5, Start intervals=1, Term=POW(X,2)

Results in:
POW(1,2)+Start interval=2
POW(2,2)+Start interval=5
POW(3,2)+Start interval=10
POW(4,2)+Start interval=17
POW(5,2)+Start interval=26

Choose either the **Time Scan** option on the **Mode** tab (for measurements at fixed wavelengths)
or the **Time controlled** option on the **Interval** tab (for measurements over a spectral region).

Activate the **Non-equidistant intervals** option.

![Non-equidistant intervals option](image)

Fig. 2-18   Entry fields for time intervals

Make the following entries:

**Waiting time (s)**  Delay time between start command and actual start of the measurement. This time can be used as incubation time for a kinetic reaction.

**Time intervals**  Number of intervals.

**Start intervals (s)**  Period of first interval.

**Term**  Mathematical term for the calculation of time intervals
Measurements with WinASPECT
Measurement parameters for SPECORDP PSxxx

<table>
<thead>
<tr>
<th>Interval times (s)</th>
<th>Display of calculated time intervals.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start request</td>
<td>If you activate this option, the measurement will not be started unless you confirmed the program query &quot;Start measurement&quot;?</td>
</tr>
</tbody>
</table>

2.4.6 Accessories tab (Measurement parameters SPECORD Sxxx)

On this tab, you can choose the accessory to be used for the measurement from the corresponding list box. For a detailed description, read the user’s manuals of the accessories. The measurement parameter options are also explained in online help.
2.5 First measurement with the SPECORD Sxxx

In this section, a survey spectrum of a sample is measured as an example for a first "acquaintance" with the operation of the SPECORD® S600. Beginning with the switch on of the device (preparation for measurement) through the entry of measurement parameters to the reference and sample measurement, all steps are explained in succession.

Which preparations are necessary for a measurement?

If you installed the device according to the user’s manual, you have already done the following actions:

- SPECORD® and PC have been interconnected via USB cable.
- SPECORD® and PC have been connected to a power outlet.
- On the PC, WinASPECT® has been loaded and started.
- The SPECORD® has been switched on and initialized.

If you have not done these steps yet, do them now. Start device initialization with the menu command Measurement / Initialize Device.

How to set the measurement parameters?

The extensive options for the selection of measurement parameters for the SPECORD® S600 have been described in more detail in Section "Measurement parameters for SPECORD S", p. 41.

- Activate menu command Measurement / Set Parameters and, in the appearing SPECORD® Sxxx Parameters dialog box, make the following settings:

<table>
<thead>
<tr>
<th>Option/Entry</th>
<th>Settings</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General tab</strong></td>
<td></td>
</tr>
<tr>
<td>Title</td>
<td>Enter a title of the measurement (optional), e.g. survey measurement</td>
</tr>
<tr>
<td>Operator</td>
<td>Enter your name. With the FDA conforming version of WinASPECT®, automatically the logged in user appears here.</td>
</tr>
<tr>
<td>Display</td>
<td>Absorbance</td>
</tr>
<tr>
<td><strong>Mode tab</strong></td>
<td></td>
</tr>
<tr>
<td>from</td>
<td>Choose the start wavelength from the list box (approx. 187 nm).</td>
</tr>
<tr>
<td>to</td>
<td>Choose the stop wavelength from the list box (approx. 1018 nm).</td>
</tr>
<tr>
<td><strong>Device tab</strong></td>
<td></td>
</tr>
<tr>
<td>Integration time</td>
<td>Let the system automatically find the optimum integration time: Click on [Monitor...] to open the SPECORD S600 Monitor dialog box. Click on [Autom.]. The adjustment of the optimum integration time starts. During this process, the [Autom.] button changes to [Stop]. When the adjustment is finished, it changes again to [Autom.]. Finally, confirm the found integration time with [OK].</td>
</tr>
</tbody>
</table>
Measurements with WinASPECT
First measurement with the SPECORD Sxxx

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Accumulation</td>
<td>5</td>
</tr>
<tr>
<td>Dark current correction</td>
<td>Activated.</td>
</tr>
<tr>
<td>Lamp switching</td>
<td>Choose the D2E + HL option from the list box.</td>
</tr>
<tr>
<td>D2E lamp automatically switched on</td>
<td>Activated.</td>
</tr>
<tr>
<td>Interface</td>
<td>USB activated.</td>
</tr>
<tr>
<td>Accessories tab</td>
<td>None</td>
</tr>
</tbody>
</table>

Save the selected measurement parameters:
- To this end, click on [Save as...] to open the Save as standard dialog box. The preset default path is \WinASPECT\ para.
- Enter the file name "Survey” and confirm it with [Save].
- Exit the SPECORD® S600 Parameters dialog box with [OK].

On having done this, the parameter file just created has been automatically activated. It is available now for the following measurements.

How to run a reference measurement?
- Put the cell with the reference into the cell holder in the beam path.

- Activate menu command Measurement / Reference or click on on the toolbar.
The reference measurement is immediately being started.

How to start the sample measurement?
- Put the cell with the sample into the cell holder in the beam path.

- Activate the menu command Measurement / Measurement or click on on the toolbar.
The sample measurement is immediately being started. The results of the measurement appear in a separate document window. To learn more about the presentation of results in WinASPECT®, read the Section “Properties and functions of document windows” p. 53.
3 Properties and Handling of Document Windows

3.1 Properties and functions of document windows

Document windows are windows displaying the contents of analytical result files. This includes major analytical parameters, measured values, measurement curves as well as user-entered information.

Fig. 3-1 WinASPECT® document window

To become familiar with the functions provided for handling document windows, you can open one of the result files stored during the WinASPECT® installation process to the folder "WinASPECT\data".

- Activate menu command File / Open to open a result file that was created with WinASPECT® or Aspect Plus.

3.1.1 Elements of the document window

Document windows contain several tabs.

Left side:

- Samples tab
- Parameter tab
- Audit Trail tab
- Notes tab

Right side:

- Tabs for graphic presentation of measured values
- Values tab
Properties and Handling of Document Windows

Properties and functions of document windows

- **Original Data** tab

  By default, both sides are displayed in the document window. If requested, you can hide the left-hand side from view, so that only the tabs for graphic presentation and the result table remain visible (→ Section "Show/hide left side (Samples, Parameters...)" p. 55).

**Samples tab**

The Samples tab contains a list of all spectra contained in the file that has been opened in the document window. The spectra are listed in the order they were measured.

To select a particular sample spectrum from the family of spectra, click on the respective sample name on the list. In the graph, it will be identified by a thicker line. Alternatively, you can also select a particular spectrum by means of menu function **Edit / Select Curve**. The thus marked spectrum appears in bold letters on the list (→ "Selecting a curve in the graph" p. 61).

**Parameters tab**

The Parameters tab contains the measurement parameters used for recording the spectra of the displayed file.

**Audit Trail tab**

On this tab, automatically all manipulations to the data of the document window will be logged. The information shown here cannot be edited by the user thus ensuring GLP-compliant work.

**Notes tab**

This field serves for displaying remarks regarding the measurement. The remarks are saved as so-called header data along with the spectra.

**Absorbance / Transmittance tabs**

On these tabs, the sample spectra are shown in absorbance, transmittance or in units of energy.

**Values tab**

The **Values** tab lists the measured values. If the document window contains a file with a family of spectra, the measured values of all spectra are listed in a common table.

You can select the unit of data presentation (transmittance or absorbance) from the list box above the table.

**Original Data tab**

On the **Original Data** tab, the original data (after the measurement or loading of a file) are presented unvaried. For the presentation, you can choose between the display of the Values table or the spectral curves.

---

Note

This function is available only with WinASPECT® Version 2.0 or higher. It is not available for results obtained with older versions of WinASPECT®.
3.1.2 Display options for document windows

Further functions for the presentation in document windows are contained on the View menu.

3.1.2.1 Show/hide left side (Samples, Parameters...)

The program allows you to hide the left side of the document window with information on the samples, parameters, Audit Trail record and notes to have a larger screen area available for the graphic presentation of the results.

- Deactivate the menu command View / Left side or click on .
  On doing so, the left side of the document window is hidden.
- To make the left side visible again, click once more on the menu command View / Left side.

3.1.2.2 Show original data

The fourth tab, Original Data, can be displayed optionally.

- Activate menu command View / Show original data. If active, the function is marked by a tick.
  The Original Data tab appears in the document window.
- If you click once more on View / Show original data, the Original Data disappears again.

Following mathematical manipulations, you may undo your most recently implemented data changes by overwriting the respective values with original data.

- Call the Edit / Overwrite with original data menu command.
  Your changes will be deleted and the settings are restored to their initial state.

3.1.2.3 Sample names, colors and marks for graphic presentation

You can define the colors for the spectral curves individually. For additional differentiation, you can mark spectra by labels and different line styles.

In a family of spectra, you can assign individual sample names to the individual spectra. On the printout, the sample names appear in the legend.

- Activate menu command Edit / Cycle Properties.
- Alternatively, right-click on the Samples tab of the document window.

This will bring up the Sample Properties dialog box.
Properties and Handling of Document Windows

Properties and functions of document windows

![Sample Properties dialog box](image)

**Fig. 3-2 Sample Properties dialog box**

<table>
<thead>
<tr>
<th>Button / Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>![OK]</td>
<td>Confirms sample names and marks.</td>
</tr>
<tr>
<td>![Cancel]</td>
<td>Exits sample name entry without saving any changes.</td>
</tr>
<tr>
<td>![Edit]</td>
<td>Importing names from an external source for the selected samples</td>
</tr>
<tr>
<td>![Name from external source]</td>
<td>Marks all curves automatically.</td>
</tr>
<tr>
<td>![Hide marks]</td>
<td>Removes all marks.</td>
</tr>
</tbody>
</table>

The sample spectra listed in the **Sample Properties** dialog box are ordered by the time of measurement.

**Assigning individual sample names**

- In the Sample Properties dialog box, right-click on the line of the table containing the sample to be renamed. On the appearing context-sensitive menu, activate the Sample Name function. This will bring up a small dialog box with a textbox and two buttons.

- In the textbox, type the desired name and confirm the entry by a click on the ![OK] button.

However, you can also enter a new name for all samples by means of an externally stored list (e.g. from Windows Notepad):

- Mark the desired spectrum with the mouse. To select several successive spectra on the list, hold the Shift key depressed while moving the cursor up or down with the arrow keys of the keyboard.

- In the **Sample Properties** dialog box, activate **Edit / Name from external source**. This will bring up the Sample Names dialog box.

- From the **New sample names** list box, choose one of the following options:
Properties and Handling of Document Windows

Properties and functions of document windows

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>From clipboard</td>
<td>Assigns a name to the selected samples from a table copied to the clipboard.</td>
</tr>
<tr>
<td>From ASCII file</td>
<td>Assigns a name to the selected samples from a table in an ASCII file. Click on [Choose] to open the standard dialog box for opening files and choose the desired file there.</td>
</tr>
<tr>
<td>Insert empty lines</td>
<td>Deletes the sample name of the selected sample.</td>
</tr>
</tbody>
</table>

Assigning colors and marks to spectral curves

- In the list of the Sample Properties dialog box, right-click on the desired spectrum.

Beside the mouse pointer, a context-sensitive menu appears with the functions Color and Mark.

Color

- Click on the Color function, if you want to assign a new color to the selected spectral curve. From the appearing toolbar, choose the desired color.

Mark

- Click on the Mark function, if you want to assign a specific line style to the selected spectral curve. From the appearing toolbar, choose the desired line style.
- Alternatively, you can automatically assign different line styles (marks) to all spectral curves by activating menu function Edit / Set all marks.
- To remove the marks again, activate menu command Edit / Hide marks.

3.1.2.4 Scaling spectrum sections

You can change the scale of the graphic presentation in the document window thus enlarging or reducing the displayed spectral curves. You can define the desired spectrum section either interactively with the mouse or digitally by the entry of scale data.

Scaling via dialog box

- Activate menu command View / Scale or click on [ ] on the toolbar.

This will bring up the Scale dialog box.

![Fig. 3-3 Scale dialog box](image)
Properties and Handling of Document Windows

Properties and functions of document windows

For scaling, three modes are available:

<table>
<thead>
<tr>
<th>Mode</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>User</td>
<td>You can define the ranges of abscissa (X) and ordinate (Y) yourself.</td>
</tr>
<tr>
<td></td>
<td>Click on the textbox of the value you want to edit and enter the desired range limits.</td>
</tr>
<tr>
<td></td>
<td>Activate the Automatic check box, if you want the software to set the minimum and maximum values of the spectrum for the abscissa or the ordinate.</td>
</tr>
<tr>
<td>Autoscale</td>
<td>The software automatically adapts the range to be displayed to the minimum and maximum values thus achieving the largest possible scale expansion.</td>
</tr>
<tr>
<td>from 0 to 100%</td>
<td>The software uses predefined values for curve presentation.</td>
</tr>
</tbody>
</table>

**Scaling with the mouse**

- Activate menu command **View / Zoom** or click on on the toolbar. When moved over the graph, the mouse pointer turns into a filled arrowhead with Zoom label.
- With the left mouse button held depressed, draw a rectangle across the graph section to be zoomed in. When you release the mouse button, the **Scale** dialog box appears which was described above.
- If necessary, edit the values and then confirm them with [OK]. The display is updated accordingly.
- To zoom out to the original scaling again, click on .
- By a double click on the graph, the **Scale** dialog box comes up again.

**3.1.2.5 Grid options for graphic presentation**

The graph can be overlaid by a grid or by horizontal and vertical lines that serve for orientation. The spacing between the lines can be automatically calculated or defined by you.

- Activate menu command **View / Grid Options**. This will bring up the **Grid Options** dialog box.
Display Gridlines field

The three option buttons serve to deactivate or activate the presentation of grid lines. Alternatively, you can also use the buttons on the toolbar of the WinASPECT® workplace.

<table>
<thead>
<tr>
<th>Option</th>
<th>Button</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal</td>
<td><img src="image" alt="Horizontal" /></td>
</tr>
<tr>
<td>Vertical</td>
<td><img src="image" alt="Vertical" /></td>
</tr>
<tr>
<td>Horizontal and vertical</td>
<td><img src="image" alt="Horizontal and Vertical" /></td>
</tr>
</tbody>
</table>

Grid Constant field

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Automatic</td>
<td>The software calculates the optimal spacing of grid lines.</td>
</tr>
<tr>
<td>User-defined</td>
<td>If activated, the dialog box is extended by an entry table below the option buttons. In this table, type the desired values.</td>
</tr>
</tbody>
</table>

3.1.3 Editing document windows

3.1.3.1 Editing header information

Header data is file information saved along with the file. For the result printout, you can activate the printing of header data via the Page Layout function.

- Activate menu command Edit / Header or click on ![Edit / Header](image) on the toolbar.

In this dialog box, you can edit the following data:
- Title
- Operator
Properties and Handling of Document Windows

Properties and functions of document windows

- Notes
  The Title and Operator entries used so far appear in the left textboxes.
  - Type the new data in the right textboxes each.

Note

If you use the FDA conf version of WinASPECT®, you cannot edit the operator. In this case, the logged in operator appears in the textbox.

- In the Notes textbox, you can type a text of optional length.
  When exiting the dialog box with [OK], the new entries will be saved. The text typed under Notes appears on the Notes tab of the document window.

3.1.3.2 Copying data to the clipboard

You can copy data from a result file to the Windows clipboard to make it available to other applications, such as Excel.

- Activate menu command Edit / Copy to clipboard.

Using this function, the measured values of the active document window are copied to the clipboard. You can paste them then into other Windows applications.

3.1.3.3 Exchanging measured values between document windows

WinASPECT® allows you to copy spectra from one document window to another one.

If the target document window already contains spectra, the spectra to be inserted must agree in the following parameters:

- Units of ordinate and abscissa
- Data point interval
- Start and end of abscissa range.

- Activate menu command Edit / Copy.

This will bring up the Copy samples dialog box.
Properties and Handling of Document Windows

Properties and functions of document windows

Fig. 3-5  Copy samples dialog box

- From the list of samples, choose the spectra to be copied by a click on the respective check boxes (tick).

- To select all spectra of the list simultaneously, click on the button. With the button, you can uncheck all check boxes simultaneously.

- Confirm your choice with [OK].

The dialog box is closed.

- Activate menu command Edit / Paste.

The selected spectra are inserted in the target window.

Note

To paste spectra in a blank document window, open a blank document window first by activating menu command File / New. Insert the selected spectra in this window as described above.

3.1.3.4 Selecting a curve in the graph

The software allows you to select and mark individual spectral curves in a document window displaying a family of spectra, created e.g. as a result of a cyclic measurement.

- On the Samples tab of the document window, click on the sample to be selected.

The selected curve is marked in the graph by a thicker line.

Alternatively, you can activate menu command Edit / Select Curve or click on the button on the toolbar.

Move the mouse pointer across the graph. The mouse pointer turns into cross hairs with DET label (for detection).

Mark the desired curve by a mouse click.

Another alternative is provided by the selection via the Values tab.
Properties and Handling of Document Windows

Properties and functions of document windows

- Mark the curve by clicking on the respective measured value of the curve of interest in the table.
- By right-clicking on the graph, the selection is undone again.

If with closely adjacent curves you want to make the course of the selected curve better visible, you may shift the curve along the ordinate.

- Activate the button.
- Click on the curve to be selected and holding the mouse button depressed move it to the desired place.

This action does not change the original spectral data.

![Graph showing shifted spectrum]

Fig. 3-6 Selected spectrum was shifted

To undo the curve shift, activate menu command Edit / Undo Curve Move or click on the button on the toolbar.

The shifted curve is inserted correctly again giving the family of spectra its original appearance.

3.1.3.5 Insertion of textboxes in a graph and textbox management

A textbox is a text frame that may be positioned in the graph and varied in size. A reference line drawn from the textbox can point to a feature, e.g. a peak, in the graph. That way, you can add notes to the graph regarding details of the spectral curve. These notes are stored together with the result file and printed (→ Fig. 0-7, p. 62).
Properties and Handling of Document Windows
Properties and functions of document windows

Inserting textboxes

- **EDIT / NEW TEX**
  - **T**

* Activate menu command Edit / New Textbox or click on the toolbar. The mouse pointer turns into cross hairs with T label (for text).

* Move the mouse pointer to the feature of the spectral curve for which you want to create a note. Click and holding the mouse button depressed move the mouse to the place, where the textbox shall appear. Then, release the mouse button. The textbox appears with program-internal numbering (Textbox0) and blinking text cursor.

* Replace the text by the desired note.

Changing the size of the textbox

- Move the cursor across the horizontal or vertical outlines of the textbox. The cursor changes to a double-headed arrow.

- While the arrow is visible, press and hold the left mouse button and move the outline into the desired direction. Then release the mouse button.

Moving the textbox

- If you want to move the textbox completely, double-click on it. The cursor turns into a four-headed arrow with the textbox “stuck” to it.

- Move the cursor to the desired place and click once more to let the textbox go. In doing this, the origin of the reference line remains unchanged.

Managing textboxes

Textboxes are managed in a separate dialog box. It is possible to delete selected textboxes or digitally define the initial coordinates of the textbox.

- **EDIT / MANAGE TEX**
  - **TEXTBOXES**

* Activate menu command Edit / Manage Textboxes. This will bring up the Manage textboxes dialog box.

![Manage Textboxes dialog box](image)

Fig.3-7 Manage Textboxes dialog boxes
Properties and Handling of Document Windows

Properties and functions of document windows

- From the Textbox list box, select the textbox you want to delete or whose initial coordinates you want to change.
  In the Page and Content fields, information is displayed on the tab where the textbox was created or on the contents of the textbox. Editing the textbox content is not possible here.

- To delete the textbox, click on the [Delete] button.

- If you want to change the initial coordinates of the textbox (not those of its reference line!), click on the [Edit] button.
  This will bring up the Editing of initial coordinates dialog box.
  Type in the desired initial coordinates (top left corner of textbox) and confirm them with [OK].

### 3.1.4 Defining a section of a spectral curve

The program allows you to define a section of a measurement curve, which will then be displayed enlarged. The regions of the measurement curve lying outside the defined section will be deleted from the document.

**Edit / Section**

- Activate menu command Edit / Section or click on on the toolbar.
  The mouse pointer turns into a vertical line with "Range" label.

- Click on the left or right boundary of the abscissa range to be cut out and holding the mouse button depressed move the mouse to the other boundary. Release the mouse button.

  The graphic presentation is instantly updated. Now, only the selected section of the measurement curve is visible. The other sections are deleted from the document.

### 3.1.5 Obtaining time-based data from a cyclic spectrum

To obtain time-based data, a so-called time section is applied to a family of curves at a particular wavelength. The three-dimensional data (absorbance data as a function of wavelength and time) is presented two-dimensionally for the selected wavelength. The resulting curve shows the change in absorbance versus time at the selected wavelength.

**Edit / Time-based data**

- Activate menu command Edit / Time-based data or click on on the toolbar.
  The mouse pointer gets an additional vertical line that extends across the entire ordinate range. The line is movable along the abscissa.

- Move the line to the place of the spectrum, from which the time-based data shall be collected. There, click the left mouse button.

  The program reads the ordinate values of the various measurement curves at this point and transfers them to a new document window.
  The new document shows the course of the measured values as a function of time.

---

**Note**

You can then evaluate the files created with this function in the Kinetics module.
3.1.6 3D-representation of a flight of spectra

A 3D-view is available for spatial representation of a flight of spectrums.

- Use File / Open in WinASPECT® to open a file containing a flight of spectrums.
- Select Edit / 3D view menu command.

The dialog window will display the flight of spectrums in 3D view.

Fig. 3-8 3D-view of flight of spectrums

This 3D-view can be tilted, rotated, repositioned or magnified by any user-selected amount.

- Activate option Position, angle, zoom.
- Move slide controllers for direction options, using the mouse, or enter a desired value directly at the input fields.

A section line may be drawn through the flight of spectrums in interactive mode (→ section "Obtaining time-based data from a cyclic spectrum" p. 64).

- Activate option Cut-direction Z.
- Click into the graphic. Move the mouse pointer onto the wavelength where the cut is to be placed, while keeping the mouse key depressed. Release the mouse key again when ready.
  - To help you make your selections, a small window provides a schematic view of the currently selected cut line at the same time.
- Answer [Yes] to the "Create new document ..." query.
  - The document containing the desired cut will be displayed in a newly opened window.

The currently selected 3D-view of a flight of spectrums can be printed.
Properties and Handling of Document Windows

Properties and functions of document windows

- Select **Print / Preview** menu command in the **3D view** dialog window to open the print preview box. Then trigger printing here.

- Alternatively, you can directly open the 3D-view window with the help of a **Print / Print** menu command.

### 3.1.7 Multi-spectrum overlay mode

Spectrum-related data of different measurements can be displayed in overlaid fashion in a co-shared document window. Each individual spectrum is organized as a file for this purpose.

Necessary preconditions for this mode of graphical representation are:

- all spectrums use the same dimension for abscissa and ordinate
- have identical starting and end values of their abscissa
- include the same number of points measured (same point-to-point distance)

**FILE / OVERLAY**

- Select the **File / Overlay** menu command. A dialog window with this name will open.

- Use **[Add]** to open the **Open** standard dialog. Mark all files you want to superimpose onto each other. To achieve multiple-marking, keep **Strg** or **shift** key depressed.

- Confirm your selections with **[Open]**. The selected file names will be displayed in the first list field of the **Overlay** dialog.

- Repeat this selection procedure, until the list field comprises all desired files.

- To remove a file from the list, mark this file and confirm your selection with **[Remove]**.

- Use **[Target file]** to open the **File save as...** standard dialog.

- Enter a file name to the new file and confirm your entry with **[OK]**.

- Exit the **Overlay** dialog window with **[OK]**. All selected spectrums will be displayed in a co-shared document window.

### 3.1.8 Signing measured data and showing signatures

In the FDA conf version of WinASPECT®, it is possible to sign files. With this action, the signing user finishes the work on a file.

The signing procedure and the available signature options are described in Section "Electronic signature" p. 213.

### 3.1.9 Overwriting measured data with original data

WinASPECT® provides a function that allows you to overwrite data in a document manipulated e.g. by a data handling function with the original data again. That way, the manipulations are completely undone.
Properties and Handling of Document Windows

Properties and functions of document windows

**EDIT / OVERWRITE WITH ORIGINAL DATA**

- Activate menu command **Edit / Overwrite with original data**.
  
The contents of the tabs for the graphic presentation of results and the Values tab are overwritten with the original data of the loaded file.

The functions for the display of original data and the overwriting of manipulated data with the original data are available only with WinASPECT® version 2.0 or higher. Therefore, this function is accessible only for measured data obtained with WinASPECT® 2.0 or higher. If you want to apply this function to older measured data, you must create a new data record of the new file format from the old data.

- Using menu command **File / Open**, load the file in a document window.
- Copy the spectra by activating menu command **Edit / Copy**.
- Activate menu command **File / New** to open a new document window.
- Insert the spectra in the new document window by means of menu command **Edit / Paste**.
- Save the new document by using menu command **File / Save as...**.

Data is now saved in the new WinASPECT® format. The functions for the display of original data and the overwriting of manipulated data are accessible.
Properties and Handling of Document Windows

Handling of document windows

3.2 Handling of document windows

For handling document windows, WinASPECT® mainly uses the standard Windows functions, such as those for opening and saving files, with which you are surely familiar. At any rate, however, you should read the Section Printing files, as WinASPECT® provides a comfortable print menu with a huge number of layout options for the result printout.

The functions for handling document windows are contained in the File and Window menus.

3.2.1 Opening files

3.2.1.1 Opening a saved file

For handling document windows, WinASPECT® uses the standard Windows functions, such as those for opening and saving files, with which you are surely familiar. At any rate, however, you should read the Section Printing files, as WinASPECT® provides a comfortable print menu with a huge number of layout options for the result printout.

The functions for handling document windows are contained in the File and Window menus.

3.2.1.1 Opening a saved file

**FILE / OPEN**

- To display result files that were created with WinASPECT® or Aspect Plus, activate menu command File / Open or click on This will bring up the standard dialog box for opening files. The default path for the selection of result files is \WinASPECT\data.

- If you have saved your results files to another folder, select this folder via the Look in list box.

- Click on the file to be opened, and then on the [Open] button. You may also double-click on the file to instantly open it.

- If you want to open several files simultaneously, hold the CTRL or Shift key depressed while clicking on the desired files.

- If you want to avoid that saved result files are overwritten inadvertently, activate the Open write protected check box.

**Note**

On the File menu, the five result files you opened last are listed. You can open these files by a click on the file name.

The measured values of the file are displayed in the document window. If the file contains several spectra, these are shown in overlaid presentation in one document window.

3.2.1.2 Opening a blank document window

If you want to separately edit a spectrum from a family of spectra, e.g. from a cyclic measurement, you must open a blank document window.

**FILE / NEW**

- Activate menu command File / New.

This will bring up a blank document window.
3.2.1.3 Displaying several files in a single document window

**FILE / OVERLAY**  
WinASPECT® also lets you overlay spectra from different files. Application of this function requires that the spectra agree in the following parameters:

- Abscissa units
- Ordinate units
- Number of data points per cycle
- First measured value
- Last measured value

- Using menu command **File / Overlay** open the standard dialog box for opening files.
- Holding the Ctrl key of the keyboard depressed, click on the files that shall be opened.
- Confirm your choice with [OK].

The spectra of the selected files are overlaid in a single document window.

3.2.2 Printing files

**FILE / PRINT**  
WinASPECT® provides a comfortable print menu for individual configuration of the result printout.

- Open the **Print** dialog box using menu command **File / Print** or by a click on 📄 .

![Print dialog box](image)

**Fig.3-9**  
Print dialog box

In the Print dialog box, you can:

- Choose printer-specific settings ([Printer Setup])
- Create the page layout ([Page Layout]) and open a preview of the printout ([Preview])
- Save and load print parameters ([Save], [Load])
3.2.2.1 Page Layout

To open the **Page Layout** dialog box, click on the corresponding button in the **Print** dialog box.

You can choose the font and font size for header and footer, the title and the contents of the printout.

In the **Contents** field, you can additionally define the grid lines for the printout of spectra.

Header and footer are subdivided each in three fields appearing flush left, centered and flush right on the printout. You can freely edit the contents of these three fields or automatically insert document information by means of the icon buttons:

- **File name**
- **Date of file creation**
- **Number of pages**
- **Title of document**
- **Operator**
- **Date of measurement**
- **Name of parameter file**

- Click on the textbox.
  The text cursor appears inside.

- Click on the desired symbol button.
  In the textbox, a placeholder of the corresponding function appears in the textbox.
  When the document is printed, the placeholder will be automatically replaced by the assigned information, e.g. the current number of the page.

To check the set page layout click on [**Preview**] in the **Print** dialog box.

3.2.2.2 Defining the contents of the printout

The data available for the printout are listed in the middle of the **Print** dialog.

- To select an item for the printout, click on it in the list of **Available Data**. Then, click the [**Add**] button.
  The selected item is appended to the list of Data to be printed.

- To delete an item from the list of **Data to be printed**, click on it. Then, click the [**Remove**] button.
  The respective item will be removed from the list of **Data to be printed**, and will not appear on the printout.
3.2.2.3 Page Preview

The page preview function lets you check the selected settings regarding the contents and the layout of the printout.

- In the Print dialog box, click the [Preview] button. This will bring up the Page Preview dialog box, which is displayed full screen showing the first page of the printout.
- If the printout contains several pages, you can navigate through the printout by using the [Next] and [Back] buttons.
- Using the [Zoom in] and [Zoom out] buttons, you can enlarge or reduce the size of the displayed page in steps of 10% each.
- Alternatively, you can zoom in the page by 10% each by left-clicking on the document. To zoom out again, right-click on the document.
- Another option is to select the desired zoom factor from the Zoom list box.
- To start the printout directly from the Page Preview dialog box, click on the [Print] button. If not, exit this dialog box by a click on the [Close] button to return to the Print dialog box.

3.2.3 Saving and closing document windows

3.2.3.1 Saving document windows

Saving a file under the existing name

FILE / SAVE

- Activate menu command File / Save or click on on the toolbar.

Any changes to the file will be saved under the existing file name.

Saving a file under a new name

FILE / SAVE AS...

- Activate menu command File / Save as.... This will bring up the standard dialog box for saving files.
- Type the new file name and confirm this action with [OK].

Any changes to the file will be saved to a new file. In the title bar of the document window, the new file name appears.

3.2.3.2 Closing a document window

FILE / CLOSE

- Activate menu command File / Close.

The active document window is being closed. If you made any changes to the file, which were not saved yet, a program query will appear asking you, if you want to save the changes.

If you opened several document windows, you need not close them individually.
Properties and Handling of Document Windows

Handling of document windows

- **WINDOW / CLOSE ALL**
  - Activate menu command **Window / Close All** or click on on the toolbar.
  - All document windows opened on the WinASPECT® workplace are being closed. If the file was changed, but you have not saved the changes yet, you will be asked, if you want to do so now.

### 3.2.4 Exporting the contents of document windows

The program provides the export of spectral data to ASCII and JCAMP files.

- **FILE / EXPORT / ASCII**
  - Activate menu command **File / Export / ASCII** or **File / Export / JCAMP** to open the standard dialog box for saving files.
  - Type the desired file name and confirm the entry with [OK].
  - Spectral data is exported to an ASCII or JCAMP file. The file name extension for ASCII files is ".csv" and for JCAMP files ".dx".

  **Note**
  - You can also copy spectral data to the Windows clipboard by activating menu command **Edit / Copy to clipboard**, thus making the data available to other Windows applications (→ Section "Copying data to the clipboard" p. 60).

### 3.2.5 Arranging document windows on the workplace

You can arrange open document windows on the workplace using the functions of the **Window** menu.

- **WINDOW / CASCADE**
  - Using menu command **Window / Cascade**, the open document windows are displayed in a cascading arrangement on the WinASPECT® workplace. The title bars of the document windows remain visible and selectable.

- **WINDOW / TILE**
  - Using menu command **Window / Tile**, the open document windows appear in a tiled arrangement.

- **WINDOW / MINIMIZE ALL**
  - By activating menu command **Window / Minimize All**, the open document windows are minimized to icon size and arranged at the bottom edge of the workplace.
4 Quantitative Analyses (Quant Module)

The Quant module is part of the standard WinASPECT® installation package. It is intended for quantitative evaluation of samples.

The Quant module includes a comprehensive set of calibration models that can be used to establish calibration curves. In addition to determining calibration curves, it can also output the differential amount or the quotient of two measured values, the baseline-corrected bandheight or band area and first-order to fourth-order derivatives.

For calculation of regression, linear regression graphs with and without a constant term and a square regression are available.

Calculation of calibration curves is accomplished in the Calibration submodule. Concentration is the module to evaluate the calibration curves which were calculated via Calibration in terms of concentration or to determine concentration with a known factor.

The Quant-Routine module has been optimized for analytical routine jobs. The module is capable of analyzing for concentration, based on a factor or a calibration curve. However, for calibration purposes, only a calculation process relying on measured values is included. Having triggered a Quant-Routine, the user can execute a method in a defined order of samples, which may include calibration if desired (→ Section "Quant Routine Module" p. 99).

4.1 Calibration

In the Calibration dialog box, you can set up calibration curves by measuring standards or entering the respective calibration data.

![Note](image)

For concentration determinations by means of a factor, directly open the dialog box for concentration determinations by activating the menu function Quant / Concentration and choose the necessary options there.

**QUANT / CALIBRATION**

- Activate the menu function Quant / Calibration.

This will bring up the Calibration dialog box.
Quantitative Analyses (Calibration)

Menu functions of the Calibration dialog box

Fig. 4-1 Calibration dialog box

This dialog box contains two tabs:

- General (parameters) (for choosing the calibration parameters)
- Calculation (parameters) (display of the calculation of calibration parameters)

A calibration curve is saved under a selected name with "*.cf" extension. Signed files receive a "*.cfs" extension. The preset path is \WinASPECT\Calib.

Note
In previous versions, the file extension was "*.cal". Files of this type can equally be opened with the Quant module.

