OPUS

Spectroscopy Software

Version 7

Quick Reference Guide

BRUKER

Table of Contents

1 Starting OPUS

1. Insert the OPUS stick into the USB port of your PC. Normally, the installation starts automatically. If the Windows *Autostart* option is disabled, you have to start the installation manually by running the *Setup* program from the stick.
2. Follow the on-screen installation instructions.
3. Restart the PC at the end of the installation procedure

Note: You may be prompted to restart your computer when you install different program components. In such a case do not restart until the OPUS setup has been completed.

4. On the Windows Start menu, click the OPUS icon when the installation has been finished.

Figure 1: Windows Start Menu

The *Login dialog* box opens.

1.1 OPUS Login

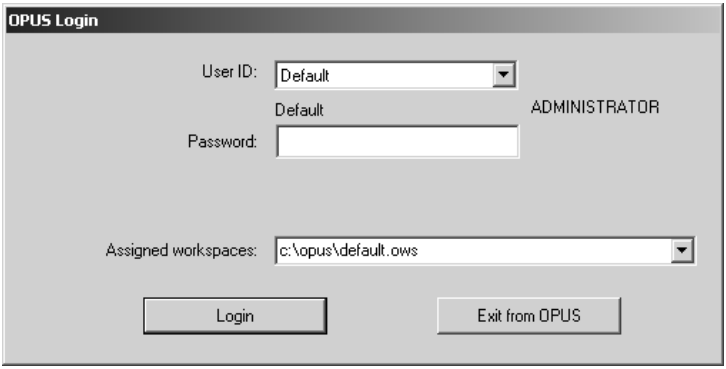


Figure 2: OPUS Login

1. Select your *User ID* from the drop-down list.
2. Enter *OPUS* in the *Password* entry field. The password is case sensitive. Once you have assigned yourself a user record in OPUS, it is possible to determine your own user ID and password.
3. Select the assigned workspace. You can always select those workspaces from the drop-down list which have been defined for your user ID. When you use OPUS for the first time, we recommend not to change the standard *default.ows* workspace. For more detailed information on the user account system refer to the OPUS Reference Manual.
4. Click the *Login* button. The *About OPUS* dialog opens.

1.2 About OPUS

This dialog contains:

- serial number of the OPUS version
- name of the licensee
- list of available OPUS packages

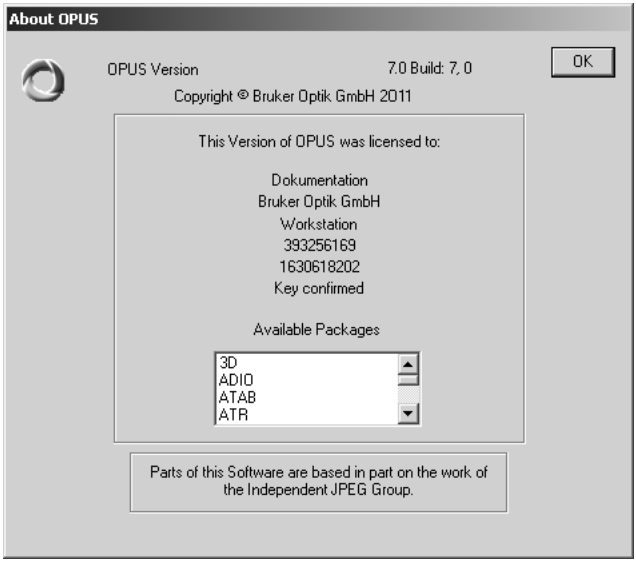


Figure 3: About OPUS

Click the *OK* button.

The OPUS user interface opens.

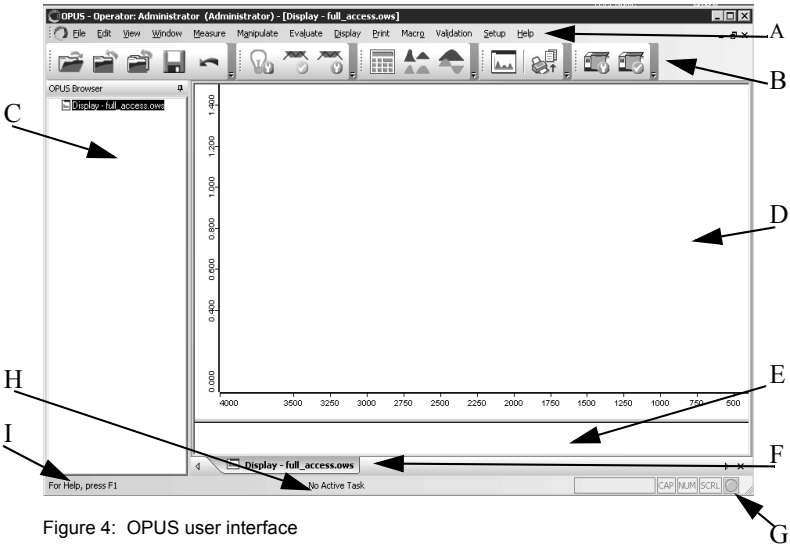


Figure 4: OPUS user interface

The OPUS user interface header shows the type and status of the operator currently logged in.

A) Menu bar
B) Toolbar
C) Browser window
D) Spectrum window
E) Overview window
F) OPUS view
G) Instrument status
H) Status bar
I) Online help

All settings (menus or icons) are individually configurable and will be reloaded when you start OPUS next time.

For detailed information on the OPUS user interface refer to the OPUS Reference Manual.

2 Working with OPUS

2.1 Acquiring a spectrum

During normal daily work you may frequently measure a single-channel reference spectrum (open-beam spectrum without any sample in the optical path). This spectrum is also called *background spectra*.

In case of routine measurements you just have to change the samples, start measurement and evaluate the results. If you turn on the spectrometer for the first time, or if you have changed the hardware (e.g. beamsplitter or detector), you have to check the instrument settings before starting the measurement.

The measurement dialogs depend on the current spectrometer configuration. Therefore, the following dialogs may be slightly different from the ones displayed on your screen.

