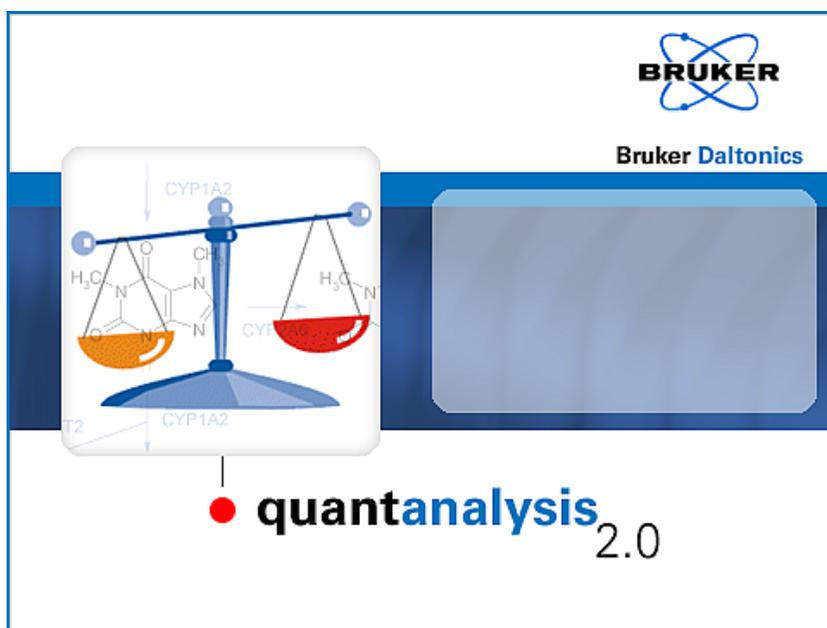

quantanalysis 2.0

Reference Manual



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Document History

QuantAnalysis Reference Manual, Version 2.0 (March 2008)

Part #: 253272

First edition: September 2002

Printed in Germany

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1 PREFACE

The *Bruker Compass QuantAnalysis 2.0* application (referred to as 'QuantAnalysis') is the state-of-art Windows XP application for quantitation of analyses acquired on Bruker Daltonics mass spectrometer instruments. QuantAnalysis is specifically designed to process analyses acquired on the *esquire/HCT* ion trap, the *micrOTOF* ESI time-of-flight and the *APEX FTMS* mass spectrometers.

QuantAnalysis is an advanced program dedicated for quantitation of MS and MSn analyses. Dynamically linked views of the spreadsheet data, the chromatogram and spectrum, and the calibration curve make quantitation faster and easier. A change in any of the views, e.g., selecting a different curve fit for calibration, is immediately reflected in all other views. QuantAnalysis processes batches acquired with *Bruker Compass HyStar* or *Agilent ChemStation*. Printed reports in various layouts are available and custom layouts can be created using the *Bruker Compass ReportDesigner*.

The QuantAnalysis Reference Manual describes the menus and commands available in QuantAnalysis 2.0. For reference on how to work with QuantAnalysis 2.0, please refer to the QuantAnalysis User Manual that is available as PDF document with your installation.

2 FILE MENU

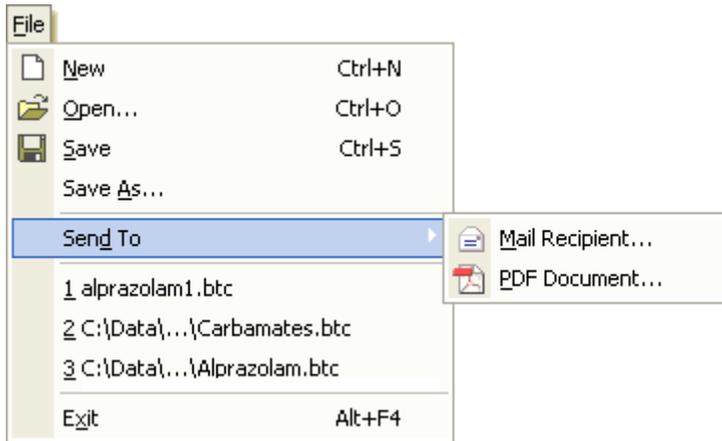


Figure 2-1 File menu

The **File** menu offers the following commands:

New	Creates a new batch file.
Open	Opens the selected batch file.
Save	Saves the open batch file under the same file name.
Save As	Saves the open batch file under a new or an existing file name.
Send To	Pops up the following commands:
Mail Recipient	Prints a selected report to a PDF file and sends this to a specified email address.
PDF Document	Prints a selected report to a PDF file.
Recent File	Opens the batch file corresponding to the file name selected.
Exit	Closes QuantAnalysis.

2.1 New Command

The **New** command is used to create a new batch file. Using this command is only required when another batch file is already open.

The command closes the currently open batch file and clears the Work Table. If the open batch file was changed but the new processing state has not been saved yet, a confirmation request to save the changed state appears first.

Shortcuts

Button:



Keys:

CTRL+N

2.2 Open Command

The **Open** command is used to open an existing batch file. QuantAnalysis writes a new, additional result file on each saving operation you perform on a batch file. Thus, for each batch file one or several result files are available. If more than one result is available for the batch file you want to open you can select either any of its previously saved results or the last saved result to be loaded. Only one batch file can be open at a time.

The command opens the **Open Batch** dialog, which allows you to specify the batch file you wish to open. The chosen batch file's Result History is displayed, and if it contains more than one result, you can select which result you want to load.

Look in and folder list

Navigate to the drive and folder that contains the batch file you wish to open. Double-click the batch file or select it and click **Open**.

File name

Enter the file name of the batch file or select a batch file from the folder list.

Files of Type

Select the type of files to be displayed in the folder list:

Batch Files (*.btc). Lists *.btc files.

(Result history)

Lists all saved results of the batch file selected in the folder list with corresponding information about the date and time it was saved (**Date**), who saved it (**Saved by**) and if it was signed (**Signed**).

From this list, you can load a previous saved result of the batch file by selecting the desired result. If no result is selected when clicking **Open**, the last saved result of the selected batch will be loaded.

You can delete a result of a batch file and remove it from the Result history using the **History** button found in the Work Table window.

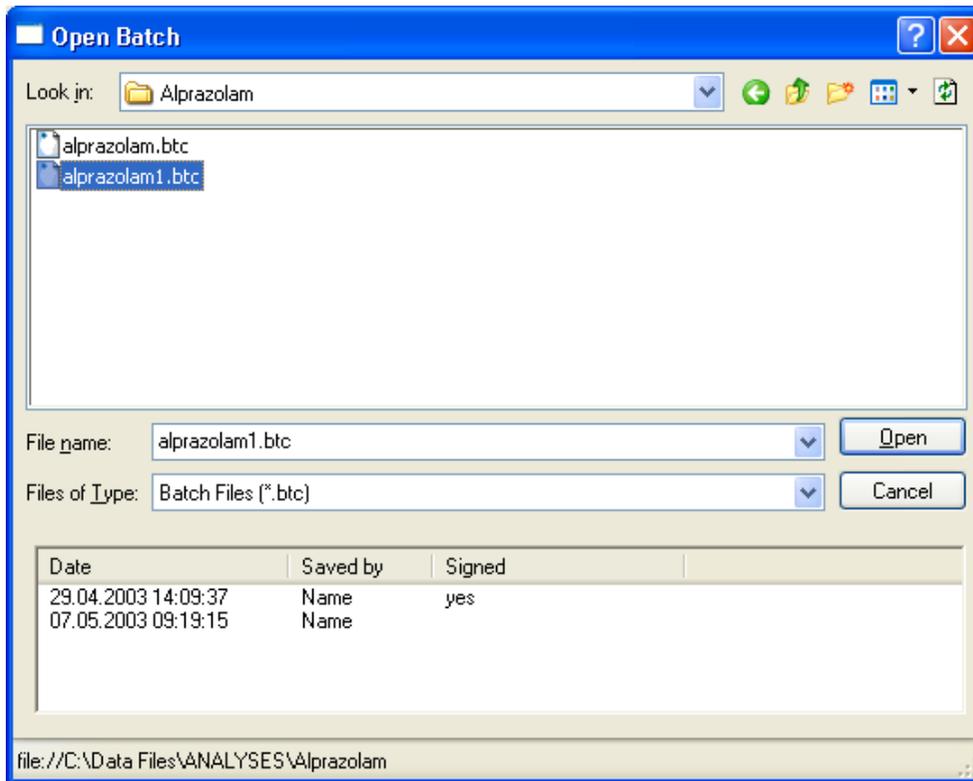


Figure 2-2 Open Batch dialog

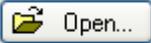
Open

If a folder is selected, opens the folder, and displays its contents in the folder list.

If a batch file is selected, opens the respective batch file in QuantAnalysis, and displays its contents in the Work Table, Chromatogram/Spectrum and Calibration windows. If for the selected batch file more than one result is available, the actually loaded data depends on the current selection in the batch file's Result history. If a previous result is selected, this result is loaded; if no result is selected the last saved result is loaded.

If another batch file is currently open and changes to it have not been saved yet, first a confirmation request to save the changed state is displayed.

Shortcuts

Buttons:  

Keys: CTRL+O

2.3 Save Command

The **Save** command is used to save the open batch file under the same file name. This includes the current state of the batch file and the parameter settings of the quantitation method used. Each saving operation results in a new, additional result file being created for the respective batch file. Existing result files are not overwritten.

The command saves the current state and the quantitation method parameter settings of the open batch file in a new result file. If the respective batch file has not been saved yet, the **Save As** dialog appears automatically to allow you to select a file name for this new batch file.

Shortcuts

Buttons:



Keys:

CTRL+S

2.4 Save As Command

The **Save As** command is used to save a batch file using a new or existing file name. When you save a batch file under a new name, a subfolder with the specified batch name is set up in the chosen target folder into which all results and later files corresponding to the respective batch file will be saved.

Note: The batch file must be saved to that folder that contains the data files to be quantified.

The command opens the **Save Batch** dialog, which allows you to specify the file name for the new batch file and the target folder.

Look in and the folder list

Navigate to the drive and folder that contains the data files to be quantified.