4.1.1 Menu functions of the Calibration dialog box

The calibration dialog box has its own menu bar providing the following functions:

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>File</td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>Creates a new calibration file</td>
</tr>
<tr>
<td>Open</td>
<td>Opens a saved calibration file</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>Copies calibration data to the Clipboard for pasting it into other Windows applications</td>
</tr>
<tr>
<td>Export to ASCII file</td>
<td>Exports calibration data to an ASCII file</td>
</tr>
<tr>
<td>Print</td>
<td>Prints calibration data.</td>
</tr>
</tbody>
</table>
Quantitative Analyses (Calibration)

Setting up a new calibration curve

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Save</td>
<td>Saves any changes to calibration data to the active file. The files with</td>
</tr>
<tr>
<td></td>
<td>calibration curve are saved under the selected name with the extension</td>
</tr>
<tr>
<td></td>
<td>&quot;*.cf&quot;. If the calibration file has been signed, the extension is &quot;cfs&quot;.</td>
</tr>
<tr>
<td>Save as</td>
<td>Saves any changes to calibration data to a new file. Brings up the</td>
</tr>
<tr>
<td></td>
<td>standard dialog box Save as (→ Section &quot;Saving document windows&quot; p. 71).</td>
</tr>
<tr>
<td>Close</td>
<td>Closes the Calibration dialog box.</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Shows Audit Trail list. Modifications to the calibration are logged and</td>
</tr>
<tr>
<td></td>
<td>shown on the Audit Trail list.</td>
</tr>
<tr>
<td>Sign document</td>
<td>Adds a signature to calibration data (→ Section &quot;Electronic signature&quot; p. 213).</td>
</tr>
<tr>
<td>View signatures</td>
<td>Shows the existing signature of an open calibration file.</td>
</tr>
<tr>
<td>To Conc.</td>
<td>Directly switches to the dialog box for concentration analysis. This button</td>
</tr>
<tr>
<td></td>
<td>becomes accessible only after you set up a calibration curve.</td>
</tr>
<tr>
<td>Close</td>
<td>Closes the Calibration dialog box.</td>
</tr>
</tbody>
</table>

4.1.2 Setting up a new calibration curve

- Activate the menu command **Quant / Calibration**.

  This will bring up the **Calibration** dialog box.

  First, enter the calibration parameters and then run the calibration by measuring standards, loading saved measurement data or entering the data.

  **Caution!**

  A calibration curve will be valid only if it at least meets the user-defined coefficient of determination ($R^2$ adjust). If the calibration curve fails to meet this criterion, it will be rejected making impossible any concentration measurements based on it!

  The value for $R^2$ adjust is to be entered in the respective textbox on the **Quant** tab of the **Options** dialog box, (accessible via menu command **Extras / Options**) (→ Section "Quant tab" p. 15).
Quantitative Analyses (Calibration)

Setting up a new calibration curve

4.1.2.1 Entry of calibration parameters

On the General (Parameters) tab, choose the following options:

Designation textbox

- In the Designation text box, you can type a text of maximally 255 characters, which describes e.g. the application of the calibration curve.

Operator textbox

- In this textbox, enter the name of the operator. Entry in this textbox is optional, too.

If you have the version WinASPECT® FDA21CFR Part 11, automatically the registered user will be entered in this textbox. This entry cannot be edited.

Regression Model list box

- From this list box, choose one of the three regression models described below:

<table>
<thead>
<tr>
<th>Math. model</th>
<th>Description</th>
<th>Number of needed standards</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y = b \times x )</td>
<td>Linear regression without absolute term</td>
<td>Minimum: 1</td>
</tr>
<tr>
<td>( y = a + b \times x )</td>
<td>Linear regression with absolute term</td>
<td>Minimum: 2</td>
</tr>
<tr>
<td>( y = a + b \times x + c \times x^2 )</td>
<td>Quadratic regression</td>
<td>Minimum: 3</td>
</tr>
</tbody>
</table>

Calibration Model list box

- From this list box, choose the desired calibration model.

Under the list box, a scheme illustrates the selected calibration model. Consider that depending on the calibration model selected you need the measured values of one to three wavelengths.

<table>
<thead>
<tr>
<th>Calibration Model</th>
<th>Calibration based on:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured value ( M(x_1) )</td>
<td>Ordinate value ( M ) at wavelength ( x_1 )</td>
</tr>
<tr>
<td>Band amplitude between ( x_1 ) and ( x_2 )</td>
<td>Automatically found band maximum between wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Difference ( (M(x_1) - M(x_2)) )</td>
<td>Difference of measured values at wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Quotient ( M(x_1) / M(x_2) )</td>
<td>Quotient of the measured values at wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Area ( (x_1, x_2) )</td>
<td>Area under the band between wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Corr. band amplitude between ( x_1 ) and ( x_2 )</td>
<td>Automatically found, baseline-corrected band maximum between wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Corr. area ( (x_1, x_2) )</td>
<td>Baseline-corrected band area under the band between wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Corr. band ( x_2 ) between ( x_1 ) and ( x_3 )</td>
<td>Baseline-corrected band at wavelength ( x_2 ) between wavelengths ( x_1 ) and ( x_3 )</td>
</tr>
<tr>
<td>Derivative, 1st order (Golay, Savitzky)</td>
<td>Band maximum of the first-order derivative of the spectrum between wavelengths ( x_1 ) and ( x_2 )</td>
</tr>
<tr>
<td>Derivative, 2nd order</td>
<td>Band maximum of the second-order derivative of the</td>
</tr>
</tbody>
</table>
Quantitative Analyses (Calibration)

Setting up a new calibration curve

<table>
<thead>
<tr>
<th>(Golay, Savitzky)</th>
<th>spectrum between wavelengths $x_1$ and $x_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Derivative, 3rd order</td>
<td>Band maximum of the third-order derivative of the spectrum between wavelengths $x_1$ and $x_2$</td>
</tr>
<tr>
<td>(Golay, Savitzky)</td>
<td></td>
</tr>
<tr>
<td>Derivative, 4th order</td>
<td>Band maximum of the fourth-order derivative of the spectrum between wavelengths $x_1$ and $x_2$</td>
</tr>
<tr>
<td>(Golay, Savitzky)</td>
<td></td>
</tr>
</tbody>
</table>

**Derivative option**

- If you decide on using one of the Derivative calibration models, additionally the Derivative dialog box will appear.

- From the **Quantity for calibration** list box, choose the quantity on which the calculation shall be based:
  - Maximum between wavelengths $x_1$ and $x_2$
  - Minimum between wavelengths $x_1$ and $x_2$
  - Maximum/minimum difference in range between $x_1$ and $x_2$.

The graph below the list box illustrates the selected principle.

- Then, from the **Derivative** list box, additionally choose the number of supporting points for the derivation.

**Wavelength 1 ... Wavelength 3 textboxes**

- In these textboxes, enter the measurement wavelengths. The number of textboxes that will be activated depends on the selected calibration model.

- If in the selected measurement parameter file you activated the **Wavelength** mode, the first three wavelengths of the parameter list will be automatically inserted in the textboxes.

**Interactive entry of wavelengths**

Alternatively, you can also select the wavelengths from a stored spectrum with the mouse.

- Click on the **[Interactive]** button.

The Calibration dialog box disappears and the standard Open dialog box for opening files appears.

- In this dialog box, select the file(s) from which you want to choose the wavelength(s).

Opening the file(s) brings up a document window with the scan. If you opened several files, they will appear in overlaid presentation.

Additionally, a small window, **Wavelength selection**, is being inserted.

The WinASPECT® toolbar is extended to the right by the following function buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Activate/Deactivate" /></td>
<td>Activates/deactivates the wavelength selection mode.</td>
</tr>
<tr>
<td></td>
<td>With this mode deactivated, you can zoom in the spectral region of interest.</td>
</tr>
<tr>
<td><img src="image" alt="Select First Wavelength" /></td>
<td>Selection of first wavelength.</td>
</tr>
<tr>
<td><img src="image" alt="Select Second Wavelength" /></td>
<td>Selection of second wavelength.</td>
</tr>
</tbody>
</table>
Quantitative Analyses ( Calibration)
Setting up a new calibration curve

Selection of third wavelength.

- To select the wavelengths, move the line cursor (Wave 1 ... 3) to the desired wavelength in the spectrum and click the left mouse button.
  The selected wavelength appears in the Wavelength selection window as Wavelength 1. You may repeat this procedure as often as necessary.
- Depending on the selected calibration model, repeat this process for the selection of Wavelengths 2 and 3. To this end, click the appropriate button of the toolbar first. Alternatively, you can also switch between the wavelengths to be selected by a click with the right mouse button.
- When you have finished interactive wavelength selection, click on [OK] in the Wavelength selection window.

On doing so, the windows are closed and the selected wavelengths appear in the Wavelength textboxes of the Calibration dialog box.

Calibration unit textbox

- In this textbox, enter the desired unit of concentration.

Ordinate list box

- From this list box, choose whether the ordinate values shall be determined in transmission or absorbance units.

Pathlength textbox

- In this textbox, type the used pathlength of the cell (optional).
  The value entered here is for information only about the used cell. It is not used for any calculations.

No. of standards textbox

- Enter the Number of standards with different concentrations to be used.
  The minimum number of standards depends on the selected regression model.

Note

If on the General Parameters tab you specified a parameter file with activated Cell Changer or Autosampler option, the number of samples chosen in the parameter file will be automatically transferred to the Number of standards textbox. You may however edit the number here.

Measure standards check box / Parameter File textbox

The standards needed for the calibration can be determined from both stored data, which will be the normal procedure, and from a direct measurement.

- Activate this check box if you want to measure the standards for the calibration instead of loading them from a file.
- In the Parameter File textbox, enter the name of the parameter file to be used for the measurement of all standards. You may also select the parameter file after acti-
Quantitative Analyses (Calibration)

Setting up a new calibration curve

vaternion of the [Choose] button. This will bring up the standard dialog box for opening files.

4.1.2.2 Entry of standard data

- After you made all necessary entries in the Calibration dialog box, click on the [Standards] button.

This will bring up the Standards dialog box.

- If you intend to measure the standards repeatedly, click on

On doing so, the dialog box will be extended by the two tables of the measurement series and the statistical data from the measurement series.

The dialog box contains three table panes:

- Standards: Name, concentration value and the source of the value
- Measurement cycles: Measured values or manually entered values
- Statistics: Statistical evaluation for the individual standards

In the tables of the standards and the measurement cycles, the selected standards or the respective measurement cycles will be displayed.

Note

In the following, repeat measurements of standards are called measurement cycles.
Quantitative Analyses (Calibration)

Setting up a new calibration curve

Menu functions / Buttons on toolbar of Standards dialog box

<table>
<thead>
<tr>
<th>Menu/Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>✅ OK</td>
<td>Confirms all entries and measurements, and exits the Standards dialog box. The results of the calibration are displayed in the Calibration dialog box on the Calculation (Parameters) tab.</td>
</tr>
<tr>
<td>✗ Cancel</td>
<td>Returns to the Calibration dialog box without calculation of the calibration curve. You can choose this button if you want to change the regression model or the number of standards on the General (Parameters) tab.</td>
</tr>
<tr>
<td>⏯ Start!</td>
<td>Opens a menu for starting the measurement of the standard with various options depending on the number of measurement cycles selected.</td>
</tr>
<tr>
<td>➡️ Reference</td>
<td>Starts the reference measurement.</td>
</tr>
<tr>
<td>📈 Statistics or No Statistics</td>
<td>Extends or reduces the dialog box by the statistics options (repeated measurement of standards).</td>
</tr>
<tr>
<td>🔎 Graph</td>
<td>Graphic display of the measured values of the selected standard (only with measurement cycles)</td>
</tr>
</tbody>
</table>

Entry of sample names and concentration values

- If you want to edit the name of the standards, click on the respective cell of the table in the Standard column and enter the desired name.
- In the Conc. column, enter the known concentrations of the standards.

Selecting repeat measurements

- Extend the Standards dialog box by the statistics field by a click on
- In the Number of series textbox, enter the desired number of repeat measurements. Enter the number directly in the textbox or select it from the list box using the arrow buttons beside the textbox.

Selecting the source of the standard data

Normally, for the measurement of the standard concentration values, the result file selected in the Calibration dialog box on the General (Parameters) tab will be used. However, you may also individually define the way in which the respective measured value is determined:

- by measurement
- from a saved file or
- by manual entry.
Quantitative Analyses (Calibration)

Setting up a new calibration curve

- Click on the standard the source of which shall be changed and then on the [Source] button.

This will bring up the **Source of selected standard** dialog box.

![Source of selected standard dialog box](image)

**Fig.4-3** Source of selected standard dialog box

- From the **Ordinate values by** list box, select the desired option:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
</table>
| Measurement     | Determination of the measured values for the calibration by direct measurement.  
|                 | Additionally, choose a parameter file for the measurement using the **[Choose]** button. If you want to use the same parameter file for all standards, activate the **Valid for all standards** checkbox.  |
| Manual input    | Entry of values via the keyboard. Click on the respective cell of the Cycle column and enter the value via the keyboard. |
| Loading from file | Loads the value(s) from a saved result file. Additionally choose a result file using the **[Choose]** button. |

**Deactivating standards or deleting measurement cycles**

The software lets you deactivate a standard thus excluding it from the calculation of the calibration curve.

- In the Standard table column, click on the respective cell and then click the below the table.

- To re-include the standard in the calculation, click once more on the [(de-)activate] button.

Furthermore, the software lets you completely delete a measurement cycle.

- Click on any value of the cycle to be deleted in the **Cycles** field. Then, click on the **[Delete]** button below the table.

**Note**

In the case of outliers within a measurement series or of a standard, you can simply measure the respective value once more:

In the result table, click on the respective standard and then activate the menu command **Start / Selected standard** or **Start / Selected standard of selected cycle**.
Quantitative Analyses (Calibration)
Setting up a new calibration curve

Statistics for measurement cycles
When running several measurement cycles, a statistical analysis is performed for every individual standard. You can choose between the calculation of the Mean or the Median by activating the corresponding option button under the Statistics table (→ Section "Statistical calculations" p. 220).

4.1.2.3 Calibration by direct measurement of standards

- On the WinASPECT® desktop, create the necessary measurement parameter file. Select the menu command Measurement / Set Parameters to activate the device driver in the SPECORD® xxx dialog box. Choose all necessary options and save the measurement parameters. Exit the measurement parameter window by a click on [OK]. On doing so, the measurement parameters will be activated.

**Note**
Ideally, you should choose the Wavelengths measuring mode when setting the measurement parameters. The first three wavelengths you selected there will be automatically adopted for the calibration settings.

- Open the Calibration dialog box using menu command Quant / Calibration.
- Activate the Measure standards check box. If not automatically entered in the respective textbox, choose the measurement parameter file by a click on the [Choose] button.
- Make the other settings as described in Section "Entry of calibration parameters" p. 76.
- By a click on the [Standards] button, switch to the Standards dialog box. The menu functions and options of this dialog box are described in Section "Entry of standard data" p. 79.
- Enter the concentrations of the standards in the respective cells of the Conc. column of the Standards table field.
- If selected accordingly in the measurement parameters, measure the reference using menu command [Reference].
- Measure the standards with the functions of the Start menu. Depending on your choice to take either single or repeat measurements of the standards, the following options are provided on this menu:

  **One measurement per standard only (without Statistics)**

<table>
<thead>
<tr>
<th>Menu command</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>Beginning with the first of the list, the standards are measured successively and the measured data entered in the respective fields.</td>
</tr>
<tr>
<td>Sel. standard</td>
<td>The currently selected standard will be measured.</td>
</tr>
</tbody>
</table>
### Quantitative Analyses (Calibration)

#### Setting up a new calibration curve

#### Several measurement cycles (with Statistics)

<table>
<thead>
<tr>
<th>Menu command</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>All – by measurement series</td>
<td>The measurement cycles are measured successively. After every measurement, the standard is to be changed until all measurement cycles are complete.</td>
</tr>
<tr>
<td>All – by standards</td>
<td>Every standard is measured n-times ( n = ) selected number of measurement cycles, before the n-times measurement of the next standard is being started.</td>
</tr>
<tr>
<td>Selected measurement series</td>
<td>With this option, only the standards of the selected measurement cycle will be measured.</td>
</tr>
<tr>
<td></td>
<td>To select a cycle, in the <strong>Measurement Cycles</strong> table, click on a result field of the respective cycle.</td>
</tr>
<tr>
<td>Selected standard</td>
<td>The selected standard will be measured for all measurement series.</td>
</tr>
<tr>
<td></td>
<td>To select a standard, in the <strong>Standard</strong> table column, click on the respective field.</td>
</tr>
<tr>
<td>Selected sample of selected series</td>
<td>Measures the selected standard of the selected measurement cycle.</td>
</tr>
<tr>
<td></td>
<td>To select the standard, in the <strong>Measurement Cycles</strong> table, click on the respective field.</td>
</tr>
</tbody>
</table>

- On completion of the measurements, confirm the standard data by a click on the [OK] button.

The **Standards** dialog box will be closed. The calibration curve and the results appear in the **Calibration** dialog box on the **Calculation Parameters** tab.

### 4.1.2.4 Calibration with saved files

- Open the **Calibration** dialog box using menu command **Quant / Calibration**.
- Make the necessary settings on the **General Parameters** tab as described in Section "Entry of calibration parameters" p. 76.
- By a click on the [Standards] button, switch to the **Standards** dialog box. The menu functions and options of this dialog box are described in Section "Entry of standard data" p. 79.
- Enter the concentrations of the standards in the respective cells of the second column (Conc.) of the **Standards** table field.
- Click on the first standard in the **Standard** table column.
- Click on the [Source] button to open the **Source of selected standard** dialog box.
- From the Ordinate values by list box, choose the **Loading from file** option.
- Click on the [Choose] button to open the standard dialog for opening files and select the desired result file.
- Repeat the procedure until you have allocated the desired file(s) to all standards used.
- Activate the menu function **Start! / All**.
Quantitative Analyses (Calibration)
Setting up a new calibration curve

The measured values of the stored file are acquired and entered in the Measurement Cycles table.

When using saved files, too, it is possible to repeat the determination in several measurement cycles. In this case, the measurement cycles for one standard each must be saved to a file of a cyclic measurement:

- Click on Statistics to extend the dialog box by the Measurement Cycles table.
- From the Number of series list box, choose the desired number of measurement cycles.
- Allocate a file to the standards as described above.
- Activate the menu command Start! / All – by standards.
- After the measured values were assigned to the standards, exit the Standards dialog box by a click on [OK].

The Standards dialog box will be closed and the calibration curve and the results appear on the Calculation Parameters tab.

4.1.2.5 Calibration with manually entered calibration data

- Open the Calibration dialog box using menu command Quant / Calibration.
- Make the necessary settings on the General Parameters tab as described in Section “Entry of calibration parameters” p. 76.
- After you have made all necessary settings in the Calibration dialog box, click on the [Standards] button to open the Standards dialog. The menu functions and options of this dialog box are described in Section "Entry of standard data" p. 79.
- Enter the concentrations of the standards in the respective cells of the second column (Conc.) of the Standards table field.
- Click on the first standard in the Standard table column.
- Click on the [Source] button to open the Source of selected standard dialog box.
- From the Ordinate values by list box, choose the Manual input option.
- In the Measurement Cycles table field, click on the respective cell(s) and enter the value(s) belonging to the standard(s).
- To run repeat measurements, extend the dialog box by a click on the [Statistics] button. From the Number of series list box, select the number of cycles to be run.
- Exit the Calibration dialog box by a click on [OK].

The Standards dialog box will be closed and the calibration curve and the results appear on the Calculation Parameters tab.
4.1.2.6 Display of calibration curve

After having finished the measurement or having assigned the measured data from a file or direct data entry, click the [OK] button on the toolbar of the Standards dialog box.

The results of the calibration appear on the Calculation Parameters tab of the Calibration dialog box.

![Calibration curve display](image)

Fig. 4-4 Display of calibration curve in Calibration dialog box

4.1.2.7 Changing calibration curves

If the calibration curve does not meet your expectations, you can make the following changes to it:

- Change the regression model used
- Change the number of standards used
- Deactivation/activation of standards
- Repeat measurement of standards

Changing the regression model used

- On the General (Parameters) tab, choose another calibration model from the Calibration Model list box.

On doing so, the program recalculates the calibration curve and directly displays the changed curve on the Calculation tab. The Coefficients of the regression curve and the Coefficient of determination, too, are recalculated and displayed on this tab.

Changing the number of standards used

- On the General (Parameters) tab, in the No. of standards textbox, enter the desired number of standards to be used.
 Quantitative Analyses (Calibration)

Printing of calibration curves and data

- Click on the [Standards] button. This will bring up the Standards dialog box again.
- Then, proceed as described in Section "Entry of standard data" p. 79.
- Subsequently, measure the additional standard(s).

Deactivation and activation of standards

Standards can be excluded from the calculation of the calibration curve by deactivating them. (→ Section "Entry of standard data" p. 79).

Repeat measurements

Standards may also be remeasured after the calculation of the calibration curve. For that, activate the menu command Start! / Selected standard of selected cycle or Start! / Selected standard (→ Section "Calibration by direct measurement of standards" p. 82). The previous results will then be overwritten by the new data.

4.1.3 Printing of calibration curves and data

- In the Calibration dialog box, activate the menu function File / Print. This will bring up the Print – Calibration.

![Print – Calibration dialog box]

The current settings of your printer appear in the top left field of this dialog box.

- By activating or deactivating the available check boxes, choose the parameters that shall appear on the printout:
  - Calibration curve
  - Parameters
  - Standards
  - Statistics
  - Audit Trail

The functions of the buttons accessible in this dialog box are described in Section "Printing files" p. 69.

- Start the printout by a click on the [Print] button.
4.2 Concentration

The Quant module allows you to determine the concentration of samples based on

- a stored calibration curve or
- already found, known factors.

The concentration determination may be performed by direct measurement of the sample spectrum or sample data or by the evaluation of saved spectra.

Note

When using a calibration curve, its coefficient of determination ($R^2_{\text{adjust}}$) must at least reach the level preset on the Quant tab of the Options dialog box. Otherwise, the calibration will be rejected, i.e. the calibration curve cannot be used for concentration measurement!

You can enter the value for $R^2_{\text{adjust}}$ in the Options dialog box on the Quant tab (menu command Extras / Options) (→ Section “Quant tab” p. 15).

The files with results of a concentration analysis are saved with the file name extension “*.coc”.

QUANT / CONCENTRATION

- Activate the menu function Quant / Concentration.
  This will bring up the Concentration dialog box.

Fig. 4-6 Concentration dialog box - Parameters tab

The dialog box contains three tabs:

- Parameters: Shows the parameters the concentration analysis is based on, such as measurement parameters, calibration file, etc.
- Concentrations: Shows the found concentrations
- Calibration Data: Graphic presentation of calibration data
Quantitative Analyses (Concentration)

Menu functions of the Concentration dialog box

### 4.2.1 Menu functions of the Concentration dialog box

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>File</strong></td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>Starts a new concentration analysis.</td>
</tr>
<tr>
<td>Open</td>
<td>Opens an existing concentration analysis, which is saved to either the database or a separate file.</td>
</tr>
<tr>
<td>Print</td>
<td>Prints the results of the current concentration analysis.</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>Copies the results of the current concentration analysis to the clipboard of the operating system thus making it available to other Windows applications.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves any changes to the active concentration analysis to the same file. The files with results of a concentration analysis are saved with the file name extension &quot;*.coc&quot;.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the results of the concentration analysis under a new name to a separate file.</td>
</tr>
<tr>
<td>Export to ASCII-File</td>
<td>Exports the results of the concentration analysis to ASCII format (*.csv)</td>
</tr>
<tr>
<td>Close</td>
<td>Exits the concentration analysis and closes the Concentration dialog box.</td>
</tr>
<tr>
<td><strong>Edit</strong></td>
<td></td>
</tr>
<tr>
<td>Measurement parameters</td>
<td>Opens the window of measurement parameters.</td>
</tr>
<tr>
<td>Setup</td>
<td>Selection of the parameters for the concentration analysis.</td>
</tr>
<tr>
<td>Show Audit Trail</td>
<td>Shows the Audit Trail edit list</td>
</tr>
<tr>
<td>Sign document</td>
<td>Sign the results of the current concentration analysis (→ Section &quot;Signing a file&quot; p. 213).</td>
</tr>
<tr>
<td>View signatures</td>
<td>Shows existing signatures.</td>
</tr>
<tr>
<td>Reference</td>
<td>Performs a reference measurement.</td>
</tr>
<tr>
<td>Start (Meas.)</td>
<td>Starts the concentration measurement of the samples.</td>
</tr>
<tr>
<td>Start (File)</td>
<td>Starts the concentration determination based on saved files.</td>
</tr>
<tr>
<td>Close</td>
<td>Exits the concentration analysis and closes the Concentration dialog box.</td>
</tr>
</tbody>
</table>

**Note**

The file name extension used in older versions of the application was "*.con". These files can also be opened with the Quant module.
Resizing the dialog box

You can customize the Concentration dialog box and the individual table columns in size to the measurement results to be displayed.

- To enlarge the Concentration dialog box, move the mouse pointer to its border until the mouse pointer changes to a double-headed arrow. Holding the left mouse button depressed drag the border to the desired size.

In order to present the measured values and especially long sample names at full length, you can also vary the width of the table columns.

- To this end, in the table head click with the mouse onto the border line between two columns and, holding the left mouse button depressed, drag the column to the desired width.

4.2.2 Selecting the parameters for concentration analysis

For the concentration analysis, it is necessary that you select e.g. the used calibration file or factor and the measurement parameters.

- Activate the menu command Edit / Setup.

This will bring up the Edit - Parameters dialog box containing the General and Factors / Calibr. Data tabs, where you can choose the respective options.

4.2.2.1 Entries on General tab

Designation / Operator

![Fig.4-7 Edit - Parameters dialog box, General tab: Designation / Operator](image)

- In the Designation textbox, you can enter a designation describing the concentration analysis. The entry of a designation is optional, but will be helpful as both the Designation and the Operator appear in the selection field of the database thus facilitating the retrieval of saved data.

- In the Operator textbox, you can enter the user name. With the FDA conf – version of WinASPECT® automatically the name of the registered user will appear. In this case, the textbox is not accessible for any entries.

Sample Table

![Fig.4-8 Edit – Parameters dialog box, General tab: Sample Table field](image)

The sample table can be used for continuous single measurements (without cell changer).

Before starting the measurement, enter the following data in the sample table:

- Sample name
Quantitative Analyses (Concentration)

Selecting the parameters for concentration analysis

- Nominal concentrations of check samples

  - Activate the Sample Table check box and, in the Number of samples check box, enter the corresponding number.

**Note**

When using a cell changer option, you need not select the Sample Table. The generated result table will show all samples chosen in the measurement parameter file.

**Repeat Measurement**

![Repeat Measurement](image)

Fig.4-9  Edit – Parameters dialog box, General tab: Repeat Measurements field

In repeat measurements, the concentration of the sample is determined from the mean of a defined number of individual measurements. Additionally it is possible to activate the Statistics option providing the calculation of the median, span or standard deviation.

Repeat measurements require that you have selected one of the Cycle Mode options (Automatic, Time-controlled or Manual) in the measurement parameter file. The time-controlled cycle can be used only with scanning spectrophotometers, but not with the SPECORD® S600.

Ideally, you should select the manual cycle mode option. When the entered number of repeat measurements have been taken, the mean value will be calculated.

Automatic or time-controlled cycles are used to advantage in conjunction with a sipper unit. With every repeat measurement, the sample will automatically be aspirated again. The number of cycles selected in the measurement parameters must agree with the selected number of repeat measurements. If the number of cycles selected is greater than the selected number of repeat measurements, only so many cycles will be considered, as repeat measurements were selected. If the number of cycles is less, an error message will appear before the measurements are started.

- Activate the Repeat Measurement check box and, if required, the Statistics option.

- In the Number of measurements per sample text box, enter a number agreeing with the number of cycles selected in the measurement parameter file.

**Note**

If you do not intend to run repeat measurements, select the "Cycle Mode: None" option in the measurement parameter file. Otherwise, only the first measured value will be considered in cyclic measurements, whereas all following results of the cycle will be rejected.

**Check Sample**

![Check Sample](image)

Fig.4-10  Edit – Parameters dialog box, General tab: Check Samples field
Check samples are samples of known concentration, which you may include in a running measurement series for verifying the correctness of the analysis.

- If you want to work with check samples, activate the Check Samples check box.
- If you want to measure the check samples each after a defined number of samples, activate the Fixed number (check sample index) option. In the corresponding textbox, enter the desired number after which a check sample shall be measured.
- If you want to variably include the check samples in the measurement series, activate the Optional (user-defined) option. WinASPECT® will then ask you after every measurement, if the current sample is to be a check sample. If so, you will be asked to enter its nominal value.

For further entries required for preparing concentration determination, change to the Factors/Calibr. Data tab.

### 4.2.2.2 Entries on Factors/Calibr. Data tab

#### Concentration determination with factors

![Factor options](image)

- Activate the Factor option, if you want to determine the concentration of your samples by means of a factor. The concentration of the sample is then determines as follows:

  \[
  \text{Concentration} = \text{factor} \times \text{ordinate value}
  \]

- In the textboxes, make the following entries:

<table>
<thead>
<tr>
<th>Textbox</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Factor (F)</td>
<td>Entry of the factor</td>
</tr>
<tr>
<td>Wavelength [nm]</td>
<td>Wavelength to be used for the concentration determination. The ordinate value measured at this wavelength will then be multiplied by the factor.</td>
</tr>
<tr>
<td>Concentration in [ ]</td>
<td>Unit of concentration</td>
</tr>
<tr>
<td>Ordinate in [ ]</td>
<td>List box for choosing the unit of the ordinate from the list box: Absorbance or Transmittance</td>
</tr>
</tbody>
</table>

#### Concentration determination with calibration file

![Calibration file](image)
The calibration file is to be created via Quant – Calibration.

- Activate the **Calibration file** option, if you want to determine the concentration of your samples based on a calibration curve.
  
  Click on the [File] button to open the Windows standard dialog box for opening files.

- In this dialog box, choose and open the desired calibration file (*.cf). The default path is “WinASPECT\Calib\.”

The program returns to the **Edit – Parameters** dialog box.

In the text box below the option button, the name of the selected file is displayed.

### Entry of the unit of concentration and of additional factors

**Concentration in [ ] textbox.** This entry is optional.

In addition to the use of a calibration curve or of the entered factor, the software lets you define two additional factors (F1 / F2) and divisors (D1 / D2) for e.g. dilution or weighed portion. These will then be taken into account additionally for the calculation of the concentration values.

- Activate the respective check boxes of factors and divisors and type the values in the corresponding textboxes.

- Activate the **Define factors individually for every sample** option, if you want to specify the factors to be used for concentration calculation individually for every sample.
  
  After the start of the measurement, you will then be prompted by WinASPECT® to enter the factors in an automatically appearing table.

The factors are taken into account in the following way:

\[
\text{Conc} = \frac{\text{Ordinate value} \times \text{Factor} \times F1 \times F2}{D3 \times D4}
\]
4.2.3 Concentration determination procedure

After you have made all entries needed for concentration determination, you can begin with the determination.

To this end, in the Concentration dialog box, switch to the Concentrations tab.

4.2.3.1 Determination by direct measurement

The currently active measurement parameter file is used for the measurement.

- If you want to change any parameters or use a different measurement parameter file, activate menu command Edit / Measurements parameters.
- Place the reference into the sample holder and start the reference measurement by the command [Reference].

Perform the sample measurement using the settings selected for concentration analysis as follows:

- Click the [Start (Meas.)] button.

  This will bring up the Sample data by measurement dialog box.

  ![Sample data by measurement dialog box](image)

  Fig.4-14 Sample data by measurement dialog box

In the sample table, you can edit the sample name and the nominal concentrations of the check samples.

- In the Name column, click on the sample name to be edited and enter the new sample name.
- On exiting the dialog box with [OK], the sample measurement is started.

If you activated the Sample Table option, a sequence of dialogs will appear informing you which sample will be measured next.

If you did not activate the Sample Table option, you can start the next sample measurement by a click on [Start (Meas.)].

All concentration values determined are then displayed on the Concentrations tab.
Quantitative Analyses (Concentration)
Concentration determination procedure

Working with check samples

Check samples are inserted in the measurement series according to the options selected for concentration analysis.

If you selected a fixed sequence of check samples (check sample index), in the Sample data by measurement dialog box, the check samples will be identified by the letter C in the first column of the table.

Example:
Check sample index: 5
Samples #6, 12, 18, etc. are marked as check samples in the table.

If you did not select a fixed check sample index, in the Sample data by measurement dialog box, click on the respective cell of the second column of the table (→ Fig. 0-16 p.93). Again, check samples are identified by a C.

With check samples, the Nominal value is set to 0.000 by default.

- Select the respective cell in the Nominal value column and enter the new nominal concentration.

Note
If you marked a sample as check sample by mistake, click once more on the respective cell in the second column thus making it a "normal" sample again.

Working with repeat measurements

The repeat measurement option is to be chosen when defining the parameters for the concentration analysis (→ Section "Entries on General tab" p. 89).

When you selected the Cycle Mode: Manual option in the measurement parameter file, follow this procedure:

- Click the [Start (Meas.)] button.
  This will bring up the Sample data by measurement dialog box. , p. 93
- On exiting the dialog box with [OK] the sample measurement is started.

When the measurement is finished, a message window will appear asking you for a manual cycle start: "Start next cycle? Yes / No".

- Start the repeat measurements with [Yes] each.
- At the end of the planned repeat measurements, click on [No].

The software calculates the concentration as mean value of all measurements and displays it in the Concentration dialog box on the Concentrations tab.

- To start the measurement of the next sample with the desired number of repeat measurements, click on the [Start (Meas.)] button again.

When you selected the Cycle Mode: Automatic or Time controlled option in the measurement parameter file, follow this procedure:

- Click the [Start (Meas.)] button.
  This will bring up the Sample data by measurement dialog box. p. 93
Quantitative Analyses (Concentration)
Concentration determination procedure

- Exit the dialog box with [OK]. On doing so, the sample measurement will be started. All repeat measurements are automatically taken in succession.
  The concentration is calculated as mean value of all measurements and displayed in the Concentration dialog box on the Concentrations tab.
- Start the measurement of the next sample with the selected number of repetitions again by a click on [Start (Meas.)].

**Note**
You can use the measurement parameter options, Cycle: Automatic and Time controlled, in connection with a sipper. In this case, after the start of the measurement the sample is aspirated and measured as often as selected under Repeat Measurements.

4.2.3.2 Determination from result file

Concentration determination with saved results is analogous to the determination by direct measurement described above.

- Click on the [Start (File)] button.
  This will bring up the standard dialog box for opening files.
- Choose the desired files and confirm your choice with [OK].
  This will bring up the Sample values from file dialog box:

![Sample values from file dialog box](image)

- If you want to edit the name of the sample, click onto the respective cell in the Name column.
- To delete a sample from the sample table, click the [Delete] button.
- If you want to change the file to be used for a sample, select the respective line of the table and click on the [Choose] button.
  Choose the desired file from the appearing standard dialog box for opening files.
- Confirm your choice and entries in the Sample values from file dialog box with [OK].
  On doing so, the selected files will be loaded for concentration determination.