2.1.1 Setting up spectrometer components

1. On the *Measure* menu, click the *Optic Setup and Service* command or use the  icon from the toolbar. The *Optic Setup and Service* dialog opens.
2. Click the *Optical Bench* tab.
3. Select the spectrometer from the *Configuration* drop-down list.
4. Click the *Save Settings* button.

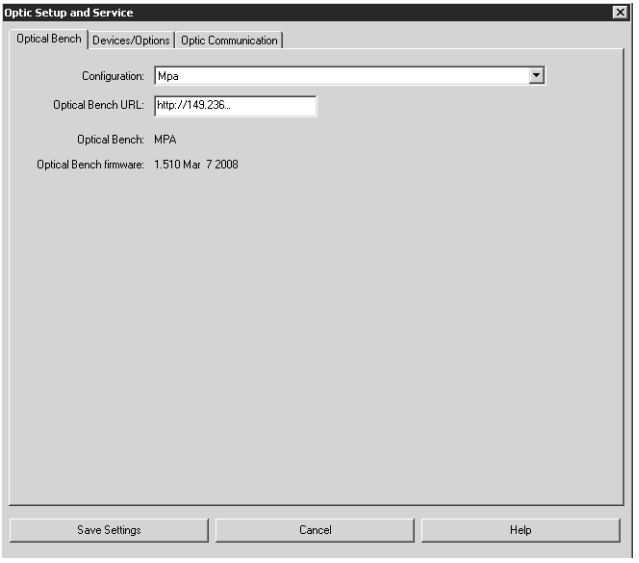


Figure 7: Optic Setup and Service - Optical Bench tab

The spectrometer is connected as soon as the spectrometer name and firmware version are displayed.

2.1.2 Setting up measurement parameters

Before starting a measurement, you have to define certain parameters.

On the *Measure* menu, click the *Measurement* command. Or use the  icon from the toolbar. The *Measurement* dialog opens:

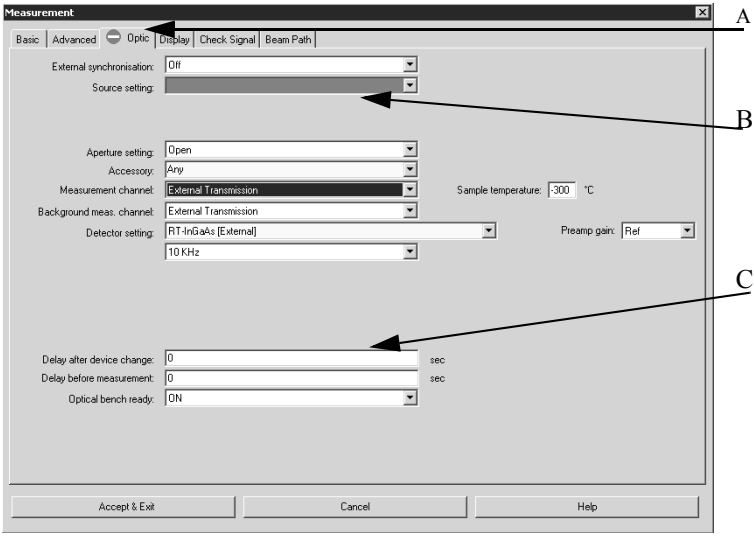


Figure 8: Erroneous setting on tab

If you open the *Measure* menu for the first time, some tabs may indicate erroneous settings by signs such as ⛔.

A) If ⛔ appears or ⚠ is displayed, you have to correct the erroneous settings first before being able to continue. In case of ⚠ it is still possible to save the configuration.
B) If the entry field is marked red, the requested parameter does not fit to the hardware used. For example, if an experiment requires an MCT detector, but a DTGS detector has been installed according to the optics configuration. In such a case, click the small arrow to have the possible setting(s) displayed. Make sure that you correct potential errors before saving the settings.
C) If an entry field is marked red, the current value for that parameter is beyond its specified range, or the value is missing completely. If you point the cursor onto a red entry field, a tooltip opens and gives an explanation.

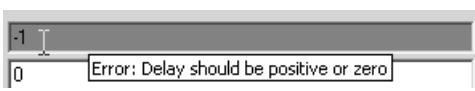


Figure 9: Error tooltip

If properly configured, the *Measurement* dialog box is displayed without any warnings:

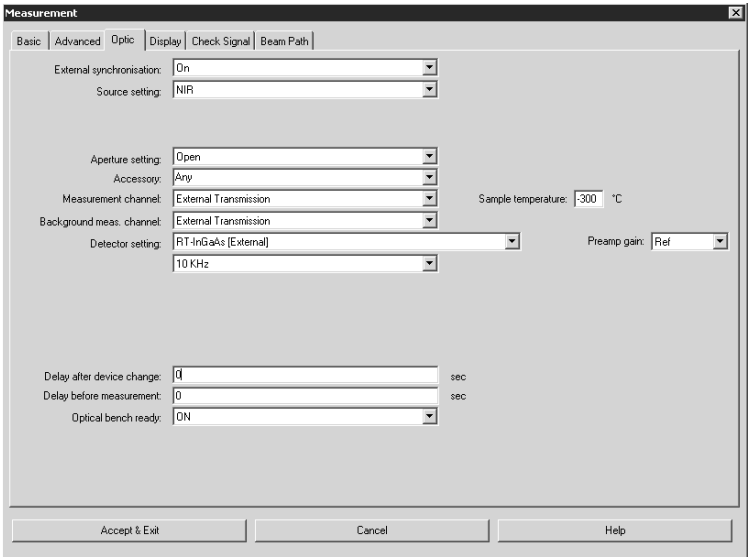


Figure 10: Measurement menu tabs without any warnings

2.1.3 Calibrating interferogram peak

Before you start the first measurement you have to determine and store the exact interferogram peak position.

You only have to repeat the peak position determination if there have been made changes in the hardware.

1. On the *Measurement* dialog, click the *Check Signal* tab. Make sure that the *Interferogram* option button is activated.