File name

Enter a new batch file name or select an existing name from the folder list to overwrite an existing batch file.

Files of Type

Select the type of files to be displayed in the folder list:

Batch Files (*.btc). Lists *.btc files.

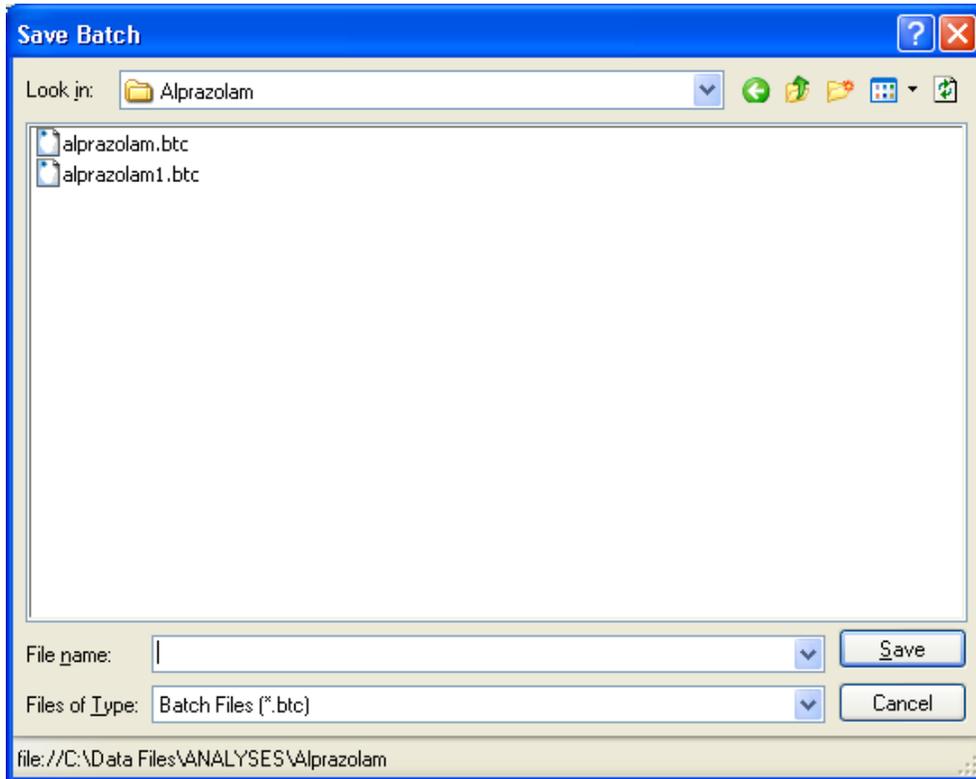


Figure 2-3 Save Batch dialog

Save

If a new file name is entered, a subfolder with the specified batch file is created in the chosen target folder, and the corresponding result file is saved to that subfolder.

If an already existing file name is selected, a confirmation request appears, informing you that a batch file of this name already exists. It asks you if you really wish to overwrite it. Clicking **Yes** results in the new file overwriting the existing result file; clicking **No** allows you to enter a new file name.

2.5 Send To Popup Command

Pointing to this submenu pops up the following commands for sending reports: **Mail Recipient** and **PDF Document**.

2.6 Send To > Mail Recipient

The **Mail Recipient** command is used to print a selected to a PDF file and send this automatically as an attachment of an email to a specified email address. The report is saved with the name of the selected layout.

The command opens the **Send To Mail Recipient** dialog, which allows you select the report to be created and the recipient to whom you want to send this report as email. If on selecting this command the current processing state of a selected analysis has not been saved yet, first a corresponding message appears that asks you about saving the respective analysis. Affirm this request, to save the analysis and open the **Send To Mail Recipient** dialog.

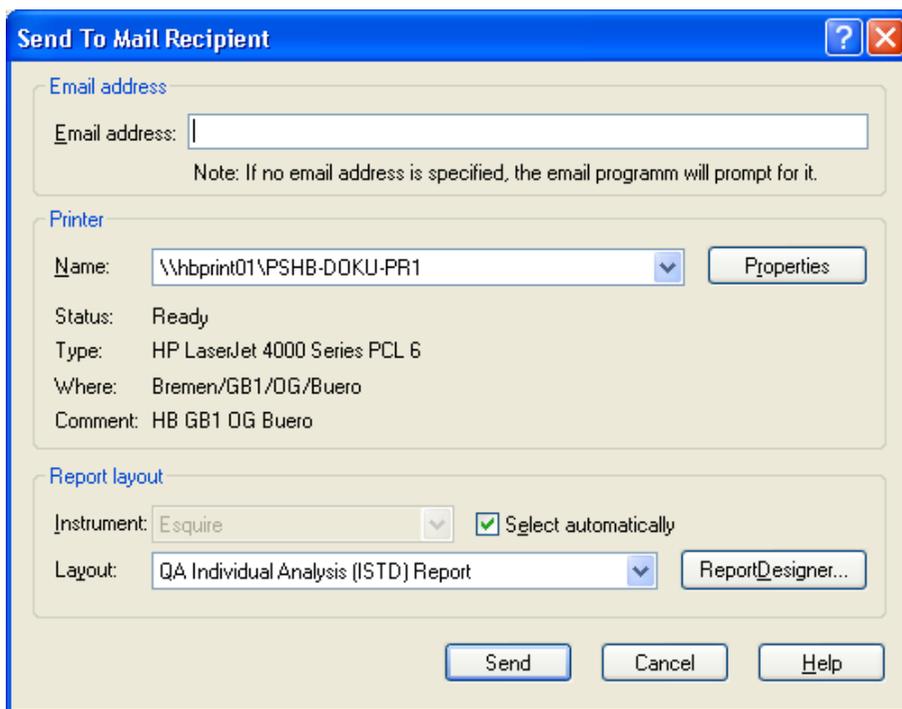


Figure 2-4 Send To Mail Recipient dialog

Email address

Enter the email address of the recipient to whom you want to send the report.

In **Printer** select the printer and print properties to be used:

Name

Displays the currently connected printer. If you wish to use another printer, select it from this list.

Properties

Allows you to define page set up and further options for the selected printer. Opens the **Properties of 'printer'** dialog, which is printer specific. Select e.g. the printer orientation to print the report in **Portrait** or **Landscape** format.

Status

Displays the status of the selected printer.

Type

Displays the type of the selected printer.

Where

Localizes the selected printer.

Comment

Displays a comment, if available.

In **Report Layout**, select the report layout you wish to print. Appropriate report layouts depending on the instrument used are listed automatically.

Instrument

Displays the instrument for which appropriate report layouts are listed in **Layout**. The instrument used for acquiring the selected analysis is selected by default. If you want to select a layout appropriate for another instrument category, uncheck **Select automatically** to enable this list box and select the desired category. This subsequently lists the corresponding layouts in **Layout**.

The following categories are available:

<all>. Lists all layouts available.

<independent>. Lists instrument-independent layouts.

Esquire. Lists Esquire layouts.

Select automatically

Check this option to list automatically report layouts appropriate for the instrument used for acquiring the selected analysis. This selects the respective instrument in **Instrument** and lists corresponding layouts in **Layout**. Uncheck this option if you want to select a layout set up for another instrument. Default is checked.

Layout

Lists the report layouts appropriate for the category selected in **Instrument**. Select from this list the type of report you want to print.

ReportDesigner

Starts the *Bruker Compass ReportDesigner* application and loads the report layout selected in **Layout**. The ReportDesigner allows you to create your own report layouts.

Note: If you want to create a new report layout, it is recommended not to modify the original layout but to save the modified layout under a new file name. Other-

wise, there is a risk that your changed layout version becomes overwritten by a later system upgrade.

Note: All QuantAnalysis report layouts must be saved to:
"C:\BDALSystemData\Report Layouts\QuantAnalysis".
Otherwise, QuantAnalysis will not list them in **Layout**.

Send

Opens the **Choose Profile** dialog (see below) to select the profile you want to use with Microsoft Exchange.

Choose Profile dialog

The **Choose Profile** dialog is used to select the profile to be used with Microsoft Exchange. In addition, this dialog allows you to set up a new profile and specify advanced options for logging on.



Figure 2-5 Expanded Choose Profile dialog (after clicking Options)

Profile Name

Select the profile you want to use.

New

Allows you to create a new profile. Opens the **Windows Messaging Setup Wizard**. To create a new profile, follow the instructions of the wizard.

Options

Expands the dialog and displays the following advanced options for logging on.

Set as default profile

Sets the selected profile as the default. You can set some messaging applications, such as Microsoft Exchange, to log on automatically using your default profile.

Show Logon screens for all information services

Displays the logon dialogs for each information service in the selected profile.

OK

Creates the selected report, saves it as PDF document, and sends it as email to the specified recipient. If no email address is specified, the email program will prompt for it.

2.7 Send To > PDF Document

The **PDF Document** command is used to print a selected report to a PDF file and save it to a chosen target folder.

The command opens the **Send To PDF Document** dialog, which allows you to select the report to be created and to specify path and name for the PDF document to be saved. If on selecting this command the current processing state of a selected analysis has not been saved yet, first a corresponding message appears that asks you about saving the respective analysis. Affirm this request, to save the analysis and open the **Send To PDF Document** dialog.