**Using check samples**

The check samples are inserted in the sample table according to the selected options.
Quantitative Analyses (Concentration)

Concentration determination procedure

If you selected a fixed sequence of check samples (check sample index), a line for the check sample will be inserted in the table after the defined number of samples.

- Click onto the line of the check sample.
- Then, click on the [Choose] button to open the standard dialog box for opening files. Choose the desired file containing the data of the check sample.
- In the corresponding cell of the Nominal value column, enter the concentration of the check sample.
- If requested, edit the name of the check sample.

If you intend to include check samples without a fixed sequence, you can either declare a sample listed in the table to be the check sample or insert new lines as check samples in the table.

- Click onto the respective cell of the second column to define the sample as check sample.
- Alternatively, you can use the buttons in the top right corner above the table to insert new check samples:
  - Inserts a check sample in the activated line of the table.
  - Appends a check sample to the end of the sample table.

- Choose the desired file for the check sample(s) by a click on the [Choose] button.
- In the Nominal value column, enter the concentration(s) of the check sample(s).

Fig.4-16 Check sample in Sample values from file dialog box

4.2.3.3 Display of results of a concentration measurement

Display of result table

The results of the concentration analysis are displayed on the Concentrations tab.
Quantitative Analyses (Concentration)

Concentration determination procedure

In the result table, you can edit the sample names. In the table, mark the sample name to be edited with the mouse, and enter the desired name. Confirm your entry with the ENTER key.

To display additional details of the sample measurement, right-click with the mouse onto the respective line of the result table. In the appearing dialog box, the results of the individual measurements (concentration and ordinate value) and the entered factors and divisors are displayed.

![Screen capture of the result table](image)

Fig. 4-18  Display of details of concentration measurement.

**Graphic presentation of results in calibration curve**

In concentration determination based on calibration curves (from *.cf file or database), you can view the position of the found concentrations with reference to the calibration curve.

To this end, in the Concentration dialog box, change to the Calibration Data tab. In the sample list, click on the desired sample.

In the graph, a horizontal line appears indicating the position of the concentration value in the calibration curve.

![Calibration curve graphic](image)

Fig. 4-19  Graphic presentation of the found concentration within the calibration curve.
4.2.4 Printing concentration measurement series

- Activate the menu command File / Print.

This will bring up the Concentration – Prepare print dialog box.

Fig.4-20 Concentration – Prepare print dialog box

The buttons are described in Section "Printing files" p. 69. In addition, this dialog box contains three check boxes. Activation/deactivation of these check boxes has the following effects on the printout:

Activated check box Printout

None Parameters, sample name, date/time of measurement, concentration data (standard printout)

Details Additional printout of results and calculated concentrations of individual measurements

Factors Additional printout of entered factors/divisors (e.g. dilution) for every individual measurement

Audit Trail Printout of Audit Trail Record
5 Quant Routine Module

The Quant routine module is mainly intended for express concentration analytical jobs. For evaluation, it uses the values that were measured for a wavelength. Concentration is determined, using the extinction value of a wavelength. A concentration routine can be performed, based on a factor or a linear or square regression model. The routine will carry out predefined sample sequences that consist of standards, concentration samples and samples. A given sequence of samples will take into account cell changers and autosamplers that are involved.

The Quant routine module allows you to prepare a given method to and save it in ready-for-use state, i.e. on subsequent selection of the same method and mounting of required samples, an analytical procedure can be triggered by just clicking the [Start!] button.

---

Note

When using a calibration curve, its coefficient of determination (R² adjust) must at least reach the level preset on the Quant tab of the Options dialog box. Otherwise, the calibration will be rejected, i.e. the calibration curve cannot be used for concentration measurement!

You can enter the value for R² adjust in the Options dialog box on the Quant tab (menu command Extras / Options) (→ Section "Quant tab" p. 15).

---

Select the Quant / Routine menu function.

The Quant Routine dialog box will open.

---

Fig.5-1 Quant Routine – Settings dialog box
5.1 Elements of Quant Routine dialog box

This dialog box includes three register tabs:

- **Settings**: displays currently valid measurement settings
- **Results**: displays measured values and values calculation for concentration
- **Measurement values**: displays single readings of a multiple measurement sequence
- **Calibration**: displays calibration result and represents measured data in calibration curve diagram.

5.1.1 Preselection screen of Quant Routine module

Fig.5-2 Express buttons in Quant Routine module

On selection of the **Quant Routine** module or a **File /New** command, a special window is displayed. It provides buttons for typically used menu commands for expedited parameter settings in Quant Routine mode.

<table>
<thead>
<tr>
<th>Button</th>
<th>Menu command / description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Measurement settings]</td>
<td>Setup / Measurement settings...&lt;br&gt;Opens measurement parameter box with setting options for analysis.</td>
</tr>
<tr>
<td>[Setup new sample table]</td>
<td>Setup / Sample table&lt;br&gt;Opens the Setup Sample table box for defining a method for concentration analysis and a sequence of samples within a given analysis.</td>
</tr>
</tbody>
</table>
[Open calibration file]  
**File / Open calibration file**  
Opens the standard Open box for loading of a calibration.
A calibration can be loaded from a Quant Routine file (*.rq) or a file of the Calibration (*.cf, *cfs) module.

[Open method file]  
**File / Open method file**  
Opens the standard Open box for loading of a method (sample table, calibration and measurement parameters).
A method can be loaded from a Quant Routine file (*.rq).

[Open result file]  
**File / Open result file**  
Opens the standard Open box for loading of a result file. A result file contains measured values, results and the content of a method.

[Close]  
Closes the preselection screen.

### 5.1.2 Menu commands in Quant Routine module

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="File" /></td>
<td><strong>File</strong></td>
</tr>
<tr>
<td>New</td>
<td>Begins new routine.</td>
</tr>
<tr>
<td>Open calibration file</td>
<td>Loads calibration from a previously saved Quant Routine file (<em>.rq) or loads calibration curve from Quant module (</em>.cf).</td>
</tr>
<tr>
<td>Open method file</td>
<td>Loads method from a previously saved Quant Routine file.</td>
</tr>
<tr>
<td>Open result file</td>
<td>Loads a complete Quant Routine file with &quot;*.rq&quot; file extension.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves changes in current Quant Routine measurement under identical file name.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the results of Quant Routine measurement in a separate file with new name.</td>
</tr>
<tr>
<td>Save measure file (.dat)</td>
<td>Saves the results of measurement in a WinASPECT® file and makes them available to other WinASPECT applications.</td>
</tr>
<tr>
<td>Export to ASCII</td>
<td>Exports the results of a concentration analysis into ASCII format (&quot;*.csv&quot;).</td>
</tr>
<tr>
<td>Sign document</td>
<td>For signing the results of a currently performed concentration analysis (→ section &quot;Electronic signature&quot; p. 213).</td>
</tr>
<tr>
<td>Signature list</td>
<td>Displays existing signatures of the current Quant Routine file.</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Displays editing list.</td>
</tr>
<tr>
<td>Changes in concentration determination are always documented and displayed in the editing list.</td>
<td></td>
</tr>
<tr>
<td>Print</td>
<td>Prints the results of a current concentration analysis.</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>Copies the results of the current concentration analysis to the clipboard of the operating system to make them available to other Windows applications.</td>
</tr>
</tbody>
</table>
### 5.2 Measurement settings in Quant Routine

Measurement settings for Quant Routine analysis can be loaded and set in different ways:

- Use measurement settings contained in the main WinASPECT® program (presets).
- Use [Measurement settings] to open the measurement settings box in the preselection screen and match settings to the specific analytical conditions.
- Use Setup / Measurement settings menu command to open the measurement settings box or use Setup / Choose parameter file in standard Open box to load a previously saved file of measurement settings.
- Use a File / Open method file menu command to load measurement settings, calibration and sample table.

For measurement mode, option **Fixed wavelengths** must be selected with a corresponding wavelength for analysis.

Automatic cell changer and autosampler settings which are contained in a set of measurement settings will be duly considered as a sample table is generated and will determine its setup.

Selected measurement settings are displayed on the **Settings** tab of the Quant Routine module.
5.3 Selection of analytical method and input of sample table in Quant Routine

Settings for analytical method and sample table can be made in a dialog box.

- Actuate the [Setup new sample table] button in the preselection screen or select the Setup / Sample table menu command.

The Quant Routine Setup sample table dialog box will open. It provides options for all required settings on three tabs: General, Method and Sample table.

**Note**

A specified sample table with analytical method can be saved as a Quant Routine method. (→ "Methods in Quant Routine" p. 118).

5.3.1 General Quant Routine settings

Settings in the Quant Routine Setup sample table / General tab dialog box are optional.

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title</td>
<td>For entering a title to the sample table.</td>
</tr>
<tr>
<td>Operator</td>
<td>For entering a user name.</td>
</tr>
<tr>
<td>Description</td>
<td>With WinASPECT® FDA21FRPart11 the logged-in user’s name is automatically applied at this point. This entry cannot be changed.</td>
</tr>
<tr>
<td></td>
<td>For entering supplementary descriptive text.</td>
</tr>
</tbody>
</table>

5.3.2 Selection of analytical method for Quant Routine

A desired analytical method can be set in the Quant Routine Setup sample table / Method tab dialog box.
Quant Routine Module

Selection of analytical method and input of sample table in Quant Routine

Fig.5-3 Dialog field for Setup sample table / Methods tab

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical parameter</td>
<td>Describes a chemical parameter which is subject to examination. If there is an established link to the AQS module, this text restores the QC regulation tab.</td>
</tr>
<tr>
<td>Selection</td>
<td>Selects the type of concentration determination: via Calibration or Factor.</td>
</tr>
<tr>
<td>Model of Regression</td>
<td>Active in the case of concentration analysis via Calibration. Select regression model: ( y = B \times x ) or ( y = A + B \times x ).</td>
</tr>
<tr>
<td>Fixed factor</td>
<td>Active in the case of concentration analysis via Factor. Enter factor.</td>
</tr>
<tr>
<td>Unit</td>
<td>Enter concentration unit for results of analysis. This unit will be displayed in the results table.</td>
</tr>
<tr>
<td>Pathlength</td>
<td>Enter cell layer thickness. This entry is only for information. It is not applied for calculation of results.</td>
</tr>
</tbody>
</table>

**Group Multi measurement**

Single samples can be measured repeatedly. Their concentration is analyzed, using the mean value of the various single samples' extinction readings (→ section "Multi Measurement with Quant Routine" p. 112).

**Multimeasurement active**

Measures single samples repeatedly if active.

**Number**

Number of repeat measurements.
Quant Routine Module

Selection of analytical method and input of sample table in Quant Routine

**Start request for single measurement**
Automatically performs repeated measurement on the same sample (same cell) if disabled.

Will not begin repeated measurement, unless a query has been answered. This mode allows you to repeat measurement with a different single sample.

Please note that some special conditions must be considered for working with cell changers and autosamplers (→ section "Multi Measurement with Quant Routine" p. 112).

**Group Automatical save**

The results of analysis can be automatically saved. To achieve this, you must enable this option and define a name and path for saving:

**Name/path for saving**

**Description**

- **Results**
  On completion of measurement, concentration values are calculated and written to the specified results file.

- **Measurement values**
  The results of measurement are saved in a WinASPECT® file with "*.dat" extension.

- **Auto-Export (ASCII)**
  The results of a concentration analysis are exported to an ASCII file on completion of measurement.

- **AQS-Link**
  Establishes link to AQS quality assurance module. This function is not yet implemented.

### 5.3.3 Entering sample table for a Quant Routine

Working in **Quant Routine Setup sample table / Sample table** tab, you can define a sample type and a sequence of samples. The **Sample table** tab includes a **Table** subtab with a sample table and a **Chart** subtab for graphical setting of a sequence of samples.

A desired sequence of standards and samples should be specified on the **Chart** subtab. Standard values and sample names can then be entered on the **Table** subtab.

Available sample type conventions are:

<table>
<thead>
<tr>
<th>Sample type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>Calibration standard</td>
</tr>
<tr>
<td>Sample (Conc.)</td>
<td>The sample for which a concentration is calculated</td>
</tr>
<tr>
<td>Sample (Meas.)</td>
<td>The sample, for which only one measured value is determined without any further calculation procedures.</td>
</tr>
</tbody>
</table>

Reference samples are measured regardless of the selected sequence of samples. They will not be included in the sample table.

Entries made for a desired sequence of samples must take into account which accessory components are involved in the process (where applicable):

- 6-cell changer
- 8-cell changer
- 2x8-cell changer
- cell carousell
- APN 40
- APG 53
- APG 100
- 50-cell carousell
Where accessory components are to be involved in analysis, you must at first define the sample number that is contained in the set of measurement settings for the given accessory component as the number of samples. If more samples need to be measured, the involved cell changers can be repeatedly refilled within a given routine. The number of multiple fills can be entered via **Number of Charges**.

If none of the accessory components listed above is involved, the total number of samples (standards + samples) must be entered.

**Input elements of sample table tab**

<table>
<thead>
<tr>
<th>Input element</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Count of charges</td>
<td>For working with PC-controlled cell changers or autosamplers. For entering the number of fill operations of changers/samplers that is required to process all samples within a given routine.</td>
</tr>
<tr>
<td>Count of samples</td>
<td>Where no cell changers or autosamplers are involved. For entering the number of samples to be processed in a given routine.</td>
</tr>
<tr>
<td>Samples [Import]</td>
<td>Loads ASCII file with sample data (→ &quot;Importing sample information to Quant Routine&quot; p. 110).</td>
</tr>
</tbody>
</table>
Quant Routine Module
Selection of analytical method and input of sample table in Quant Routine

**Table tab**
Displays table of samples.
The sample table is intended for defining a desired sequence of samples, assigning sample names and defining standard values.
The various columns on display can be configured.

**Chart tab**
Graphical display of sequence of samples.
A desired sequence of samples can be defined with a mouse-click in the graphical display screen. The sample positions will be displayed for samplers/changers.
A sample is represented as a circle with colored background in accordance with its assigned sample type.

- **[Standard]**, **[Sample (Conc)]**, **[Sample (Meas.)]**  
  Turns sample type to be assigned active.

- **[AQS sample] buttons**  
  *These elements have not been assigned a function as yet.*

- **View Charge**  
  Where samples/changers are included, View Charge allows you to set a sample lot for which a given sequence of samples is defined.

### 5.3.3.1 Graphical setup of sample table

![Sample table tab dialog field with graphic input tool for working with cell carousell](image)

**Fig.5-5** Setup sample table / Sample table tab dialog field with graphic input tool for working with cell carousell
Enter the total number of samples in the **Count of samples** field.

If you are working with a sample feeder/sample changer, specify the required number of fill operations of your accessory component in the **Count of charges** field.

Turn the button of that sample type on, to which you want your samples assigned.

Mark the samples of this sample type with a mouse-click. Icons located one beside the other can be jointly marked by dragging a frame around the sample icons in question while keeping the left mouse-key depressed.

Selected sample icons will be marked with a background that is colored in accordance with their assigned sample type:
- Standards – light-blue
- Concentration samples – dark-blue
- Samples for which measured values are determined – gray.

If you are working with a sample feeder/sample changer, you can use **View Charge** to set the next fill operation of your accessory component and assign a sample type to these samples in the same way.

### 5.3.3.2 Specifying samples in the sample table

Graphical entries made for sample type and sample sequence are transferred from the **Chart** subtab to the **Table** subtab. Regardless of that, sample types can also be directly assigned in the sample table.

Assign the desired properties to the sample cells you have marked. Sample cells which are located one below the other can be marked together by running the mouse pointer over these cells while keeping the left mouse-key depressed. You can also mark single cells with a mouse-click while keeping the shift key depressed.

<table>
<thead>
<tr>
<th>Table</th>
<th>Chart</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Pos.</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

Fig.5-6  Sample table for Quant Routine

**Columns of sample table**

- **Pos.**  The number of a sample in a sequence of samples. Numbers are automatically assigned.
- **Charge**  For working with cell changers and autosamplers. Designates the number of accessory fill number (→ section "Entering sample table for a Quant Routine" p. 105). Numbering occurs automatically.
- **Type**  Sample type
- **Name**  For input instructions, see further below.
Quant Routine Module

Selection of analytical method and input of sample table in Quant Routine

For input instructions, see further below

Nom. val.
Concentration of standard
To define a nominal value, click onto the respective table cell and enter the desired value.

Notes
Sample-related annotation
This entry is optional. Click into the respective table cell and type in a desired sample-related annotation.

Init weight, Dilution, Factor, Divisor
Takes specific sample coefficients into consideration where concentration is calculated.

Defining sample types
A required sample type can be declared in column Type.

- Use a mouse-click onto those sample cells in the Type column you want to mark for type definition.
- With a right mouse-click you can open a special context menu with the three sample types available for definition. Select a desired sample type from this context menu. This sample type will appear in your previously marked cells.

Defining sample names
Sample names can be entered in the Name column. You may assign identical names to a succession of samples in automatic mode, including with incrementing numbers if so desired. In the case of numbering in ascending order, the last numeral in a chain of characters will be incremented.

Example: sample1, sample2 / 1sample, 2sample / sample2203Pat13In; sample2203Pat14In

- Use a double click onto the sample cell in column Name. The content of this cell can be marked for overwriting with a new sample name.
- For a collective name assignment, you should assign the particular collective name to the first sample or the first standard. All subsequent numbers of this assignment will also include its starting number. Mark the name cells which are located one below the other. Open the context menu by clicking onto the marked cells with the right mouse-key. Trigger a fill bottom context menu command. The first sample’s name will appear in each marked name cell. If you trigger a fill bottom increased context menu command, the first sample’s name will appear in each marked name cell in ascending order of numbers.

Defining specific sample coefficients
Besides fixed factors for concentration analysis, further individual coefficients may be set for inclusion in calculation procedures for a given sample. These coefficients must be defined separately for each sample in the four columns: Init weight, Dilution, Factor and Divisor.

Unhiding and hiding sample table columns, matching size and sequence
Sample table columns can be turned on or off as required.
Quant Routine Module

Selection of analytical method and input of sample table in Quant Routine

- Click with the right mouse-key onto the sample table header to open a context menu with column headings.

- Turn the columns you want displayed with a checker mark. The sample table will be adjusted to your settings.

- The width of a table column can be modified by positioning the mouse between two columns in the table header. The mouse-pointer will convert to a double arrow. Draw the column to the desired width while keeping the mouse-key depressed.

- To make changes in the order of columns, use drag-and-drop. Click onto the header of a given column. The left boundary of this column will be marked by a somewhat bolder line. Keep the mouse-key depressed as you drag the column to a desired position. Then release the mouse-key.

5.3.3.3 Importing sample information to Quant Routine

Sample information can be imported from an ASCII file.

If the first line of an ASCII file is found to consist of valid code words, it will be interpreted as a header and its data will be assigned to the appropriate columns. Columns must be separated by semicolon.

Valid code words and their related data types:

<table>
<thead>
<tr>
<th>Column</th>
<th>Code word</th>
<th>Data type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>&quot;typ&quot;</td>
<td>Integer number (1 calibration, 2 concentration, 3 measurement, 4 QC, 5 QC standard, 6 QC blank value)</td>
</tr>
<tr>
<td>Name</td>
<td>&quot;name&quot;</td>
<td>Text</td>
</tr>
<tr>
<td>Nom.val.</td>
<td>&quot;nomvalue&quot;</td>
<td>Decimal number</td>
</tr>
<tr>
<td>Notes</td>
<td>&quot;notes&quot;</td>
<td>Text</td>
</tr>
<tr>
<td>Init weight</td>
<td>&quot;initweight&quot;</td>
<td>Decimal number</td>
</tr>
<tr>
<td>Dilution</td>
<td>&quot;dilution&quot;</td>
<td>Decimal number</td>
</tr>
<tr>
<td>Factor</td>
<td>&quot;factor&quot;</td>
<td>Decimal number</td>
</tr>
<tr>
<td>Divisor</td>
<td>&quot;divisor&quot;</td>
<td>Decimal number</td>
</tr>
</tbody>
</table>

Example:

notes;name;typ;dilution;initweight;nomvalue;
notes1;is1:1;12.1;8,51:0;
notes2;is2:1;12.2;8,52:1;
notes3;is3:1;12.3;8,53:2;
notes4;is4:1;12.4;8,54:3;

- Mark those samples of the sample table, the information of which you want to import.

- Use [Import] to call up the standard window for file loading.

- Select the text file (*.txt) that contains the given sample information.
5.4 Measurement with Quant Routine

For Routine measurement, a set of measurement settings, a sequence of samples and conditions or a factor for calibration must have been specified.

Note

Once recorded, a reference measurement will be temporarily stored. It can be applied in all modules of WinASPECT®, provided that no changes are made in the measurement settings. Consequently, a set of measurement settings can be prepared and a reference measurement be performed before a Quant Routine run is triggered. In this case, no measurement settings need to be set and no reference measurement to be carried out as part of the Quant Routine. Instead, you may directly proceed to sample table compilation and trigger measurement as soon as the table is complete.

Measurement of a sample table

- Use a [Reference] menu command to measure the reference if this was defined in the measurement settings.
- Launch measurement, using the functions of menu Start!/All Samples.
- Follow screen prompts regarding the order of samples. Measurement will occur in accordance with the configuration set in the sample table and the selected accessory settings. The results will be shown in a table on the Results tab in the Quant Routine box.

Repeating sample measurement

If no changer/sampler was involved, a measurement of samples can be repeated.

- Mark those samples in the results table you want to re-measure.
- Use a right mouse-click onto the line of a sample to be re-measured. A context menu opens.
- Trigger a repeated sample measurement with the help of a Measure marked sample context menu command. Follow the screen prompts.

The previously measured sample values will be corrected. Where a standard is re-measured, its concentration will be calculated again and added to the editing list (Audit Trail).

Measuring further samples

On completion of measurement of the samples in a sample table, more samples can be "supplemented" as part of a Routine.

- Select the Start! / Append samples menu command. A sample table opens.
- Enter the new samples as described in section "Specifying samples in the sample table" p. 108.
5.5 Multi Measurement with Quant Routine

Multiple measurement of a given sample uses the mean value of all individual readings to calculate that sample's concentration.

A multi-measurement sequence may selectively refer to the same sample or to individual samples of the same series of samples. The standard deviation may optionally be tested for excession of a given limit value. Outliers in a series of samples can be marked and excluded from the concentration calculation procedure.

A multi measurement and the number of repeat measurements can be defined on the Methods tab of the QuantRoutine – Setup sample table window (→ section "Selection of analytical method for Quant Routine" on page 103).

![Quant Routine - Setup sample table](image)

Fig.5-7 Dialog field for settings regarding sample series / Methods tab; selection of multiple measurement

Make parameter settings on the Methods tab as described hereafter:

- Mark the Multi measurement active checkbox.
- Type in a desired number of repeat measurements for each sample at the Number input field.
- By disabling or enabling the Start request for single measurement checkbox, you can define if you want multiple measurement performed on the same sample or on different samples of a given series of samples. The order in which measurements will actually be performed also depends on what accessory items are involved in the process (see further below).

Measurement is triggered as described in section "Measurement with Quant Routine" p. 111.

Measurement without accessories

For accessories, the measurement parameter set provides two options: none or Sipper. Starting query disabled: Once measurement has started, it will automatically be repeated as many times as necessary to execute the preset repeat number for that same sample.
Starting query **enabled**: Once measurement has started, measurement will be performed on a given sample. This sample can then be replaced with another sample from the same series of samples. The next measurement will not begin, before the starting query has been acknowledged.

**Measurement with cell changer**

For accessory settings, a set of measurement parameters may contain a cell changer or also two cell changers in the case of a two-beam spectral photometer.

Starting query **disabled**: Once measurement has started, as many repeat cycles will automatically be performed on the first sample as necessary to execute the preset repeat number. On completion thereof, the next samples in the cell changer will automatically be picked and measured in the same way.

Starting query **enabled**: Sample measurement is repeated by lines. Initially, the first single samples are placed into the cell holder of the cell changer in accordance with the sample table (sample 1/1, sample 2/1, sample 3/1...). Once started, measurement will be performed for all samples. During the pause that follows, samples for the next line can be inserted (sample 1/2, sample 2/2, sample 3/2...). Measurement of this second line of samples will not begin, before the starting query has been acknowledged. Measurement then continues in the same manner until the last repeat cycles is reached.

**Measurement with autosampler**

No starting query is involved when working with an autosampler.

Prior to each measurement, the autosampler will dip the cannula into the same sample container and pump sample liquid into the flow-through cell.

**Display of measured results**

The results for single measurement, related mean values and standard deviations can be looked up on the *measurement results* results tab.

Optionally, a limit value can be defined for standard deviation. A standard deviation which is greater than the limit value will appear in bold lettering and marked in blue color.

- Use **File / Extras** menu command to call up the **Quant-Routine – Extras** window.
- Mark the checkbox **Warning if standard deviation too great**.
Quant Routine Module

Maintaining result files in Quant Routine

- Define a desired limit value for permissible standard deviation at the Limit value input box.

Single readings of a series of sample (outliers) may be excluded from calculation of the mean value and, hence, from the concentration analysis. This manipulation will be documented in the audit trail.

- Click onto the table cell that contains the particular single reading with the right mouse key.

- Acknowledge the “Disable single reading?” query with [Yes].

- To reset a disabled state, click the table cell again with the right mouse key and confirm the “Enable single reading?” query with [Yes].

5.6 Maintaining result files in Quant Routine

5.6.1 Quant Routine result file display resources

The results are displayed in a sample table on the Results tab.

Adaptation of results table

The various results table columns may be configured in much the same way as the columns of the sample table before measurement starts. A right mouse-click onto the table header will open a context menu with the table columns to be displayed. The width of a column can be altered by positioning the mouse-pointer onto the separation line of two columns in the table header. The mouse-pointer will change into a double arrow. Keep the mouse-key depressed as you drag the column to a desired width.

Enabling/disabling samples/standards

Samples and standards can be disabled in the results table. A disabled sample is distinguished by a lighter color of its script. The results of such samples are enclosed in brackets.
Once a standard has been disabled, the regression coefficients of calibration and the sample concentrations resulting therefrom will be re-calculated.

**Note**

The calibration model can be changed on the **Calibration** tab.

### Changing sample coefficients

After measurement, you may modify a given sample individually via the four columns: **Init weight**, **Dilution**, **Factor** and **Divisor**. The sample concentration will then be calculated again.

### 5.6.2 Graphical representation of results measured in Quant Routine

The **Calibration** tab:

- displays the selected regression model
- displays the calculated regression coefficients and $R^2$
- displays a list of samples measured
- provides a graphical view diagram of the calibration curve.

![Graphical representation of results](image)

**Fig.5-10** Calibration curve and sample concentration values display screen

Sample and standard values are shown in the graphical view screen of the calibration curve. A given sample that was selected from the list of **Samples** will be marked in bold lettering.

### New selection of model of regression

A regression model can be selected. On completion of measurement, it may also be redefined via the **Model of Regression** list. Following selection of another model of regression, the regression coefficients and related sample concentration values will be recalculated. Recalculated calibration results are added to the Audittrail.
5.6.3 Saving and opening result files in Quant Routine

The data of the Quant Routine module are saved in binary format in a result file. For this reason, no extra file signing is required for encoding of the results.

A result file contains the complete set of information about selected measurement settings, measured data, the sample table and the analytical method. The calibration curve and the method can be extracted from a results file for inclusion in further analytical procedures.

Result files of the Quant Routine contain a "*.rq" extension and signed result files a "*.rqs" extension.

Saving result files

Results can be saved even while measurement is still going on. In this case, you should specify the (→ “Selection of analytical method for Quant Routine” p. 103) memory path as part of method setting action.

On completion of measurement, you can save a result file with standard menu commands.

- Select the File / Save as... menu command in the Quant Routine dialog box. The standard Save dialog opens.
- Enter a file name and click onto the [Save] button.

Alternatively, you may also use the File / Save menu command.

If the same data had already been saved as a file, the revisions will be saved under the previously assigned name. Otherwise, the Save standard box opens.

Opening result files

On opening of a result file, you will load the entire set of information that relates to this result file (method, calibration, sample table, measured results, measurement settings).

- For a Quant Routine restart, you use [Open result file] to open the Open standard dialog in the preselection screen.

Alternatively, you can also use the File / Open result file menu command for this purpose.

- Select a desired file and open this file with a click onto the [Open] button.

The result file will appear in the result box of the Quant Routine.

By triggering a Start! / Append samples menu command, more samples can be appended to an existing result file for measurement with the same method and with identical measurement settings. The results of such appended measurements will be added at the end of the result list.

5.6.4 Printing Quant Routine results

- Select the File / Print menu command.

The Quant Routine – Print dialog box opens.

Related control buttons are described in section "Printing files" p. 69. Use the checker boxes for setting those components which you want to print:
### Quant Routine Module

Maintaining result files in Quant Routine

---

<table>
<thead>
<tr>
<th>Active checkerbox</th>
<th>Printout</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration curve</td>
<td>Calibration curve graphic</td>
</tr>
<tr>
<td>Measurement parameter</td>
<td>Measurement settings for concentration analysis</td>
</tr>
<tr>
<td>Method parameters</td>
<td>Parameters for concentration analysis (inputs in Quant Routine dialog box, General and Method tabs)</td>
</tr>
<tr>
<td>Result table</td>
<td>Results of measurement and concentration analysis</td>
</tr>
<tr>
<td>Measurement values</td>
<td>Prints single readings, mean values and standard deviation in the case of multi measurement</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Additional output of editing logsheet.</td>
</tr>
</tbody>
</table>

Configured inputs regarding the contents of printing can be saved as preselections via [Save] and called up again via [Load].

**Defining result table contents in printout**

A result table contains the various sample data printed in vertical order. Up to five columns and three lines can be configured for each sample. The content of cells can be defined in the **Setup sample table** dialog box.

![Setup sample table](image)

**Fig.5-11** Dialog box for printed result table in Quant Routine module

- Use beside the **Result table** checker box to open the **Setup sample table** dialog box.
- Select a desired line number in the **Count of lines for sample** list (max. 3).
- The individual cells can be filled via "drag-and-drop". Click onto a desired element in the list on the left and drag it to the required cell while keeping the mouse-key depressed. Release the mouse-key. The dragged element will "drop" into this cell. You may also shift a given element from one cell to another in the same way. To remove an element from the list, you need to shift it back to the list.
5.7 Methods in Quant Routine

A method can be extracted and loaded from a previously created result file.

A method contains the parameters that are required to perform routine measurement. These comprise:

- the measurement settings, including accessory equipment assignments
- calibration coefficients or fixed factors for concentration analysis
- sample table with sampling sequence.

Once a method has been loaded and accessory components been filled, measurement may begin immediately.

If a sample table specifies that standards are to be measured, no calibration coefficients will be loaded. In this case, the coefficients are determined as part of measurement.

The preset sample table can be re-specified.

As part of a calibration load procedure only the calibration coefficients will be loaded and displayed on the Calibration tab.

Creating and saving a method

- Open a new file by triggering a File / New menu command or perform a Quant Routine restart.
  The preselection screen will show in the Quant Routine working window.

- Use [Measurement settings] in the preselection screen to open the measurement settings box and set the required values for later routine measurement. Once your measurement settings were acknowledge or saved, you will return to the preselection screen.

- To load previously obtained calibration coefficients, open the Open standard dialog box with the help of an [Open calibration file] command. Select a result file or calibration file for extraction of required calibration coefficients. The calibration data will be displayed in the Import calibration file dialog box. After confirmation of your selections, the Quant Routine Setup sample table will open.

- If you have loaded no calibration coefficients, use [Setup new sample table] to open the Quant-Routine Setup sample table dialog box and make necessary settings for analytical method and sample table in this box. Having acknowledged your settings, you will return to the Quant Routine working screen.

- Save the selected method with a File / Save as.... menu command. The file with the method you have just created will be saved with an "*.rq" extension.

Loading a method

- In the event of a Quant Routine restart, you may use [Open a method file] in the preselection screen to open the Open standard dialog.
Alternatively, you may also trigger a File / Open method file command for this purpose.

- Select a desired method file and click the [Open] button to open this file. The method will be loaded and the Quant Routine Setup sample table dialog box opens.

### 5.8 Calibration in Quant Routine

To compose a Quant Routine method, you may load calibrations. A load procedure of this type will either extract the regression coefficients from available result files or load a calibration set previously recorded in the Quant calibration module (*.cf-file).

As part of a calibration load procedure, the software checks that the analytical calibration wavelength matches the analytical wavelength of the measurement settings being loaded.

- Use [Open calibration file] in the preselection screen to open the Open standard dialog.

Alternatively, you may also trigger a File / Open calibration file menu command for this purpose.

- Select a desired file and open this file by clicking onto the [Open] button. The calibration curve of this file with related parameters will be displayed in the Import calibration data dialog box.

Fig. 5-12 Display screen for calibration file to be loaded in Quant Routine

- On acknowledgement of your selection, the Setup sample table dialog box will open for specifying a desired sample table.
6 Methods for Water Analysis

The Water Analysis method package is another additional option of the Quant module. The package includes the optimized measurement parameters and calibration data for the Merck Spectroquant test kits.

Based on the German standard methods for water, waste water and sludge examination, these test kits were developed in direct cooperation with the users for the analysis of surface, ground and drinking water, rainwater, boiler feeding and waste water. Appropriate sample preparation provided, they also permit complex sample materials (e.g. soil, solids or organic substances) to be analyzed.

The methods for water analysis are to be started from the Quant-Concentration module. For their use it is indispensable that you know about the function of the Quant module.

Safety notes

Achtung!
Pay attention to the safety notes given in the user's manual of the SPECORD®.

In particular, observe the safety notes as well as the information on handling, storage and disposal of reagents given on the labels, reaction cells and the package inserts provided with the Merck test kits.

Installation notes

During installation, a folder with calibration files and a folder with measurement parameter files are installed. By default, the folders carry the following names:

- C:\Programs\WinASPECT\calib\Wateranalysis\*.cf – Folder with calibration files
- C:\Programs\WinASPECT\para\Wateranalysis\*.par – Folder with measurement parameter files

6.1 Selection of a Water Analysis method

For every Water Analysis method, there is a calibration file and a measurement parameter file. Select the method-specific measurement parameter file and the calibration file to be used.

When working with check samples, activate the respective options.

Selection of measurement parameter file

Activate the menu command Measurement / Open Parameter File to bring up the standard dialog box for opening files.

The parameter files for the water analysis methods are saved to the folder \WinASPECT\para\Wasseranalytik by default. The filename extension is *.par.