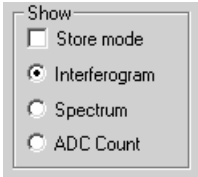


Figure 11: Check Signal tab - Select interferogram

2. If no interferogram peak is displayed, move the scan region to the left or right using the arrow buttons to find the peak.

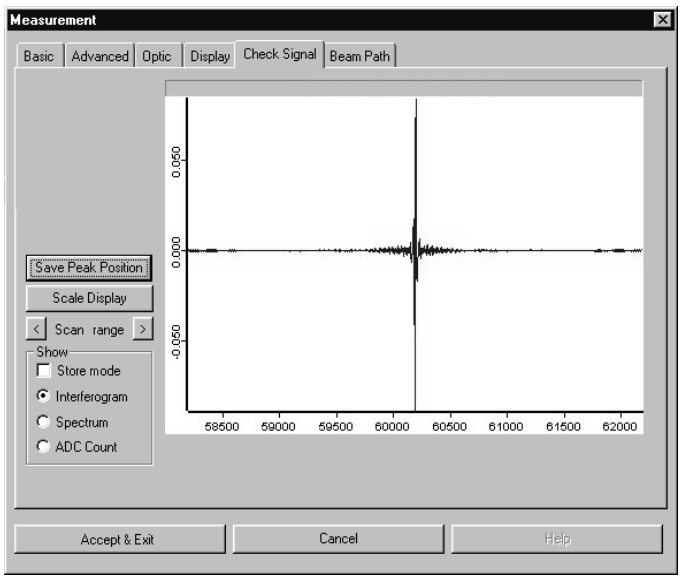


Figure 12: Measurement - Interferogram calibration

3. Once the interferogram peak has been found, click the *Save Peak Position* button. The exact peak position is required to perform Fourier Transformation.

2.1.4 Storing experiment file

1. On the *Measurement dialog*, click the *Advanced* tab.

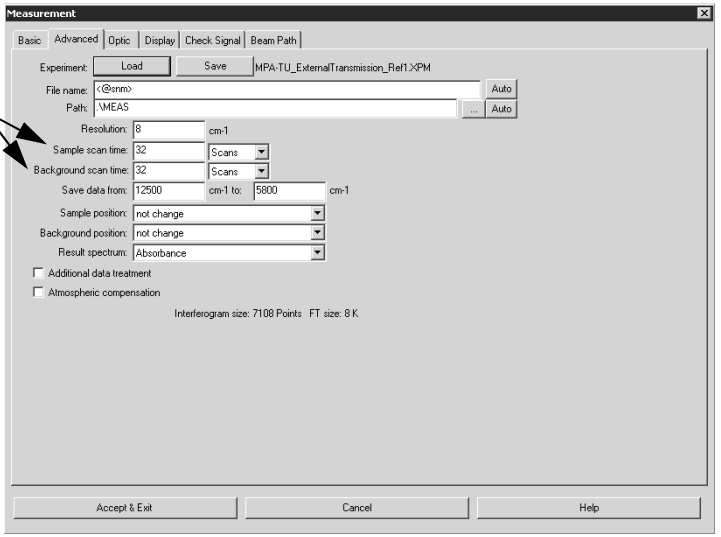


Figure 13: Measurement - Advanced tab

2. Define the number of scans in the *Sample/Background Scan Time* entry fields.
3. Enter the data path to automatically store the measurement. If you want to change this path, select the new path by the ... button.
4. Determine the data type for the result spectrum. It is recommended to select *Absorbance* as a common result spectrum type.

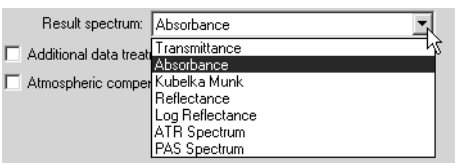


Figure 14: Measurement - Select result spectrum type

If you later want to work with a different kind of data type for the result spectrum, you can change the type of result spectrum at any time.

5. Click the *Save and Exit* button. Define an appropriate file name. It is recommended to repeatedly use the experiment files. They are essential when working with macros.

2.1.5 Background Measurement

Except for emission, Raman, and single-channel measurements, it is always necessary to acquire a background spectrum before measuring the sample. This spectrum reflects the effects that the spectrometer itself has on measured spectra.

For example, the performance of the light source varies at some frequencies, or the optics absorbs light stronger at a certain wavelength.

1. On the *Optic* tab, set the aperture to the same value used to acquire a sample spectrum.
2. To start the background measurement select the *Basic* tab and click the *Background Single Channel* button.

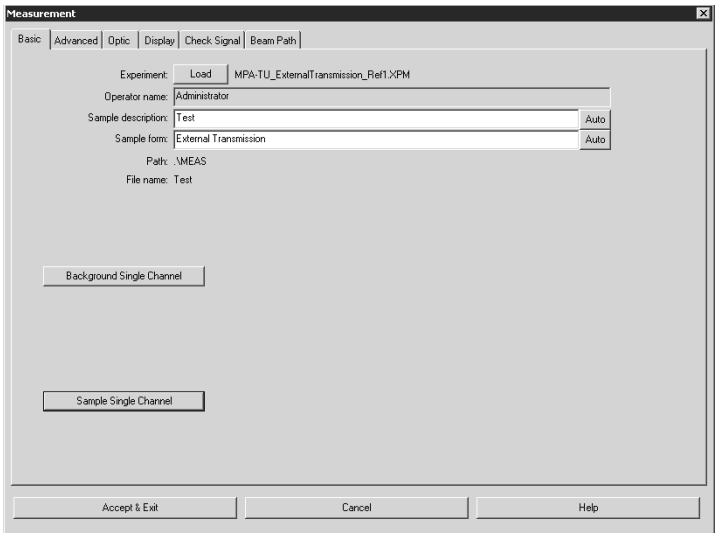
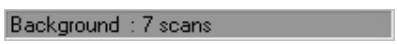


Figure 15: Measurement - Basic tab

The status bar below the OPUS spectrum window indicates the measurement progress, the number of scans performed by the optical bench and the OPUS application which is currently running:



Right click on the status bar to interrupt measurement. If the data acquisition has been finished, the status bar indicates that *No Active Task* is performed.