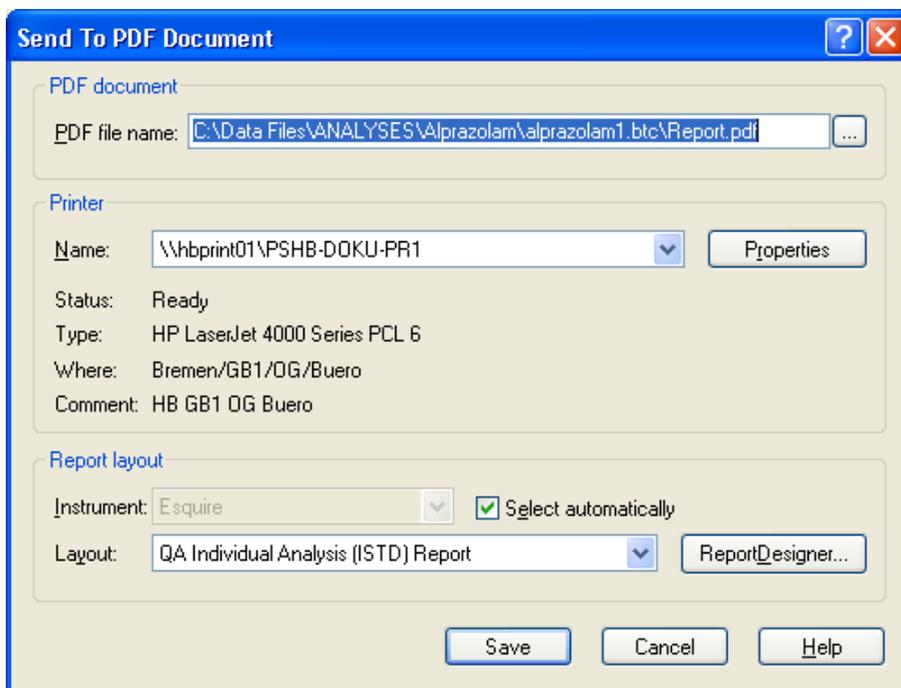


Figure 2-6 Send To PDF Document dialog

PDF file name

Enter path and name for the PDF document to be saved. The folder of the active analysis and the name 'Report.pdf' are suggested by default. If you want to save the PDF

document with another name, change the name as desired. If you want to save the document to another folder, either enter the respective path or click  and select the desired folder in the appearing dialog.

Save

Creates the selected report and saves it as PDF document with the specified name in the chosen target folder.

For the other parameters, please refer to section 2.6.

2.8 Recent File List

You can use the numbers and batch file names listed in the recent file list at the bottom of the **File** menu to open quickly one of as many as ten previous closed files. Select the number that corresponds to the batch file you want to open. This loads the last saved result available for the batch file. When pointing on a recent file, corresponding full path name is displayed in a tool tip.

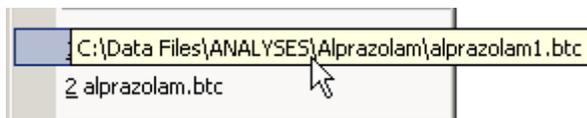


Figure 2-7 Tool tip displaying full path name of selected recent file

2.9 Exit Command

The **Exit** command closed your current QuantAnalysis session. It automatically stores the current user interface settings for the current user logged into Windows. If changes made to the currently open batch file have not been saved yet when closing QuantAnalysis, a request appears asking you about saving the current state. After answering this request, QuantAnalysis is closed.

Shortcuts

Keys: ALT+F4

Mouse: Click the application's **Close**  or double-click the application's Control menu button.

3 EDIT MENU



Figure 3-1 Edit menu

The **Edit** menu offers the following commands:

- Undo** (Not yet implemented.)
- Cut** Cuts the current selection and puts it on the Clipboard.
- Copy** Copies the selection and puts it on the Clipboard.
- Paste** Inserts the current Clipboard contents.

3.1 Undo Command

The **Undo** command is not yet implemented.

Shortcut

Keys: CTRL+Z

3.2 Cut Command

The **Cut** command cuts the current selection and puts it onto the Clipboard.

Shortcuts

Button: 

Keys: CTRL+X

3.3 Copy Command

The **Copy** command copies the current selection and puts it onto the Clipboard.

Shortcuts

Button:



Keys:

CTRL+C

3.4 Paste Command

The **Paste** command pastes the current Clipboard contents to the selected position.

Shortcuts

Button:



Keys:

CTRL+V

4 VIEW MENU

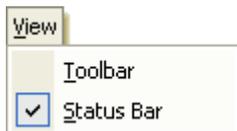


Figure 4-1 View menu

The **View** menu offers the following commands:

Toolbar Shows/Hides the toolbar.

Status Bar Shows/Hides the status bar.

4.1 Toolbar Command

The **Toolbar** command shows/hides the toolbar. The toolbar is hidden by default.

4.2 Status Bar Command

The **Status Bar** command shows/hides the status bar. The status bar is shown by default.

5 METHOD MENU



Figure 5-1 Method menu

The **Method** menu offers the following commands:

- Open** Opens the selected quantitation method.
- Save As** Saves the open quantitation method under a new or an existing file name.
- Edit** Edits the open quantitation method.

5.1 Open Command

The **Open** command is used to open a quantitation method and attach it to the loaded batch file in place of the previously attached quantitation method. This overwrites the previous QuantAnalysis part of the method with the new one. You can view and process the current parameter settings of the active method via the **Edit** command from the **Method** menu.

In Compliance mode, methods can be saved as SOP or non-SOP methods (SOP = standard operating procedure) if the UserManagement administrator has turned on SOP method handling. All operators can load methods with an SOP flag but only operators with a special right can also load non-SOP methods. If the current operator does not have this right, the **Open Method** dialog shows SOP methods only. The SOP/non-SOP status of a selected method is indicated by the **SOP method** check box. If the UserManagement administrator has defined an SOP method folder, methods can be loaded only from that default folder except the operator has the special right to use non-default method folders, too.

The command opens the **Open Method** dialog, which allows you to select the desired quantitation method.

Look in and folder list

Navigate to the drive and folder that contains the method you want to open. Double-click the method or select it and click **Open**.

If SOP method handling is turned on and you do not have the right to open non-SOP

methods, the folder list shows SOP methods only. If an SOP method folder has been defined and you do not have the right to use non-default method folders, you can load methods only from the default folder.

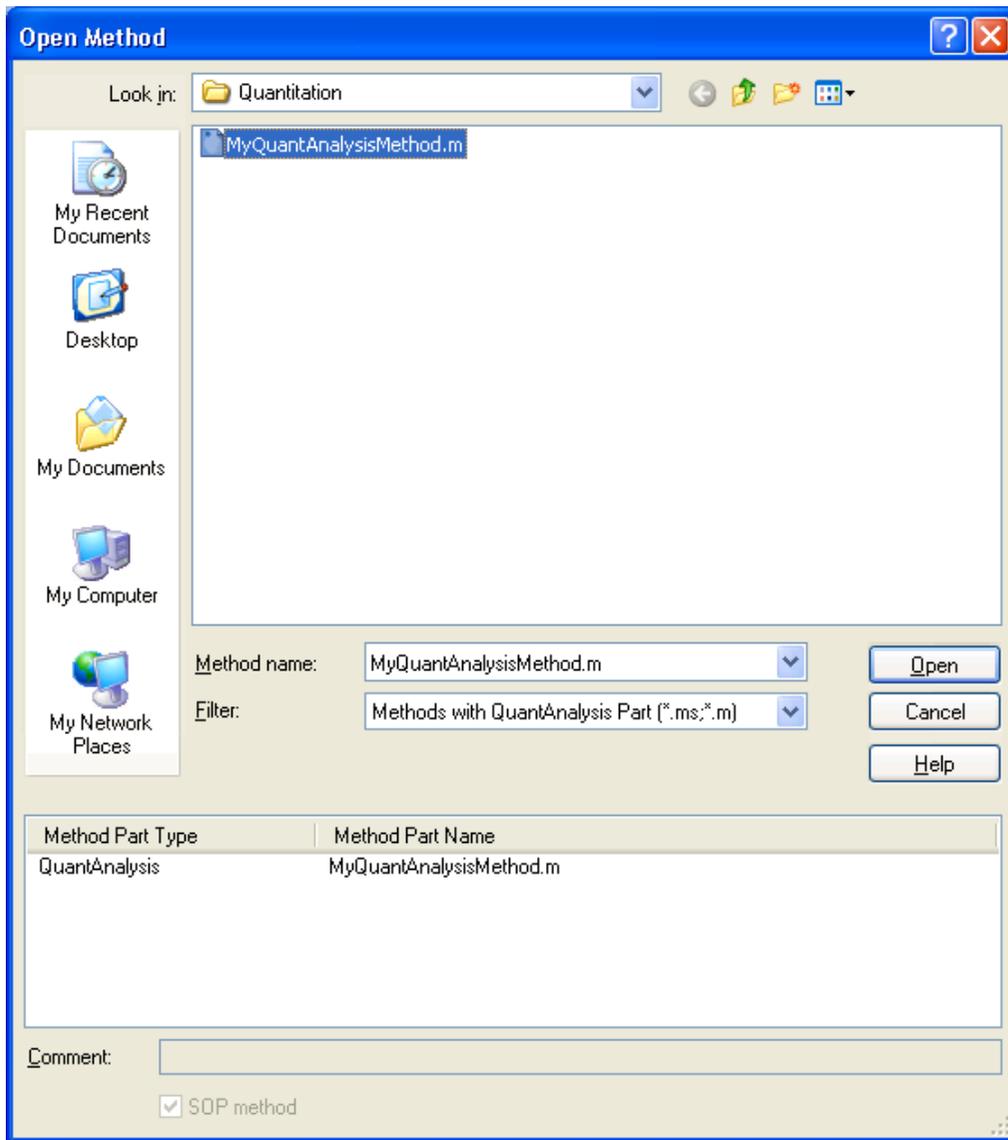


Figure 5-2 Open Method dialog (when in Compliance mode with SOP method handling being enabled)

Method name

Enter the name of the desired method or select a method from the folder list.

Filter

Select the type of methods to be displayed in the folder list:

Methods with QuantAnalysis Part (*.ms, *.m). Filters methods containing a QuantAnalysis part.

All (*.*). Lists all data files available.

(Method part list)

Lists under **Method Part Type** all application method parts currently contained in the selected method and under **Method Part Name** the corresponding part names.

Comment

Displays the comment for the selected method if available. A comment can be entered when the method is saved using the **Save As** command from the **Method** menu. A comment applies to the entire method.

SOP method

Note: This option is available when SOP method handling is activated.

Indicates the SOP/non-SOP status of the selected method.

Open

Opens the selected quantitation method and attaches it to the loaded batch file.

If SOP method handling is turned on and you have selected another folder than the default SOP method folder but do not have the corresponding right a corresponding message will appear.