The filename is composed of the method name and the method number (→see 3rd column in "Overview of implemented Spectroquant test kits" pg. 123):
e.g. \Wateranalysis\Ammonium-14965.par

- Choose the parameter file you need for the desired method. On confirmation of your choice with [OK], the file will be loaded. The parameters defined in this file will then be applied to all following measurements. The workplace of WinASPECT® appears again.

Selection of calibration file

- Activate the menu command Quant / Concentration to open the Concentration dialog box.
- There, click on the menu command Edit / Setup. This will bring up the Edit - Parameters dialog box with the following tabs: General and Factors / Calibr. Data.

General tab

- On the General tab, make the necessary entries as described in the Section "Selecting the parameters for concentration analysis" p. 89.

Factors / Calibr. Data tab

- Activate the Calibration file option.
- Then, click on the [File] button. This will bring up the standard Open dialog box.
- Choose the desired calibration file. The default path for calibration files of water analysis in WinASPECT® is \WinASPECT\Calib\Wateranalysis\.
- The filenames are composed of the method name, the method number (→see 2nd and 3rd column in "Overview of implemented Spectroquant test kits" pg. 123), the used cell and the measuring range. They are identified by the extension *.cf:

  Lead14333_16mm_0.1-5mg_I cf
  Extension for calibration files
  Measurement range
  Pathlength of cell
  Method number
  Method name

- After having chosen the file, exit the dialog box by a click on the [Open] button. The program returns to the Edit – Parameters dialog box.

After you have made all entries in the Edit – Parameters dialog box, exit it with [OK] to return to the Concentration dialog box.
6.2 Measurement with a Water Analysis method

After you have made all necessary entries in the Edit – Parameters dialog box, you can begin with the concentration determination:

Reference measurement
- Place the reference cell in the sample beam.

Sample measurement
- Replace the reference cell by the first sample cell.
- To start the sample measurement, click on the Start (Meas.) button.

Depending on the selected options regarding the use of sample tables, repeat measurements or check samples, proceed as described in → Section "Determination by direct measurement" p. 93.

6.3 Overview of implemented Spectroquant test kits

The Water Analysis method package comprises optimized measurement parameter files and calibration data for the following Spectroquant® test kits:

<table>
<thead>
<tr>
<th>No.</th>
<th>Parameter</th>
<th>Type No.</th>
<th>Measuring Range</th>
<th>Unit</th>
<th>Cell</th>
<th>Wavelength</th>
<th>Measurement against</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Alcohol KT</td>
<td>1,14965</td>
<td>0.4-5.00 g/L C2H5OH</td>
<td>16 mm</td>
<td>340 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Aluminium Test</td>
<td>1,14825</td>
<td>0.20-1.20 mg/L Al</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Ammonium</td>
<td>1,14739</td>
<td>0.010-2.000 mg/L NH4-N</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Ammonium</td>
<td>0.01-2.58 mg/L NH4+</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Ammonium</td>
<td>1,14558</td>
<td>0.20-8.00 mg/L NH4-N</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Ammonium</td>
<td>0.26-10.30 mg/l NH4+</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Ammonium</td>
<td>1,14544</td>
<td>0.5-16.0 mg/L NH4-N</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Ammonium KT</td>
<td>0.6-20.6 mg/L NH4+</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Ammonium</td>
<td>1,14559</td>
<td>4.0-80.0 mg/L NH4-N</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Ammonium</td>
<td>5.2-103.0 mg/L NH4+</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Ammonium Test</td>
<td>1,14752</td>
<td>0.05-3.00 mg/L NH4-N</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Ammonium Test</td>
<td>0.010-0.500 mg/L NH4-N</td>
<td>50 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Ammonium Test</td>
<td>0.06-3.86 mg/L NH4+</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Ammonium Test</td>
<td>0.012-0.644 mg/L NH4+</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Ammonium Test</td>
<td>1,00683</td>
<td>2.0-75.0 mg/L NH4-N</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>Ammonium Test</td>
<td>5-150    mg/L NH4-N</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>Ammonium Test</td>
<td>2.6-96.6 mg/L NH4+</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## Methods for Water Analysis

Overview of implemented Spectroquant test kits

<table>
<thead>
<tr>
<th>No.</th>
<th>Test</th>
<th>Code</th>
<th>Range</th>
<th>Unit</th>
<th>Filter Size</th>
<th>Wavelength</th>
<th>Blank Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>Ammonium Test</td>
<td>1,14833</td>
<td>0.10-5.00</td>
<td>mg/L NH₄⁺</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>19</td>
<td>Lead KT</td>
<td>1,14833</td>
<td>0.10-5.00</td>
<td>mg/L Pb</td>
<td>16 mm</td>
<td>525 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>20</td>
<td>Lead-Test</td>
<td>1,09717</td>
<td>0.10-5.00</td>
<td>mg/L Pb</td>
<td>10 mm</td>
<td>525 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>21</td>
<td>Lead-Test</td>
<td>1,14833</td>
<td>0.010-1.000</td>
<td>mg/L Pb</td>
<td>50 mm</td>
<td>525 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>22</td>
<td>Boron KT</td>
<td>1,00826</td>
<td>0.05-2.00</td>
<td>mg/L B</td>
<td>16 mm</td>
<td>405 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>23</td>
<td>Boron Test</td>
<td>1,14839</td>
<td>0.050-0.800</td>
<td>mg/L B</td>
<td>10 mm</td>
<td>565 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>24</td>
<td>Bromine Test</td>
<td>1,00605</td>
<td>0.20-7.50</td>
<td>mg/L Br₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water-for-analysis</td>
</tr>
<tr>
<td>25</td>
<td>Bromine Test</td>
<td>1,14839</td>
<td>0.020-1.500</td>
<td>mg/L Br₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>26</td>
<td>BOD KT</td>
<td>1,00687</td>
<td>0.5-3000</td>
<td>mg/L BSB</td>
<td>16 mm</td>
<td>500 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>27</td>
<td>Cadmium KT</td>
<td>1,14834</td>
<td>0.025-1.000</td>
<td>mg/L Cd</td>
<td>16 mm</td>
<td>550 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>28</td>
<td>Calcium Test</td>
<td>1,14815</td>
<td>10-160</td>
<td>mg/L Ca</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>29</td>
<td>Cadmium Test</td>
<td>1,00602</td>
<td>0.10-15.0</td>
<td>mg/L Cd</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>30</td>
<td>Chlorine KT</td>
<td>1,00595</td>
<td>0.05-7.50</td>
<td>mg/L Cl₂</td>
<td>16 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>31</td>
<td>Chlorine KT</td>
<td>1,00597</td>
<td>0.05-7.50</td>
<td>mg/L Cl₂</td>
<td>16 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>32</td>
<td>Chlorine Test</td>
<td>1,00598</td>
<td>0.10-7.50</td>
<td>mg/L Cl₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>33</td>
<td>Chlorine Test</td>
<td>1,14732</td>
<td>0.010-1.500</td>
<td>mg/L Cl₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>34</td>
<td>Chlorine Test</td>
<td>1,00599</td>
<td>0.10-7.50</td>
<td>mg/L Cl₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>35</td>
<td>Chlorine Test</td>
<td>1,00602</td>
<td>0.010-1.500</td>
<td>mg/L Cl₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>36</td>
<td>Chlorine Test</td>
<td>1,14828</td>
<td>0.10-7.50</td>
<td>mg/L Cl₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>37</td>
<td>Chlorine Test</td>
<td>1,14828</td>
<td>0.010-1.500</td>
<td>mg/L Cl₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>38</td>
<td>Chlorine Test</td>
<td>1,14732</td>
<td>0.10-5.00</td>
<td>mg/L Cl₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>39</td>
<td>Chlorine Test</td>
<td>1,14732</td>
<td>0.010-1.500</td>
<td>mg/L Cl₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>40</td>
<td>Chlorine Test</td>
<td>1,14732</td>
<td>0.10-5.00</td>
<td>mg/L Cl₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>41</td>
<td>Chlorine Test</td>
<td>1,00608</td>
<td>0.20-7.50</td>
<td>mg/L ClO₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>42</td>
<td>Chlorine dioxide Test</td>
<td>1,00608</td>
<td>0.20-7.50</td>
<td>mg/L ClO₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>43</td>
<td>Chlorine dioxide Test</td>
<td>1,14732</td>
<td>0.020-1.500</td>
<td>mg/L ClO₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>44</td>
<td>Chlorine dioxide Test</td>
<td>1,14732</td>
<td>0.10-5.00</td>
<td>mg/L ClO₂</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>45</td>
<td>Chlorine dioxide Test</td>
<td>1,14732</td>
<td>0.020-1.000</td>
<td>mg/L ClO₂</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>46</td>
<td>Chloride KT</td>
<td>1,14730</td>
<td>5-125</td>
<td>mg/L Cl⁻</td>
<td>16 mm</td>
<td>525 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>47</td>
<td>Chloride Test</td>
<td>1,14897</td>
<td>2.5-25.0</td>
<td>mg/L Cl⁻</td>
<td>10 mm</td>
<td>445 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>48</td>
<td>Chloride Test</td>
<td>1,14758</td>
<td>10-250</td>
<td>mg/L Cl⁻</td>
<td>10 mm</td>
<td>500 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>49</td>
<td>Chromate KT</td>
<td>1,14552</td>
<td>0.05-2.00</td>
<td>mg/L Cr</td>
<td>16 mm</td>
<td>550 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>50</td>
<td>Chromate Test</td>
<td>1,14552</td>
<td>0.05-3.00</td>
<td>mg/L Cr</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>51</td>
<td>Chromate Test</td>
<td>1,010-0.600</td>
<td>mg/L Cr</td>
<td>50 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>CSB KT</td>
<td>1,14560</td>
<td>4.0-40.0</td>
<td>mg/L CSB</td>
<td>16 mm</td>
<td>340 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>53</td>
<td>CSB KT</td>
<td>1,14540</td>
<td>10-150</td>
<td>mg/L CSB</td>
<td>16 mm</td>
<td>445 nm</td>
<td>Own blank</td>
</tr>
</tbody>
</table>
## Methods for Water Analysis

Overview of implemented Spectroquant test kits

<table>
<thead>
<tr>
<th>#</th>
<th>Test</th>
<th>Code</th>
<th>Range</th>
<th>Units</th>
<th>Diameter</th>
<th>Wavelength</th>
<th>Blank</th>
</tr>
</thead>
<tbody>
<tr>
<td>54</td>
<td>CSB KT</td>
<td>1,14895</td>
<td>15-300 mg/L CSB</td>
<td>16 mm</td>
<td>445 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>55</td>
<td>CSB KT</td>
<td>1,14690</td>
<td>50-500 mg/L CSB</td>
<td>16 mm</td>
<td>445 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>56</td>
<td>CSB KT</td>
<td>1,14541</td>
<td>25-1500 mg/L CSB</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>57</td>
<td>CSB KT</td>
<td>1,14691</td>
<td>300-3500 mg/L CSB</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>58</td>
<td>CSB KT</td>
<td>1,14555</td>
<td>500-10000 mg/L CSB</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>59</td>
<td>CSB KT (Hg-free)</td>
<td>1,09772</td>
<td>10-150 mg/L CSB</td>
<td>16 mm</td>
<td>445 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>60</td>
<td>CSB KT (Hg-free)</td>
<td>1,09773</td>
<td>100-1500 mg/L CSB</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Water-for analysis.</td>
</tr>
<tr>
<td>61</td>
<td>Cyanide KT</td>
<td>1,14561</td>
<td>0.010-0.500 mg/L CN-</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>62</td>
<td>Cyanide Test</td>
<td>1,09701</td>
<td>0.010-0.500 mg/L CN-</td>
<td>10 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>63</td>
<td>Cyanide Test</td>
<td></td>
<td>0.002-0.100 mg/L CN-</td>
<td>50 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>64</td>
<td>Cyanide Test</td>
<td>1,14800</td>
<td>0.025-0.500 mg/L CN-</td>
<td>10 mm</td>
<td>585 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>65</td>
<td>Cyanide Test</td>
<td></td>
<td>0.002-0.100 mg/L CN-</td>
<td>50 mm</td>
<td>585 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>66</td>
<td>Iron KT</td>
<td>1,14549</td>
<td>0.05-4.00 mg/L Fe</td>
<td>16 mm</td>
<td>565 nm</td>
<td></td>
<td>Packing blank</td>
</tr>
<tr>
<td>67</td>
<td>Iron KT</td>
<td>1,14896</td>
<td>1.0-50.0 mg/L Fe</td>
<td>16 mm</td>
<td>525 nm</td>
<td></td>
<td>Packing blank</td>
</tr>
<tr>
<td>68</td>
<td>Iron Test</td>
<td>1,14761</td>
<td>0.05-5.00 mg/L Fe</td>
<td>10 mm</td>
<td>565 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>69</td>
<td>Iron Test</td>
<td></td>
<td>0.005-1.000 mg/L Fe</td>
<td>50 mm</td>
<td>565 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>70</td>
<td>Iron Test</td>
<td>1,00796</td>
<td>0.10-5.00 mg/L Fe</td>
<td>10 mm</td>
<td>500 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>71</td>
<td>Iron Test</td>
<td></td>
<td>0.010-1.000 mg/L Fe</td>
<td>50 mm</td>
<td>500 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>72</td>
<td>Fluoride KT</td>
<td>1,14557</td>
<td>0.10-1.50 mg/L F-</td>
<td>16 mm</td>
<td>620 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>73</td>
<td>Fluoride Test</td>
<td>1,14598</td>
<td>0.10-2.00 mg/L F-</td>
<td>10 mm</td>
<td>635 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>74</td>
<td>Fluoride Test</td>
<td></td>
<td>1.0-20.0 mg/L F-</td>
<td>10 mm</td>
<td>635 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>75</td>
<td>Formaldehyde KT</td>
<td>1,14500</td>
<td>0.10-8.00 mg/L HCHO</td>
<td>16 mm</td>
<td>565 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>76</td>
<td>Formaldehyde Test</td>
<td>1,14678</td>
<td>0.10-9.00 mg/L HCHO</td>
<td>10 mm</td>
<td>565 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>77</td>
<td>Formaldehyde Test</td>
<td></td>
<td>0.02-1.50 mg/L HCHO</td>
<td>50 mm</td>
<td>565 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>78</td>
<td>Gold Test</td>
<td>1,14821</td>
<td>0.5-12.0 mg/L Au</td>
<td>10 mm</td>
<td>550 nm</td>
<td></td>
<td>Own blank</td>
</tr>
<tr>
<td>79</td>
<td>Hydrazine Test</td>
<td>1,09711</td>
<td>0.02-2.00 mg/L N2H4</td>
<td>10 mm</td>
<td>445 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>80</td>
<td>Hydrazine Test</td>
<td></td>
<td>0.005-0.400 mg/L N2H4</td>
<td>50 mm</td>
<td>445 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>81</td>
<td>Iodine Test</td>
<td>1,00606</td>
<td>0.20-7.50 mg/L I2</td>
<td>10 mm</td>
<td>550 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>82</td>
<td>Iodine Test</td>
<td></td>
<td>0.020-1.500 mg/L I2</td>
<td>50 mm</td>
<td>550 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>83</td>
<td>Potassium KT</td>
<td>1,14562</td>
<td>5.0-50.0 mg/L K</td>
<td>16 mm</td>
<td>690 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>84</td>
<td>Copper KT</td>
<td>1,14553</td>
<td>0.05-8.00 mg/L Cu</td>
<td>16 mm</td>
<td>605 nm</td>
<td></td>
<td>Packing blank</td>
</tr>
<tr>
<td>85</td>
<td>Copper Test</td>
<td>1,14767</td>
<td>0.10-6.00 mg/L Cu</td>
<td>10 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>86</td>
<td>Copper Test</td>
<td></td>
<td>0.02-1.20 mg/L Cu</td>
<td>50 mm</td>
<td>605 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>87</td>
<td>Manganese KT</td>
<td>1,00816</td>
<td>0.10-5.00 mg/L Mn</td>
<td>16 mm</td>
<td>445 nm</td>
<td></td>
<td>Packing blank</td>
</tr>
<tr>
<td>88</td>
<td>Manganese Test</td>
<td>1,14770</td>
<td>0.50-10.00 mg/L Mn</td>
<td>10 mm</td>
<td>445 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
<tr>
<td>89</td>
<td>Manganese Test</td>
<td></td>
<td>0.01-2.00 mg/L Mn</td>
<td>50 mm</td>
<td>445 nm</td>
<td></td>
<td>Water for analysis</td>
</tr>
</tbody>
</table>
### Methods for Water Analysis

**Overview of implemented Spectroquant test kits**

| Issue 05/2008 | WinASPECT® |

<p>| 90 | Molybdenum KT | 1.00860 | 0.02-1.00 | mg/L Mo | 16 mm | 620 nm | Own blank |
| 91 | Sodium KT (Dün.) | 1.0085 | 10-300 | mg/L Na | 16 mm | 550 nm | Water for analysis. |
| 92 | Nickel KT | 1.14554 | 0.10-6.00 | mg/L Ni | 16 mm | 445 nm | Packing blank |
| 93 | Nickel Test | 1.14785 | 0.10-5.00 | mg/L Ni | 10 mm | 445 nm | Water for analysis |
| 94 | Nickel Test | 0.02-1.00 | mg/L Ni | 50 mm | 445 nm | Water for analysis |
| 95 | Nitrate KT | 1.14542 | 0.5-18.0 | mg/L NO3-N | 16 mm | 525 nm | Own blank |
| 96 | Nitrate KT | 2.2-79.7 | mg/L NO3-N | 16 mm | 525 nm | Packing blank |
| 97 | Nitrate KT | 1.14563 | 0.5-25.0 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 98 | Nitrate KT | 2.2-110.7 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 99 | Nitrate Test | 1.14764 | 1.0-50.0 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 100 | Nitrate Test | 4-221 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 101 | Nitrate KT | 1.00614 | 23-225 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 102 | Nitrate KT | 102-996 | mg/L NO3-N | 16 mm | 340 nm | Packing blank |
| 103 | Nitrate Test | 1.14773 | 0.5-20.0 | mg/L NO3-N | 10 mm | 525 nm | Own blank |
| 104 | Nitrate Test | 2.2-88.5 | mg/L NO3-N | 10 mm | 525 nm | Own blank |
| 105 | Nitrate Test | 1.09713 | 1.0-25.0 | mg/L NO3-N | 10 mm | 340 nm | Own blank |
| 106 | Nitrate Test | 0.10-5.00 | mg/L NO3-N | 50 mm | 340 nm | Own blank |
| 107 | Nitrate Test | 4.4-110.7 | mg/L NO3-N | 10 mm | 340 nm | Own blank |
| 108 | Nitrate Test | 0.4-22.1 | mg/L NO3-N | 50 mm | 340 nm | Own blank |
| 109 | Nitrate KT (Seaw.) | 1.14556 | 0.10-3.00 | mg/L NO3-N | 16 mm | 500 nm | Own blank |
| 110 | Nitrate KT (Seaw.) | 0.3-13.3 | mg/L NO3-N | 16 mm | 500 nm | Own blank |
| 111 | Nitrate Test (Seaw.) | 1.14942 | 0.2-17.0 | mg/L NO3-N | 10 mm | 500 nm | Water for analysis |
| 112 | Nitrate Test (Seaw.) | 1.0-75.0 | mg/L NO3-N | 10 mm | 500 nm | Water for analysis |
| 113 | Nitrite KT | 1.14547 | 0.010-0.700 | mg/L NO2-N | 16 mm | 525 nm | Packing blank |
| 114 | Nitrite KT | 0.03-2.30 | mg/L NO2-N | 16 mm | 525 nm | Packing blank |
| 115 | Nitrite Test | 1.14776 | 0.02-1.00 | mg/L NO2-N | 10 mm | 525 nm | Own blank |
| 116 | Nitrite Test | 0.005-0.200 | mg/L NO2-N | 10 mm | 525 nm | Own blank |
| 117 | Nitrite Test | 0.07-3.28 | mg/L NO2-N | 50 mm | 525 nm | Own blank |
| 118 | Nitrite Test | 0.016-0.657 | mg/L NO2-N | 50 mm | 525 nm | Own blank |
| 119 | Ozone Test | 1.00607 | 0.10-7.50 | mg/L O3 | 10 mm | 550 nm | Water for analysis. |
| 120 | Ozone Test | 0.010-1.500 | mg/L O3 | 50 mm | 550 nm | Water for analysis |
| 121 | Ozone Test | 1.14732 | 0.10-5.00 | mg/L O3 | 10 mm | 550 nm | Water for analysis |
| 122 | Ozone Test | 0.010-1.000 | mg/L O3 | 50 mm | 550 nm | Water for analysis |
| 123 | Phenol KT | 1.14551 | 0.10-2.50 | mg/L Phenol | 16 mm | 500 nm | Packing blank |
| 124 | Phenol KT | 0.025-1.000 | mg/L Phenol | 50 mm | 500 nm | Own blank |
| 125 | Phosphate KT | 1.14543 | 0.05-5.00 | mg/L PO4-P | 16 mm | 690 nm | Packing blank |</p>
<table>
<thead>
<tr>
<th>Product Code</th>
<th>Test Description</th>
<th>Range of Measurement</th>
<th>Blank</th>
<th>Wavelength</th>
<th>Blank Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>126</td>
<td>Phosphate KT (PMB)</td>
<td>0.2-15.3 mg/L PO₄⁻</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>127</td>
<td>Phosphate KT (PMB)</td>
<td>0.11-11.46 mg/L P₂O₅</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>128</td>
<td>Phosphate KT (PMB)</td>
<td>1.14729 mg/L PO₄⁻P</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>129</td>
<td>Phosphate KT (PMB)</td>
<td>1.5-76.7 mg/L PO₄⁻</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>130</td>
<td>Phosphate KT (PMB)</td>
<td>1.1-57.3 mg/L P₂O₅</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>131</td>
<td>Phosphate KT (PMB)</td>
<td>1,00616 mg/L PO₄⁻P</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>132</td>
<td>Phosphate KT (PMB)</td>
<td>9-307 mg/L PO₄⁻</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>133</td>
<td>Phosphate KT (PMB)</td>
<td>7-229 mg/L P₂O₅</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>134</td>
<td>Phosphate Test (PMB)</td>
<td>1,14848 0.05-5.00 mg/L PO₄⁻P</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>135</td>
<td>Phosphate Test (PMB)</td>
<td>0.010-1.000 mg/L PO₄⁻P</td>
<td>50 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>136</td>
<td>Phosphate Test (PMB)</td>
<td>0.2-15.3 mg/L PO₄⁻</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>137</td>
<td>Phosphate Test (PMB)</td>
<td>0.03-3.07 mg/L PO₄⁻</td>
<td>50 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>138</td>
<td>Phosphate Test (PMB)</td>
<td>0.11-11.46 mg/L P₂O₅</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>139</td>
<td>Phosphate Test (PMB)</td>
<td>0.02-2.29 mg/L P₂O₅</td>
<td>50 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>140</td>
<td>Phosphate Test (PMB)</td>
<td>1,00798 1.0-100.0 mg/L PO₄⁻P</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>141</td>
<td>Phosphate Test (PMB)</td>
<td>3-307 mg/L PO₄⁻</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>142</td>
<td>Phosphate Test (PMB)</td>
<td>2-229 mg/L P₂O₅</td>
<td>10 mm</td>
<td>690 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>143</td>
<td>Phosphate KT (VM)</td>
<td>1,14546 0.5-25.0 mg/L PO₄⁻P</td>
<td>16 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>144</td>
<td>Phosphate KT (VM)</td>
<td>1.5-75.0 mg/L PO₄⁻</td>
<td>16 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>145</td>
<td>Phosphate KT (VM)</td>
<td>1.1-57.3 mg/L P₂O₅</td>
<td>16 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>146</td>
<td>Phosphate Test (VM)</td>
<td>1,14842 1.0-30.0 mg/L PO₄⁻P</td>
<td>10 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>147</td>
<td>Phosphate Test (VM)</td>
<td>3.1-92.0 mg/L PO₄⁻</td>
<td>10 mm</td>
<td>410 nm</td>
<td>Own blank</td>
</tr>
</tbody>
</table>
## Methods for Water Analysis

Overview of implemented Spectroquant test kits

<table>
<thead>
<tr>
<th>Test</th>
<th>Method</th>
<th>Concentration</th>
<th>Unit</th>
<th>Tube Length</th>
<th>Wavelength</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphate Test (VM)</td>
<td>2.3-68.7</td>
<td>mg/L P2O5</td>
<td>10 mm</td>
<td>410 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Residual Hardness KT</td>
<td>1,14683</td>
<td>0.50-5.00</td>
<td>mg/L Ca</td>
<td>16 mm</td>
<td>565 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Oxygen KT</td>
<td>1,14694</td>
<td>0.5-12.0</td>
<td>mg/L O2</td>
<td>16 mm</td>
<td>565 nm</td>
<td>Water for analysis.</td>
</tr>
<tr>
<td>Silver Test</td>
<td>1,14831</td>
<td>0.50-3.00</td>
<td>mg/L Ag</td>
<td>10 mm</td>
<td>550 nm</td>
<td>Water for analysis</td>
</tr>
<tr>
<td>Silicate Test</td>
<td>1,14794</td>
<td>0.10-5.00</td>
<td>mg/L Si</td>
<td>10 mm</td>
<td>665 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Silicate Test</td>
<td>0.005-0.750</td>
<td>mg/L Si</td>
<td>50 mm</td>
<td>820 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Silicate Test</td>
<td>0.21-10.70</td>
<td>mg/L SiO2</td>
<td>10 mm</td>
<td>665 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Silicate Test</td>
<td>0.01-1.60</td>
<td>mg/L SiO2</td>
<td>50 mm</td>
<td>820 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Silicate Test</td>
<td>1,00857</td>
<td>0.5-50</td>
<td>mg/L Si</td>
<td>10 mm</td>
<td>405 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Silicate Test</td>
<td>5-500</td>
<td>mg/L SiO2</td>
<td>10 mm</td>
<td>405 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Silicate Test</td>
<td>11-1070</td>
<td>mg/L SiO2</td>
<td>10 mm</td>
<td>405 nm</td>
<td>Own blank</td>
<td></td>
</tr>
<tr>
<td>Nitrogen (ges.) KT</td>
<td>1,00613</td>
<td>0.5-15.0</td>
<td>mg/L N</td>
<td>16 mm</td>
<td>340 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>Nitrogen (ges.) KT</td>
<td>1,14537</td>
<td>0.5-15.0</td>
<td>mg/L N</td>
<td>16 mm</td>
<td>525 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Nitrogen (ges.) KT</td>
<td>1,14763</td>
<td>10-150</td>
<td>mg/L N</td>
<td>16 mm</td>
<td>340 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>Sulphate KT</td>
<td>1,14548</td>
<td>5-250</td>
<td>mg/L SO42-</td>
<td>16 mm</td>
<td>520 nm</td>
<td>Sample without reagent, filtered</td>
</tr>
<tr>
<td>Sulphate KT</td>
<td>1,00617</td>
<td>50-500</td>
<td>mg/L SO42-</td>
<td>16 mm</td>
<td>525 nm</td>
<td>Sample without reagent, filtered</td>
</tr>
<tr>
<td>Sulphate KT</td>
<td>1,14564</td>
<td>100-1000</td>
<td>mg/L SO42-</td>
<td>16 mm</td>
<td>690 nm</td>
<td>Sample without reagent, filtered</td>
</tr>
<tr>
<td>Sulphate Test</td>
<td>1,14791</td>
<td>25-300</td>
<td>mg/L SO42-</td>
<td>10 mm</td>
<td>525 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Sulphide Test</td>
<td>1,14779</td>
<td>0.020-0.500</td>
<td>mg/L S2-</td>
<td>50 mm</td>
<td>665 nm</td>
<td>Water for analysis.</td>
</tr>
<tr>
<td>Sulphite KT</td>
<td>1,14394</td>
<td>1.0-20.0</td>
<td>mg/L SO32-</td>
<td>16 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>Sulphite KT</td>
<td>1,14394</td>
<td>0.05-3.00</td>
<td>mg/L SO32-</td>
<td>50 mm</td>
<td>410 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Surfactants (anion.) KT</td>
<td>1,14697</td>
<td>0.05-2.00</td>
<td>mg/L MBAS</td>
<td>16 mm</td>
<td>665 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>TOC KT</td>
<td>1,14878</td>
<td>5.0-80.0</td>
<td>mg/L TOC</td>
<td>16 mm</td>
<td>585 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Hydrogen peroxide KT</td>
<td>1,14731</td>
<td>2.0-20.0</td>
<td>mg/L H2O2</td>
<td>16 mm</td>
<td>410 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>Hydrogen peroxide KT</td>
<td>0.25-5.00</td>
<td>mg/L H2O2</td>
<td>50 mm</td>
<td>410 nm</td>
<td>Water for analysis</td>
<td></td>
</tr>
<tr>
<td>Zinc KT</td>
<td>1,14566</td>
<td>0.20-5.00</td>
<td>mg/L Zn</td>
<td>16 mm</td>
<td>500 nm</td>
<td>Packing blank</td>
</tr>
<tr>
<td>Zinc KT</td>
<td>1,14832</td>
<td>0.05-2.50</td>
<td>mg/L Zn</td>
<td>10 mm</td>
<td>565 nm</td>
<td>Own blank</td>
</tr>
<tr>
<td>Tin KT</td>
<td>1,14622</td>
<td>0.10-2.50</td>
<td>mg/L Sn</td>
<td>16 mm</td>
<td>660 nm</td>
<td>Water for analysis.</td>
</tr>
</tbody>
</table>
7 Kinetics Module

After its installation, the Kinetics module is fully integrated into the WinASPECT® workplace. Its functions are accessible via the Kinetics menu.

The Kinetics module provides evaluation of time-dependent measurement curves for the determination of kinetic reactions. The program calculates the rate of the kinetic reaction by linear regression based on measured values from a user-defined range. The slope of the line of regression may be additionally multiplied by a factor.

Moreover, the Kinetics module provides diverse options for the presentation of measurement curves.

You may save the results of the calculation and the graph and print them out. By copying them to the Windows clipboard, you can also make them available to other Windows applications (e.g. Office software).

The preset path for files containing the results of a kinetic evaluation procedure is \WinASPECT\Kinetic. A kinetics file is saved under a selected name with an extension as follows:

"*.cir" File with evaluation of kinetics
"*.cirs" Signed file with evaluation of kinetics

On the WinASPECT® workplace, activate the menu function Kinetics / Routine. The WinASPECT® application window becomes inactive and the following dialog box becomes visible (without graph and table):

![Kinetics Module](image)

Fig.7-1 Kinetics – Routine dialog box
## Menu functions of the Kinetics dialog box

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>New</strong></td>
<td>Starts a new kinetic analysis.</td>
</tr>
<tr>
<td><strong>Open</strong></td>
<td>Opens a stored kinetic analysis.</td>
</tr>
<tr>
<td><strong>Copy to clipboard</strong></td>
<td>Copies the results of the kinetic analysis to the clipboard thus making them available to other Windows applications.</td>
</tr>
<tr>
<td><strong>Print</strong></td>
<td>Prints the results of the kinetic analysis.</td>
</tr>
<tr>
<td><strong>Export</strong></td>
<td>Exports the files to the *.csv format (Excel).</td>
</tr>
<tr>
<td><strong>Save</strong></td>
<td>Saves any changes to the kinetic analysis file.</td>
</tr>
<tr>
<td><strong>Save as...</strong></td>
<td>Saves any changes to the kinetic analysis file under a new file name.</td>
</tr>
<tr>
<td><strong>Close</strong></td>
<td>Closes the <strong>Kinetics</strong> module and returns to the WinASPECT® application window.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Measurement parameters</strong></th>
<th>Opens the measurement parameters window.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Properties of selected measure</strong></td>
<td>To be activated for defining the options for the kinetic analysis (designation, factor and range limits for regression calculation).</td>
</tr>
<tr>
<td><strong>Sign document</strong></td>
<td>Signs kinetics data. (→ Section “Signing a file” p. 213)</td>
</tr>
<tr>
<td><strong>View signatures</strong></td>
<td>Shows the existing signatures of the open kinetics file.</td>
</tr>
</tbody>
</table>

| **Line of regression**     | Activates/deactivates the display of the line of regression in the graph. The line of regression is displayed as continuous line in the same color as the sample curve. |
| **Ranges**                 | Activates/deactivates the display of the abscissa range limits in the graph as vertical lines.                                               |
| **Grid**                   | Displays a grid in the graph.                                                                                                                |
| **Abscissa in minutes/seconds** | Converts the abscissa values from seconds to minutes and vice versa.                                                                      |
| **Scaling**                | Allows you to enlarge or reduce the curve section in the graph.                                                                             |
| **Audit trail**            | Displays the Audit Trail record of the active kinetic analysis.                                                                             |

| **Reference**              | Starts the reference measurement.                                                                                                           |
| **Start!**                 | Starts kinetic analysis of a file saved in *.dat format.                                                                                     |
| **Load from file**         | Starts a sample measurement with following kinetic analysis.                                                                                 |
| **Measure**                |                                                                                                                                             |
| **Close**                  | Closes the Kinetics – Routine dialog box.                                                                                                     |
Buttons and textboxes of the Kinetics dialog box

<table>
<thead>
<tr>
<th>Buttons / textboxes</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title</td>
<td>Entry of a title of the currently active kinetic analysis. The title is saved along with the kinetics data. The entry is optional.</td>
</tr>
<tr>
<td>Operator</td>
<td>Entry of a user name. The entry is optional. If you use the FDA conf version of WinASPECT®, the logged in user will be entered automatically.</td>
</tr>
<tr>
<td></td>
<td>Activates the mouse pointer for the interactive selection of the range limits for the regression calculation. The range limits are to be defined with the mouse button held depressed.</td>
</tr>
<tr>
<td></td>
<td>Serves to zoom in a section of the graph.</td>
</tr>
<tr>
<td></td>
<td>Returns to the original scaling of the graph.</td>
</tr>
<tr>
<td>Color fields left of the sample table</td>
<td>Serves to select a sample for kinetic analysis and display in the graph.</td>
</tr>
<tr>
<td></td>
<td>The selected sample is marked by &quot;!&quot; and shown in the respective color in the graph.</td>
</tr>
<tr>
<td>All buttons</td>
<td>When activating one of these buttons, the same presentation properties are applied to all sample curves in the graph (colored, gray, or hidden).</td>
</tr>
</tbody>
</table>

7.1 Measuring a kinetic reaction

Taking the reference measurement

You must take a reference measurement, if you activated this correction option in the parameter file.

- Place the reference in the sample beam.
- Start the reference measurement by activating menu command Reference.

In the reference measurement, a correction value is determined at the defined wavelength. The measured values obtained afterwards will then be corrected by this value.