2.1.6 Sample Measurement

1. Having measured the background spectrum, place the sample into the optical path of the spectrometer. This procedure depends on your specific hardware setup.
2. On the *Basic* tab, enter the sample name and define the sample form. This information is stored together with the spectrum.
3. Click the *Sample Single Channel* button to start measurement.

The *Measurement* dialog closes and the spectrum window opens.You can monitor the progress of the measurement on the status bar at the bottom of the OPUS window.

If the measurement has been finished, the measured spectrum is displayed in the spectrum window.

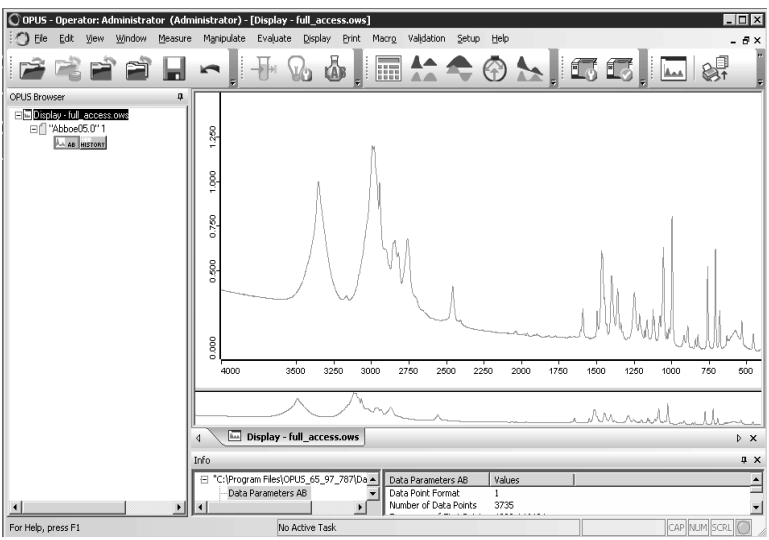


Figure 16: Spectrum Window - Showing the spectrum measured

Strictly speaking, the spectrometer measures an interferogram rather than a spectrum. Using Fourier Transformation this interferogram is transferred into a single-channel spectrum. On the basis of this single-channel spectrum and the background spectrum measured, a result transmission spectrum is calculated.

This is done automatically and apart from short descriptions in the status bar you cannot see any of these steps.

To get an idea of the different types of spectra, figure 17 shows the single-channel spectrum, background spectrum and the calculated transmission spectrum. Each data block is displayed in the browser. For further details on the data blocks, refer to the OPUS Reference Manual.

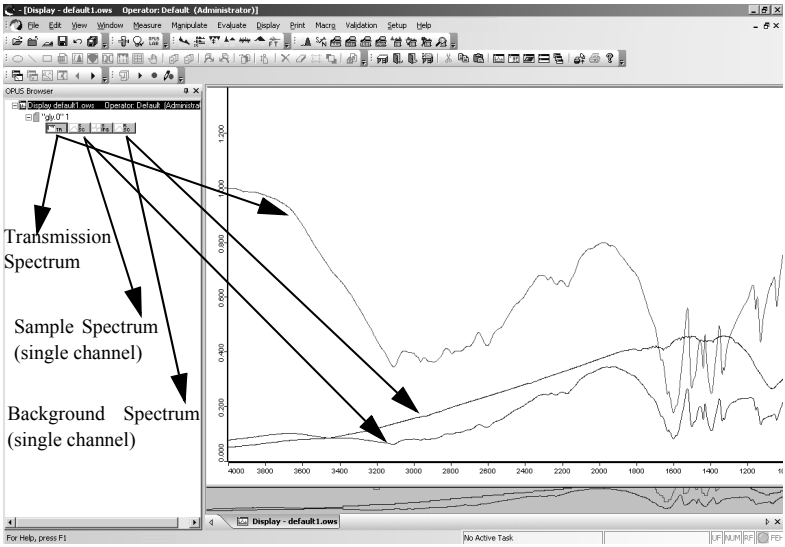


Figure 17: Spectrum Window - Showing different types of spectra

2.2 Baseline Correction

If the baseline of your spectrum is sloped, curved or significantly below 100% transmission, the sample preparation might have been insufficient. Instead of measuring the sample again, perform a baseline correction. In many cases, this will solve the problem.

The baseline correction is useful to manipulate spectra which could not have been measured very well due to the sample material.

However, you should always try to prepare the samples properly to get good spectra, instead of correcting them later.

Figure 18 shows an example of a baseline correction: the second spectrum is the original, whereas the first one is baseline corrected.

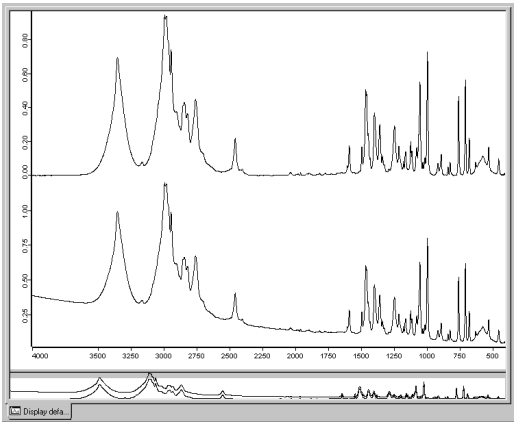


Figure 18: Spectrum Window - Baseline correction results

How to perform baseline correction?