Shortcut

Button:



5.2 Save As Command

The **Save As** command is used to save the quantitation method as 'QuantAnalysis part' either into an existing method with replacing the current QuantAnalysis part or into a new method. The latter creates a new method with only the QuantAnalysis part being contained whereas saving into an existing method results in modifying the selected original method. Each method can contain only one QuantAnalysis part.

In Compliance mode, methods can be saved as SOP or non-SOP methods (SOP = standard operating procedure) if the UserManagement administrator has turned on SOP method handling. Methods with an SOP flag cannot be modified. Only operators who have the special right can mark SOP methods. If the UserManagement administrator has defined an SOP method folder for saving/loading SOP methods operators need a special right to use non-default method folders, too.

The command opens the **Save QuantAnalysis Method Part As** dialog, which allows you to select the file name and target folder in which the method should be stored.

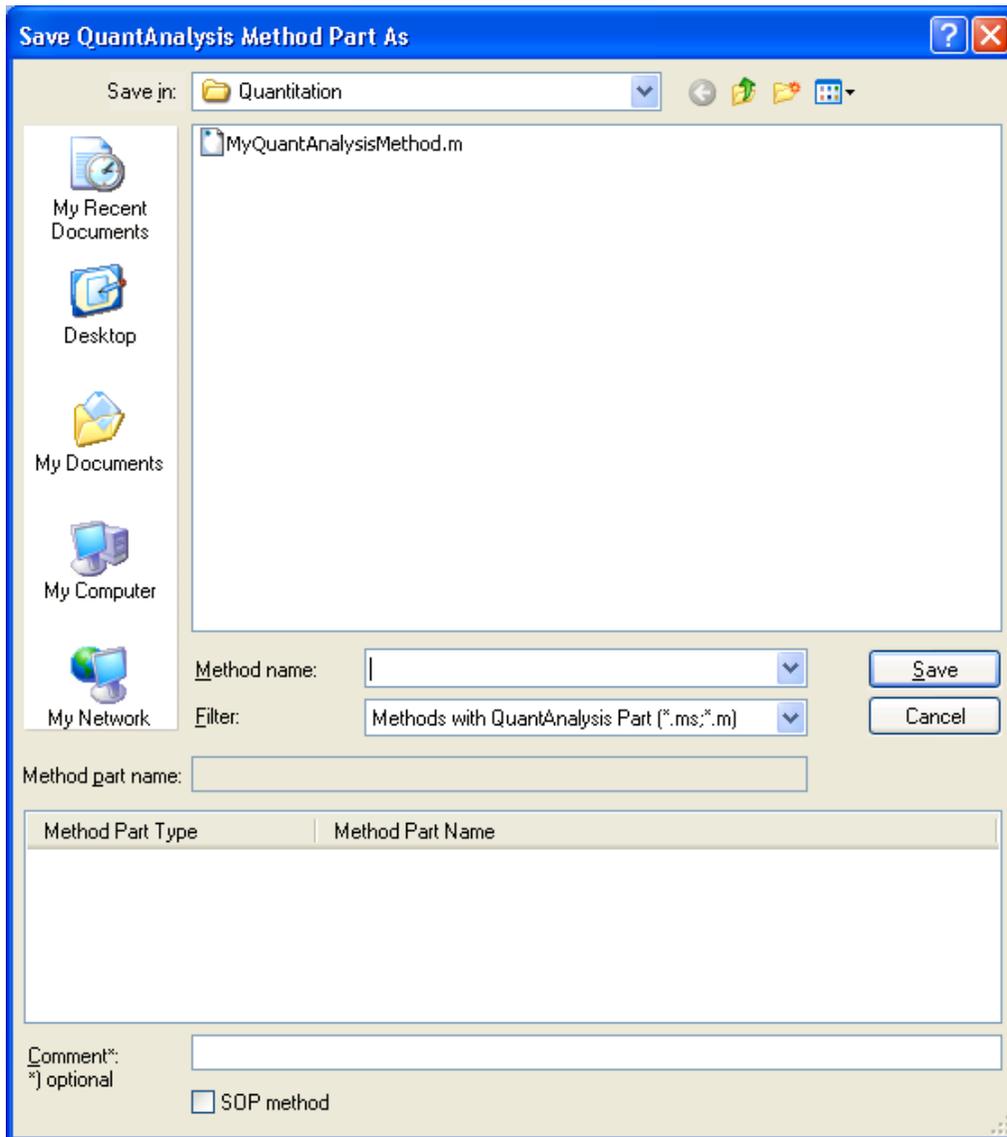


Figure 5-3 Save QuantAnalysis Method Part As dialog (when in Compliance mode with SOP method handling being enabled and the operator has the right to mark methods as SOP)

Save in and folder list

Navigate to the drive and folder in which you want to save the method. Navigate to the drive and folder in which you want to save the method. If SOP method handling is

turned on and an SOP method folder has been defined, you have to save the method in the default folder if operators without the right to use non-default method folders should use the method. To save the method to another folder you need the corresponding right.

Method name

Enter the name of the method into which the QuantAnalysis part should be saved. If you want to overwrite an existing method, enter its name or select it from the folder list. If you wish to create a new method, enter the desired new name.

Filter

Select the type of methods to be displayed in the folder list:

Methods with QuantAnalysis Part (*.ms, *.m). Lists methods containing a QuantAnalysis part.

All (*.*). Lists all data files available.

Method part name

Enter the name the QuantAnalysis part should be saved with in the specified method. A part name can be entered in a sense of a comment. If no name is entered, the QuantAnalysis part will get a part name that is the same as the method name.

(Method part list)

Lists under **Method Part Type** all application method parts currently contained in the specified method and under **Method Part Name** the corresponding part names.

Comment

Optionally enter a comment for the method. A comment applies to the entire method.

Method is SOP

Note: This option is available when SOP method handling is turned on. It is enabled when the operator has the right to mark a method as SOP.

Check this option if you want to mark the method as SOP. This sets the SOP flag, which allows loading the method by all operators. If the flag is not set only operators with the right to load non-SOP methods can load the method. Default is not checked.

Save

Depending on whether a new or an existing method name is chosen, the current parameter settings of the QuantAnalysis part are saved into a new or an existing method file together with the specified part name and comment, if available. If the QuantAnalysis part should be saved into an existing method, the previous QuantAnalysis part of this method becomes overwritten after you have confirmed the corresponding request. If the QuantAnalysis part should be saved into a new method, the new method is created that contains only the QuantAnalysis method part.

The specified new (or modified) method is automatically attached to the loaded batch file.

If SOP method handling is turned on with an SOP method folder being defined and you

do not have the right to use non-default method folders, a message will appear if the default folder is not selected.

5.3 Edit Command

The **Edit** command is used to edit the parameter settings for the quantitation procedure you wish to use. Selecting this command starts the Method Editor and guides you through the set up of a method. The Method Editor's **General** dialog appears automatically.

Shortcut

Buttons:  

5.3.1 Edit Command - General

The **General** dialog is used to define the default injection volume used, an accuracy limit, if the dilution factor should be applied to ISTD compounds, too, and whether mass spectra should be recalculated when loading an analysis.

Default Injection Volume

Enter the default injection volume used during data acquisition.

Accuracy limit (%)

Enter a limit value for the **Accuracy** parameter that is calculated for 'Calib' and 'QC' samples. All calculated accuracy values that exceed this defined limit will be displayed in the Work Table in red color. This allows quick assessment of those integrations where problems may have occurred and which should be checked whether a manual reintegration is necessary. Default is 20.

Apply dilution factor to ISTD compounds

Check this option to apply the dilution factor set in the Work Table's **Dil. Factor** column also to ISTD compounds. If this option is not checked, the dilution factor will be applied to the target compounds only.

Load calibration from DataAnalysis results

Check this option if the mass spectra in an analysis being loaded in QuantAnalysis should be calibrated using the calibration coefficients stored in the last DataAnalysis result of the respective analysis.

Next

Switches forward to the method editor's **Chromatograms** dialog.

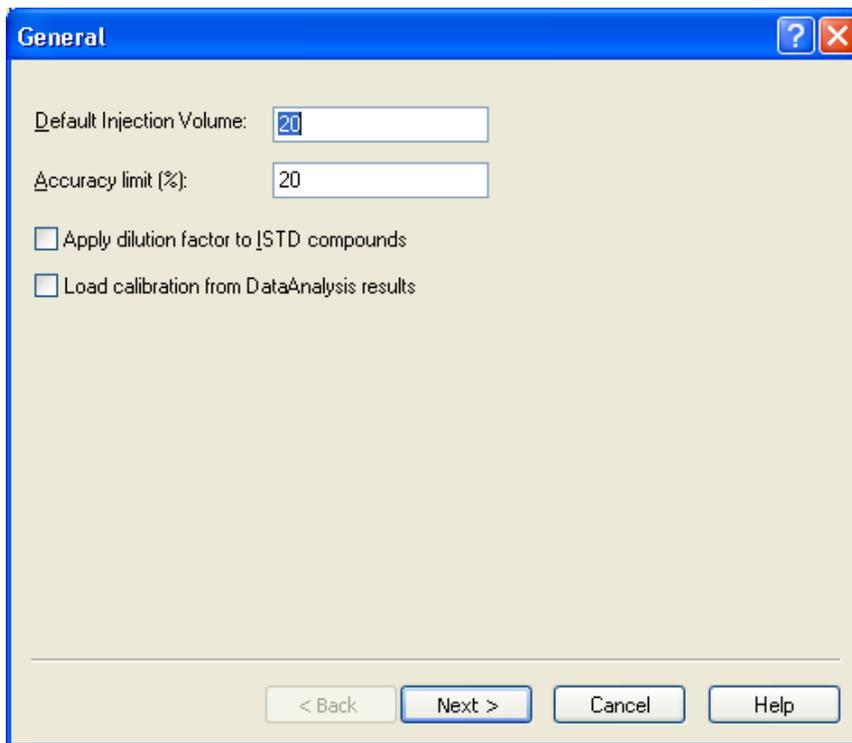


Figure 5-4 Method Editor's General dialog

5.3.2 Edit Command - Chromatograms

The **Chromatograms** dialog is used to define the chromatogram traces for the compounds to be quantified and for the internal standards used. The traces are defined in the same way as in DataAnalysis.