Taking the sample measurement

- Place the sample in the sample beam.
- Start preparing the measurement by activating the menu command Start! / Measure.
  On doing so, the following query appears: "Start time cycle? [OK]".
- Start the kinetic measurement by a click on [OK]. The measurement is being executed.
Note

With a click on the [Pause] button, you can interrupt the measurement. On scanning spectrophotometers, you can open the sample compartment cover afterwards (e.g. to add further reagents to the sample). To continue the measurement, click on the [Continue] button.

7.1.1 Parameter settings for kinetic measurements on scanning spectrophotometers

- Activate menu command Edit / Measurement Parameters to open the device driver software.
- For the entry of parameters, observe the following:
  - For the measurement of sample batches, it is necessary that you activate the Cycle mode - Manual option on the Settings tab. If the Cycle mode - None option has been activated, the results of the measurement and of the following kinetic analysis will be saved to separate files each for every sample.
  - On the Mode tab, the Time Scan option must have been selected.
  - When using a cell changer, you can choose between normal mode and Slow time scan mode.
  - For the kinetic analysis that automatically follows the measurement, the measurement result must always be a curve measured versus time (abscissa).

With time-controlled measurements of spectra over a defined wavelength range, it is necessary to determine the time-based data by applying a time section through the family of spectra at the desired wavelength. These measured values must have been acquired and stored before the start of the Kinetics module. They can then be loaded as file for kinetic analysis.

Example of selected measurement parameters for a kinetic measurement:

<table>
<thead>
<tr>
<th>Option/Textbox</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Settings tab</strong></td>
<td></td>
</tr>
<tr>
<td>Title</td>
<td>Enter a title of the measurement (optional), e.g. &quot;Survey measurement&quot;.</td>
</tr>
<tr>
<td>Cycle</td>
<td>Manual (or None)</td>
</tr>
<tr>
<td>Display</td>
<td>Absorbance</td>
</tr>
<tr>
<td>Min.</td>
<td>0</td>
</tr>
<tr>
<td>Max.</td>
<td>2</td>
</tr>
<tr>
<td>Correction</td>
<td>Reference</td>
</tr>
<tr>
<td><strong>Device tab</strong></td>
<td></td>
</tr>
<tr>
<td>Lamp change at</td>
<td>320*</td>
</tr>
<tr>
<td>D2E automatically</td>
<td>To be activated</td>
</tr>
<tr>
<td>COM Port</td>
<td>Choose the COM port of your PC to which the SPECORD® has been connected.</td>
</tr>
</tbody>
</table>
7.1.2 Parameter settings for kinetic measurements on SPECORD Sxxx

- Activate menu command **Edit / Measurement parameters** to open the device driver software.

- For the entry of parameters, observe the following:
  - On the **Mode** tab, you must have selected the **Time Scan** option with a fixed wavelength.
  - When using a cell changer, the normal mode and the **Slow time scan mode** can be used.
  - For the kinetic analysis that automatically follows the measurement, the measurement result must always be a curve measured versus time (abscissa). With time-controlled measurements of spectra over a defined wavelength range, it is necessary to determine the time-based data by applying a time section through the family of spectra at the desired wavelength. These measured values must have been acquired and stored before the start of the Kinetics module. They can then be loaded as file for kinetic analysis.

Example of measurement parameters for a kinetic measurement without accessory:

<table>
<thead>
<tr>
<th>Option/Entry</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General tab</strong></td>
<td></td>
</tr>
<tr>
<td>Title</td>
<td>Enter a title of the measurement (optional), e.g. &quot;Survey measurement&quot;</td>
</tr>
<tr>
<td>Operator</td>
<td>Enter your name.</td>
</tr>
<tr>
<td></td>
<td>With the FDA conforming version of WinASPECT®, the logged in user will automatically be entered here.</td>
</tr>
<tr>
<td>Display during measure-</td>
<td>Activate the <strong>Absorbance</strong> and <strong>Autoscale</strong> options.</td>
</tr>
<tr>
<td>ment</td>
<td></td>
</tr>
<tr>
<td><strong>Device</strong></td>
<td></td>
</tr>
<tr>
<td>Integration time</td>
<td>Search for the optimum time using the Monitor mode (→ Section &quot;Selecting the integration time in Monitor mode&quot; p. 44).</td>
</tr>
<tr>
<td>Accumulation</td>
<td>Enter 5.</td>
</tr>
<tr>
<td>Dark current correction</td>
<td>To be activated.</td>
</tr>
<tr>
<td>Lamp switching</td>
<td>Choose the <strong>D2E+HL</strong> option.</td>
</tr>
</tbody>
</table>
7.2 Loading a file for kinetic analysis

For a kinetic analysis, you can also load a file measured and saved in the WinASPECT® main window.

The files must meet the following requirements:

- The abscissa must have a time scale.
- Spectra measured with the Cycle option "time controlled", must be subjected to a time section first to obtain time-based data (menu function Edit / Time-based data).

- Activate the menu function Start! / Load from file.
  This will bring up the standard dialog box for opening files.
- Choose the desired file and click on [Open].
  The measured data of the file and the kinetic analysis appear in the dialog box.

7.3 Evaluating kinetic reactions

In the sample table, the kinetic analysis is displayed directly after the measurement and the loading of the file.

In the table, the following parameters are presented:

- Designation of the sample
- Start and end of the regression range
- Factor
- Slope
- Coefficient of determination $R^2_{\text{adj}}$
- Result of the kinetic analysis
• Markings for the graphic presentation of the measured curves.

A linear regression is calculated for the selected ranges according to the parameters set for the kinetic analysis. The result of the kinetic analysis (Result) is the product of the slope of the line of regression and the entered factor:

\[ \text{Result} = \text{Factor} \times \text{Slope}. \]

### 7.3.1 Selecting a sample for kinetic analysis

When you measure serial samples or work with the cell changer, the measured curves are displayed altogether on the screen. You can optionally assign common parameters for the kinetic analysis or select individual curves for analysis.

In the table, every sample is identified by a colored field. The measured curve of this sample in the graph (broken line) is identified by the same color.

- To select a measured curve, click on the colored field left of the table entry.

The colored field selected that way is marked by an exclamation mark "!". Under the table, a note appears on the selected sample, e.g. "Selected measurement series 2"

![Fig.7-2 Selecting a measured curve in Kinetics – Routine](image)

### 7.3.2 Defining the parameters for the kinetic analysis

- Choose the desired sample by a click on the corresponding colored field left of the field with the designation of the sample. Activate the menu command Edit / Properties of selected measurement.

- Alternatively, right-click on the row containing the desired sample. For that, the sample need not be selected before.

This will bring up the Settings dialog box.

![Fig.7-3 Settings dialog box](image)

- Make the following settings:
Kinetics Module

Graphic presentation of sample data in the Kinetics module

<table>
<thead>
<tr>
<th>Textbox / check box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Designation</td>
<td>Sample name</td>
</tr>
<tr>
<td>Range start</td>
<td>Start of the range in which the regression calculation shall be performed.</td>
</tr>
<tr>
<td>Range end</td>
<td>End of the range in which the regression calculation shall be performed.</td>
</tr>
<tr>
<td>Factor</td>
<td>Factor with which the calculated slope is multiplied.</td>
</tr>
<tr>
<td>for all samples</td>
<td>If these check boxes are activated, the settings are applied to all samples of the measurement series.</td>
</tr>
</tbody>
</table>

Confirm the entries with [OK].

The results of the kinetic analysis are being updated in the table.

Interactive selection of range limits

You can also select the range limits for the regression calculation in the graph interactively. The thus selected limits apply to all samples.

- Click on this button: ![Image]
  The mouse pointer turns into a vertical line with RANGE label.
- In the graph, click on the desired start of the range and, holding the mouse button depressed, move the mouse to the desired end of the range. Release the mouse button.

The new range limits are being transferred and the data in the table updated accordingly.

7.4 Graphic presentation of sample data in the Kinetics module

The graph shows the measured curves of the samples. A specific color is assigned to every sample. The color fields left of the sample table serve as color code.

The View menu provides options for the display of additional information:

- Presentation of the line of regression as continuous line in the same color as the sample curve
- Display of the limits of the regression range as broken vertical lines
- Display of a grid in the background

7.4.1 Displaying measured kinetic curves

If you select a single sample by a click on the colored field beside the table, its curve and, if this option was activated, also the corresponding line of regression are shown in colors in the graph, whereas all other curves appear in gray.

You can also define for every curve individually, whether it shall appear colored, gray or whether it shall be hidden. For that, mark the corresponding fields of the "mark", "un-mark" or "hide" columns of the table. The functions being active for the sample are
marked by (x) in the field.

<table>
<thead>
<tr>
<th></th>
<th>mark</th>
<th>unmark</th>
<th>hide</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td></td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 7-4 Marking the curves for graphic presentation

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>mark</td>
<td>The curve of this sample appears colored.</td>
</tr>
<tr>
<td>unmark</td>
<td>The curve appears in gray.</td>
</tr>
<tr>
<td>hide</td>
<td>The curve is hidden.</td>
</tr>
</tbody>
</table>

The All check boxes below the columns facilitate marking. By activation one of the check boxes, the function specified in the column head is assigned to all samples simultaneously.

7.4.2 Scaling of kinetic curve presentation

Setting the scaling via entries in a dialog box

- Activate the menu command View / Scaling.
  This will bring up the Kinetics – Zoom dialog box.

Fig. 7-5 Kinetics – Zoom dialog box

- In the corresponding textboxes, type the desired limits for abscissa and ordinate presentation. By a click on the [Apply] button, you can reset the original scaling of the graph.

- Confirm your entries with [OK].
  The selected section of the graph appears.

Interactive selection of the displayed section of the graph

- Click on the button (top left above the graph).
  In the graph, the mouse pointer turns into a full arrowhead.
With the mouse button held depressed, draw a rectangle across the section to be zoomed in.
When you release the mouse button, the selected section appears.

By a click on the software automatically resets the original scaling of the graph.

### 7.5 Printing a kinetic analysis

- Activate menu command File / Print.
  This will bring up the dialog box for preparing the printout.

![Print Kinetics - Routine dialog box](image)

Fig.7-6 Print Kinetics - Routine dialog box

- Activate the check boxes of the items you want to include in the printout and choose the desired layout and printer options.
  The functions of Page Layout and Printer Setup are described in Section "Printing files" pg. 69.

- Start the printout of the kinetic analysis by a click on [Print].
8 Biochemical Analysis (Bio Module)

After installation, the Bio module is fully integrated in the WinASPECT® desktop and its functions are accessible via the Bio menu.

The Bio module allows the measurement of proteins, DNA and RNA and result analysis according to the following methods:

<table>
<thead>
<tr>
<th>Method name</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorbance 260 nm</td>
<td>(x = A(260\text{nm}))</td>
</tr>
<tr>
<td>DNA Purity A260/A280</td>
<td>(x = A(260\text{nm}) / A(280\text{nm}))</td>
</tr>
<tr>
<td>Absorbance 260 nm, Factor 33</td>
<td>(x[\mu\text{g/ml}] = A(260\text{nm}) \times 33)</td>
</tr>
<tr>
<td>Absorbance 260 nm, Factor 40</td>
<td>(x[\mu\text{g/ml}] = A(260\text{nm}) \times 40)</td>
</tr>
<tr>
<td>Absorbance 260 nm, Factor 50</td>
<td>(x[\mu\text{g/ml}] = A(260\text{nm}) \times 50)</td>
</tr>
<tr>
<td>Warburg and Christian (DNA)</td>
<td>(x[\text{mg/ml}] = (A(260\text{nm}) \times 62.9) - (A(280\text{nm}) \times 36))</td>
</tr>
<tr>
<td>Warburg and Christian (Protein)</td>
<td>(x[\text{mg/ml}] = (A(280\text{nm}) \times 1.55) - (A(260\text{nm}) \times 0.76))</td>
</tr>
<tr>
<td>Absorbance 280 nm</td>
<td>(x = A(280\text{nm}))</td>
</tr>
<tr>
<td>Absorbance 205 nm, Factor 31</td>
<td>(x[\mu\text{g/ml}] = A(205\text{nm}) \times 31)</td>
</tr>
<tr>
<td>Scopes Formula</td>
<td>(x[\text{mg/ml}] = \left(\frac{A(280\text{nm})}{A(205\text{nm})}\right) \times 120 + 27)</td>
</tr>
<tr>
<td>Whitaker and Granum</td>
<td>(x[\text{mg/ml}] = \left(\frac{A(235\text{nm})}{A(280\text{nm})}\right) \times 2.51)</td>
</tr>
<tr>
<td>Absorbance 215nm, 225nm</td>
<td>(x[\text{mg/ml}] = \left(\frac{A(215\text{nm})}{A(225\text{nm})}\right) \times 144)</td>
</tr>
<tr>
<td>Kalb and Bernlohr</td>
<td>(x[\mu\text{g/ml}] = A(230\text{nm}) \times 183 - A(280\text{nm}) \times 75.8)</td>
</tr>
<tr>
<td>Absorbance 280 nm, Factor 1.38</td>
<td>(x[\text{mg/ml}] = A(280 \text{nm}) \times 1.38)</td>
</tr>
<tr>
<td>Kalckar and Shafran</td>
<td>(x[\text{mg/ml}] = A(280\text{nm}) \times 1.45 - A(260\text{nm}) \times 0.74)</td>
</tr>
</tbody>
</table>

In addition, you can recall result records created with the Bio Module for later review and printout.

The preset path for files created with the Bio module is \\WinASPECT\\Bio. Result files are saved under the selected name with the following filename extensions:

"*.bio" Bio method file
"*.bios" Signed Bio method file

In older WinASPECT® versions, the extension "*.bix" was used.

In the Bio module, only files that have been created with this module can be opened and edited. The evaluation of spectra that have already been measured and stored (".dat" files) is not possible.

The measurement parameters used are saved together with the analytical results of a measurement series. When re-loading this file, the corresponding measurement parameters are available for further measurements. The measurement results will then be appended to the existing measurement record.

- Activate the menu function Bio / Method.

On doing so, the WinASPECT® becomes inactive and the Method dialog box appears.
Biochemical Analysis (Bio Module)

Printing a kinetic analysis

Fig. 8-1 Method dialog box

This dialog box has two tabs:

- **Setup** with the current measurement and analysis parameters
- **Results** with result analysis.

**Functions of the menu bar of the Bio Module**

The Method dialog box provides the following menu functions and buttons:

<table>
<thead>
<tr>
<th>Menu function / Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>File</strong></td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>Starting new analyses.</td>
</tr>
<tr>
<td>Open</td>
<td>Opening a file created with the <strong>Bio</strong> module. The filename extension for files of the <strong>Bio</strong> module is &quot;.bio&quot; or &quot;**bios&quot;.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves the results and settings under the currently valid filename.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the results and settings to a new file.</td>
</tr>
<tr>
<td>Print</td>
<td>Saving is via the Windows standard dialog box for saving files.</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>Starts the printout of results and settings. Copies the results to the Windows clipboard. Thus, the results are accessible to other Windows applications.</td>
</tr>
<tr>
<td>Close</td>
<td>Closes the current <strong>Bio</strong> module session.</td>
</tr>
<tr>
<td><strong>Setup</strong></td>
<td>Selection of the settings for an analysis with the <strong>Bio</strong> module.</td>
</tr>
</tbody>
</table>
Biochemical Analysis (Bio Module)

Measurement settings in Bio module

| Sign Document | Providing the results with a signature (→ Section "Electronic signature" p. 213). |
| View signatures | Shows the existing signature of an open calibration file. |
| Audit Trail | Shows the Audit Trail list. |
| Start | Starts the measurement. |
| Reference | Starts the reference measurement. |
| Help | Activating online help. |
| Close | Closes the Bio module session and the Method dialog box. |

8.1 Measurement settings in Bio module

Measurements with the Bio Method module require you to choose a method formula and individual measurement parameters among various options. First, choose the measurement parameters and the method.

You can also load a saved result record and continue taking measurements. For these measurements, the program will use the same measurement settings as those used in the previous measurements. The new results will then be appended to the result record.

- Activate the menu function Setup to open the Method – Setup dialog box.

The dialog box has four tabs:

- General
- Method
- Measurement settings
- Cell changer

- On the tabs, make the necessary entries.
- Confirm the entries with [OK]. On doing so, the buttons Start! and Reference become accessible.

General tab

![Fig.8-2 Method - Setup dialog box: General tab](image)

- In the Description and Operator textboxes, you can enter a description and the name of the operator to ensure GLP compliance.
Biochemical Analysis (Bio Module)

Measurement settings in Bio module

Entered data will appear on the result record. They will be saved along with the results.

Method tab

![Method tab](image)

- On the displayed list, mark the methods to be used for the analyses by a tick. You may choose several methods at the same time.

Measurement Settings tab

![Measurement Settings tab](image)

The program will automatically set the wavelengths and the measuring mode appropriate for the selected method. The cell changer may be used optionally as accessory.

- The following measurement parameters are variable:

### Scanning SPECORD®

<table>
<thead>
<tr>
<th>Function</th>
<th>Settings</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integration time</td>
<td>0.1 to 50 s</td>
<td>Time for the registration of a measured value</td>
</tr>
<tr>
<td>Correction</td>
<td>Reference</td>
<td>Reference measurement</td>
</tr>
<tr>
<td></td>
<td>Standard</td>
<td>Only for SPECORD® 50 / 200 / 205 / 210 / 250</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Correction with internally stored baseline</td>
</tr>
<tr>
<td>Slit setting</td>
<td>Device-dependent</td>
<td>Only for SPECORD® 200 / 205 / 210 / 250</td>
</tr>
</tbody>
</table>
8.2 Measurement procedure in the Bio Method module

Reference measurement
If in method setup you selected the baseline correction option, **Correction: Reference**, you must measure the reference value first.

- Place the cell with the reference in the sample beam of the spectrometer.
- Start the reference measurement using the **Reference** function on the menu bar of the **Method** dialog box.

Sample measurement
- Put the sample into the sample beam.
- Start the sample measurement by a click on [**Start!**] in the menu bar of the **Method** dialog box.
Biochemical Analysis (Bio Module)

Measurement procedure in the Bio Method module

Fig.8-5 Method dialog box: Results tab

The measurement and analysis results are displayed on the Results tab of the Method dialog box.

The measurement results are consecutively numbered. The result table contains the following data:

- Sample name
- Date and time of measurement
- Result of calculation
- Measured values
- Additionally, with activated zero correction option, the uncorrected measured values and the zero point

- Sample names can be edited individually. To this end, click onto the respective field and type the desired name of the sample.

- To run further measurements, click the Start button again. The results will be added to the result record.

You can vary the width of the table columns so that the results and particularly long sample names are displayed unclipped.

- To this end, in the table head, click on the border line between two columns and holding the left mouse button depressed drag the column to the desired width.
The **Formula** module is accessible via the **Quant** menu or the **Bio** menu.

The **Formula** module allows you to link measurement results of a wavelength measurement with a mathematical formula.

Result protocols of a formula calculation can be recalled for later viewing and be supplemented by further measurements.

The preset path for files created with the Formula module is `\WinASPECT\Formula`. Result files of this module are saved under the selected name with the following filename extensions:

- `*.fom` Formula method file
- `*.foms` Signed formula method file

In older WinASPECT® versions, the extension `*.bre` was used.

In the **Formula module**, only files that have been created with this module can be opened and edited. The evaluation of spectra that have already been measured and stored (".dat" files) is not possible.

The measurement parameters used are saved together with the analytical results of a measurement series. When re-loading this file, the corresponding measurement parameters are available for further measurements. The measurement results will then be appended to the existing measurement record.

Start the **Formula** module by activating the menu functions **Quant / Formula** or **Bio / Formula**.

The main window of WinASPECT® becomes inactive and the **Formula** dialog appears.

The **Formula** dialog box contains two tabs with the settings and the results of the measurements.
## Menu commands of the Formula module

The menu bar of the **Formula** dialog box contains the following functions:

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
</table>
| **File**           | **New**  
> Starts a new analysis.  
Open  
> Opens a file created with the **Formula** module.  
Files created with the **Formula** module have the extension “*.fom”.  
Save  
> Saves results and settings to the currently active file.  
Save as...  
> Saves results and settings to a new file.  
For that, the Windows standard dialog box for saving files is used.  
Print  
> Prints results and settings.  
Copy to clipboard  
> Copies the results to the clipboard of the operating system.  
That way, the results are accessible to other Windows applications.  
Close  
> Closes the **Formula** module session. |
| **Edit**           | Measurement parameters  
> Opens the measurement parameters window.  
Settings  
> Entry of formula and selection of measurement parameter file.  
Audit Trail  
> Displays the Audit Trail record.  
Sign document  
> Signs the settings and results in the Formula module.  
View signatures  
> Displays the signature(s) of settings and results in the Formula module. |
| **Start**          | **Reference**  
> Starts the measurement.  
Help  
> Activates online help.  
Close  
> Exits the **Formula** module session and closes the Formula dialog box. |

### 9.1 Measurement parameters in Formula module

- Activate menu command **Edit / Measurement parameters** to open the measurement parameters window.
- Select the required settings and options and exit the measurement parameters window with [OK].
Alternatively, you can activate a measurement parameters file before starting the Formula module. The corresponding parameters record will then be active also in the started module.

**Note**

The **Formula** module evaluates the results at discrete wavelengths. Therefore, it is necessary that you activate the measurement at fixed wavelengths option in the measurement parameters record.

### 9.2 Entry of formula

Before taking a measurement in the **Formula** module, you must define the evaluation parameters (formula).

However, it is also possible to open a file with results obtained with the **Formula** module by activating menu command **File / Open** and continue the measurements with this file. In this case, the program will use the same measurement settings as in the previous measurements. The new results will be appended to the existing measurement record.

- Activate the menu command **Edit / Settings** to open the **Formula – Setup** dialog box.
- After you have entered all parameters in the **Formula – Setup** dialog box, confirm the settings with **[OK]**. On doing so, the measurement functions **Start** and **Reference** in the **Formula** dialog box become accessible.

**General settings in Formula module**

In the two textboxes, **Description** and **Operator**, type a short description characterizing the measurement and the name of the user. These data will be printed on the result record and be stored.

Entry in these textboxes is optional. If you use the FDA-conf version of WinASPECT®, automatically the program will enter the logged in user as operator.

**Result**

In the textbox **Result**, type the unit of measurement for result presentation.
Formula Module

Entry of formula

Factors

<table>
<thead>
<tr>
<th>Factors</th>
<th>Factors</th>
<th>Factors</th>
<th>Factors</th>
</tr>
</thead>
<tbody>
<tr>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
</tr>
<tr>
<td>÷</td>
<td>÷</td>
<td>÷</td>
<td>÷</td>
</tr>
</tbody>
</table>

Fig.9-4 Formula – Setup dialog box: Factors field

In the Factors textboxes, you can define a factor for every wavelength selected in the parameter record. The measurement result obtained at a specific wavelength will then be multiplied by the respective factor. The product of this operation will then be transferred to the calculation of the formula (A1, A2 ... A10).

- Click on the textbox and type the desired factor. The default factor setting is 1.

Method

In the Method field, you can define the calculation formula to be used. For this, various buttons are available. Alternatively, you can also type the formula directly after a click on the textbox below the buttons. At any rate, it is advisable to check the formula for correctness by means of the [Test] button.

Fig.9-5 Formula – Setup dialog box: Method field

- By clicking the buttons of the numerical keypad, you can add digits, e.g. factors or summands, to the formula.

- Using the Operator buttons, you can add mathematical operators to the formula. The following operators are available:

<table>
<thead>
<tr>
<th>Button label</th>
<th>Operator/Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>Addition</td>
</tr>
<tr>
<td>-</td>
<td>Subtraction</td>
</tr>
<tr>
<td>*</td>
<td>Multiplication</td>
</tr>
<tr>
<td>/</td>
<td>Division</td>
</tr>
<tr>
<td>x²</td>
<td>Square</td>
</tr>
</tbody>
</table>
**Formula Module**

**Entry of formula**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sqrt</td>
<td>Square root</td>
</tr>
<tr>
<td>sin</td>
<td>Sine</td>
</tr>
<tr>
<td>cos</td>
<td>Cosine</td>
</tr>
<tr>
<td>ln</td>
<td>Natural logarithm</td>
</tr>
<tr>
<td>pi</td>
<td>π constant</td>
</tr>
<tr>
<td>( )</td>
<td>Brackets</td>
</tr>
</tbody>
</table>

**Option buttons RAD, DEG**
Selection of either radian or degrees for angle functions

- With the [A1], [A2] … [A10] buttons, you can include the product of the measured value at a selected wavelength and the corresponding factor (See above: Factors field).

**Note**

The number of buttons available agrees with the number of wavelengths selected in the parameter file. The numbering of the buttons corresponds to the sequence of the wavelengths in the parameter file. Hence, [A1] corresponds to the first wavelength selected in the parameter file, [A2] to the second wavelength, etc.

The [Clear] and [Back] buttons serve to facilitate editing the formulas.
- [Clear] deletes the complete formula.
- [Back] deletes the last term of the formula.

**Saving and loading formulas**

The finished formula can be saved and reloaded for use in other methods.
- To save the formula, click on [Save].
- The formula to be loaded must be selected from the list of stored formulas using the [Load] button. This will bring up the Formula - Selection dialog box.

**Fig.9-6 Formula Selection dialog box**

- To choose a formula from the list, click on it. Then click the [OK] button.
- To delete a selected formula from the list click on the [Delete] button.
- To exit the list without choosing a formula, click on [Cancel].
Note

For reasons of clarity, formulas are saved along with the date and time of saving, the entered description and the operator's name, the factors (though not visible in the table) and the units DEG or RAD for angle functions (not visible either).

You can use a saved formula as the basis for a new method and edit it. When you save the formula again, it will be appended to the list. The original formula will not be overwitten by this operation.

9.3 Measurements in the Formula module

Reference measurement in the Formula module

If in the parameter file you selected the Correction – Reference option, you must first measure this correction value.

- Start the measurement of the correction data by a click on the [Reference] button on the toolbar of the Formula dialog box.
- If you should not have initialized the device yet, it will automatically be done now.

Sample measurement in the Formula module

- Start the measurement by a click on the [Start!] button on the toolbar of the Formula dialog box.

The measurement and analysis results are displayed on the Results tab of the Formula dialog box.

![Figure 9-7](image)

Fig. 9-7 Formula dialog box with activated Results tab

The top line of this tab shows the calculation formula.

The first line of the result table contains the factors with which the results were multiplied before their inclusion in the calculation formula.

The measurement results are consecutively numbered.

The result table lists the sample name, the date and the time of measurement, the result of calculation, as well as the measured values.
You can edit sample names individually. For this, click onto the corresponding field of the table and type the desired name.

Start further measurements by a click on the [Start!] button. The results of the measurements will be appended to the result record.
Formula Module

Measurements in the Formula module
10 Color Measurement

Module description

The color measurement module of WinASPECT® evaluates the transmission spectrums of solid or liquid samples, as well as reflexion spectrums (remission spectrums) of non-transparent solid or powder samples for colorimetric features.

The following color data can be calculated:

Color coordinates

- Tristimulus values for: X, Y, Z
- Chromaticity coordinates: x and y
- Color spaces: CIELAB and CIELUV with derived magnitudes:
  - L (lightness)
  - \(c_a\) and \(c_u\) (chroma)
  - \(h_a\) and \(h_u\) (hue angle)
  - \(S_u\) (saturation)

Color coordinates can be calculated for field of view 2° and 10° and for CIE illuminants of types A, C and D65.

- White and yellow index according to STM E313-67

Color numbers for transparent solutions

- Platinum cobalt to DIN ISO 6271
- Jodine to DIN EN 1557
- Gardner to DIN ISO 4630

Triggering and terminating a color measurement module session

This application is triggered from the main WinASPECT® program.

- To perform color measurement, turn the SPECORD® on and trigger an initialization routine.
- Select Color measurement / Color coordinates/Color numbers menu command in WinASPECT®.

The Color measurement dialog window opens.

There are different ways for closing the Color measurement module.

- Select File / Close menu command in Color measurement dialog window or click onto Close in the toolbar.
10.1 Tools in Color Measurement Dialog Window

Tabs in color measurement dialog window

The dialog window provides four tab cards:

- **Settings**: Displays current measurement settings and color coordinates that were selected for calculation
- **Spectra**: Represents sample spectrums
- **Color view**: Outputs tristimulus color portions (x, y) with related positions within a coordinate grid
- **Results**: Displays resulting color coordinates and color numbers

Pre-measurement view

On triggering of the Color measurement module or selection of the File / New menu command, a window appears with control buttons containing typically required menu commands to facilitate parameter settings for color measurement.

<table>
<thead>
<tr>
<th>Control button</th>
<th>Menu command / description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Measurement settings]</td>
<td>Setup.../ Measurement settings</td>
</tr>
<tr>
<td></td>
<td>Opens the window with measurement options for parameter settings as required for analysis.</td>
</tr>
<tr>
<td>[Setup new sample table]</td>
<td>Setup.../ Sample series</td>
</tr>
<tr>
<td></td>
<td>Opens the Color measurement - setup window for definition of the parameters for color measurement and the sequence of samples to be analyzed.</td>
</tr>
</tbody>
</table>
### Color Measurement

**Tools in Color Measurement Dialog Window**

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Open file (*.dat)]</td>
<td><strong>File / Open</strong>&lt;br&gt;Opens the Open standard window for loading a file of previously measured values for colorimetric evaluation.</td>
</tr>
<tr>
<td>[Close]</td>
<td><strong>Close</strong>&lt;br&gt;Closes the pre-measurement screen.</td>
</tr>
</tbody>
</table>

**Menu commands available in "Color measurement" module**

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>File</strong></td>
<td></td>
</tr>
<tr>
<td>New</td>
<td><strong>Starts new color measurement.</strong></td>
</tr>
<tr>
<td>Open</td>
<td><strong>Loads a previously saved file of spectrums for color analysis.</strong></td>
</tr>
<tr>
<td></td>
<td>Also allows evaluation of spectrums recorded in the main program of WinASPECT® provided they cover the relevant range of 380 nm to 780 nm for colorimetry.</td>
</tr>
<tr>
<td>Save</td>
<td><strong>Saves measured values.</strong></td>
</tr>
<tr>
<td>Save as...</td>
<td><strong>Saves measured values under a new name.</strong></td>
</tr>
<tr>
<td>ASCII-Export</td>
<td><strong>Exports results of color measurement to ASCII format.</strong></td>
</tr>
<tr>
<td>Print</td>
<td><strong>Prints the results of latest color measurement, currently selected color spectrums and Fourier-transformed and/or measurement settings.</strong></td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td><strong>Copies the results of latest color measurement to the clipboard of the operating system to make them available for other Windows applications.</strong></td>
</tr>
<tr>
<td>Audit Trail</td>
<td><strong>Displays processing list.</strong> Any change in color analysis will be documented and displayed in a processing list.</td>
</tr>
<tr>
<td>Settings</td>
<td><strong>Activates an option that will automatically display a dialog window for selection of color coordinates and color numbers to be analyzed when a file of measured data is opened.</strong></td>
</tr>
<tr>
<td>Close</td>
<td><strong>Terminates color measurement and closes Color measurement dialog window.</strong></td>
</tr>
<tr>
<td><strong>Setup...</strong></td>
<td></td>
</tr>
<tr>
<td>Measurement settings...</td>
<td><strong>Opens the measurement parameters menu for setting of new parameters to be determined by color measurement.</strong></td>
</tr>
<tr>
<td>Open parameter file</td>
<td><strong>Opens the Open standard window for loading a previously saved file of measurement settings.</strong></td>
</tr>
<tr>
<td>Sample series</td>
<td><strong>Opens the Color measurement -setup dialog window. It provides options for defining the color coordinates and color numbers that need to be calculated and for specifying a sequence in which the various samples are to be analyzed.</strong></td>
</tr>
<tr>
<td>Start!</td>
<td><strong>Starts color measurement on samples.</strong></td>
</tr>
<tr>
<td>Reference</td>
<td><strong>Performs reference measurement.</strong></td>
</tr>
</tbody>
</table>
Color Measurement
Settings for Color Measurement

Terminates color measurement and closes the **Color measurement** dialog window.

### 10.2 Settings for Color Measurement

**Note**

Make selections for measurement settings at first, then open the **Color measurement - setups** dialog window. Sample table settings depend on accessory settings contained in the various measurement parameters.

#### 10.2.1 Measurement parameter settings for color measurement

- Use the **[Measurement settings]** button in the pre-measurement view screen or the **Setup.../ Measurement settings...** menu command to open the measurement parameters window.

For color measurement, transmission and reflexion spectrums must be available. Their measuring range must at least cover the spectral region from 380 nm to 780 nm.

For measurement, the following parameter settings should be observed:

<table>
<thead>
<tr>
<th>Option/input</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Settings tab</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Display</strong></td>
<td>Transmission or remission when working with integration sphere.</td>
</tr>
<tr>
<td><strong>Correction</strong></td>
<td>Reference</td>
</tr>
<tr>
<td><strong>Device tab</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Slit</strong></td>
<td>SPECORD® 200/210/250 only Set greatest possible slit size.</td>
</tr>
<tr>
<td><strong>Mode tab</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Meas.mode</strong></td>
<td>Scan mode or step mode</td>
</tr>
<tr>
<td><strong>Integration time</strong></td>
<td>Setting as great as possible, max. 5s.</td>
</tr>
<tr>
<td><strong>Range [nm]</strong></td>
<td>At least from 380 nm to 780 nm</td>
</tr>
<tr>
<td><strong>Accessories tab</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Accessories</strong></td>
<td>With clear solutions in cells: none For solid samples: integration sphere</td>
</tr>
</tbody>
</table>

#### 10.2.2 Selection of chromaticity values and settings for sample series

- Use **[Setup new sample table]** or the **Setup.../ Sample series** menu command to open the **Color measurement – setup** dialog window.
General tab

Settings available in Color measurement - setup / General tab are optional.

- **Input field**
  - **Title**: For entering a name of a sample series.
  - **Operator**: For user name entry. With WinASPECT® FDA21CFR Part 11, the name of the currently logged user is automatically validated at this point. This entry cannot be changed.

- **Description**: For entry of additional descriptive text.

Automatic data saving / exporting

Spectrum data belonging to a sample series can be automatically saved and the results of a series of sample color measurements be exported to an ASCII file.

- Activate **Results and measurement** option in **Automatical save** sub-screen in order to save the spectrum values as a "*.dat" file, or select **Auto Export(ASCII)** to export the results of color measurement to a "*.txt" file.

- Use the control button beside this option to open the **Open** standard dialog field and enter a file name for saving or exporting.

Chromaticity values (Color Data) tab

Working with the **Color data** tab, you can specify the chromaticity values you want determined.
Activate checker boxes to match your desired options.