1. On the *Manipulate* menu, click the *Baseline Correction* command, or use the  icon from the toolbar. The following dialog box opens:

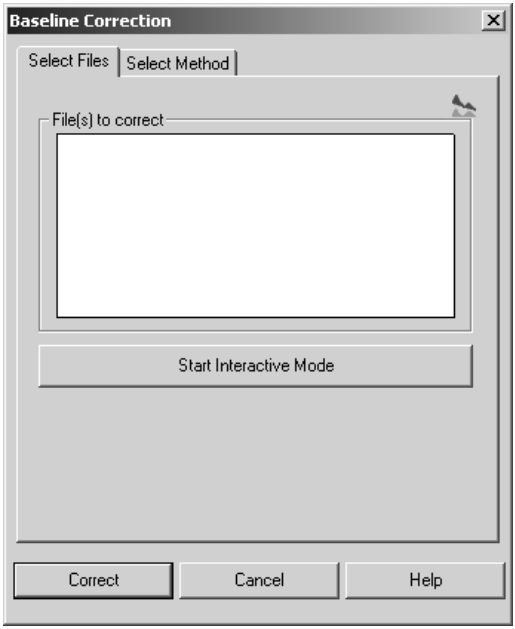


Figure 19: Baseline Correction - Select Files tab

2. On the browser, select the spectrum block (AB or TR) and drag it to the *File(s) to correct* selection field while pressing the left mouse button. Alternatively, double click on the spectrum block. If you release the left mouse button, the file selected will be displayed in the selection field:

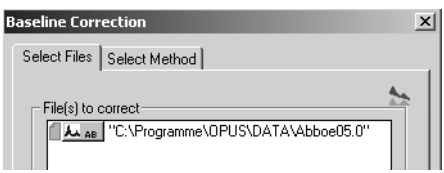


Figure 20: Baseline Correction - File selected

3. To define a particular baseline correction method, click on the *Select Method* tab.

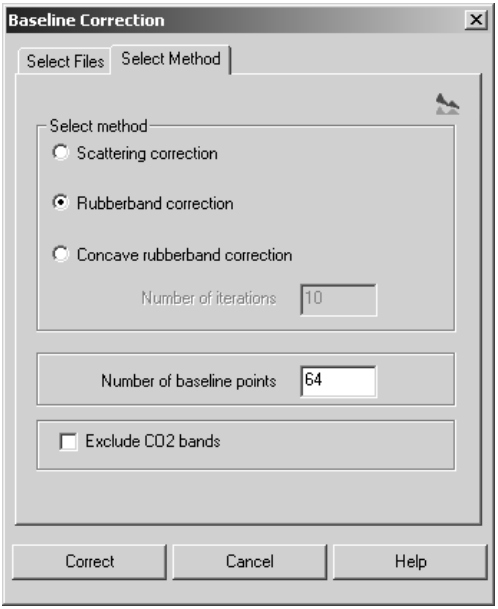


Figure 21: Baseline Correction - Select Method tab

4. Select a method type. For detailed information on the different method types refer to the OPUS Reference Manual.
5. Set the number of baseline points manually. Click the corresponding entry field and change the number. A value of 64 is generally recommended.
6. To exclude the CO_2 range during baseline correction, activate the *Exclude CO_2 Bands* check box.
7. Click the *Correct* button to immediately start baseline correction.

Now, the OPUS browser window shows a red document symbol which indicates that the file has been manipulated. The red symbol is on top of the blue one (raw data).

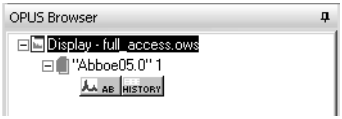


Figure 22: Spectrum file displayed in browser after baseline correction

After baseline correction is complete...

... the spectrum has not yet been saved to disk and exists only as a temporary file. Store the file on the disk as a separate file to prevent the original file from being overwritten.

To undo baseline correction...

1. On the OPUS browser, right click the red document symbol. A menu pops up.

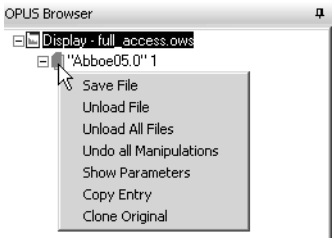


Figure 23: Pop-up menu used to undo function

2. Select the *Undo all Manipulations* command. The following dialog opens:

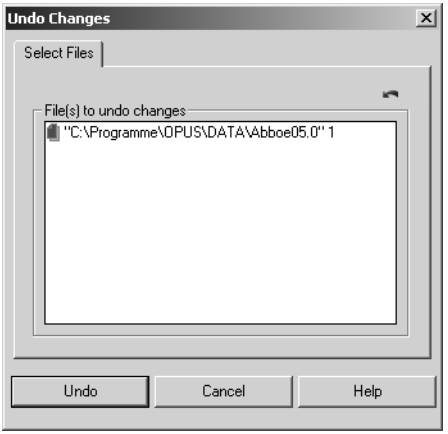


Figure 24: Undo changes - Select Files tab

3. Click the *Undo* button. The red document symbol disappears in the OPUS browser and the original data are available again.

2.3 Data File History

Any spectrum manipulations and measurement parameter changes are recorded in a non-editable, non-deletable history data block (HISTORY).

Figure 25 shows a file of a spectrum with several types of manipulations performed:

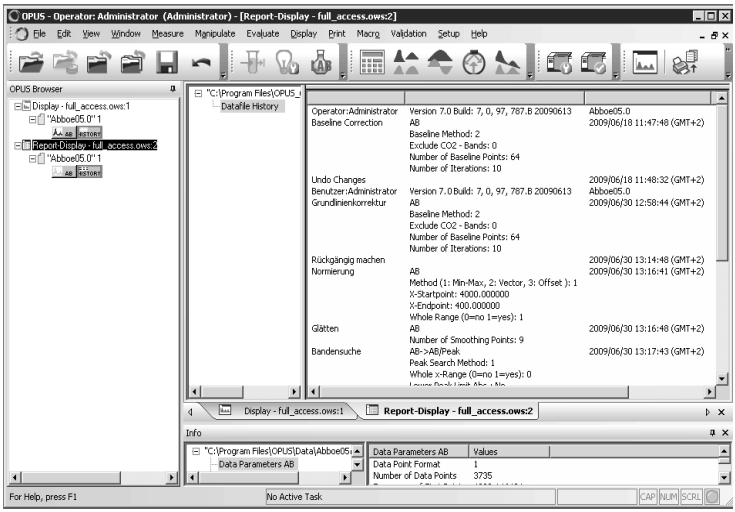


Figure 25: Report window showing the data file history

The first line of the data file history contains the user ID, OPUS version and the spectrum name. All manipulations and their parameters are listed in the order of performance.