Note: To define the chromatogram traces you have to know the MS details of the analysis.

In the example shown in the dialog below, a target analysis was performed. The target compound Alprazolam and its d5-derivative, used as internal standard, both form $[M+H]^+$ compound ions ($m/z = 309$ and 314) which give two specific fragment ions in MS/MS experiments ($m/z 309 \rightarrow m/z 274$ and 281 ; $m/z 314 \rightarrow m/z 279$ and 286). During the chromatographic run alternating MS/MS experiments for both compounds were performed. The fragments were scanned and used for quantitative analysis. For quantitation, you have to define the chromatogram traces for the target compound and for the internal standard.

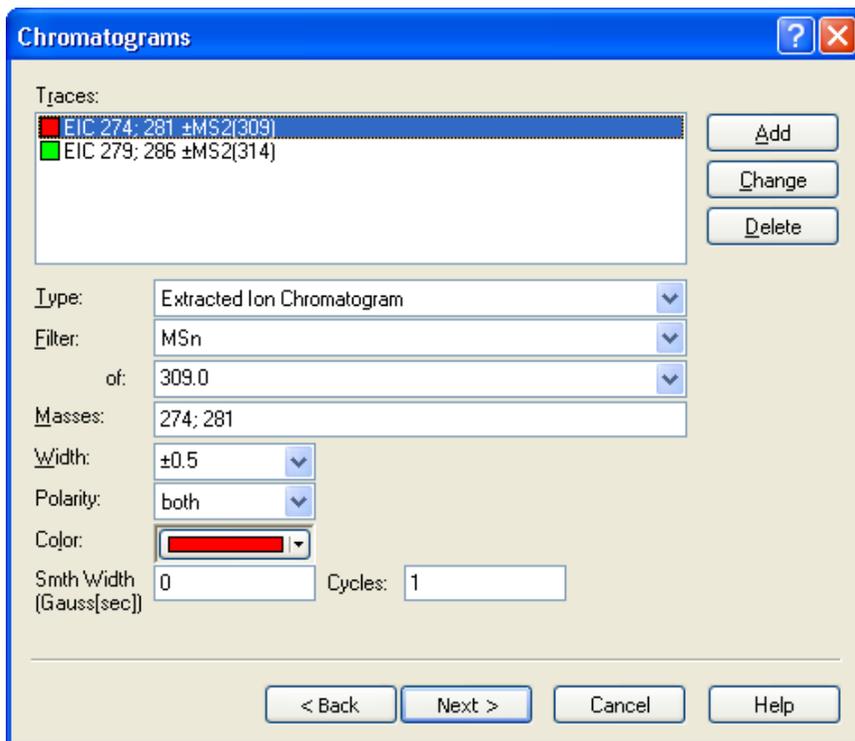


Figure 5-5 Method Editor's Chromatograms dialog showing parameter settings for an already defined chromatogram trace

Traces

Lists all chromatogram traces currently defined. Each chromatogram trace is represented by a short description and a color box that indicates the color the respective chromatogram is displayed with in the Chromatogram view of the Chromatogram/Spectrum window after quantitation has been performed. For changing or deleting an already defined chromatogram trace, select it from this list.

Type

Select the type of chromatogram trace to be edited.

Total Ion Chromatogram. (Default) This calculates a chromatogram by summing up the intensities of all masses contained in the mass spectra of the selected MS/MS type. Abbreviation is 'TIC'.

Extracted Ion Chromatogram. This calculates a chromatogram by summing up the intensities of the specified mass(es) contained in the mass spectra of the selected MS/MS type. Abbreviation is 'EIC'.

Base Peak Chromatogram. This calculates a chromatogram by using the intensity of the most abundant of the specified masses contained in the mass spectra of the selected MS/MS type. Abbreviation is 'BPC'.

Depending on the selected type, specific options for defining the chromatogram trace

are displayed below this list box.

Filter

Select the type of mass spectra to be filtered for calculating the respective chromatogram trace.

All (MS and MSn). (Default) Uses all mass spectra (no filter).

All MS. Uses all MS spectra.

All MSn. Uses all MSn spectra.

MSn. Uses only MSn spectra of the precursor ion specified in **of**.

of

For **MSn** filter chosen, select the precursor ion mass to be used for calculating the chromatogram trace. The list includes all isolated and fragmented masses, which have been collected during data acquisition.

Masses

For an **Extracted Ion Chromatogram** or **Base Peak Chromatogram** enter the mass values or mass ranges to be used for calculating the respective chromatogram trace. Default is full mass range.

Single masses: Separate each mass value by a comma, semicolon or plus sign.

Mass ranges: Separate starting and ending masses by a hyphen "-". Leaving starting (or ending) mass empty results in the first (or last) measured mass of the chromatographic run to be chosen. Entering only a hyphen selects the full mass range.

Note: Exclusion masses are not included in the respective calculation.

Width

For an **Extracted Ion Chromatogram** or **Base Peak Chromatogram**, select a mass precision range from the list of pre-defined precision ranges or enter a customized range. The precision range to be used depends on how precise the respective measurement was. Normally it is not necessary to change the default value but in the case of mass shifts during analysis, this width can be adjusted. Default is ± 0.5 .

Polarity

For an **Extracted Ion Chromatogram** or **Base Peak Chromatogram**, select the polarity of the ions to be used for calculating the respective chromatogram trace. If the chromatogram traces were acquired in alternating mode, i.e. alternating scans in positive and negative ionization mode were performed, you have to select the right polarity for trace definition:

both (\pm). (Default) Uses both positive and negative ions.

positive (+). Uses positive ions only.

negative (-). Uses negative ions only.

Color

Select the color the selected chromatogram trace should be displayed with.

Smth Width (Gauss[sec])

If you want to smooth the chromatogram trace because it is very noisy, enter an appropriate smoothing width (in seconds). An entry of '0' will result in no smoothing. Default is '0'.

Cycles

Enter the number of smoothing cycles to run. Default is '1'.

Add

Adds the new defined chromatogram trace to **Traces**.

Change

Changes the chromatogram trace selected in **Traces** according to the new settings.

Delete

Deletes the selected chromatogram trace from **Traces**.

Next

Switches forward to the Method Editor's **ISTD Compounds** dialog.

Back

Switches back to the Method Editor's **General** dialog.

5.3.3 Edit Command - ISTD Compounds

The **ISTD Compounds** dialog is used to define the internal standard compound(s) used. For each ISTD compound, you have to enter its name and the corresponding chromatographic and concentration data.

Note: In the case of a quantitation with external calibration, you can skip this dialog and proceed with the **Target Compounds** dialog.

ISTD Compounds

Lists all ISTD compounds currently defined. For changing or deleting an already defined ISTD compound, select the respective ISTD compound from this list.

Name

Enter the name of the ISTD compound.

CAS No.

Enter the CAS number of the ISTD compound (optional).

Chrom.

Select the chromatogram trace that corresponds to the ISTD compound.

The screenshot shows a dialog box titled "ISTD Compounds". At the top left, there is a list box containing "Alprazolam D5". To the right of the list box are three buttons: "Add", "Change", and "Delete". Below the list box are several input fields: "Name:" with "Alprazolam D5", "CAS No.:" (empty), "Chrom.:" with a dropdown menu showing "EIC 279; 286 ±MS2(314)", "Retention time [min]:" with "1.2", "Window [min]:" with "0.5", "Default Concentration:" with "10", and "Concentration units:" with "pg/µl". At the bottom of the dialog are four buttons: "< Back", "Next >", "Cancel", and "Help".

Figure 5-6 Method Editor's ISTD Compounds dialog showing parameter settings for an already defined ISTD compound

Retention time [min]

Enter the retention time (in minutes) of the ISTD compound peak.

Window [min]

Enter the width of the time window (in minutes) for the software to search for the ISTD compound peak.

Default Concentration

Enter the default concentration of the ISTD compound.

Concentration units

Enter the concentration units of the default concentration.

Add

Adds the new defined ISTD compound to **ISTD Compounds**.

Change

Changes the ISTD compound selected in **ISTD Compounds** according to the new settings.

Delete

Deletes the ISTD compound selected in **ISTD Compounds**.

Next

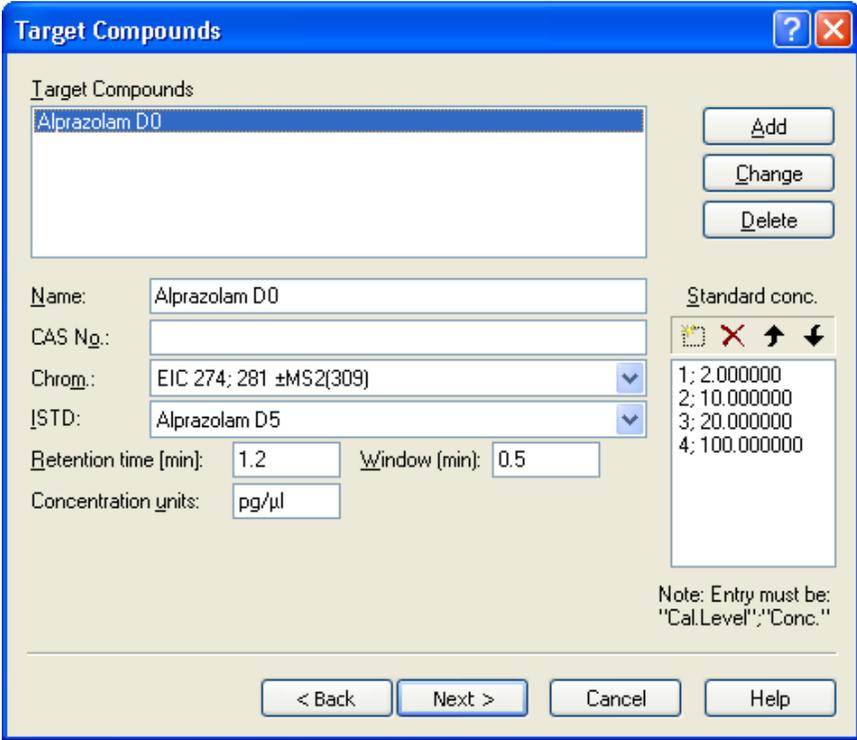
Switches forward to the Method Editor's **Target Compounds** dialog.