If **Color coordinates all** or **Color numbers** were set, all options in this group will be marked.

**Color coordinates**

For each activated field of view \((2° / 10°)\) and each activated standard CIE illuminant \((A / C / D65)\), values will be calculated according to the preselected color data for:

- tristimulus value \((X,Y,Z)\)
- chromaticity coordinates \((x,y)\)
- color spaces **CIELAB 76** and **CIELUV 76** with derived magnitudes
  - \(L\) (lighness)
  - \(C_{ab}\) and \(C_{UV}\) (chroma)
  - \(h_{ab}\) and \(h_{UV}\) (hue angle) and
  - \(S_{UV}\) (saturation)

According to ASTM E313-98, white index and yellow index values are only calculated for standard CIE illuminant C and 2° field of view.

**Color numbers**

For transparent solutions such as paints or bonding agents, the following color numbers can be determined:

- **Platinum cobalt** to DIN ISO 6271
- **Iodine** to DIN EN 1557
- **Gardner** to DIN ISO 4630
For calculation of color numbers, a cell path length must be defined in addition [in cm].
Color numbers are calculated for a layer thickness of 1 cm as specified in these standards. Other layer thickness will be mathematically adjusted.

**Sample table tab**

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of samples</td>
<td>Defines number of samples in a sample series.</td>
</tr>
<tr>
<td>Table</td>
<td>Enter sample name here.</td>
</tr>
<tr>
<td>[Import]</td>
<td>Import sample name from a ASCII file.</td>
</tr>
</tbody>
</table>

On actuation of this control button, the Open standard dialog will open. Select a desired file.

With liquid samples, autosamplers or automatic sample changers may be used. The sample number which was preset for accessories in a set of measurement parameters must be initially defined as sample number in such cases. Where multiple samples are measured, the sample changers can be repeatedly refilled within a given routine. The number of multiple reloadings must be entered as **Number of Charges**.

### 10.3 Sample Measurement Performed with Color Measurement Module

**Reference measurement**

- Place reference sample into measuring beam path.
- Trigger reference measurement, using a **Reference** menu command.

**Note! Reference standard!**

For the integration sphere, a reference standard of the same surface material as that of the sphere (teflon) is included in delivery. However, this reference standard is not certified.

**Sample measurement**

- Place sample into measuring beam path.
- Trigger sample measurement, using a **Start** menu command!
- In case of a series of several samples, place the next sample into the measuring beam path when prompted to do so. Then trigger next measurement with [OK].
- Continue this procedure, until all samples have been measured.

On completion of all measurement cycles, the measured results will be displayed by the **Results** tab of the **Color measurement** dialog window.
10.4 Display of Results in Color Measurement Module

On completion of color measurement or opening of a respective file, the results of color measurement will be displayed.

Fig. 10-4 Window Color measurement

For a sample which was selected in the sample table (left subarea of dialog window), the following data will be displayed by the tabs listed below:

<table>
<thead>
<tr>
<th>Tab</th>
<th>Display</th>
</tr>
</thead>
<tbody>
<tr>
<td>Settings</td>
<td>Settings regarding measurement parameters, and color coordinates or color numbers to be determined.</td>
</tr>
<tr>
<td></td>
<td>(This display feature is independent of the selected sample.)</td>
</tr>
<tr>
<td>Spectra</td>
<td>Graphical representation of measured spectrums.</td>
</tr>
<tr>
<td></td>
<td>On activation of option Mark selected sample, the spectrum of a selected sample will be highlighted with a somewhat bolder line.</td>
</tr>
<tr>
<td>View of colors</td>
<td>Displays tristimulus value portions (x, y) and their positions within a coordinate grid.</td>
</tr>
<tr>
<td></td>
<td>The two selection lists Illuminant and Field of view allow you to vary the type of standard CIE illuminant and the angle of observation.</td>
</tr>
<tr>
<td>Results</td>
<td>Displays color coordinates that were obtained.</td>
</tr>
</tbody>
</table>
10.5 Management of Result Files in Color Measurement Module

The table below provides an overview of the types of files used by the Color measurement module:

<table>
<thead>
<tr>
<th>File extension</th>
<th>File content</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>*.dat</td>
<td>Spectral data</td>
<td>File with results of spectral measurement.</td>
</tr>
<tr>
<td>*.par</td>
<td>Measuring program</td>
<td>Program file containing measurement parameter set.</td>
</tr>
<tr>
<td>*.txt</td>
<td>Sample table with color measurement results</td>
<td>File is created on ASCII exporting of results.</td>
</tr>
</tbody>
</table>

Spectral data which has been obtained in a Color measurement module session will be saved as a "*.dat" file. For a series of multiple samples, the spectrums will be collectively saved as a flight of spectrums in a cyclic file.

In addition to actually measured values, this file will keep information about calculated in the audit trail.

Saving / exporting results

After measurement, you can use standard menu commands available in the Color measurement dialog window to save a spectrum file with related information about calculated color values.

- Select File / Save as... menu command. The Save standard dialog opens.
- Enter a file name and click the [Save] control button.
- Alternatively, you may trigger a File / Save menu command.
  If these data had previously been saved in a file, the latest changes will be saved under the previously selected name.

The results table with calculated color coordinates can be exported as an ASCII file.

- Select File / ASCII-Export menu command. The Save standard dialog opens.
- Enter a file name and click the [Save] control button. The results will be exported to the ASCII file.

Note

The saving of spectrum data and exporting of data can also be defined to happen automatically during measurement of a sample series (→ Section "Selection of chromaticity values and settings for sample series" p. 156).

Opening files

Working in the Color measurement module, you can open spectrums that contain at least the wavelength range (380 to 780 nm) of relevance to color measurement.
Color Measurement
Management of Result Files in Color Measurement Module

- On restarting the Color measurement module, you can use [Open file (*.dat)] in the pre-measurement view to open the Open standard dialog.

- Alternatively, you can trigger a File / Open menu command for the same purpose.

- Select a desired spectrum file (*.dat) and open this file by clicking onto the [Open] button.

- If the related spectrum data were recorded in a previous session of the Color measurement module, this "*.dat" file will contain information about the originally calculated color coordinates. In this case you will be questioned if a change in the selection of color coordinates is wanted.

  If the data in question were measured in a previous main program session of WinASPECT®, a dialog screen for selection of color coordinates will open. Activate the measurement dialog window (→ section "Display of results in color measurement module" on page 160).

<table>
<thead>
<tr>
<th>Option</th>
<th>Print</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectra</td>
<td>Sample spectrums and Fourier transforms</td>
</tr>
<tr>
<td>Parameters</td>
<td>Measurement parameters</td>
</tr>
<tr>
<td>Results</td>
<td>Results of color measurement</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Audit trail of measured data</td>
</tr>
</tbody>
</table>

- Note
  The query function for changes in previous information regarding color coordinates can be turned on and off with the help of a File / Settings menu command.

Printing results

- Select File / Print menu command to open the Color data – Print dialog window.
  Its control buttons are explained in section "Printing files" p. 69.

- Highlight option boxes as necessary for printing of desired result contents:

- Note
  Use the print preview screen ([Preview] button) for a preview of the printed sheet of results.
11 Film Thickness Measurement

The **Film Thickness Measurement** module facilitates calculation of a thin transparent layer in a thickness range from 1 µm to 200 µm.

It uses a non-contact procedure that is based on the evaluation of a sample’s spectrum of interference which is generated by mutual superposition of two beams reflected from the front face and the rear face of a thin film with a certain shift in phase. This optical path difference in wave phasing is caused by the phase jumps occurring at the film’s boundaries and by the thickness of the film. The particular optical film thickness (nd) can be calculated by evaluation of the positions of points of maximum interference and points of minimum interference.

The following view illustrates this operating principle:

![Diagram of film thickness measurement](image)

- **S** Incident light beam
- **a, b** Reflected light beams
- **α** Angle of incidence
- **β** Angle of refraction
- **δ** Shift in phase
- **n₀** Refractive index of film
- **n₁** Refractive index of component
- **n₂** Refractive index of component
- **d** Film layer
- **1** Component surface
- **2** Film layer

A geometrical film thickness can be calculated if the dispersion value \( n = n(\lambda) \) is known. For dispersion graph setting, – wavelength/refractive index – value pairs must be entered. Where only the mean refractive index is known, only an average value can be obtained for a selected range of evaluation.

Subject to measurement is the interference of white light in reflection with preferentially orthogonal incidence of light or with transparent plane-parallel base layers (for example, glass plates) in transmission.

The lower limit of the measuring range around \( d = 1 \mu m \) is defined by the minimum number of interference maximums that are required to reliably determine a given film thickness. The upper limit around \( d = 200 \mu m \) is defined by the spectral resolution capability of the selected spectrometer.

**Triggering and terminating a film thickness measurement cycle**

- Select **Film Thickness Measurement / Thickness measurement** menu command.

  The **Film Thickness Measurement** dialog window opens.
11.1 Tools in Film Thickness Measurement Dialog Window

Tabs available in Film Thickness Measurement dialog window

This dialog window provides three tabs:

- **Measurement settings**: Displays current measurement parameters
- **Results**: Displays resulting film thickness values
- **Spectra**: Displays interference spectrums that were measured with related Fourier transforms.

Pre-measurement view

On triggering a session of the Film Thickness Mesasurement module or selection of the File / New menu command, a window opens with control buttons containing typically required menu commands to expedite parameter settings for film thickness measurement.

<table>
<thead>
<tr>
<th>Control button</th>
<th>Menu command / description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Measurement settings]</td>
<td>Set / Measurement settings... Open the measurement settings window for making settings as required for a particular analytical job.</td>
</tr>
<tr>
<td>[Setup new sample table]</td>
<td>Set / Sample series Open the Set sample series window for defining required values for film thickness analysis and a desired sequence of samples to undergo analysis.</td>
</tr>
<tr>
<td>[Open file (*.dat)]</td>
<td>File / Open Open the Open standard window which allows you to load a required file of measured values for film thickness analysis.</td>
</tr>
</tbody>
</table>
**Film Thickness Measurement**

Tools in Film Thickness Measurement Dialog Window

[Close] Closes the pre-measurement view.

**Menu commands in "Film thickness" module**

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>File</strong></td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>Triggers new film thickness analysis</td>
</tr>
<tr>
<td>Open</td>
<td>Loads previously created file of measured values for film thickness analysis.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves measured values.</td>
</tr>
<tr>
<td>Save as</td>
<td>Saves measured values under new name.</td>
</tr>
<tr>
<td>ASCII-Export</td>
<td>Exports results of film thickness analysis to ASCII format (*.csv).</td>
</tr>
<tr>
<td>Print</td>
<td>Prints the results of latest film thickness analysis, prints interference spectrums and/or measurement settings.</td>
</tr>
<tr>
<td>Copy to clipboard</td>
<td>Copies the results of the latest film thickness analysis to the clipboard of the operating system to make it available to other Windows applications.</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Displays processing list. Any change in film thickness analysis will be documented and reflected in the processing list.</td>
</tr>
<tr>
<td>Settings</td>
<td>Activates an option that will automatically display a dialog window for entry of a materials file when a file of measured values is opened.</td>
</tr>
<tr>
<td>Close</td>
<td>Terminates film thickness analysis and closes the <strong>Film thickness</strong> dialog window.</td>
</tr>
</tbody>
</table>

**Measurement settings...**

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open parameter file</td>
<td>Opens the <strong>Open</strong> standard window for loading a previously saved file of measurement settings.</td>
</tr>
<tr>
<td>Sample series</td>
<td>Opens the <strong>Film thickness - settings</strong> dialog window. Allows definition of material-related data (dispersion graph or refractive index) and desired sequence in which samples are to be analyzed.</td>
</tr>
</tbody>
</table>

**Start!**

<table>
<thead>
<tr>
<th>Reference</th>
<th>Performs reference measurement.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Close</strong></td>
<td>Terminates film thickness measurement and closes the <strong>Film Thickness Measurement</strong> dialog window.</td>
</tr>
</tbody>
</table>
11.2 Settings for Film Thickness Analysis

**Note**

Before you make settings in the *Film thickness - settings* dialog window, you should specify the required measurement settings in the measurement settings window (→Section "Sample Measurement with Film Thickness Module" p. 167).

11.2.1 Settings for film thickness measurement

- Click the [Measurement settings] control button in the pre-measurement view or use a *Setup... / Measurement settings* menu command to open the measurement settings window.

To be able to perform film thickness measurement, transmittance and reflectance spectrums must be available. A selected measuring range must contain two or more points of maximum interference.

The following items should be taken into account for measurement settings:

<table>
<thead>
<tr>
<th>Option/Input</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Settings tab</strong></td>
<td></td>
</tr>
<tr>
<td>Display</td>
<td>Transmittance or reflectance when working with reflectance measurement inserts</td>
</tr>
<tr>
<td>Correction</td>
<td>Reference</td>
</tr>
<tr>
<td><strong>Mode tab</strong></td>
<td></td>
</tr>
<tr>
<td>Meas. mode</td>
<td>Registration or step mode</td>
</tr>
<tr>
<td>Range [nm]</td>
<td>Analytical range with points of maximum interference.</td>
</tr>
<tr>
<td><strong>Accessories tab</strong></td>
<td></td>
</tr>
<tr>
<td>Accessory</td>
<td>“none” or reflectance measurement inserts</td>
</tr>
</tbody>
</table>

11.2.2 Settings for sample series and material-related data

- Click [Setup new sample table] or use a *Setup... / Sample series* menu command to open the *Film thickness – settings* dialog window.

**General tab**

Settings in the *Film thickness – settings / General* tab dialog window are optional.

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title</td>
<td>Enter name of sample series.</td>
</tr>
<tr>
<td>Operator</td>
<td>Enter user name. With WinASPECT® FDA21CFR Part 11, the currently logged user will be selected at his point. This entry cannot be changed.</td>
</tr>
<tr>
<td>Description</td>
<td>For entering additional descriptive text.</td>
</tr>
</tbody>
</table>
Automatic saving / exporting of data

Spectral data of a sample series can be automatically saved and the results of film thickness measurement performed for a sample series can automatically be exported to an ASCII file.

- Use the Automatic save subarea to activate either option Measure values to save the spectral values as a "*.dat" file or select Auto-Export(ASCII) to export the results of film thickness measurement to a "*.txt" file.

- Click button which is located beside this option to open the Open standard dialog field and enter a file name for saving or exporting.

Refractive index tab

The Refractive index tab is available for entering a refractive index for the film material to be examined. Preferentially, information inputs should provide for a maximum in details regarding the shape of a dispersion graph (the dependence of a refractive index from the wavelength), i.e. for value pairs consisting of wavelength/refractive index over the entire selected spectral range under evaluation. One value pair must be known as a minimum requirement.

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>Enter name of film material. This input is optional.</td>
</tr>
<tr>
<td>Number of refractive indices</td>
<td>Enter wavelength/refractive index value pairs to be used for description of a dispersion graph.</td>
</tr>
<tr>
<td>Table</td>
<td>Enter wavelength/refractive index value pairs in the appropriate columns.</td>
</tr>
</tbody>
</table>

Alternatively to defining wavelength/refractive index value pairs, you may also load a previously saved material file (→ Section "Creating a Material File" on page 171).

- Use button beside this option to open the Open standard dialog field and select a desired material file.

Table of samples tab

<table>
<thead>
<tr>
<th>Input field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of samples</td>
<td>Enter number of samples for a sample series.</td>
</tr>
<tr>
<td>Table</td>
<td>Enter sample name.</td>
</tr>
<tr>
<td>[Import]</td>
<td>Import sample name from an ASCII file.</td>
</tr>
</tbody>
</table>

By actuation of this control button you will open the Open standard dialog screen. Select a desired file here.

11.3 Sample Measurement with Film Thickness Module

Reference measurement

- Place reference into the measuring beam path.
- Trigger reference measurement with a Reference command.
Sample measurement

- Place sample into the measuring beampath.
- Trigger sample measurement with a Start! menu command.
- If processing a series of multiple samples, you place the next sample into the beam path when prompted to do so by the software, then trigger measurement via [OK].
- Continue until all samples have been measured.

On completion of measurement, all measured results will be displayed by the Results tab in the Film Thickness measurement dialog window.

11.4 Display of Results in Film Thickness Module

The results of film thickness measurement can be viewed in the Results tab of the Film Thickness measurement dialog window.

A sample table output contains the results for optical (nd) and geometrical (d) film thickness in μm.

<table>
<thead>
<tr>
<th>Measurement settings</th>
<th>Results</th>
<th>Spectra</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Name</td>
<td>Date/Time</td>
</tr>
<tr>
<td>1</td>
<td>Probe 1</td>
<td>18.06.2007 10:37</td>
</tr>
</tbody>
</table>

Fig. 11-2 Film thickness dialog window / results (displays results)

The Spectra tab shows sample spectrums and their Fourier transforms.
11.5 Management of Result Files in Film Thickness Module

The following table provides an overview of the types of files that are used by the film thickness module:

<table>
<thead>
<tr>
<th>File extension</th>
<th>File content</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>*.dat</td>
<td>Spectral data</td>
<td>File with results of spectral measurement.</td>
</tr>
<tr>
<td>*.mat</td>
<td>Material file</td>
<td>Dispersion graph of known materials can be created as a material file.</td>
</tr>
<tr>
<td>*.par</td>
<td>Measuring program</td>
<td>Program file with measurement settings.</td>
</tr>
<tr>
<td>*.txt</td>
<td>Sample table with results of film thickness analysis</td>
<td>File is created on exporting resulting to ASCII file.</td>
</tr>
</tbody>
</table>

Spectral data obtained in a Film Thickness Measurement module session will be saved in a "*.dat" file. For a series of multiple samples, related spectra are saved in a collective cyclical file.

In addition to measured values, this file stores material-related data. This makes it possible to restore the results of film thickness measurement. On opening of a spectrum in the main WinASPECT® window, you will find a "Settings thickness..." entry with related material data in the audit trail part.
Film Thickness Measurement
Management of Result Files in Film Thickness Module

Saving / exporting results

On completion of measurement, you can use standard menu commands to save spectral data with related material data.

- Select File / Save as... menu command in the Film thickness measurement dialog window.
  The Save standard dialog opens.

- Enter a file name and click onto [Save].

- Alternatively, you can select File / Save menu command.
  If these data had previously been saved as a file, changes will be saved under the previously assigned name.

A sample table with resulting optical and geometrical film thickness details can be exported as an ASCII file.

- Select File / ASCII-Export menu command in the Film Thickness Measurement dialog window.
  The Save standard dialog opens.

- Enter a file name and click [SAve].
  The results are exported to a ASCII file.

Opening files

Working in the Film thickness measurement module, you can open and evaluate *.dat files of WinASPECT® software.

- When restarting the Film thickness measurement module, you can use [Open file (*.dat)] in the pre-measurement view to open the Open standard dialog.

- Alternatively, you can trigger a File / Open menu command for this purpose.

- Select a desired spectrums file (*.dat) and open this file with a clock onto [Open].

- If these spectral data were previously acquired in a film thickness measurement module session, all information regarding material data will be contained in the "*.dat" file. In this case, you will be asked if the material data are to be changed.

  If the spectral data had been measured in a main program session of WinASPECT®, a special dialog screen for input of material data will appear. These will be used for calculation of film thickness. Enter wavelength/ refractive index pairs as required here.

  The results will be shown in the sample table of the Film thickness window (→ section "Display of Results in Film Thickness Module " on page 168).

Note

The query function for changes in previously created material data can be turned on and off with a File / Settings menu command.

Printing results

- Use a File / Print menu command to open the Print – Film Thickness dialog window.

  Related control buttons are explained in section "Printing files" on page 69.

- Highlight option boxes as necessary for the contents you want to print:
11.6 Creating a Material File

In connection with Film Thickness Measurement a material file is understood to contain details regarding the dispersion graph of a film material. A dispersion graph is described by paired value inputs for wavelength/refractive index.

The dispersion graph of a given film material can be saved in a material file for subsequent use in analytical jobs (→ Section “Settings for Film Thickness Analysis” p.166).

- Select Film Thickness Measurement / Material constants menu command in WinASPECT® program.

A dialog window of identical name opens.

![Material constants dialog window](image)

**Fig.11-4 Material file dialog window for input of wavelength/refractive index value pairs**

- Required data entries are:

  **Input field**  
  **Description**
  
  **File name**  
  Shows under what name the material file was saved.
  
  **Material**  
  Enter a name for film material.
  
  **Number of refractive indexes**  
  Enter number of value pairs.
  
  **Table**  
  Enter wavelength/refractive index value pairs.

- Save the material file by triggering a [Secure] menu command.
Film Thickness Measurement

Creating a Material File
12 Mathematical Data Handling

After installation, the Data Handling module is fully integrated in the WinASPECT® desktop and its functions are accessible via the Data Handling menu.

Note

Directly after the start of WinASPECT® only the Two spectra function is available on the Data Handling menu. The other functions become accessible only after you opened a document window.

12.1 Mathematical operations with two spectra

The Data Handling / Two spectra menu function provides the following options of mathematical data treatment of two original spectra:

- Addition
- Subtraction
- Multiplication
- Division
- Normalization
- Adaptation
- Link

Mathematical data treatment operations are performed in a separate dialog box.

Mathematical operations with two spectra require the two source spectra to have the same units of abscissa and ordinate.

If the data-point intervals of abscissa values of both spectra are different, the data of the spectrum scanned at a wider data-point interval will be recalculated by interpolation. To this end, the abscissa values will be recalculated first by adopting the data of the spectrum scanned at the smaller data-point interval. If the spectrum to be interpolated should cover a wider wavelength range (or time range), new abscissa values will be generated based on the smaller data-point interval. Interpolation will be performed then with these new abscissa values.

DATA HANDLING / TWO SPECTRA

- Activate the menu command Data Handling / Two spectra.

This will bring up the Data Handling dialog box:
Mathematical Data Handling

Mathematical operations with two spectra

![Data Handling - Two spectra dialog box](image)

This dialog box contains three spectrum windows:

- Two windows for the source spectra (top) and
- one for the result spectrum.

Each of these windows has its own toolbar.

**Toolbar buttons of spectrum windows:**

<table>
<thead>
<tr>
<th>Button</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Open File" /></td>
<td>Opening a file via the Windows standard dialog box.</td>
</tr>
<tr>
<td><img src="image" alt="Enlarged Presentation" /></td>
<td>Enlarges the presentation of the window and changes the arrangement of the three spectrum windows as illustrated on the button label.</td>
</tr>
<tr>
<td><img src="image" alt="Delete Source Spectrum" /></td>
<td>Deletes the data of the source spectrum from the active window. By doing so, the data of the result spectrum, if existing, will be deleted, too.</td>
</tr>
<tr>
<td><img src="image" alt="Open Menu" /></td>
<td>Available only in the window of source spectrum 1: Opens a menu providing functions available for mathematical treatment of two source spectra.</td>
</tr>
<tr>
<td><img src="image" alt="Copy Spectrum" /></td>
<td>Available only in the window of the result spectrum: Copies the result spectrum for further processing with all its data to a new document window and closes the Data Handling dialog box.</td>
</tr>
</tbody>
</table>

**Selection of spectra and display of results**

- In the **Spectrum 1** window, click on the button ![Open File](image) to open the standard dialog for opening files.
- Choose the file containing the source spectrum 1 and open this file.
The spectrum appears in the corresponding window. If the file to be opened contains cyclic spectra, a small dialog box will appear first for the selection of a defined cycle.

- In the same way, in the Spectrum 2 window, open the file containing source spectrum 2.

After you have opened the source spectra, you may treat them with the available functions.

Every spectrum window provides a **zoom function**. Define the area to be zoomed in with the left mouse button held depressed. When you release the mouse button, the display will be updated. By double-click you may reset the display to the original state.

If you want to save the result of the operation or copy it for further processing to a new document window, click on [ ] in the result window. The manipulated spectrum appears in a new document window with the following note under the measured curve: „processed by data handling module“.

### 12.1.1 Addition

Adds Spectrum 1 and Spectrum 2.

If the abscissa ranges of the two spectra do not fully agree, the ordinate values of the spectrum region existing only in the other spectrum will be entered in the calculation with the value '0'.

- Activate the menu function [ ] / Addition.

  The result of the operation instantly appears in the Result window.

### 12.1.2 Subtraction

Subtracts Spectrum 2 from Spectrum 1.

The result spectrum only contains the values of the abscissa region common to both source spectra.

- Activate the menu function [ ] / Subtraction.

  The result of the operation instantly appears in the Result window.

### 12.1.3 Multiplication

Multiplies Spectrum 1 by Spectrum 2.

If the abscissa ranges of the two spectra do not fully agree, the ordinate values of the spectrum region existing only in the other spectrum will be entered in the calculation with the value '1'.

- Activate the menu function [ ] / Multiplication.

  The result of the operation instantly appears in the Result window.
12.1.4 Division

Divides Spectrum 1 by Spectrum 2.

The generated result spectrum only contains values of the abscissa region common to both source spectra.

- Activate the menu function / Division.

The result of the operation instantly appears in the Result window.

12.1.5 Normalization

Normalizes Spectrum 2 to Spectrum 1 by means of interactively defined supporting points.

This option allows the comparison of spectra having different backgrounds. Normalization uses a normalization factor that is calculated by means of the following formula:

\[ \tilde{f} = \frac{1}{n} \sum_{i=1}^{n} \frac{E_{2i}}{E_{1i}} \]

- Normalization factor
- Number of supporting points
- Index
- Ordinate values at the supporting points in Spectrum 2
- Ordinate values at the supporting points in Spectrum 1

The normalization factor calculated in this way constitutes the correction value used to correct Spectrum 2.

- Activate the menu function / Normalization.

On activation of the function, a vertical-line cursor appears in Spectrum 1.

- Move the vertical-line cursor to the first desired supporting point and mark it by a click with the left mouse button.
- Mark the other desired supporting points as described above.
- Finish selecting the supporting points by a click with the right mouse button.

The normalized curve is calculated and displayed in the Result window.

12.1.6 Adaptation

Allows adaptation of Spectrum 2 to Spectrum 1.

Based on supporting points that were interactively defined in Spectrum 1, the software calculates a baseline. The values of Spectrum 2 will then be corrected with this baseline.

As a result, Spectrum 2 tallies with Spectrum 1 at the supporting points. Unlike normalization, this function does not use a constant normalization factor.

- Activate the menu function / Adaptation.

On activation of the function, a vertical-line cursor appears in Spectrum 1.
### 12.1.7 Link

Links two spectra to a new spectrum.

In this way, you can produce a total spectrum based on two individual spectra. By repeated application of this function, it is possible to produce a spectrum from more than two single spectra.

- Move the vertical-line cursor to that point on the abscissa at which the left section of the spectrum (Spectrum 1) shall be linked to the right section of the other spectrum (Spectrum 2).
- Define this point by a click with the left mouse button.

The result of the operation instantly appears in the Result window.

### 12.2 Mathematical operations with a single spectrum

The mathematical operations with a single spectrum will be applied to the spectrum of the active document window.

Open the file containing the spectrum to be treated. The operation is applied to the spectrum of the active document window. The following options are provided:

- Offset
- Smooth
- 1st to 4th order derivative
- Baseline correction
- Integration
- Peaklist
- Values of defined wavelengths

- In the graph pane of the document window, activate the tab with the ordinate unit (e.g. %T or A) on which the mathematical operation shall be based.

The mathematical operation has an effect on both measuring curves and the value table of the document window (Transmission / Absorbance).

The performed manipulation will be logged on the Audit Trail tab of the document window.
You can undo mathematical operations with a single spectrum by overwriting the data in the active document window with the original data (menu command Edit / Overwrite with original data).

### 12.2.1 Offset

An offset shifts the complete measuring curve uniformly by adding a constant to the measured values.

By the entry of either positive or negative values, the shift is possible in both directions. In this way, interfering quantities can be simulated or compensated.

**DATA HANDLING / OFFSET**
- Activate the menu function Data Handling / Offset.
  
  This will bring up a dialog box for the entry of the offset value.
  
  - In the Summand textbox, type the desired value.
  
  - Confirm the entry by a click on [OK].

The spectrum is corrected by the entered offset value and the display updated accordingly.

### 12.2.2 Factor

Multiplies the measured values by a constant.

By this operation, the spectrum is either expanded or contracted.

The multiplication of an absorbance spectrum by a constant theoretically corresponds to a variation of the pathlength and/or the concentration of the sample.

**DATA HANDLING / FACTOR**
- Activate the menu function Data Handling / Factor.
  
  This will bring up a dialog box for the entry of the desired factor.
  
  - In the Factor textbox, type the desired value.
  
  - Confirm your entry with [OK].

The spectrum is multiplied by the factor and the display updated accordingly.

### 12.2.3 Smooth

Smoothes a spectrum according to the Savitzky-Golay algorithm

**DATA HANDLING / SMOOTH**
- Activate the menu function Data Handling / Smooth.
  
  This will bring up a small dialog box with the Supporting points list box.
  
  - Choose the number of Supporting points for smoothing the spectrum.
  
  - Confirm your choice with [OK].

The spectrum is smoothed and the display updated accordingly.
12.2.4 Derivative, 1\textsuperscript{st} to 4\textsuperscript{th} order

First to fourth-order derivative according to Savitzky-Golay with simultaneous smoothing operation. The derivative spectrum can suppress background signals overlaying the measured spectrum and make specific absorption stand out more clearly.

This function can be applied only to single spectra. A family of spectra must be separated first into single spectra (Select the desired spectrum using the Edit / Select Curve function and copy it to a blank document window. \(\rightarrow\) Section "Selecting a curve in the graph" p. 61). A spectrum can be derived several times. However, as the algorithm is specifically adapted to every type of derivation, the ordinate values of the 4\textsuperscript{th} derivative do not agree with the values obtained by applying the 1st derivative function four times to the spectrum. For quantitative analysis, you should therefore always use the same method to obtain comparable results.

**DATA HANDLING / DERIVATIVE**

- Activate the menu function Data Handling / Derivative. This will bring up the Derivative dialog box.
- In the Derivation field, click on the desired option.
- From the list on the right, choose the number of supporting points to be used for the derivative spectrum. Supporting points are measuring points of the spectrum the software will include in the calculation of the derivative.
- Confirm your choice with [OK].

The derivative spectrum appears in a new document window. On the Audit Trail tab of the new document window, you can find the information on the type of derivation, the number of supporting points used for the calculation, and the name of the original spectrum.

12.2.5 Interpolation

This function interpolates the step size (sampling-point-to-sampling-point interval) of a spectrum. For interpolation, one linear option and one spline cubic option are available.

**DATA HANDLING / INTERPOLATION**

- Select the Data handling / Interpolation menu function. A dialog box of this name appears.
- Mark a desired algorithm to be used for interpolation (Linear or Spline Cubic).
- Type the new step size value into the input field.
- Confirm your inputs via [OK].

The data of this spectrum will be interpolated for the new step size, and the recalculated spectrum will be shown in a new document window.

12.2.6 Baseline correction

This function allows you to define points in the graph of the spectrum by mouse clicks that mark the corrected baseline.
Activate the menu function **Data Handling / Baseline Correction**. The mouse cursor appears with a 'B' label.

- In the spectrum, choose the points to be used for baseline correction by clicks with the left mouse button.
- Finish selecting the correction points by a click with the right mouse button. This will bring up the **Base Points** dialog box with a table of abscissa (X) and ordinate (Y) values of the correction points. These values may be edited.
- To this end, click onto the desired field of the table and edit the value as desired.
- Confirm your choice and possible corrections with **[OK]**.

The spectrum is corrected and the display updated accordingly.

**Note**

If you activated the Baseline Correction function by mistake, you can instantly exit the function again by a click with the right mouse button.

### 12.2.7 Integration

Calculation of the area between a baseline defined by two measuring points and the measuring curve.

- Activate the menu command **Data Handling / Integration / New**. The mouse pointer turns into cross hairs.
- With the mouse pointer, click on the first measuring point and holding the mouse button depressed move it to the second measuring point. On release of the mouse button, the **Integral Settings** dialog box will appear.

**Fig. 12-2** Integral Settings dialog box

- Change the coordinates, if necessary:
  - Choose the X coordinates for the start (x1) and the end of the baseline (x2) from the list. Transfer the values to the respective textboxes by a click on the button.
  - After a corresponding request, transfer the Y coordinates automatically, too, or enter the values directly in the respective textboxes.
Mathematical Data Handling
Mathematical operations with a single spectrum

- Click on [Calculate].
  The values for Area and Integral appear in the display field.

To show or hide the integrated area in the graph, activate or deactivate the menu function Data Handling / Integration / Display.

Definitions of Area and Integral

If a baseline intersects several peaks, areas above and below the baseline are enclosed by the measured curve and the baseline.

Integral:
The Integral is the difference of the areas above the baseline and the areas below the baseline.

Area:
The Area is the sum of the areas enclosed between baseline and curve.

![Graph showing areas enclosed by curve and baseline](image)

Fig. 12-3 Areas enclosed by curve and baseline

12.2.8 Peaklist

Automatic detection and display of peaks in the active spectrum. The result is a peaklist. You can then edit the list, add peaks to it or delete the list.

The Peaklist function has a submenu providing the following functions:
- Search automatically
- Add manually
- Edit
12.2.8.1 Search automatically

Automatic peak search.

With this search option, you can choose both a threshold value for the relative display of extreme values and a limit value for the absolute display.

Relative display means that the ordinate range between the minimum and the maximum measured value is set to 100%, and only those extrema will be displayed whose relative amplitude is above the threshold value.

Example threshold value:

The absorbance spectrum covers an ordinate range from 0.1 to 1.0 A. Hence, the ordinate range coverage is 0.9 A. With a threshold value of 20 % of the range coverage, only those extrema will be displayed whose relative amplitude is above 0.18 A.

However, if you enter a limit value, those extrema will be displayed that are above the entered limit value.

- Activate the menu function Data Handling / Peaklist / Search automatically.

The Peaklist - Parameters dialog box appears.

- Make the following entries:

<table>
<thead>
<tr>
<th>Option / Textbox</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threshold value</td>
<td>Entry of threshold value in ordinate units.</td>
</tr>
<tr>
<td>Maxima</td>
<td>Choice of extrema to be displayed in the list.</td>
</tr>
<tr>
<td>Minima</td>
<td></td>
</tr>
<tr>
<td>Max. and Min.</td>
<td></td>
</tr>
<tr>
<td>Limit value</td>
<td>Optional entry of an absolute ordinate value, above or below which the found extrema shall be displayed.</td>
</tr>
<tr>
<td>above limit value</td>
<td>Choose whether peaks above or below the entered limit value shall be listed.</td>
</tr>
<tr>
<td>below limit value</td>
<td></td>
</tr>
</tbody>
</table>

- Confirm your choice with [OK].