Data information is always stored in the data block in one single spectrum file, together with the processed spectrum. This ensures that all data manipulations are recorded, e.g. manipulation method, time and operator.

2.4 Save File

The original spectrum is automatically saved in the path defined in section 2.1.4.

1. Right click on the red document symbol in the OPUS browser.
2. On the pop-up menu, select the *Save File* command. Alternatively, click the *Save* icon or select *Save File* from the *File* menu.

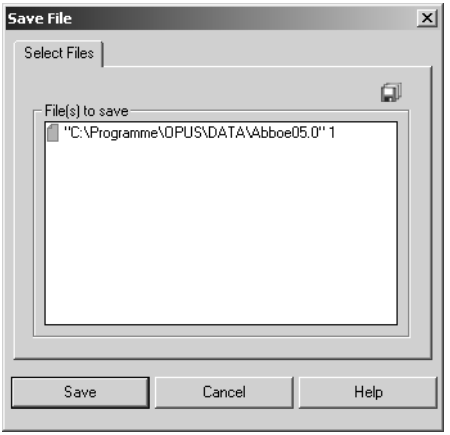


Figure 26: Save File - Select Files tab

3. The spectrum file has to be listed in the *File(s) to save* selection field.
4. Click the *Save* button. The original file is overwritten and cannot be restored anymore.

2.5 Save File As

Use this command if you want to save the spectrum files by a different file name, or in a different directory.

1. Click the *Save File As* icon , or select the *File* menu and click the *Save File As* command. The *Save File As* dialog opens.

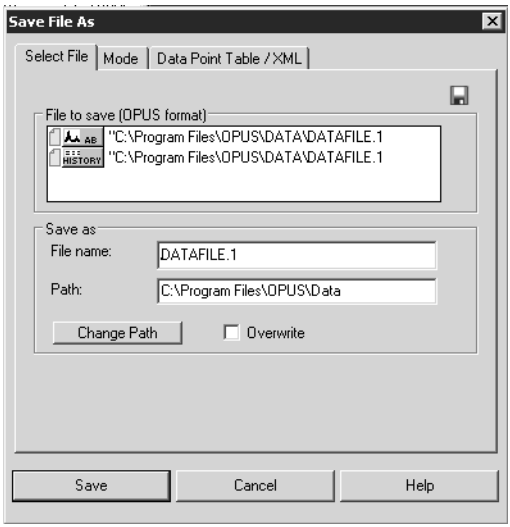


Figure 27: Save Spectrum - Select File tab

2. Enter the new file name into the *File* name entry field. OPUS always suggests a file name.
3. Enter the new path directly into the *Path* entry field. Alternatively, you can browse the directories by clicking on the *Change Path* button.
4. Activate the *Overwrite* check box, if you want to overwrite a previous file. Otherwise, an increment will be added to the file name. The *Overwrite* option is not available in validation mode.
5. Click the *Save* button.

The spectrum file is normally saved in OPUS format. However, the *Mode* and *Data Point Table* tabs allow to save the file in JCAMP-DX or XML format, as a plain X-Y data table, in Pirouette (DAT) or in GALACTIC format (SPC).

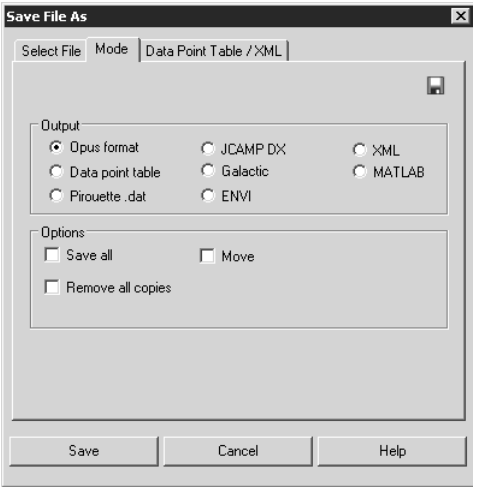


Figure 28: Save Spectrum - Mode tab

2.6 Load File

1. On the *File* menu, click the *Load File* command. Alternatively, click the icon from the toolbar. The *Load Spectrum* dialog opens.
2. Select a spectrum file.
3. Click the *Open* button.

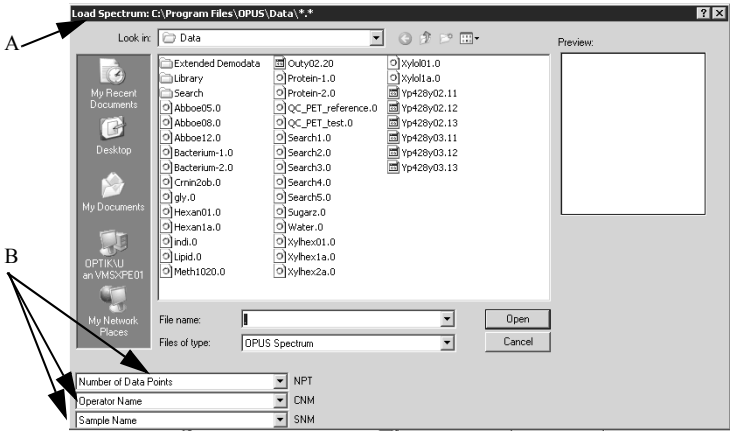


Figure 29: Load Spectrum - No file selected

A) The title bar shows the directory in which the spectrum files are located.
B) Three parameters of a spectrum file are shown by default. You can select the specific parameters from the drop-down lists. As no file has been selected yet in figure 29, only the parameter abbreviations are shown.