Back

Switches back to the Method Editor's **Chromatograms** dialog.

5.3.4 Edit Command - Target Compounds

The **Target Compounds** dialog is used to define the target compounds to be used in quantitation and their standard concentrations.



The screenshot shows the 'Target Compounds' dialog box. The title bar is blue with a question mark and a close button. The main area has a list box containing 'Alprazolam D0'. To the right of the list are three buttons: 'Add', 'Change', and 'Delete'. Below the list box are several input fields: 'Name:' with 'Alprazolam D0', 'CAS No.:', 'Chrom.:' with a dropdown menu showing 'EIC 274; 281 ±MS2(309)', 'ISTD:' with a dropdown menu showing 'Alprazolam D5', 'Retention time [min]:' with '1.2', 'Window [min]:' with '0.5', and 'Concentration units:' with 'pg/µl'. To the right of these fields is a 'Standard conc.' section with a list box containing four entries: '1; 2.000000', '2; 10.000000', '3; 20.000000', and '4; 100.000000'. Above this list are four icons: a square, a red X, an up arrow, and a down arrow. Below the list is a note: 'Note: Entry must be: "Cal.Level"; "Conc."' At the bottom of the dialog are four buttons: '< Back', 'Next >', 'Cancel', and 'Help'.

Figure 5-7 Method Editor's Target Compounds dialog showing parameter settings for an already defined target compound

Target Compounds

Lists all target compounds currently defined. For changing or deleting an already defined target compound, select the respective compound from this list.

Name

Enter the name of the target compound.

CAS No.

Enter the CAS number of the target compound (optional).

Chrom.

Select the chromatogram trace that corresponds to the target compound.

ISTD

Select the ISTD compound that should be assigned to the target compound.

Retention time [min]

Enter the retention time (in minutes) for the target compound peak.

Window [min]

Enter the width of the time window (in minutes) for the software to search for the target compound peak.

Concentration units

Enter the concentration units for the standard concentrations of the target compound.

Standard conc.

Define the standard concentrations for the calibration levels given in the Work Table's **Calib Level** column. For this, level ID and corresponding concentration value pairs must be entered.

- To enter a new calibration level/concentration pair, click . Then enter the level ID and concentration value separated by a semicolon (;) and click on the list box or press the Enter key. This adds the new pair at the bottom of the list.
- To delete a calibration level/concentration pair, select it and click .
- To move a calibration level/concentration pair to another position in the list, click  or  until the desired position is reached.

Add

Adds the new defined target compound to **Target Compounds**.

Change

Changes the target compound selected in **Target Compounds** according to the new settings.

Delete

Deletes the target compound selected in **Target Compounds**.

Next

Switches forward to the Method Editor's **Integration Parameters** dialog.

Back

Switches back to the Method Editor's **Target Compounds** dialog.

5.3.5 Edit Command - Integration Parameters

The **Integration Parameters** dialog is used to define the parameter settings to be used for peak detection and mass spectrum calculation. Normally the default values allow good integration results but if necessary, the parameters can be given independently for each individual chromatogram.

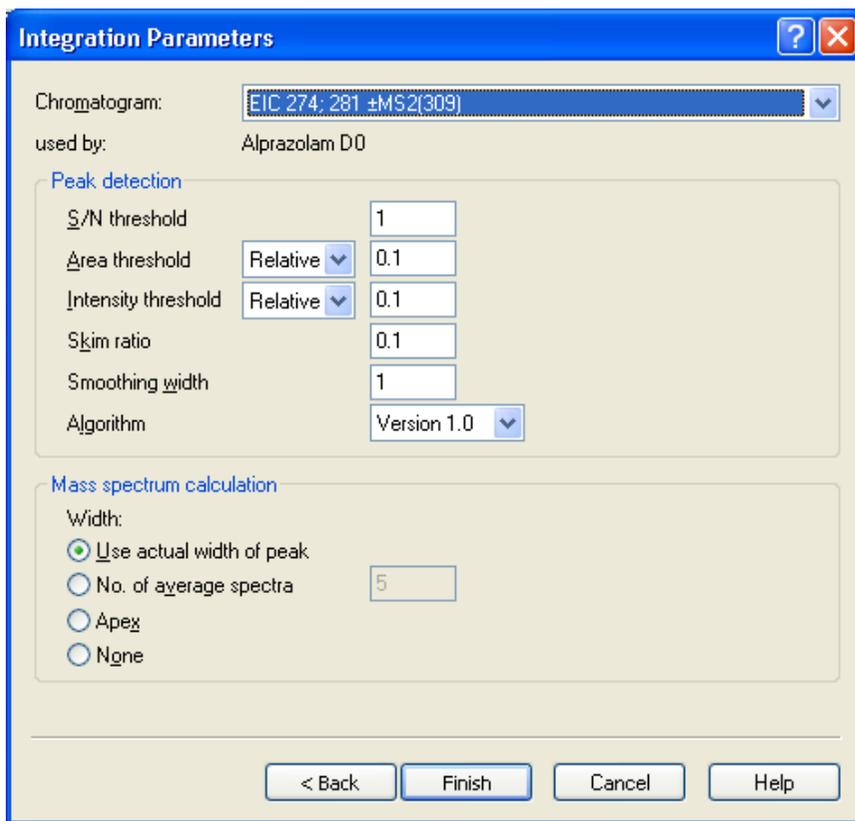


Figure 5-8 Method Editor's Integration Parameters dialog

Chromatogram

Select the chromatogram trace you will define for the peak detection and mass spectrum calculation parameters.

used by

Displays the target or ISTD compound the selected chromatogram trace is assigned to.

In **Peak detection**, define the parameters for peak detection:

S/N threshold

Enter the S/N (signal-to-noise) threshold a signal must exceed to be used in peak detection. Values from 0.001 to 1000 are allowed. Default is '1'.

The S/N is defined as the height of the mass peak above its baseline, relative to the noise. The noise level is defined as 5 x sigma (sigma = standard deviation) and is calculated on the full mass spectrum except the regions of peaks.

The steps included in the signal-to-noise ratio determination depend on the selected chromatographic peak finder version, **Version 1.0** or **Version 2.0**.

For Version 1.0: The S/N determination includes the following steps:

1. The third derivative of the chromatogram is calculated using the *Savitsky Golay* algorithm with a smoothing width m as set.

$$y' = \sum_{t=-m}^m \frac{(2m-1)(2m+3)t}{Norm} f(t)$$

$$Norm = m(4m^2 - 1)(2m + 3)(m + 1)/3$$

2. The maximum value of a histogram of the absolute of the third derivative y''' determines the internal threshold T for the next step.
3. The standard deviation σ' of all values of the third derivative y''' which absolute is smaller or equal the internal threshold T is determined.

$$\sigma' = \sqrt{\frac{\sum_{i=1}^N y_i''''^2}{N}}, \text{ with } |y_i''''| \leq T$$

4. The standard deviation is corrected with the smoothing width giving the noise σ for signal-to-noise ratio calculation:

$$\sigma = \sigma' \cdot m^3, \text{ with } m = \text{smoothing width}$$

5. The signal-to-noise ratio S/N of each peak is then calculated as:

$$S/N = S/5\sigma, \text{ with } S = \text{peak height above the peak baseline.}$$

The noise N is determined as 5σ ; statistically 99% of the noise values are within this range.

The following drawing illustrates the *Signal* and the *Noise* values.

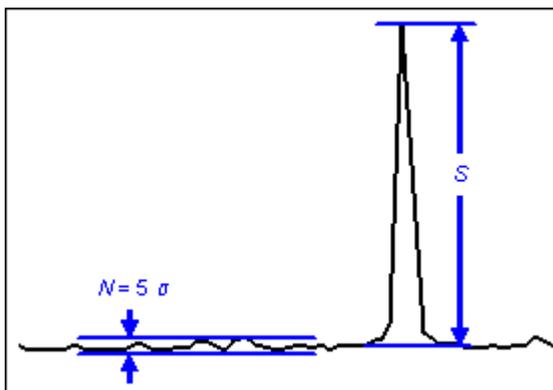


Figure 5-9 Illustration of the *Signal* and the *Noise* values

For Version 2.0: The S/N determination is done in the following way:

1. Determination of local maxima.
2. Splitting of spectrum in segments according to number of local maxima.
3. Per segment:
 - a. Sorting of intensity values of local maxima (histogram).
 - b. Calculation of first derivative using the *Savitsky Golay* algorithm with a smoothing width of 1/10 of the number of local maxima in the segment (formula see above).
 - c. Determination of points of minimal and maximal derivative of the histogram, which give the turning points of the distribution.
 - d. Use the noise obtained from the intersection of the tangents at the appropriately selected turning points.

Area threshold

Define the area threshold a signal must exceed to be detected as a peak. Select the threshold type and enter the desired threshold value:

Absolute. Uses an absolute threshold value.

Relative. (Default) Uses a threshold value relative to the 100% (base) peak.

(Area Threshold). Enter the relative or absolute area threshold value. Default is '0.1'.

Intensity threshold

Define the intensity threshold a signal must exceed to be detected as a peak. Select the threshold type and enter the desired threshold value.

Absolute. Uses an absolute threshold value.

Relative. (Default) Uses a threshold value relative to the 100% (base) peak.

(Intensity Threshold). Enter the relative or absolute intensity threshold value. Default is '0.1'.

Skim ratio

Enter the skim ratio to influence the calculation of peak areas of overlapping peaks. Default is '0.1'.

Smoothing width

Enter the number of mass spectra to be used for smoothing. Values from 1 to 20 are allowed. Default is '1'.

In **Mass spectrum calculation**, define how the mass spectrum corresponding to a detected peak should be calculated:

Width

Select which mass spectrum/spectra should be included in calculating the resulting mass spectrum for a detected peak:

Use actual peak width. (Default). Calculates the mass spectrum by averaging all mass spectra contained in the actual peak width.

No. of average spectra. Calculates the mass spectrum by averaging a specified number of mass spectra. Enter the desired number of mass spectra in the related text box. Default is '5'.