This will bring up the Peaklist dialog box.
Mathematical Data Handling

Mathematical operations with a single spectrum

Fig. 12-5  Peaklist dialog box

The Peaklist dialog box contains a table with abscissa (X) and ordinate (Y) values of the found peaks. The right column shows the cycle number.

The buttons and the check box have the following functions:

<table>
<thead>
<tr>
<th>Buttons / Check box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>✓ OK</td>
<td>Exits the dialog box and displays the extrema in the graph according to the selected options.</td>
</tr>
<tr>
<td>✗ Cancel</td>
<td>Exits the dialog box rejecting the peaklist.</td>
</tr>
<tr>
<td>📜 Print</td>
<td>Opens the Print menu with the following functions: Set Printer, Set Page, Preview and Print (→ Section “Printing files” p. 69).</td>
</tr>
<tr>
<td>🥷 Help</td>
<td>Starts the interactive help function.</td>
</tr>
<tr>
<td>[Remove]</td>
<td>Deletes the selected line of the table. The corresponding extreme value is removed from the peaklist.</td>
</tr>
<tr>
<td>Mark</td>
<td>On exiting the dialog box with [OK], the found extrema will be marked in the graph by textboxes. The textboxes show the coordinates of the corresponding extreme value. After a double-click on the textbox, you can move the textbox holding the left mouse button depressed.</td>
</tr>
</tbody>
</table>

Note

In the case of outliers within a measurement series or a standard, you can simply re-measure the respective value following this procedure:

In the result table, click on the respective standard and then activate the menu command Start / Selected standard or Start / Selected standard of selected cycle.

After you have created the peak list as described in the previous section, the other functions of the Peaklist submenu become accessible.
12.2.8.2 Add peaks manually

This function allows you to manually add peaks to the peaklist by mouse clicks in the graph.

- Activate the menu function Data Handling / Peaklist / Add manually.
- On activation, the cross-hairs cursor additionally appears with a "double peak" label.
- Define the peaks you want to add to the peaklist by left-clicking on the desired point in the spectrum.
- Exit this function by a click with the right mouse button.

This will bring up the Peaklist dialog box again (→ Fig. 0-5 p. 183). The added peaks are identified by the designation "manual" in the first column of the table.

- If you want to accept the edited peaklist, click on [OK].

The dialog box is being closed.

Note

If in the textboxes of manually added peaks the ordinate value should not be visible, enlarge the textbox by moving the cursor onto the right frame and then pulling it to the right with the left mouse button held depressed.

12.2.8.3 Editing the peaklist

- Activate the menu function Data Handling / Peaklist / Edit.

On doing so, the Peaklist dialog box reappears. In this dialog box, the options described above are available (→ Fig. 0-5 p. 183).

12.2.8.4 Deleting the peaklist

- Activate the menu function Data Handling / Peaklist / Delete list.

The existing peak list will be deleted and the peak labels removed from the graph without any program query to confirm this action.

12.2.9 Values of defined wavelengths

Determines the ordinate values at one or several wavelengths.

- When this function is applied to cyclic spectra, the values will be simultaneously determined for every single spectrum.

The wavelengths can be selected either

- interactively (via the graph of the spectrum by means of the mouse pointer) or
- numerically (selection via dialog box).
Selection with mouse pointer

Activate the menu function Data Handling / Values of defined wavelengths / Interactive.

In the graph, the cursor changes into a vertical line with W label.

Move the cursor to the desired point and press the left mouse button. Select additional wavelengths in the same way, if desired.

To finish selecting wavelengths, press the right mouse button.

This will bring up the Values of defined wavelengths dialog box:

![Values of defined wavelengths dialog box](image)

Fig. 12-6 Values of defined wavelengths dialog box

In this dialog box, the standard buttons for the printout are available (→ Section "Printing files" p. 69). The printout includes the graph with the set marks and the found ordinate values at the selected wavelengths.

Selection via dialog box

Activate the menu function Data Handling / Values of defined wavelengths / Numerical input.

This will bring up the Value of selected Waves.

![Value of selected Waves dialog box](image)

Fig. 12-7 Value of selected Waves dialog box
In the Available Wavelengths list, highlight the wavelength the ordinate value of which shall be displayed. Then, click on the [Add] button to transfer the wavelength to the Selected Wavelengths list.

You may also type the desired wavelength in the Looking for textbox and transfer it to the Selected Wavelengths list by a click on [Add].

To remove a wavelength from the Selected Wavelengths list again, select it by a mouse click and then click on the [Remove] button.

When you have transferred all wavelengths of interest to the selection list, exit the dialog box with [OK]. On doing so, the selected wavelengths and the pertaining measured values will appear in the Values of defined wavelengths dialog box.
13 Validation

For quality assurance of analyses with the SPECORD®, the device must be regularly validated.

The Validation software is a supplementary option of the WinASPECT® software, Version 1.7 or higher. It is customized to the hardware parameters of the following devices:

- SPECORD® 40
- SPECORD® 50
- SPECORD® 200
- SPECORD® 205
- SPECORD® 210
- SPECORD® S600
- SPECORD® S300 UVVIS
- SPECORD® S300 VIS
- SPECORD® 250

Validation is strictly based on the regulations of Ph.Eur. The Validation software makes it easy for you to meet the standards of Good Laboratory Practice (GLP).

Note

The complete validation process takes approx. 150 min.

Result files of validation are saved under the selected name with the filename extensions: ".v06".

13.1 Starting the Validation module

Starting the validation process

- On the Windows taskbar, click on the [Start] button.
- Activate the menu function Programs / WinASPECT / Validxxx.

This will bring up the Validation SPECORD XXX application window:

![Validation SPECORD XXX application window](image)

Fig. 13-1 Validation SPECORD® XXX application window

The parameters to be tested can be selected under Setup / Setup.

In the list field Part of validation a parameter group each can be selected for display.
Validation
Starting the Validation module

For every parameter to be tested, a separate parameter sheet is available. On the Results sheet, the digital test results are displayed; the Measured Values sheet shows a graph of the scanned spectra.

Note
Bei der Validierung des SPECORD® S600 does not exist the list field Part of validation. All cards of tested parameters are announced in common.

Functions of the toolbar of the Validation SPECORD dialog box

The toolbar of the Validation - SPECORDxxx dialog box provides the following functions:

<table>
<thead>
<tr>
<th>Menu function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>File</td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>Starts a new analysis.</td>
</tr>
<tr>
<td>Open</td>
<td>Opens a file created with the Validation module. The extension used for files of the Validation module is &quot;*.val&quot;.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the results and settings to a new file or a file of a different name. For that, the Windows standard dialog box for saving files is used.</td>
</tr>
<tr>
<td>Print</td>
<td>Prints the results and settings.</td>
</tr>
<tr>
<td>Exit</td>
<td>Exits the session in the Validation module.</td>
</tr>
<tr>
<td>Setup</td>
<td>Choose the COM or USB port of the PC to which the SPECORD® has been connected.</td>
</tr>
<tr>
<td>Interface</td>
<td>To be activated to select the parameters to be validated and set the calibration standards to be used for device validation.</td>
</tr>
<tr>
<td>Initialization</td>
<td>Starts initialization of the device.</td>
</tr>
<tr>
<td>Wavelength Correction</td>
<td>Runs a wavelength correction.</td>
</tr>
<tr>
<td>Validation</td>
<td>Runs the validation measurement.</td>
</tr>
<tr>
<td>INFO</td>
<td>Displays the version of the installed Validation software.</td>
</tr>
<tr>
<td>Exit</td>
<td>Exits the session in the Validation module.</td>
</tr>
</tbody>
</table>

On the parameter sheets, the test results are presented. For every parameter to be tested, a separate parameter sheet is available.
13.2 Test parameters and required aids

13.2.1 Test parameters

Some of the parameters are tested only on devices covering the UV region or on double-beam devices. These parameters are specially marked. The following parameters are tested:

**Transmission zero**

Measurement with blocked sample path and open reference path (only on SPECORD® 200) from 200 to 1000 nm. From the result, the minimum and the maximum values of the transmission measurement of the device will be calculated.

**Baseline stability**

Records the baseline in absorbance mode in the range 200 nm to 800 nm.

**Baseline noise**

Measures 61 data points at an integration time of 1 s at the wavelength of 500 nm. Determines the difference between the minimum and the maximum results on the SPECORD® 30 / 40 / 50. On the SPECORD® 200 / 205 / 210, this test determines the RMS noise.

**100%T uncorrected** (not available for SPECORD® 40 and SPECORD® S600 / 300)

Measures the transmission baseline without any correction.

**Photometric accuracy in VIS region**

Performs three measurement series with a certified set of standard filters. Determination of the difference of the measured absorbance values from the nominal absorbance values of the standard filter set.

**Photometric accuracy with potassium dichromate**

Measures the absorbance of the potassium dichromate solution in the range from 235 nm to 350 nm and at 430 nm. Determines the difference of the measured absorbance values from the nominal absorbance values certified for the potassium dichromate solutions.

**Wavelength tests**

Takes five measurements of a standard holmium filter or a holmium perchlorate solution with certified values for the wavelengths. Determines the wavelength accuracy and wavelength reproducibility in the range from 250 nm to 650 nm.

**Stray light test**

Determines the maximum stray light value in transmission mode by using different edge filters in the following regions:
Validation

Test parameters and required aids

<table>
<thead>
<tr>
<th>Edge filter</th>
<th>Measuring range</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCl filter cell</td>
<td>200 nm (does not apply to SPECORD® 30)</td>
</tr>
<tr>
<td>NaJ filter cell</td>
<td>220 nm – 240 nm (does not apply to SPECORD® 30)</td>
</tr>
<tr>
<td>NaNO₂ filter cell</td>
<td>340 nm</td>
</tr>
</tbody>
</table>

SPECORD® S300 UVVIS

<table>
<thead>
<tr>
<th>Edge filter</th>
<th>Measuring range</th>
</tr>
</thead>
<tbody>
<tr>
<td>GG 495</td>
<td>450 nm</td>
</tr>
<tr>
<td>RG 695</td>
<td>550 nm</td>
</tr>
<tr>
<td>BG 3</td>
<td>630 nm</td>
</tr>
</tbody>
</table>

**Resolution test** (does not apply to SPECORD® 30, SPECORD® S300)

Test of optical resolution using a toluene solution in n-hexane by determining the absorbance ratio of the following wavelengths: 269 nm and 266 nm (A₂₆₉/A₂₆₆).

**Long-term stability test**

Repeated measurements of the baseline over a period of one hour and calculation of the gradient of the measured values at 500 nm.

### 13.2.2 Required aids

- Certified filter set for the photometric measurement in the visible spectral region and certified holmium oxide glass filter for wavelength measurement.
- Holmium perchlorate standard solution for wavelength accuracy test acc. to DAB and Ph.Eur. (alternative to holmium oxide glass filter)
- Potassium dichromate standard solution for UV photometry test acc. to DAB and Ph.Eur.
- Sodium nitrite standard solution for stray light measurement acc. to DAB and Ph.Eur.
- Sodium iodide standard solution for stray light measurement acc. to DAB and Ph.Eur.
- Potassium chloride solution for stray light measurement acc. to DAB and Ph.Eur.
- 0.02% toluene in hexane for resolution test and hexane as reference (does not apply to SPECORD® 30)
- Filter GG 495, RG 695, BG 3 (only for stray light test on SPECORD® S300 VIS)
13.3 Entry of validation parameters

Before starting the validation, you must define the validation parameters.

- Click on the Setup button.

This will bring up the Preferences dialog box.

The Preferences dialog box contains the following tabs:

<table>
<thead>
<tr>
<th>Tab</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>General</td>
<td>Selection of parameters to be tested.</td>
</tr>
<tr>
<td>Limit values</td>
<td>Adjustment of limit values and tolerances of the parameters to be tested.</td>
</tr>
<tr>
<td>VIS, Potassium Dichromate, Wavelength, Stray light, Resolution</td>
<td>Parameters of test aids (designation, test wavelength, standard data, etc.) to be used for the validation procedure.</td>
</tr>
</tbody>
</table>

The entries on the respective tabs must be made, if on the General tab the corresponding test parameter has been selected.

- Confirm the settings of the parameter limits with [OK].

The program returns to the Validation main window. The [Start!] button is accessible now.

13.3.1 Selection of validation parameters to be tested: General tab

![Preferences dialog box](image)

Fig. 13-2 Dialogfenster Preferences – General tab

You can optionally choose the tests to be performed and their parameters, thus creating your own validation routine for your spectrophotometer.
Validation
Entry of validation parameters

Textbox/check box  Entry
According to European Pharmacopoeia  Checks the SPECORD® for compliance with the requirements of European pharmacopeia
Test items of pharmacopeia which are not applicable to the particular SPECORD® (e.g. resolution of SPECORD® S300 UVVIS) are not subject to testing.
Operator  Enter your or the operator's name.
This entry is compulsory.
Note  Here, you can enter a brief comment.
The entry is optional.
Selection of measurements to be performed  Activate the check boxes of the tests to be performed for validation (tick).

Option  Tested parameters
General  Transmission zero, Baseline stability, Baseline noise; 100%T uncorrected
VIS-Photometry  Photometrie at VIS range

Photometry with potassium dichromate  Photometrie at the range from 235 nm to 350 nm and at the wavelength 430 nm
Wavelength  Determines the wavelength accuracy and wavelength reproducibility in the range from 250 nm to 650 nm.

Stray light  Maximum stray light value in transmission mode
Resolution  Optical resolution using a toluene solution in n-hexane by determining the absorbance ratio of the following wavelengths: 269 nm and 266 nm (A269/A266).
Long term stability  Repeated measurements of the baseline over a period of one hour and calculation of the gradient of the measured values at 500 nm.

Note
If you have selected the VIS or UV photometry test, the Wavelength, Stray light and/or Resolution test, it is absolutely necessary to make the test-specific entries on the respective tabs (→ See below).
13.3.2 Selection of limit values: Limit values tab

Fig. 13-3 Preferences dialog box – Limit Values tab

The Validation module of WinASPECT® allows you to test the device both with the parameter limits and tolerances guaranteed by the manufacturer and with user-defined range limits. In the latter case it can be ensured, that the device is suitable for a specific analysis.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default values</td>
<td>Use of preset parameter limits and tolerances guaranteed by the manufacturer.</td>
</tr>
<tr>
<td></td>
<td>The validation parameters will be displayed in the entry fields of the table. They cannot be edited.</td>
</tr>
<tr>
<td>Values from file</td>
<td>Use of user-defined parameter limits and tolerances.</td>
</tr>
<tr>
<td></td>
<td>In the entry fields of the parameter table, define the new tolerance limits.</td>
</tr>
<tr>
<td></td>
<td>You can save the entered tolerance limits using the [Save] button. The file name extension of limit-value files is &quot;.vag&quot;.</td>
</tr>
<tr>
<td></td>
<td>To load a file with saved limit values, click on the [Open] button.</td>
</tr>
<tr>
<td></td>
<td>You can edit the loaded set of limit values and save them again.</td>
</tr>
<tr>
<td></td>
<td>To enter a new set of limit values, click on the [New] button.</td>
</tr>
</tbody>
</table>

13.3.3 Entry of the data of the used standards

On the VIS, UV, Wavelength, Stray light and Resolution tabs, the names/ID numbers and the certified data of the used test aids must be entered. Entry of data on these tabs is necessary, if you selected the respective tests on the General tab.

VIS tab

Name/ID

Enter the identification number of your certified standard filter set (neutral-density filters) as specified on the datasheet.

Filter parameters F4

Enter the wavelengths to be tested and the certified absorbance values respectively the data shied of filter F4 in the table. The test must always include the measurement at five wavelengths.
Validation

Validation procedure

**Potassium dichromate tab**

Entry of the data of the potassium dichromate standard solution (versus its reference) according to the specifications on the datasheet.

Reference (UV photometry)  ID numbers of the reference

Potassium dichromate  ID number of potassium dichromate.

Test wavelengths and nominal absorbance values  In the first line of the table, Test wavelength [nm], enter the wavelengths to be tested. The test must always include four wavelengths.

In the second line, Nominal values [A], enter the certified absorbance values at the respective test wavelengths.

**Wavelength tab**

Standard filter set  ID number of the used wavelength standard.

Name/ID  Here, enter the ID number of the holmium perchlorate standard solution or, if you intend to use the Hellma glass filter set, that of the holmium oxide filter.

Test wavelengths  In the table, enter the certified values of the spectral peaks according to the datasheet provided with the standard.

**Stray light tab**

Potassium chloride  ID number of the potassium chloride standard solution

Sodium iodide  ID number of the sodium iodide standard solution

Sodium nitrite  ID number of the sodium nitrite solution

**Resolution tab**

Reference (resolution)  ID number of the reference solution

Toluene/Hexane  ID number of the toluene standard solution

13.4 Validation procedure

After you have defined the validation parameters in the Preferences dialog box, the Start menu becomes accessible.

Note for validation of double beam spectrometers

All filters and cells with standard solutions, also the references must always be placed in the sample beam path. In all measurements, the reference beam path must remain free!
13.4.1 Switching on and calibration of SPECORD

**Note**

To obtain optimum results, observe the following notes:

- Start the validation only after a warm-up of two hours with both lamps switched on.
- Perform a wavelength calibration immediately before the validation procedure.

If you had switched on the spectrometer with the deuterium lamp yet before starting the validation program, initialize the SPECORD® now.

- Start device initialization using the menu command **Start! / Initialize Device**.

The program checks the connected device and the device driver used. If a fault is detected, the program will display an error message.

**For scanning SPECORD®:**

- After device initialization, wait two hours before starting wavelength calibration.
- Start device calibration by activating the menu command **Start! / Wavelength correction**.

13.4.2 Running the validation tests

You are prompted by dialog boxes through the validation process. The measurements are performed successively depending on your choice of tests in the **Preferences** dialog box.

- Start validation by activating menu command **Start / Validation**.
- Follow the prompts for the use of filters or cells appearing in the dialog boxes.

![Fig. 13-4 Dialog box with the prompt to insert a filter](image)

- After a click on [OK] in the dialog boxes, the respective reference or device parameter measurement will be performed.

The following measurements are performed to test the device parameters:

<table>
<thead>
<tr>
<th>Device parameter</th>
<th>Measurement</th>
<th>Used standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmission zero</td>
<td>Reference</td>
<td>Empty sample compartment</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Block sample path, e.g. with a sheet of black cardboard</td>
</tr>
<tr>
<td>Baseline noise</td>
<td>Reference and parameter measurement</td>
<td>Empty sample compartment</td>
</tr>
<tr>
<td>100%T, uncorrected (only for )</td>
<td>Parameter measurement</td>
<td>Empty sample compartment</td>
</tr>
</tbody>
</table>
### Validation

**Validation procedure**

<table>
<thead>
<tr>
<th>Device parameter</th>
<th>Measurement</th>
<th>Used standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength accuracy</td>
<td>Reference</td>
<td>Empty sample compartment</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Filter F1 )*</td>
</tr>
<tr>
<td>Wavelength reproducibility</td>
<td>Reference</td>
<td>Empty sample compartment</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Filter F1 )*</td>
</tr>
<tr>
<td>VIS Photometry</td>
<td>Reference</td>
<td>Filter F0 )*</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement (ca. 1A)</td>
<td>Filter F4 )*</td>
</tr>
<tr>
<td>Photometry with potassium dichromate</td>
<td>Reference</td>
<td>Reference solution (UV photometry test)</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Potassium dichromate standard solution for UV photometry</td>
</tr>
<tr>
<td></td>
<td>Reference</td>
<td>Reference solution (430 nm)</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Potassium dichromate standard solution for UV photometry</td>
</tr>
<tr>
<td>Stray light</td>
<td>Reference</td>
<td>Reference solution or double distilled water</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement (does not apply to SPECORD® 30)</td>
<td>Potassium dichromate standard solution</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement (does not apply to SPECORD® 30)</td>
<td>Sodium iodide standard solution</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Sodium nitrite standard solution</td>
</tr>
<tr>
<td>Resolution (does not apply to SPECORD® 30)</td>
<td>Reference</td>
<td>Reference standard solution (hexane)</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Toluene standard solution</td>
</tr>
<tr>
<td>Long-term stability</td>
<td>Reference</td>
<td>Empty sample compartment</td>
</tr>
<tr>
<td></td>
<td>Parameter measurement</td>
<td>Empty sample compartment</td>
</tr>
</tbody>
</table>

Summar table 2  Validation measurements and necessary standards

)* When using the secondary calibration standards for spectrophotometers from HELLMNA

At the end of every individual test of the validation process, a dialog box informs of the obtained test results and the pre-selected tolerances.
Validation

Printing the results of validation

Fig. 13-5  Display of validation results while validation is running

The dialog box with the test results and the available buttons provides the following options for the further validation procedure:

- **Repeat**: Starts the repetition of the test. The previously recorded results of this test will be rejected.
- **Continue**: Starts the measurement of the next test parameter.
- **Abort**: Aborts the validation procedure. However, the measured values obtained so far will be stored temporarily and displayed on the tabs in the Validation main window.

13.4.3 Presentation of validation results

After completion of validation, the results are displayed on the index cards of the Validation application window.

- Among the parameter tabs, choose the test parameter, the results of which you want to see.
- On the **Results** card, the digital measurement results are shown compared to the permissible tolerances.
- For a graphic presentation of the measurement results, click on the **Measured values** tab.
  
  The **Wavelength accuracy** test includes several spectra. To navigate through various graphs, use the displayed arrow keys (◀ ▶).

13.5 Printing the results of validation

- Activate the menu command *File / Print* to bring up the **Validation SPECORD xxx - Print** dialog box.

  For the printout of validation results, the Print dialog box provides various templates.

  **Template options**  **Description**
  
  **Short protocol**  Printout with the assessment of compliance with tolerances, measured parameter value as well as permissible tolerances of all parameters under test.
Validation

Printing the results of validation

<table>
<thead>
<tr>
<th>Detailed</th>
<th>Printout with the assessment of compliance with tolerances, detailed list of measured parameter values and permissible tolerances</th>
</tr>
</thead>
<tbody>
<tr>
<td>Individual values</td>
<td>(only accessible in combination with activated Detailed option) Printout as with Detailed option and additional presentation of the graphs of the measurements.</td>
</tr>
</tbody>
</table>

The Validation SPECORDxxx – Print dialog box provides the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Set Printer]</td>
<td>Opens the Windows standard dialog box for printer setup.</td>
</tr>
<tr>
<td>[Preview]</td>
<td>Shows a preview of the validation protocol to be printed according to the selected template options.</td>
</tr>
<tr>
<td>[Print]</td>
<td>Starts the printout of the protocol.</td>
</tr>
<tr>
<td>[Close]</td>
<td>Closes the dialog box.</td>
</tr>
</tbody>
</table>
14 Service Check for scanning SPECORD®

The SPECORD Service Check software is a diagnostic utility that is installed together with the device driver software. However, it is not started from the WinASPECT® workplace, but as individual application.

The SPECORD Service Check allows you to check the functionality of your SPECORD. The results of the diagnosis may be printed out and saved to a file. You may then send the printout as fax for evaluation to the Service Department of Analytik Jena AG. If you have an online connection, you may also send the results of the diagnosis by e-mail directly to our Service Department.

Service check of scanning SPECORD®

For scanning SPECORD® operation, program checks include (but are not limited to):

- Energy in sample and reference beam (Diagnosis) (not accessible for SPECORD 30)
- 100%-T line (Diagnosis)
- Wavelength accuracy (Diagnosis)
- Energy of deuterium lamp (not accessible for SPECORD 30)
- Energy of halogen lamp

The file extension of a service check file is “*.drs”.

Service check for simultaneously measuring SPECORD®

For operation of a simultaneously measuring SPECORD® Sxxx, the following parameters are determined:

- Energy in sample beam (Diagnosis)
- 100%-T line (Diagnosis)
- Wavelength accuracy (Diagnosis)
- Energy of deuterium lamp or halogen lamp (depend on instrument type)

The file extension of a service check file is “*.sv3” or “*.sv6”, respectively.

14.1 Activating Service Check

- On the Windows taskbar, click the [Start] button.
- Activate the menu function Programs / WinASPECT / Service xxx.
- This will bring up the SPECORD– Service-Check dialog box.

Functions of the toolbar of the SPECORD– Service-Check dialog box

The toolbar of the SPECORD– Service-Check dialog box provides the following functions:
Service Check for scanning SPECORD®P

Performing the diagnosis

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Close</td>
<td>Closes the Service Check utility.</td>
</tr>
<tr>
<td>Diagnosis</td>
<td>Starts the diagnosis.</td>
</tr>
<tr>
<td>Start!</td>
<td>Opens a file created with the Service Check utility.</td>
</tr>
<tr>
<td>Open</td>
<td>The file name extension for files created with the Service Check utility is &quot;*.drs&quot;.</td>
</tr>
<tr>
<td>Save as...</td>
<td>Saves the results and settings under a new file name via the Windows standard dialog box for saving files.</td>
</tr>
<tr>
<td>Print</td>
<td>Printout of results.</td>
</tr>
<tr>
<td>E-mail to Service</td>
<td>Sends the results of the service check by e-mail to the Service Department of Analytik Jena AG.</td>
</tr>
<tr>
<td>Lamp Check</td>
<td>Checks the lamp energy.</td>
</tr>
<tr>
<td>Zerth Order</td>
<td>Only for scanning spectrometers. Sets the zeroth order of the spectrum for adjustment.</td>
</tr>
<tr>
<td>Wavelength corr.</td>
<td>Only for scanning spectrometers. Starts wavelength correction.</td>
</tr>
<tr>
<td>Beam position</td>
<td>Only for SPECORD® Sxxx. Releases beam passage into sample space for alignment of accessory components in beam position.</td>
</tr>
</tbody>
</table>

14.2 Performing the diagnosis

Activate the menu function Diagnosis /Start! in the SPECORDxxx – Service-Check dialog box.

The program initializes the spectrophotometer and checks whether the device has been connected correctly to the serial port of the PC.

Observe the prompts and error messages possibly appearing in the dialog box. The checking routine is running automatically with predefined parameters. The following measurements are taken:

- Energy measurement in sample beam.
- Energy measurement in reference beam (not available on SPECORD 30/40).
- Reference measurement with subsequent scanning of the 100% T line.
- Scan of the spectral line at 485.9 nm and spectral line at 656.1 nm emitted by the deuterium lamp (not available on SPECORD 30 and SPECORD S300 VIS)

While the measurement is running, a dialog box appears showing the progress of the measurements. On completion of the diagnosis, the scans appear on four tabs in the Service Check dialog box.
14.3 Printing the results of diagnosis

To print out the results of the diagnosis, follow this procedure:

- Activate the menu function Diagnosis / Print to open the Print dialog box.
- Activate the function Print to start the printout.

14.4 Sending the results of diagnosis by e-mail

If you have a registered e-mail account of an e-mail service provider, you may directly send the results of diagnosis by e-mail to the Service Department of Analytik Jena AG. For that, configure the e-mail connection first and then send the data:

- By activating menu command Diagnosis / E-mail to Service / Configure to open the Configuration dialog box.
- In the textboxes, type the necessary data and confirm the entries with [Apply].

Note

If you do not know the name of the mail server and the port, ask your system administrator.

- To send the results of the diagnosis by e-mail, activate the menu function Diagnosis / E-mail to Service / Send.
Service Check for scanning SPECORDP®

Lamp Check

Note
For sending the results of the diagnosis, it is not necessary to save them before as file.

14.5 Lamp Check

The Lamp Check function allows you to check the energy emitted by halogen and deuterium lamp (not available for SPECORD 30) thus obtaining information on bulb ageing and further usability of the lamps.

- Click on the Lamp Check button.

![Configuration dialog box (for e-mail connection)](image)

Fig. 14-2 Configuration dialog box (for e-mail connection)

The program initializes the device and starts checking the deuterium lamp in the wavelength range 220 … 260 nm. The energy scan is displayed in a window (not available for SPECORD 30).

Afterwards, the program measures the energy emitted by the halogen lamp at a defined wavelength. On conclusion of both measurements, two bar graph charts appears in the Service Check dialog box to inform you of the measurement results of both lamps. Under the bar graphs, the system will inform you, whether

- the energy of the lamp lies within the normal range,
- the lamp approximates the end of its service life,
- or the lamp needs replacement.

- If necessary, replace the lamp(s) (→ Description of SPECORD®).
14.6 Zeroth order

With the Zeroth Order function, the monochromator drive is moved in such a position that undispersed light of the used halogen or mercury lamps (on the SPECORD 30: of the halogen lamp) passes through the sample compartment. This intense beam can easily be observed and is thus especially suitable for the alignment of the lamps or of the accessory units in the beam path (e.g. microcells).

- Activate the menu function Zeroth Order / D2E Lamp or Zeroth Order / Halogen lamp.

The program initializes the device and moves the wavelength drive into a position, where the light of the zeroth order (“white” light) becomes visible in the sample compartment.

Now, you can check the position of the cells in the sample compartment relative to the beams and correct it, if necessary.

14.7 Beam position

Only for SPECORD® Sxxx.

With the Beam position function, the shutter to the sample compartment is opened. The shutter zum Probenraum geöffnet. This intense beam can easily be observed and is thus especially suitable for the alignment of the lamps or of the accessory units in the beam path (e.g. microcells).

- Activate the menu function Beam position / D2E Lamp or Beam position / Halogen lamp auf.

The shutter is opened and lamp-selector slider is moved in such a position that undispersed light of the used lamp passes through the sample compartment.
Service Check for scanning SPECORDP®P

Beam position
15 User Management and Electronic Signatures

The FDA conf version of WinASPECT® includes a User Management module and the possibility of electronic signature of measurement results.

15.1 User Management

15.1.1 Hierarchy and access to functions

The user management provides four access levels.

These levels have the following hierarchy:

Level 1 > Level 2 > Level 3 > Level 4.

Access to WinASPECT® functions

Administrator level

An administrator has full access rights to user administration resources. He/she may set and change any of these resources. He/she has no access to WinASPECT® functions.

Level 1

Level 1 users have unrestricted access to all functions of WinASPECT®. In addition, a level 1 user may inspect user administration setups, but is prevented from making any settings or changes therein.

Level 2

Level 2 users have access to all functions except for the menu function Extras / User Management.

Level 3 and Level 4

For the individual WinASPECT® functions the following rules apply:

+ The function can be executed.
– The function is denied for users of the respective level.

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>File menu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>New</td>
<td>+</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>Open</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Close</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Overlay</td>
<td>+</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>Save</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Save as...</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Print</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>
## User Management and Electronic Signatures

### User Management

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exit</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

### Measurement menu

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initialize Device</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Open Parameter File</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Set Parameters</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>View current parameters</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Standard Correction</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Wavelength Correction</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Reference Measurement</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Measurement Settings</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
</tbody>
</table>

*The restrictions applicable here also apply to the Quant module as well as to the optional modules Bio, Formula, Water Analysis and Kinetics.*

### Extras menu

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Options</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>User Management</td>
<td>−</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Logout / New login</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Change Password</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

*Level 3 and Level 4 users may open the Options dialog box, but are not authorized to change any options.*

### Data Handling

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>All menu functions that change the spectra</td>
<td>+</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Peaklist</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Values at defined wavelengths</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

### Quant

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setting up a new calibration curve</td>
<td>+</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Editing a stored calibration curve</td>
<td>+</td>
<td>−</td>
<td></td>
</tr>
<tr>
<td>Viewing a stored calibration curve</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>Executing a concentration determination</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

*All functions provided in Quant / Concentration are accessible to Level 3 and Level 4 users.*
User Management and Electronic Signatures

User Management

<table>
<thead>
<tr>
<th>Menu function / Module function</th>
<th>Level 3</th>
<th>Level 4</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quant/Bio Formula</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Creating a new method</td>
<td>+</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>Loading a stored method and continuing measurements</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Water Analysis</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>All functions (as Quant / Concentration)</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bio</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Creating a new method</td>
<td>+</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>Loading a stored method and continuing measurements</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Kinetics</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>All functions</td>
<td>+</td>
<td>+</td>
<td>Level 4 users must not vary parameters.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Method</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Recording a method</td>
<td>–</td>
<td>–</td>
<td>Accessible only to Level 1 and Level 2 users.</td>
</tr>
<tr>
<td>Playing a method</td>
<td>+</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

15.1.2 Configuration of User Management / Activating the login list

The User Management may only be configured by Level 1 users.

Level 2 users have the right to view the entries made in User Management.

Level 3 and Level 4 users do not have any access to the User Management.

For every user, a user account is created, to which the user profile is stored. If a user account is no longer needed, it can be deactivated or blocked. It is not possible to delete user accounts!

**EXTRAS / USER MANAGEMENT**

- Activate the menu command **EXTRAS / USER MANAGEMENT**.

This will bring up the **User Management** dialog box.
User Management and Electronic Signatures

User Management

Fig. 15-1 User Management dialog box

The dialog box contains a list with the entered users and the corresponding passwords. On the right side of the dialog box, the details of the user profile of the selected user are displayed.

In the User Management dialog box, you can

- establish a new user account
- edit an existing user account and
- call the login list.

15.1.2.1 Establishing a new user account

Only Level 1 users are authorized to establish a new user account.

To establish a new user account, click on the [New] button of the User Management dialog box.

This will bring up the User account properties dialog box.
In the textboxes, make the following entries:

For the entry of user names and passwords, observe the conventions described in → Section “Passwords and login names” p. 212.

<table>
<thead>
<tr>
<th>Textbox</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Login name</td>
<td>Name under which the user logs in to WinASPECT®.</td>
</tr>
<tr>
<td></td>
<td>Max. number of characters: 20</td>
</tr>
<tr>
<td>Full name</td>
<td>User’s full name.</td>
</tr>
<tr>
<td></td>
<td>Max. number of characters: 30</td>
</tr>
<tr>
<td>Description</td>
<td>Additional note on the user.</td>
</tr>
<tr>
<td></td>
<td>This entry is displayed in the User Management dialog box for the selected user.</td>
</tr>
<tr>
<td></td>
<td>The entry is optional.</td>
</tr>
<tr>
<td>Level</td>
<td>Select the desired authorization level.</td>
</tr>
<tr>
<td>Password</td>
<td>Password used by the user to log in to WinASPECT®.</td>
</tr>
<tr>
<td></td>
<td>Min. number of characters: 5; max. number of characters: 20</td>
</tr>
<tr>
<td>Confirm password</td>
<td>Exactly repeated entry of the password.</td>
</tr>
</tbody>
</table>

The check boxes serve to activate various states regarding the validity of the password, or of the entire user account.