If you select a spectrum file, the *Load Spectrum* dialog will change as follows:

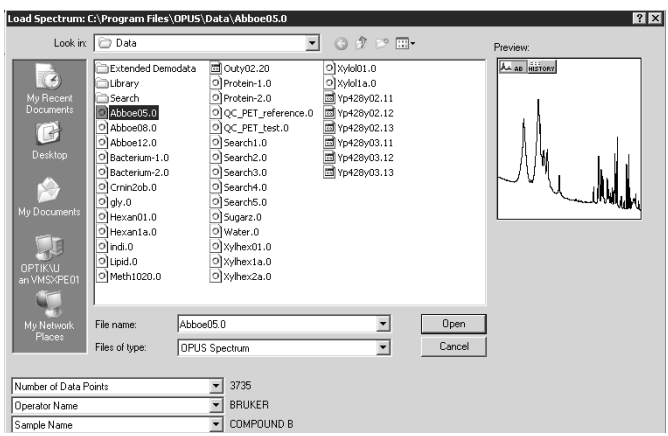


Figure 30: Load Spectrum - Active preview

A preview of the spectrum without the axes is displayed. The absorption data block () on the top left corner is displayed as a small icon. The spectrum parameters are now defined.

As normally not all parameters have been specified for each spectrum file, some of the parameters may be missing.

To load the spectrum into the OPUS spectrum window click the *Open* button.

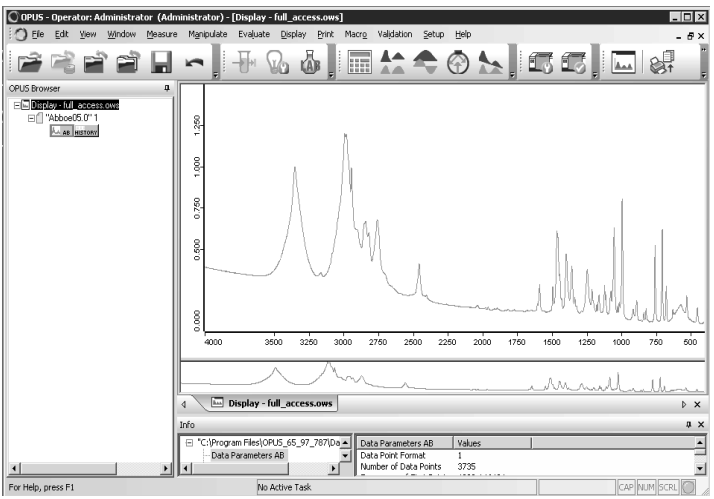


Figure 31: OPUS spectrum and browser window

As the spectrum cannot be displayed in full size within the spectrum window, you can scale the spectrum using the *Scale* icon ().

2.7 Print Spectra

OPUS provides two possibilities to quickly and easily print recorded spectra.

1. *Quick Print* icon () from the toolbar:
   OPUS selects an appropriate plot layout depending on the window type currently used. For example, if you work in the spectrum window, the spectrum will be printed within a frame. If you search a spectrum library, the results as well as a hit list, spectral information and the structure of the product will be printed. For details on default layout plots available, refer to the OPUS Reference Manual.
2. *Print Spectra* command on the *Print* menu:
   using this command allows to define further basic printout options, e.g. frames and frequency range.

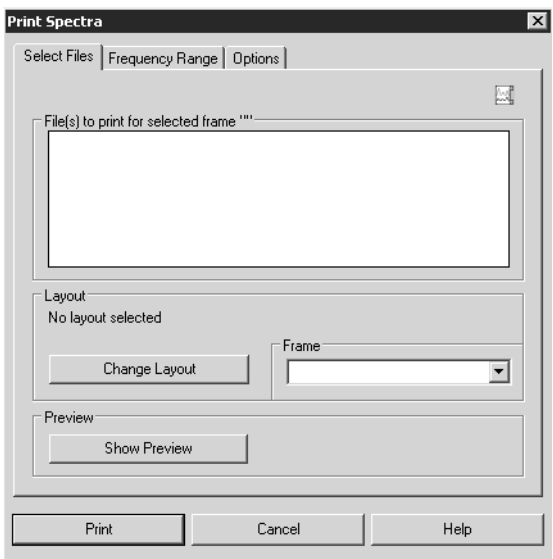


Figure 32: Print Spectra - Select Files tab

For details on printing data refer to chapter 3.

3 Analysis Report

OPUS allows to depict sample parameters and evaluation results for one or several spectrum files in an analysis report. The spectra files need to contain the data block of the respective evaluation. Evaluation data blocks are e.g. PEAK, INTEG, QUANT, IDENT, SEARCH, CT.

Figure 33: Example of a spectrum file with data blocks of different types of evaluation

3.1 Report Layout

To generate the report there are three different types of layout options available:

- **Single sample report:** one report for each spectrum file
- **Multi sample report:** one report for all spectrum files
- **Paper strip report:** one report for each spectrum file, with fewer report data than with the single sample report

To generate a single sample or paper strip report you can use several spectra files at once. In this case, a separate report is generated for each spectrum file separately.

A multi sample report lists all spectrum files with the respective data in one report.

3.2 Report Structure

The structure of an analysis report is similar with all three report types. The report can contain:

- general report data
- sample-specific data
- spectrum frame of each sample

3.2.1 Spectrum Frame

The spectrum frame is displayed below the general report data and product-specific data. This kind of report data is optional and displayed either always, never or only if the evaluation result is not ok.

3.3 Standard Template

When generating an analysis report for the very first time OPUS uses the *Default.art* standard template. The data provided in this template considers the typical setting options available for the three different report layouts, with regard to e.g. sample parameters and evaluation results.

The standard template is stored in the <*Program Files\OPUS*> directory and can be edited. Detailed information on how to edit the standard template are provided in the OPUS Reference Manual.