Apex. Calculates the mass spectrum using the Apex algorithm, taking the mass spectrum at the peak apex.

None. Calculates no mass spectrum.

Finish

Finishes the Method Editor.

Back

Switches back to the Method Editor's **Target Compounds** dialog.

6 COMPASS MENU

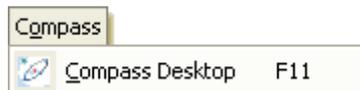


Figure 6-1 Compass menu

The **Compass** menu offers the following command:

Compass Desktop Launches Compass Desktop.

6.1 Compass Desktop Command

The **Compass Desktop** command launches Compass Desktop which allows switching to other Bruker Compass applications. The buttons enabled depend on the programs currently installed on your computer.



Figure 6-2 Compass Desktop

Shortcut

Button: 

7 HELP MENU

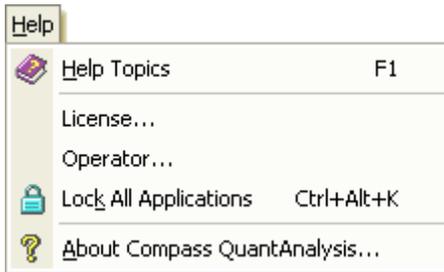


Figure 7-1 Help menu (when in Compliance mode)

The **Help** menu offers the following commands:

Help Topics	Launches QuantAnalysis help.
License	Registers your Bruker Daltonics applications licenses.
Operator	Logs in the specified operator.
Lock All Applications	Locks all Bruker Daltonics applications.
About Compass QuantAnalysis	Provides information about your current QuantAnalysis copy.

7.1 Help Topics Command

The **Help Topics** command is used to start the QuantAnalysis help program in order to get information about specific topics. QuantAnalysis help operates as a standard Windows help program.

Shortcut

Button: 

Key: F1

7.2 License Command

The **License** command is used to view, add and/or delete licenses for Bruker Daltonics applications. The command opens the **Bruker Daltonics LicenseManager** dialog that shows any license currently available for any of the Bruker Daltonics applications and how long it will be valid.

To add a new license, enter the license key you received in **New license key** and click **Add**. A new line is added to **Existing licenses** with the key you have entered, the product name and the date until the license will be valid. To delete an existing license select it in **Existing licenses**, click **Delete** and confirm the corresponding request.

Note: If QuantAnalysis is running in Compliance mode, only operators who have the special right can add or delete licenses.

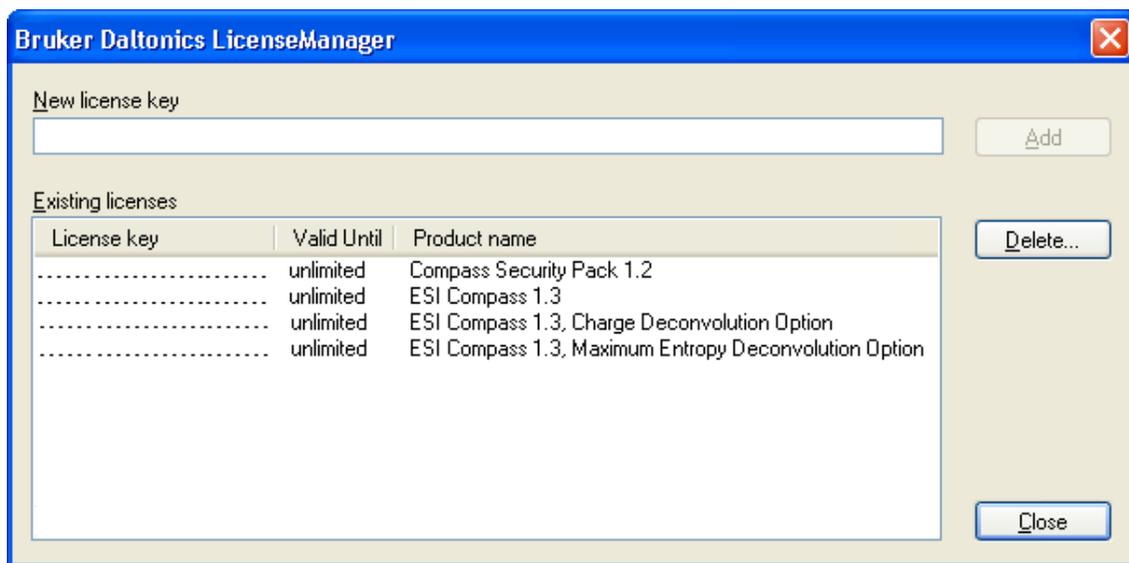


Figure 7-2 Bruker Daltonics LicenseManager dialog with 'ESI Compass 1.3' license needed for QuantAnalysis being present (example)

New license key

Enter the submitted license key.

Existing licenses

Lists already existing licenses.

License key

Lists the license keys for the existing licenses.

Valid until

Permanent licenses are indicated as 'unlimited'.

For temporary licenses, the date until the respective license is valid is shown. An expiration warning will inform you automatically about the forthcoming expiration of a temporary license firstly 30 days before the respective expiration will expire. If for one product more than one license is present, this warning concerns to the longest valid license. An expiration warning will appear once per 24 hours and can be skipped by the operator.

Product name

Lists the names of the products for which licenses already exist.

Add

When in Non-Compliance mode, it licenses the product and adds the license key you entered in **New license key** to the list of existing licenses.

When in Compliance mode, it opens the **Re-enter Your Password** dialog (see below) to re-enter the password for the current operator account. The license key is added after re-entering the correct password and if the operator has the required right.

This button is enabled after the license key has been entered completely.

Delete

When in Non-Compliance mode, it deletes the license key selected in the **Existing licenses** list after affirming corresponding confirmation request.

When in Compliance mode, it opens, after affirming confirmation request, the **Re-enter Your Password** dialog to re-enter the password for the current operator account. The license key is deleted after re-entering the correct password and if the operator has the required right.

Re-enter Your Password dialog

This dialog is used to re-enter the password for the current operator account.



Figure 7-3 Re-enter Your Password dialog

Password

Enter the password for the current operator account.

OK

If the password is correct for the current operator account and the operator has the right to add/delete licenses the entered license key is added to or the selected license key is deleted from the LicenseManager's **Existing licenses** list.

If the password is incorrect or the operator does not have the required right a corresponding error message will inform you.

7.3 Operator Command

The **Operator** command is used to change the operator during a QuantAnalysis session. When QuantAnalysis is running in Compliance mode, you can also use this command to change your current password.

Note: There can only be one operator at a time logged into Bruker Daltonics applications on a specific computer.

The command opens the **QuantAnalysis** dialog, which allows you to log in or change your password. Depending on the current mode, Non-Compliance or Compliance, this dialog may appear different. In Non-Compliance mode, you can log in without identifying yourself, while in Compliance mode you must identify yourself by operator ID and password.

Note: This dialog appears automatically whenever you start-up of your QuantAnalysis application unless you are currently logged in another Bruker Daltonics application (for both Non-Compliance and Compliance mode) or the corresponding option for skipping this dialog is set (for Non-Compliance mode only).

Operator

Enter your operator ID. The ID of the current operator will automatically be entered if the UserManagement administrator has set the corresponding option. The operator ID is not case-sensitive.

Password

Enter your password. The password is not displayed as you type it.

Note: Passwords are case-sensitive. The operator will be locked if the number of wrong login tries exceeds a number set by the UserManagement administrator. Only the UserManagement administrator can unlock a locked operator.

Note: This entry field is available in Compliance mode only.

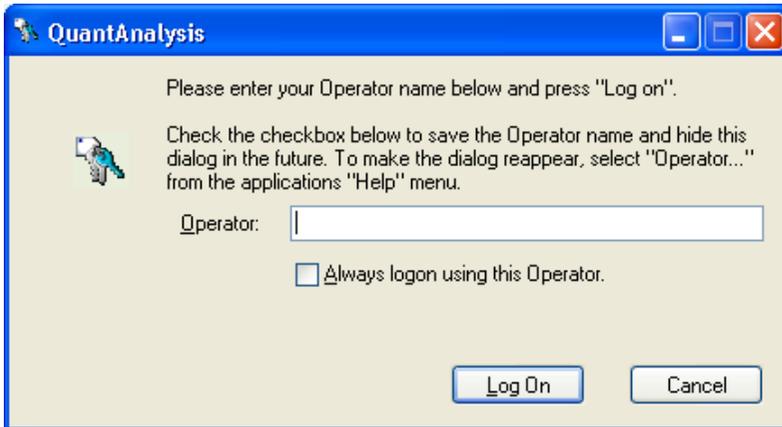


Figure 7-4 QuantAnalysis dialog for logging in the operator in Non-Compliance mode



Figure 7-5 QuantAnalysis dialog for logging in the operator in Compliance mode

Always login using this Operator

Check this option to have the operator named in **Operator** logged in automatically. This will skip this dialog when starting QuantAnalysis in future.

Note: This check box is available in Non-Compliance mode only.

Change Password

Allows you to change your current password before logging in. Opens the **Change Password** dialog.

Note: This button is available in Compliance mode only.

Log On

Logs in the (specified) operator.

In Compliance mode, log in will be successful only if operator ID and password match. If both do not match an error message will appear. Successive wrong password inputs

can cause locking of an operator by UserManagement. If a new created operator tries to log into a Bruker Daltonics application for the first time, the program requires for changing the password. Quitting the request opens the **Change Password** dialog.

Change Password dialog

The **Change Password** dialog is used to change the current password for the operator named in **Operator**. The new password must comply with the password policy settings defined by the UserManagement administrator.



Figure 7-6 Change Password dialog

Operator

Displays the ID of the operator whose password can be changed. If the password for another operator should be changed, click **Cancel** and enter the desired operator in the previous dialog.

Old password

Enter your current password. The password is not displayed as you type it.

Note: Passwords are case-sensitive.

New password

Enter the new password. The password is not displayed as you type it.

Note: Passwords are case-sensitive. Make sure, that the new password complies with the current password policy settings.

Confirm new password

Confirm your new password. You must enter the same password as above.