<table>
<thead>
<tr>
<th>Check box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>User has to change password with next start.</td>
<td>Password is always valid only for a single login. User has to enter a new password when logging in for the next session.</td>
</tr>
<tr>
<td>User can't change password.</td>
<td>The function Extras / Change Password is deactivated for this user.</td>
</tr>
<tr>
<td>Password limited in time</td>
<td>When you activate this check box, you must enter the number of days this password shall be valid in the appearing textbox.</td>
</tr>
</tbody>
</table>
Account deactivated. The account was deactivated by a Level 1 user.
User account blocked. The account was automatically blocked after the wrong password had been entered three times in succession.

- Click on [OK] to confirm the properties of the new user account.

15.1.2.2 Editing an existing user account

- In the table of the User Management dialog box, click on the user account to be edited and then on the [Edit] button.

   This will bring up the User Account Properties dialog box showing the properties of the selected account. The Login name, Full name as well as the Description textboxes are not accessible. All other entries and options can be changes as desired (→ Section "Establishing a new user account" p. 208).

15.1.2.3 Activating the Login List

The Login List stores all login actions to WinASPECT® software (only with FDA conf version).

- In the User Management dialog box, click on the [Login List] button. This will bring up the LoginList dialog box.

![Login List dialog box](image)

Fig. 15-3 Login List dialog box

The Login List saves the following data:

- Date and time of login
- Login name
- Full name used in User Management
- Access level
User Management and Electronic Signatures
User Management

The buttons below the list serve to navigate through the entries or delete the selected entry:

- Moves to first entry of list.
- Moves to the previous entry.
- Moves to the next entry.
- Moves to the end of the list.
- Deletes the selected entry.

Before, a safety query appears asking you if you really want to delete the entry.

Searching the list with a filter

The software allows you to search the login list for any entries with a filter.

- In the Login List dialog box, activate the menu command Search / Define filter.

![Define filter dialog box](Fig.15-4)

You can select and combine the following filter settings:

<table>
<thead>
<tr>
<th>Check box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Search data range</td>
<td>Displays the entries within a defined period. In the respective textboxes, enter the dates of the beginning and the end of the period to be searched for in the format corresponding to the Windows &quot;Regional Settings&quot;.</td>
</tr>
<tr>
<td>Name of user</td>
<td>Displays all entries of a defined name. You can optionally scan the database for the login name or the full name entered in the user account.</td>
</tr>
<tr>
<td>User level</td>
<td>Displays all entries of a defined user level.</td>
</tr>
</tbody>
</table>

- Using the menu command Search / Filter reset, you can reset the default settings.
15.1.3 Passwords and login names

Conventions for passwords and login names

The following conventions apply to the use of passwords and login names:

- The login name must have at least one and maximally twenty characters. The entry is not case-sensitive.
- The password must contain at least five and maximally 20 characters. The entry is case-sensitive.
- Login name and password must not be the identical.
- After three faulty login attempts, the corresponding user account will be blocked. The blocking can only be undone by a Level 1 user.

Changing the password

Depending on the user account settings, the user may be authorized to access his/her password. In this case, he/she may also change the password, if required.

**EXTRAS / CHANGE PASSWORD**

- Activate the menu command Extras / Change Password.
  
  This will bring up the Change Password dialog box.

![Change Password dialog box](image)

In the textbox, type the new password and click on [OK]. This will bring up a dialog box asking you to repeat password entry for confirmation.

- Type the password once more and confirm the entry with [OK].

If the entry was faultless, the following message will appear: "Password has changed".

Defining minimum password length

A minimum length for passwords can be defined in the User management dialog box.

- Use a Settings menu command to open a dialog field of this name.
- Enter desired minimum length value for passwords in the input field (Minimum length of password).
- Confirm your entry with [OK].
15.2 Electronic signature

In the FDA conf version of WinASPECT®, it is possible to sign files. With the signature, the signing user will finish his/her work on the file. By the signing the files, the files will be

- encrypted,
- provided with a signature state and the data of the signing user,
- protected from further modifications,
- saved under the same name and the extension "*dat*".

Signed files can be opened for viewing. Files can be signed repeatedly by different users.

15.2.1 Setting the signature status

- Activate the menu command Extras / Options to open the Options dialog box and activate the Signature tab.

On the Signature tab, you can define your own signature remarks, such as "Read" or "Concluded". That way, you can create an option list for the signatures:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Add]</td>
<td>Adds a new option to the list. By a click on [Add], a textbox appears. Type the desired remark and confirm the entry with the ENTER key of the keyboard. The note will be transferred to the list.</td>
</tr>
<tr>
<td>[Edit]</td>
<td>Edits list entry. On the list, mark the entry to be edited and click on [Edit]. Edit the respective entry in the appearing textbox and confirm the edited entry with the ENTER key of the keyboard. The altered entry appears on the list.</td>
</tr>
<tr>
<td>[Delete]</td>
<td>Deletes an entry from the list. On the list, mark the entry to be deleted and click on [Delete]. The entry will be deleted from the list.</td>
</tr>
</tbody>
</table>

15.2.2 Signing a file

To sign files after a measurement taken in a module other than Quant or Kinetics, activate the menu command Edit / Sign Document. To sign files in optional modules, activate the corresponding commands in these modules. The further procedure is the same for all modules.

- Activate the menu command Edit / Sign Document.

After the display of a warning message, the Signature dialog box appears.
15.2.3 Viewing signatures

The software also lets you review the signatures of a file.

- Activate the menu command Edit / View Signatures.

This will bring up the List of signatures dialog box. The following data regarding the signatures are displayed:

- Login name
- Full name
- Status of signature
- Date and time of signing
- Comment on the signature, if entered.
Additional settings to ensure FDA conformity according to 21 CFR Part 11

16 Additional settings to ensure FDA conformity according to 21 CFR Part 11

16.1 Authorization settings in the operating system

The WinASPECT Version 2.0 UV VIS device control software is a file-based system. This system provides the advantage of relatively easy portability of data to other systems. To meet the higher safety requirements, the Microsoft Windows 2000 or XP (Professional) operating system must be used with the appropriate configuration options. The combination of WinASPECT and Windows 2000/XP represents a closed system meeting the technical requirements of FDA conformity according to 21 CFR Part 11.

That way, permissions can be defined for every folder for all users registered to the operating system. This refers to the creation of files, overwriting of existing files, opening of files and many things more. These settings should be made by an authorized system administrator.

Example setting of the denial for the overwriting of files (Windows XP)

- Open Windows Explorer.
- Search for the desired folder and right-click on it.
- On the appearing submenu, select the Properties function. This will bring up the Properties dialog box.
- Activate the Security tab.
- Click on [Advanced]. This will bring the Advanced security settings dialog box. In the upper part, different Windows(!) users can be selected.
- Choose the group of Windows users to whom the settings shall apply.
- Deactivate the check box Inherit from parent the permission entries that apply to child objects. Include these with entries explicitly defined here.
- The following warning message appears: "Selecting this option means that the parent permission entries that apply to child objects with no longer applied to this object...". Click on [Copy].
- On the Permission tab, click on [Edit]. This will bring up the Permission Entry dialog box.
- Choose the options shown below or those meeting your requirements:
Additional settings to ensure FDA conformity according to 21 CFR Part 11

Authorization settings in the operating system

Confirm the selected options with [OK]. The software will take you back to the Advanced security settings dialog box.

Click on [Apply] and then on [OK] to return to the Properties dialog box.

In the Properties dialog box, click on [Apply] and then close the dialog box with [OK].

The selected user/user group now has the following access privileges:

**The user is authorized to:**

- Traverse Folder / Execute File
- List Folder / Read Data
- Read Attributes
- Read Extended Attributes
- Create Files / Write Data
- Write Attributes
- Write Extended Attributes
- Read Permissions
Additional settings to ensure FDA conformity according to 21 CFR Part 11

Additional supporting functions of WinASPECT to achieve FDA conformity according to 21 CFR Part 11

- Change Permissions
- Take Ownership.

The user is not authorized to:
- Create Folders / Append Data
- Delete subfolders and files
- Delete

In particular, this means that files may be created, but not overwritten or deleted independent of the calling application or the logged in user.

For a detailed description, you are advised to read the extensive documentation of the operating system.

16.2 Additional supporting functions of WinASPECT to achieve FDA conformity according to 21 CFR Part 11

WinASPECT provides the possibility to save the results of a measurement automatically to a freely selectable folder at the end of each measurement. This is done independent of the used module. You can activate this function in the Measurement Settings dialog box in the Save results field (menu command Measurement / Measurement Settings). In this field, you can also define the storage path. In the selected folder, the software automatically creates a subfolder for every day. The name of this subfolder contains the date, e.g. "2004-01-13". The individual files will then be saved to this folder. The file names are created from the time at the end of the measurement.

![Measurement Settings dialog box](image)

Fig.16-2 Selecting the folder for automatic result storage
That way it is possible, for instance, to save the original data to a server initially not accessible to the user. The access to the server is to be defined by the respective system administrator, too.
17 Appendix

17.1 New Features in WinASPECT®

New features in WinASPECT® 2.2
- Integration of SPECORD S300 UVVIS and SPECORD S300 VIS
- Integration of Spekol 1300 / 1500 / 2000
- Service check SPECORD S600 und S300
- Automatic Initialisation on startup of WinASPECT
- Changes in the control of the Autosamplers APG 53 and 100
- Control of the Peltier-tempered accessories implemented, supports the temperature display
- Online-Display
- Implementation of Routine Quant
- Implementation of macro programming
- Connection to AJAQC (AJ Blome control card module)
- Connection to other LIMS – Systems possible
- Serial measurement:
  - Field for “notes” added
  - Transfer to document window possible
- Overlay from different folders
- Data export as JCAMP
- Kinetic module: colour changes
- Optional Auto start function of the individual modules in Extras/Options
- Fixed scale, specification of the display region separately for all dimensions (settings in Extras/Options)
- Changes in the FDA-Version:
  - New User Admin in, only authorized user-management can be carried out
  - Minimum password length can be set
  - Warning before password expiration
- Window Management – All windows accessible from “Window” in the menu bar
- Error elimination

New features in WinASPECT® 2.3.
- 3D view of flight of spectra
- Color measurement module
- Film thickness module
17.2 Statistical calculations

The following formulas are used for the statistical calculations in WinASPECT®:

**Median**

The list of ordinate values is sorted.

For an odd number of values, the median is exactly in the middle of the list, e.g.

Median ([1, 2, 3, 20, 21]) = 3

For an even number of values, the median is the mean value of the two values in the middle of the list, e.g.

Median ([1, 2, 3, 4, 20, 21, 22, 25]) = (4+20)/2 = 12

**R – Range**

Difference between minimum and maximum of measured values.

\[ R = y_{\text{max}} - y_{\text{min}} \]

\( y_{\text{max}} \) Maximum measured value

\( y_{\text{min}} \) Minimum measured value

**RR – Relative Range**

\[ RR = \frac{y_{\text{max}} - y_{\text{min}}}{\bar{y}} \]

\( \bar{y} \) Mean value

**Mean value**

\[ \bar{y} = \frac{\sum y_i}{n} \]

\( y_i \) Measured value

\( n \) Total number of measured values

**SD – Standard Deviation**

\[ SD = \sqrt{\frac{n\sum y_i^2 - (\sum y_i)^2}{n(n-1)}} \]

**RSD – Relative Standard Deviation**

\[ RSD = \frac{SD \times 100}{\bar{y}} \]

**\( R^2 \) (adjust) – Coefficient of determination (quality of regression)**

\[ r^2 = 1 - \frac{(n-1)\sum (y_i - f(x_i))^2}{(n-1)\sum (y_i - \bar{y})^2} \]

\( f(x_i) \) Value of the function of regression at \( x_i \)
17.3 Determination of sample data and acquisition of reference data

This section gives a brief introduction into the determination of sample data and explains the significance of the baseline and of its correction.

In an absorbance measurement, the system measures the energy $I_0$ incident on the sample (reference value) and the energy $I$ emerging from and attenuated by the sample. Measurement is in arbitrary units, as only the ratio of both energy values is of interest. Quantitatively, the absorption behavior is expressed in transmittance $T[\%]$ or absorbance $A$:

$$D = \frac{I}{I_0}$$

$D$ Transmission

$I_0$ Energy without attenuation (basic value)

$I$ Energy emerging from the sample

$T[\%] = D \times 100$ $T[\%]$ Transmission in percent

$A = -\log D$ $A$ Absorbance

**Determination of sample data on single-beam spectrometers**

On single-beam spectrometers, sample data is determined as described by the formulas above.

First, the system measures the energy $I_0$ attenuated by the reference and then the energy $I$ attenuated by the sample. The ratio of both energy values is formed and the transmittance and absorbance calculated.

**Determination of sample data on double-beam spectrometers**

Double-beam spectrometers were designed to reduce measuring errors caused by energy variations during the measurement (drift). For that, the lamp spectrum is "observed" by means of a reference beam. The two energy values of sample and reference beam, the ratio of which is determined, are used to compensate for any variations in lamp energy.

Calculation of the reference value (also: baseline):

$$D_R = \frac{I_{MR}}{I_{VR}}$$

$D_R$ Transmission of reference

$I_{MR}$ Energy of reference beam

$I_{VR}$ Energy of sample beam
Appendix

Determination of sample data and acquisition of reference data

Calculation of the sample value

\[
D_p = \frac{I_{VP}}{I_{VP}} \frac{D}{D} \frac{I_{MP}}{I_{VP}} \frac{D}{D} \quad \text{Transmission of sample}
\]

\[
I_{VP} \quad \text{Energy of reference beam}
\]

\[
I_{VP} \quad \text{Energy of sample beam}
\]

Calculation of the measured value

\[
D = \frac{D_p}{D_R} \frac{D}{D} \quad \text{Transmission}
\]

\[
D \quad \text{Transmission of sample}
\]

\[
D_R \quad \text{Transmission of reference}
\]

Where to place the reference in double-beam spectrometers?

On single-beam spectrometers, placing the reference is quite easy. Just place it in the beam path of the spectrometer.

Depending on the following sample measurement, however, on double-beam spectrometers, there are various combinations possible for placing the reference. Unfortunately, this involves the risk of making mistakes:

The following combinations are possible and yield correct results:

<table>
<thead>
<tr>
<th>Combination</th>
<th>Reference measurement</th>
<th>Sample measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Reference</td>
<td>Reference</td>
</tr>
<tr>
<td></td>
<td>Sample</td>
<td>Reference</td>
</tr>
<tr>
<td>1</td>
<td>Reference</td>
<td>Empty</td>
</tr>
<tr>
<td></td>
<td>Empty</td>
<td>Sample</td>
</tr>
<tr>
<td>2</td>
<td>Empty</td>
<td>Empty</td>
</tr>
<tr>
<td></td>
<td>Sample</td>
<td>Empty</td>
</tr>
<tr>
<td>3</td>
<td>Empty</td>
<td>Empty</td>
</tr>
<tr>
<td></td>
<td>Sample</td>
<td>Reference</td>
</tr>
</tbody>
</table>

Combination 1 can be chosen, if the references, too, already have a high absorbance. Then, the gain of the detector diodes is set to a higher level so that the measurement is taken with an improved energy ratio. With that, the so-called dynamic range of the detector diode is utilized better.

Which types of reference correction are available on the double-beam spectrometers?

The WinASPECT® software provides three different options for the measurement of the reference:

- Standard
- Reference
- Special

Reference

This type of reference measurement you will use in most cases. Before the measurement of the sample, the reference is measured at the same measurement parameters used afterwards also for the sample measurements. Thus, any al-
Determination of sample data and acquisition of reference data

In Special Correction, you can use any stored file as source of reference data.

For the use of the Special reference option, the following requirements must be met:

- The values of the reference file must have been measured with the following measurement parameter option:
  
  **Correction - No**

- A correction value must exist for every measured value. Thus, it is possible to measure the correction data with a data point interval (Delta lambda) that is less than that used for the sample measurement. The inverse case, however, is not permissible, i.e. you must not acquire the reference data with a data point interval that is greater than that of the sample measurement.

- Accessories that restrict the beam path must already be used when measuring the reference data.

This type of reference measurement is suited to survey measurements taken with a special accessory unit. Compared to the Reference option, this type of correction is less accurate because of the possible time difference between reference and sample measurements.
Appendix

Determination of sample data and acquisition of reference data
### Table of figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fig. 1-1</td>
<td>User Login dialog box</td>
<td>9</td>
</tr>
<tr>
<td>Fig. 1-2</td>
<td>Safety program query</td>
<td>10</td>
</tr>
<tr>
<td>Fig. 1-3</td>
<td>WinASPECT® workplace</td>
<td>10</td>
</tr>
<tr>
<td>Fig. 1-4</td>
<td>Options dialog box</td>
<td>14</td>
</tr>
<tr>
<td>Fig. 2-1</td>
<td>Serial Measurement dialog box</td>
<td>20</td>
</tr>
<tr>
<td>Fig. 2-2</td>
<td>Serial measurement settings</td>
<td>21</td>
</tr>
<tr>
<td>Fig. 2-3</td>
<td>Measurement Configuration dialog box</td>
<td>25</td>
</tr>
<tr>
<td>Fig. 2-4</td>
<td>Device driver dialog box</td>
<td>27</td>
</tr>
<tr>
<td>Fig. 2-5</td>
<td>Measurement parameters – Scanning SPECORD® Settings tab</td>
<td>28</td>
</tr>
<tr>
<td>Fig. 2-6</td>
<td>Measurement parameters – Scanning SPECORD® - Device tab</td>
<td>31</td>
</tr>
<tr>
<td>Fig. 2-7</td>
<td>Mode tab - Activated Scan Mode</td>
<td>32</td>
</tr>
<tr>
<td>Fig. 2-8</td>
<td>Mode tab – Activated Step Mode</td>
<td>33</td>
</tr>
<tr>
<td>Fig. 2-9</td>
<td>Mode tab – Activated Time Scan</td>
<td>34</td>
</tr>
<tr>
<td>Fig. 2-10</td>
<td>Mode tab – Activated Wavelengths mode</td>
<td>35</td>
</tr>
<tr>
<td>Fig. 2-11</td>
<td>Sample compartment with sample beam path</td>
<td>39</td>
</tr>
<tr>
<td>Fig. 2-12</td>
<td>Measurement parameters for SPECORD® S600 – General tab</td>
<td>42</td>
</tr>
<tr>
<td>Fig. 2-13</td>
<td>Measurement parameters for SPECORD® S600 – Device tab</td>
<td>43</td>
</tr>
<tr>
<td>Fig. 2-14</td>
<td>Monitor display of the current intensity curve of the measured signal I(M)</td>
<td>45</td>
</tr>
<tr>
<td>Fig. 2-15</td>
<td>Measurement parameters for SPECORD® S600 – Mode tab</td>
<td>45</td>
</tr>
<tr>
<td>Fig. 2-16</td>
<td>S600 measurement parameters – Interval tab</td>
<td>47</td>
</tr>
<tr>
<td>Fig. 2-17</td>
<td>Entry fields for time intervals</td>
<td>48</td>
</tr>
<tr>
<td>Fig. 2-18</td>
<td>Entry fields for time intervals</td>
<td>49</td>
</tr>
<tr>
<td>Fig. 3-1</td>
<td>WinASPECT® document window</td>
<td>53</td>
</tr>
<tr>
<td>Fig. 3-2</td>
<td>Sample Properties dialog box</td>
<td>56</td>
</tr>
<tr>
<td>Fig. 3-3</td>
<td>Scale dialog box</td>
<td>57</td>
</tr>
<tr>
<td>Fig. 3-4</td>
<td>Grid Options dialog box</td>
<td>59</td>
</tr>
<tr>
<td>Fig. 3-5</td>
<td>Copy samples dialog box</td>
<td>61</td>
</tr>
<tr>
<td>Fig. 3-6</td>
<td>Selected spectrum was shifted</td>
<td>62</td>
</tr>
<tr>
<td>Fig. 3-7</td>
<td>Manage Textboxes dialog boxes</td>
<td>63</td>
</tr>
<tr>
<td>Fig. 3-8</td>
<td>3D-view of flight of spectrums</td>
<td>65</td>
</tr>
<tr>
<td>Fig. 3-9</td>
<td>Print dialog box</td>
<td>69</td>
</tr>
<tr>
<td>Fig. 4-1</td>
<td>Calibration dialog box</td>
<td>74</td>
</tr>
<tr>
<td>Fig. 4-2</td>
<td>Standards dialog box with several measurement cycles</td>
<td>79</td>
</tr>
<tr>
<td>Fig. 4-3</td>
<td>Source of selected standard dialog box</td>
<td>81</td>
</tr>
</tbody>
</table>
### Table of figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fig.4-4</td>
<td>Display of calibration curve in Calibration dialog box</td>
<td>85</td>
</tr>
<tr>
<td>Fig.4-5</td>
<td>Print – Calibration dialog box</td>
<td>86</td>
</tr>
<tr>
<td>Fig.4-6</td>
<td>Concentration dialog box - Parameters tab</td>
<td>87</td>
</tr>
<tr>
<td>Fig.4-7</td>
<td>Edit - Parameters dialog box, General tab: Designation / Operator</td>
<td>88</td>
</tr>
<tr>
<td>Fig.4-8</td>
<td>Edit – Parameters dialog box, General tab: Sample Table field</td>
<td>89</td>
</tr>
<tr>
<td>Fig.4-9</td>
<td>Edit – Parameters dialog box, General tab: Repeat Measurements field</td>
<td>90</td>
</tr>
<tr>
<td>Fig.4-10</td>
<td>Edit – Parameters dialog box, General tab: Check Samples field</td>
<td>90</td>
</tr>
<tr>
<td>Fig.4-11</td>
<td>Edit – Parameters dialog box, Factors/Calibr. Data tab: Factor options</td>
<td>91</td>
</tr>
<tr>
<td>Fig.4-12</td>
<td>Edit – Parameters dialog box, Factors/Calibr. Data tab: Calibration file</td>
<td>91</td>
</tr>
<tr>
<td>Fig.4-13</td>
<td>Edit – Parameters dialog box, Factors/Calibr. Data tab: Additional factors</td>
<td>92</td>
</tr>
<tr>
<td>Fig.4-14</td>
<td>Sample data by measurement dialog box</td>
<td>93</td>
</tr>
<tr>
<td>Fig.4-15</td>
<td>Sample values from file dialog box</td>
<td>95</td>
</tr>
<tr>
<td>Fig.4-16</td>
<td>Check sample in Sample values from file dialog box</td>
<td>96</td>
</tr>
<tr>
<td>Fig.4-17</td>
<td>Result display of concentration analysis</td>
<td>96</td>
</tr>
<tr>
<td>Fig.4-18</td>
<td>Display of details of concentration measurement</td>
<td>97</td>
</tr>
<tr>
<td>Fig.4-19</td>
<td>Graphic presentation of the found concentration within the calibration curve</td>
<td>97</td>
</tr>
<tr>
<td>Fig.4-20</td>
<td>Concentration – Prepare print dialog box</td>
<td>98</td>
</tr>
<tr>
<td>Fig.5-1</td>
<td>Quant Routine – Settings dialog box</td>
<td>99</td>
</tr>
<tr>
<td>Fig.5-2</td>
<td>Express buttons in Quant Routine module</td>
<td>100</td>
</tr>
<tr>
<td>Fig.5-3</td>
<td>Dialog field for Setup sample table / Methods tab</td>
<td>104</td>
</tr>
<tr>
<td>Fig.5-4</td>
<td>Setup sample table / Sample table tab with Table subtab dialog box</td>
<td>106</td>
</tr>
<tr>
<td>Fig.5-5</td>
<td>Setup sample table / Sample table tab dialog field with graphic input tool for working with cell carousell</td>
<td>107</td>
</tr>
<tr>
<td>Fig.5-6</td>
<td>Sample table for Quant Routine</td>
<td>108</td>
</tr>
<tr>
<td>Fig.5-7</td>
<td>Dialog field for settings regarding sample series / Methods tab; selection of multiple measurement</td>
<td>112</td>
</tr>
<tr>
<td>Fig.5-8</td>
<td>Results tab – values measured in Routine Quant module</td>
<td>113</td>
</tr>
<tr>
<td>Fig.5-9</td>
<td>Representation of results in Quant Routine module</td>
<td>114</td>
</tr>
<tr>
<td>Fig.5-10</td>
<td>Calibration curve and sample concentration values display screen</td>
<td>115</td>
</tr>
<tr>
<td>Fig.5-11</td>
<td>Dialog box for printed result table in Quant Routine module</td>
<td>117</td>
</tr>
<tr>
<td>Fig.5-12</td>
<td>Display screen for calibration file to be loaded in Quant Routine</td>
<td>119</td>
</tr>
<tr>
<td>Fig.7-1</td>
<td>Kinetics – Routine dialog box</td>
<td>129</td>
</tr>
<tr>
<td>Fig.7-2</td>
<td>Selecting a measured curve in Kinetics – Routine</td>
<td>135</td>
</tr>
<tr>
<td>Fig.7-3</td>
<td>Settings dialog box</td>
<td>135</td>
</tr>
<tr>
<td>Fig.7-4</td>
<td>Marking the curves for graphic presentation</td>
<td>137</td>
</tr>
<tr>
<td>Fig.7-5</td>
<td>Kinetics – Zoom dialog box</td>
<td>137</td>
</tr>
<tr>
<td>Fig.7-6</td>
<td>Print Kinetics - Routine dialog box</td>
<td>138</td>
</tr>
<tr>
<td>Fig.</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>-----</td>
<td>-----------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>8-1</td>
<td>Method dialog box</td>
<td>140</td>
</tr>
<tr>
<td>8-2</td>
<td>Method - Setup dialog box: General tab</td>
<td>141</td>
</tr>
<tr>
<td>8-3</td>
<td>Method – Setup dialog box: Method tab</td>
<td>142</td>
</tr>
<tr>
<td>8-4</td>
<td>Method – Setup dialog box: Measurement Settings tab</td>
<td>142</td>
</tr>
<tr>
<td>8-5</td>
<td>Method dialog box: Results tab</td>
<td>144</td>
</tr>
<tr>
<td>9-1</td>
<td>Formula dialog box</td>
<td>145</td>
</tr>
<tr>
<td>9-2</td>
<td>Formula Setup dialog box: General field</td>
<td>147</td>
</tr>
<tr>
<td>9-3</td>
<td>Formula – Setup dialog box: Result field</td>
<td>147</td>
</tr>
<tr>
<td>9-4</td>
<td>Formula – Setup dialog box: Factors field</td>
<td>148</td>
</tr>
<tr>
<td>9-5</td>
<td>Formula – Setup dialog box: Method field</td>
<td>148</td>
</tr>
<tr>
<td>9-6</td>
<td>Formula Selection dialog box</td>
<td>149</td>
</tr>
<tr>
<td>9-7</td>
<td>Formula dialog box with activated Results tab</td>
<td>150</td>
</tr>
<tr>
<td>10-1</td>
<td>Colour measurement dialog window</td>
<td>154</td>
</tr>
<tr>
<td>10-2</td>
<td>Color measurement – setups</td>
<td>157</td>
</tr>
<tr>
<td>10-3</td>
<td>Color measurement – setups dialog window</td>
<td>158</td>
</tr>
<tr>
<td>10-4</td>
<td>Window Color measurement</td>
<td>160</td>
</tr>
<tr>
<td>11-1</td>
<td>Film thickness measurement dialog window</td>
<td>164</td>
</tr>
<tr>
<td>11-2</td>
<td>Film thickness dialog window / results (displays results)</td>
<td>168</td>
</tr>
<tr>
<td>11-3</td>
<td>Film thickness dialog window / spectra (displays interference spectrums)</td>
<td>169</td>
</tr>
<tr>
<td>11-4</td>
<td>Material file dialog window for input of wavelength/refractive index value</td>
<td>171</td>
</tr>
<tr>
<td></td>
<td>pairs</td>
<td></td>
</tr>
<tr>
<td>12-1</td>
<td>Data Handling - Two spectra dialog box</td>
<td>174</td>
</tr>
<tr>
<td>12-2</td>
<td>Integral Settings dialog box</td>
<td>180</td>
</tr>
<tr>
<td>12-3</td>
<td>Areas enclosed by curve and baseline</td>
<td>181</td>
</tr>
<tr>
<td>12-4</td>
<td>Peaklist – Parameters dialog box</td>
<td>182</td>
</tr>
<tr>
<td>12-5</td>
<td>Peaklist dialog box</td>
<td>183</td>
</tr>
<tr>
<td>12-6</td>
<td>Values of defined wavelengths dialog box</td>
<td>185</td>
</tr>
<tr>
<td>12-7</td>
<td>Value of selected Waves dialog box</td>
<td>185</td>
</tr>
<tr>
<td>13-1</td>
<td>Validation SPECORD® XXX application window</td>
<td>187</td>
</tr>
<tr>
<td>13-2</td>
<td>Dialogfenster Preferences – General tab</td>
<td>191</td>
</tr>
<tr>
<td>13-3</td>
<td>Preferences dialog box – Limit Values tab</td>
<td>193</td>
</tr>
<tr>
<td>13-4</td>
<td>Dialog box with the prompt to insert a filter</td>
<td>195</td>
</tr>
<tr>
<td>13-5</td>
<td>Display of validation results while validation is running</td>
<td>197</td>
</tr>
<tr>
<td>14-1</td>
<td>Service Check dialog box after a diagnosis</td>
<td>201</td>
</tr>
<tr>
<td>14-2</td>
<td>Configuration dialog box (for e-mail connection)</td>
<td>202</td>
</tr>
<tr>
<td>15-1</td>
<td>User Management dialog box</td>
<td>208</td>
</tr>
<tr>
<td>15-2</td>
<td>User account properties dialog box</td>
<td>209</td>
</tr>
</tbody>
</table>
Table of figures

Fig.15-3  Login List dialog box ................................................................. 210
Fig.15-4  Define filter dialog box ............................................................ 211
Fig.15-5  Change Password dialog box .................................................. 212
Fig.15-6  Signature dialog box ................................................................. 214
Fig.16-1  Example of selected permission entries for the selected folder .... 216
Fig.16-2  Selecting the folder for automatic result storage ..................... 217
Index

19  Index

3

3D-view 65

A

Accessories
  Selection 36
  Audit Trail 54

C

Calibration
  Repeat measurements 80
Calibration curve
  Graphic presentation 97
  Print 86
  Setting up a new c. 75
Calibration file 92
Calibration model 76
Check sample index 96
Color measurement
  Exporting results 157
COM port
  Selection of COM port on PC 31
Concentration determination
  By direct measurement 93
  With factors 91
Concentration measurement series
  Print 98
Concentration Measuring Series
  Print 116
Correction
  Reference 222
  Special 223
  Standard 223
Cycle Mode
  Selection for measurement 28

D

D2E lamp 31
Data Handling 173
  Adaptation of spectra 176
  Addition of spectra 175
  Baseline Correction 179
  Division of spectra 176
  Linking of spectra 177
  Multiplication by a factor 178
  Multiplication of spectra 175
  Normalization of spectra 176
  Offset 178
  Peaklist 181
  Smooth 178
  Subtraction of spectra 175
  Two spectra 173
  Two spectra (toolbar) 174
  Values of defined wavelengths 184
Delta lambda 33, 34
Deuterium lamp 31
Diagnosis
  Spektrometer 200
  Diagnosis / Start 200
Display
  Results during measurement 29
Document window
  Notes tab 54
  Parameters tab 54
  Samples tab 54

E

Edit
  Paste 61
  Copy 60
  Copy to clipboard 60
  View Signatures 214

F

FDA conf – Version 205
FDA21FR Part11 – software version 6
File
  Exit 9
  New 61
  Print 69
Film thickness
  Export results 167
  Material data 171

G

graphic
  grid options 58

H

Halogen lamp 31

I

Installation
  WinASPECT 7
Integration time 33, 34, 35

K

Kinetics
Index

Loading a file 134

Lamp change
  Wavelength for I. 31
LoginList 210

Measurement
  Reference Measurement 18
  Standard Correction 37
Measurement at preselected wavelengths 35
Measurement window buttons 17
Measuring mode
  Scan mode 32
  Selection 32
  Step Mode 33
  Time Scan 34
  Wavelengths 35
Measuring time 34
Menu command Bio
  Formula 145
  Method 139
Menu Command Color measurement
  Color coordinates/Color numbers menu command 153
Menu command Data Handling
  Baseline Correction 180
Menu command Data Handling
  Derivative 179
  Factor 178
  Integration / Display 181
  Interpolation 179
  Offset 178
  Peaklist / Adding peaks manually 184
  Peaklist / Delete list 184
  Peaklist / Edit 184
  Peaklist / Search automatically 182
  Smooth 178
  Two spectra 173
  Values of defined wavelengths / Numerical input 185
  Values of defined wavelengths I Interactive 185
Menu Command Data Handling
  Integration / New 180
Menu command Edit
  Section 64
Menu command Edit
  3D view 65
  Header 59
Menu command Edit / Cycle Properties
  55
Menu command Extras
  Change Password 212
  Options 13
  User Management 207
Menu command File
  Close 71
  Export / ASCII 72
  Export / JCAMP 72
  New 68
  Open 68
  Overlay 69
  Overlay 66
  Save 71
  Save as... 71
Menu command Film thickness measurement
Menu command Film Thickness measurement
Menu command File
  Initialize Device 18
  Measurement 19
  Serial Measurement 19
  Set Parameters 24
Menu command Quant
  Concentration 87
  Formula 145
  Routine 99
Menu command View
  Left side 55
  Scale 57
  Show original data 55
  Zoom 58
Menu command Window
  Cascade 72
  Close All 72
Index

Minimize All 72
Tile 72

Notes 60

Online help 13

Peaklist
Adding peaks manually 184
Deleting 184
Editing 184

Printing
Contents of printout: 70
Page Layout 70
Page Preview 71

Quant
Calibration 73

Regression model
Change 85
Result presentation
Decimals 15

Savitzky-Golay algorithm 178
Scan Mode 32
Scanning speed 33
Service Check 199
Lamp Check 202
Zeroth order 203
Slit 31
Slit width, spectral 31
Spectral curves
Colors and marks 57
Spectroquant test kits 121
Spectrum
scaling 57
Spectrum smoothing 178
Spracheneinstellungen 14
Statistics
Measurement cycles 82
Step Mode 33
Strahlposition
Halogenlampe 203
Supporting points 176

Textbox 62
Time Scan 34

Wait time 34
Wavelength 34
Wavelength range 32
Wavelength range 33
WinASPECT
Desktop 10
Exiting 9
FDA21FR Part11 Version 6
Help 13
Menu bar 11
Starting 9
Status bar 13
Toolbar 11

Zeroth order
Halogen lamp 203
Zeroth Order
D2ELamp 203