3.4 Report Output

There are different possibilities for the report output:

- printer
- file (either as PDF or csv file)
- clipboard (to integrate the report into other types of documents)

3.5 Generating Report

1. Load the spectrum file(s).
2. On the *Print* menu, select the *Generate Analysis Report* command.
3. Drag & drop the spectrum file(s) into the *File(s) for report generation* selection field.

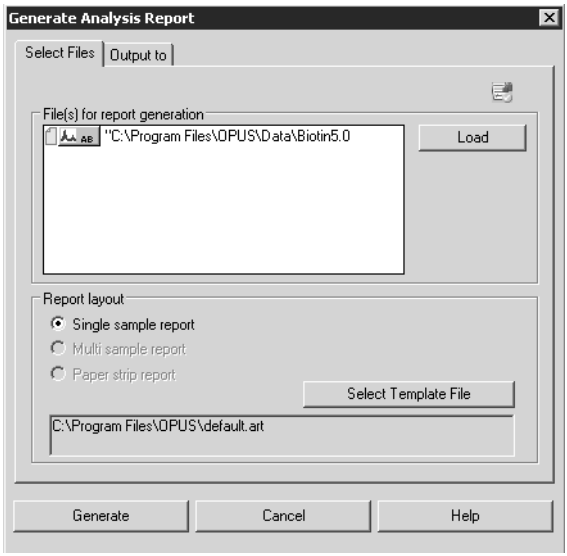


Figure 34: Generate Analysis Report - Select Files

4. Select the report layout. The report template file previously used is always defined.
5. Click the *Output to* tab to define how the report is to be printed.

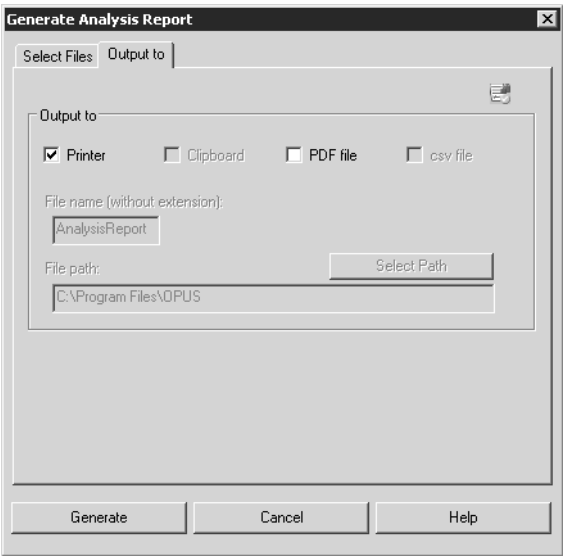
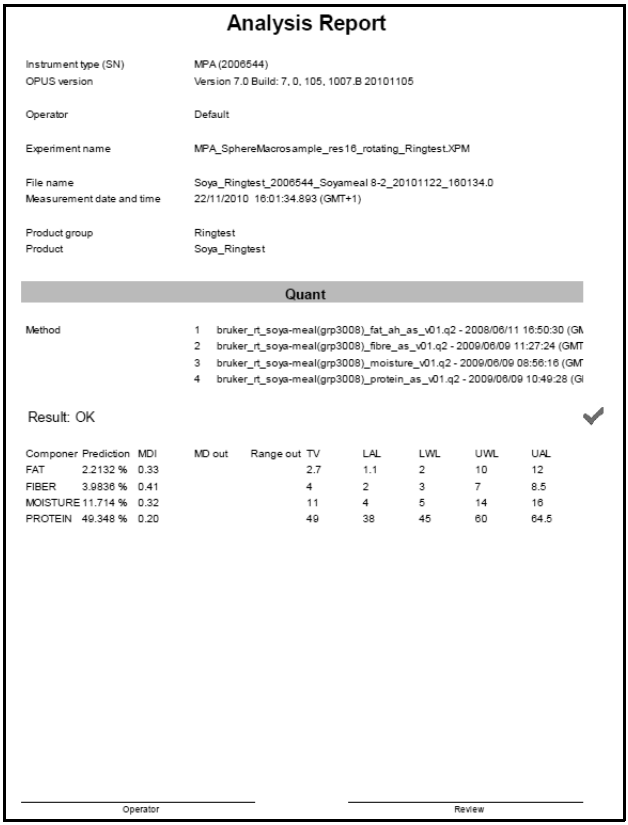


Figure 35: Generate Analysis Report - Output to

If you activate the *PDF* or *csv file* option button, the *File name* and *path* entry fields are enabled. To save the report define the file name and path or edit the path, using the *Select Path* button.

6. Click the *Generate* button.

3.6 Example of analysis report



Analysis Report

Instrument type (SN)	MPA (2006544)
OPUS version	Version 7.0 Build: 7, 0, 105, 1007.B 20101105
Operator	Default
Experiment name	MPA_SphereMacros:sample_res16_rotating_Ringtest.XPM
File name	Soya_Ringtest_2006544_Soyameal 8-2_20101122_160134.0
Measurement date and time	22/11/2010 16:01:34.893 (GMT+1)
Product group	Ringtest
Product	Soya_Ringtest

Quant

Method

1 bruker_rt_soya-meal(grp3008)_fat_ah_as_v01.q2 - 2008/06/11 16:50:30 (GM
2 bruker_rt_soya-meal(grp3008)_fibre_as_v01.q2 - 2009/06/09 11:27:24 (GMT
3 bruker_rt_soya-meal(grp3008)_moisture_v01.q2 - 2009/06/09 08:56:16 (GM
4 bruker_rt_soya-meal(grp3008)_protein_as_v01.q2 - 2009/06/09 10:49:28 (G

Result: OK

Componer	Prediction	MDI	MD out	Range out	TV	LAL	LWL	UWL	UAL
FAT	2.2132 %	0.33			2.7	1.1	2	10	12
FIBER	3.9836 %	0.41			4	2	3	7	8.5
MOISTURE	11.714 %	0.32			11	4	5	14	16
PROTEIN	49.348 %	0.20			49	38	45	60	64.5

Operator

Review

Figure 36: Example of a single analysis report with 4 components