OK

If the new password and its repetition are the same, and the new password complies with the password policy settings, it changes the password. A dialog appears informing you that your password was changed successfully. Quitting this dialog returns you to the **QuantAnalysis** dialog.

If the new password and its repetition are different or the chosen password does not comply with the password policy settings, a corresponding message appears. Repeat the respective entries.

If the old password is incorrect, a message appears informing you that the password was not changed. Quitting this message returns you to the **QuantAnalysis** dialog.

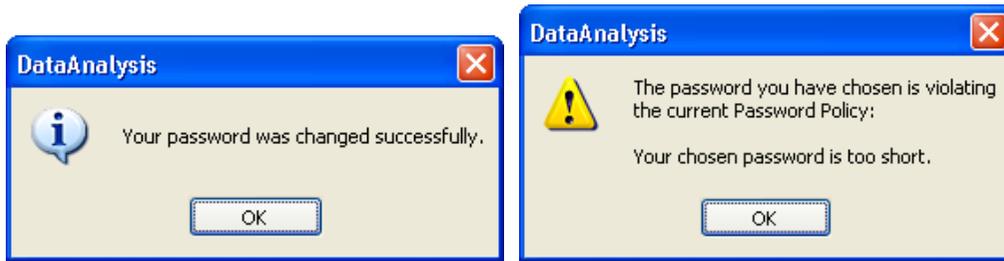


Figure 7-7 Messages on successful password change (left) and chosen password is violating password policy (right)

7.4 Lock All Applications Command

Note: The **Lock All Applications** command is available only in Compliance mode.

The **Lock All Applications** command is used to lock all Bruker Daltonics applications. This includes QuantAnalysis as well as all other Bruker Daltonics applications currently installed on your system.

Note: Only the previous operator or someone with the special right to unlock applications can unlock a locked application.

Note: All UserManagement-using Bruker Daltonics applications will be locked automatically if one of these applications has not been used for a certain period as defined by the UserManagement administrator.

The command opens the **QuantAnalysis** dialog which informs you that QuantAnalysis has been locked, by whom (displays full name of operator) and how it can be unlocked. You must enter the required entries to unlock the application.

Operator

Enter the operator ID of the operator who has locked QuantAnalysis. The respective operator ID will automatically be entered if the UserManagement administrator has set the corresponding option.

If an operator other than the previous one wants to unlock the applications, enter the other operator ID.

Note: This respective operator must have the right to unlock applications.



Figure 7-8 QuantAnalysis dialog when QuantAnalysis has been locked

Password

Enter the corresponding password.

Note: Passwords are case-sensitive. The operator will be locked if the number of wrong login tries exceeds a number set by the UserManagement administrator. Only the UserManagement administrator can unlock a locked operator.

Change Password

Allows you to change your current password before logging in. Opens the **Change Password** dialog.

Log On

If operator ID and password match, and the respective operator is allowed to unlock applications, it unlocks Bruker Daltonics applications and logs in the specified operator.

Shortcuts

Button: 

Key: Ctrl+Alt+K

7.5 About Compass QuantAnalysis Command

The **About Compass QuantAnalysis** command is used to display the version number of your current copy of DataAnalysis and QuantAnalysis with the copyright notice, the user-specific license information as well as the information on how to contact Bruker Daltonik GmbH. The command opens the **About Bruker Daltonics QuantAnalysis** dialog.

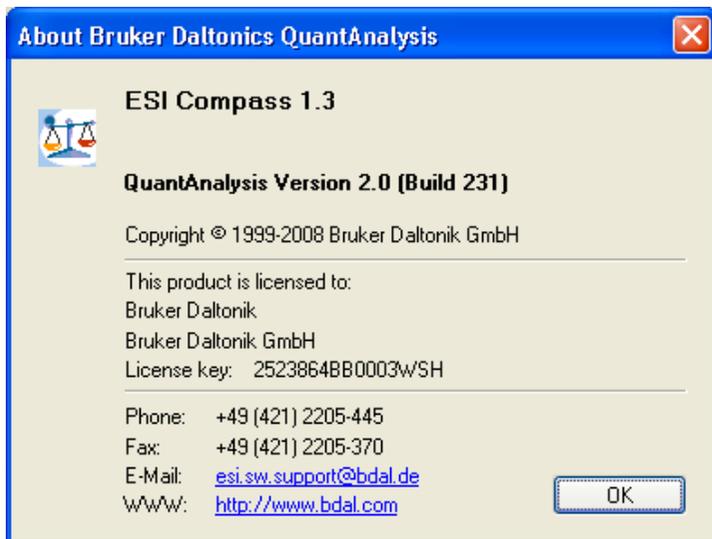


Figure 7-9 About Bruker Daltonics QuantAnalysis dialog

Shortcut

Button:



8 COMMANDS ACCESSIBLE FROM BUTTONS ONLY

In addition to the commands accessible from the menus, QuantAnalysis provides other commands that are accessible from buttons only. These commands can be found in the Work Table window and Chromatogram/Spectrum window. For example, processing of a batch is performed by clicking the **Process** button in the Work Table window, or to print a specific quantitation report use the **Report** button in the Work Table window.

8.1 Process Command (Work Table Window)

The **Process** command is used to process the open batch file according to the current parameter settings defined in the selected quantitation method, and to save the quantitation results and the method used with the processed batch file. The batch file to be processed can be either a not-yet-processed or an already-processed batch file.

Before processing a batch file, the quantitation method to be used must be opened or created.

Clicking  **Process** in the Work Table window starts batch processing. First, the batch file is automatically saved. In the case of a not-yet-processed batch file, the **Save As** dialog will appear to allow you to save the processed batch file under a new file name and to keep the original batch file unprocessed for performing further processing operations on it, such as by using another quantitation method. In the case of an already-processed batch file no saving dialog will appear. After saving has occurred, the processing operation really starts. Usually, processing a batch file takes only a few seconds. A blue bar at the bottom of the screen shows the progress of this process.

After processing is finished you should save the processed batch file. Then you can review the quantitation results obtained.

8.2 Report Command (Work Table Window)

The **Report** command is used to print a QuantAnalysis report containing specific quantitation data from the open batch file. All layouts can be printed in portrait and landscape format. You can preview the report before printing it.

Note: With older printer models (with insufficient firmware performance), there might

be the problem that printing of a report takes a very long time. To overcome this, a registry switch now supports faster printing on such printers (see below).

Clicking  **Report...** in the Work Table window opens the **Print** dialog, which allows you to select the report layout you want to print and to specify the destination printer, other printer setup options and the number of copies.

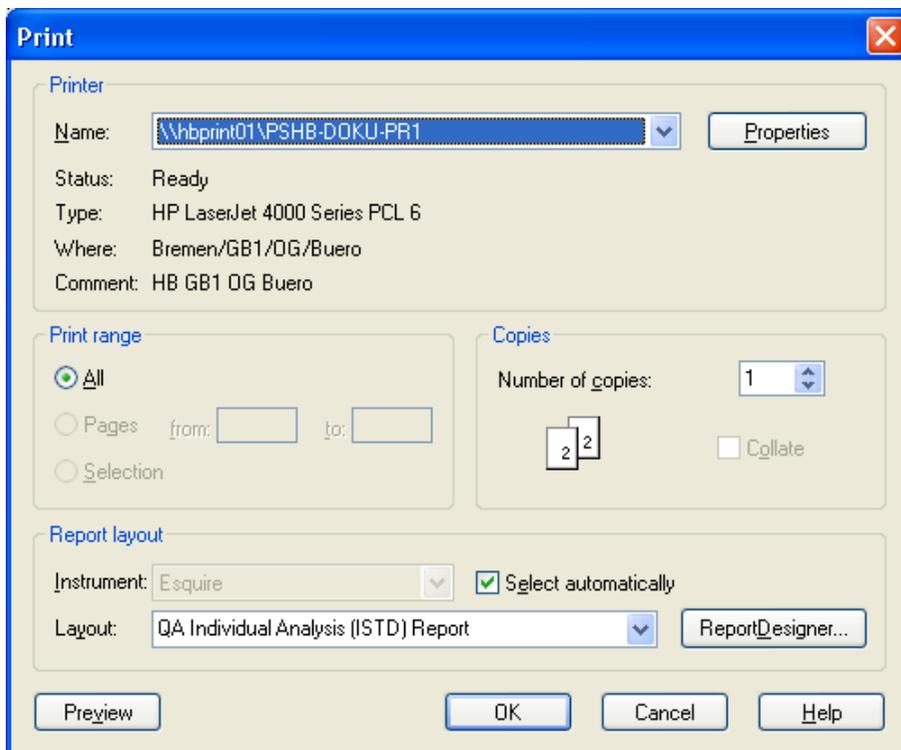


Figure 8-1 Print dialog

For description of parameters, please refer to section 2.6.

Preview

Allows you to preview the selected report before printing it. It creates the report and shows in the **Preview** window how the report will look if you print it.

If you want to print the report, you can start printing directly from the preview by clicking its . Otherwise, click the preview's  to close it and return to the **Print** dialog.

OK

Creates the selected report and prints it on the specified printer.

Support for printing on older printer models

With older printer models, there might be the problem that printing of a report takes a very long time since the firmware is too slow when converting the vector graphic into a bitmap graphic. To overcome this problem a registry switch is now available which lets DataAnalysis create the bitmap already and thus speeds up printing on such printers.

Note: NT administrator privileges are required for setting the registry key.

1. Click .
2. Click **Run**. This opens the **Run** dialog.
3. In **Open**, type in "regedit" and click **OK**. This opens the Registry Editor.
4. Navigate to "Computer\HKEY_LOCAL_MACHINE\SOFTWARE\Bruker Daltonik".
5. Right-click the key "Bruker Daltonik" and from the context-sensitive menu (CSM) select **New > Key**. Overwrite the default key name with "Printer".
6. Right-click the key "Printer" and from the CSM select **New > Key**. Overwrite the default key name with the name of the printer for which you want to set the registry key, e.g. "HP LaserJet 5000 Series PCL". You must type in the name the respective printer is referred with in the DataAnalysis **Print** dialog.
7. Right-click the key "[printer name]" and from the CSM select **New > DWORD Value**. This enters a double word (dword) value for the key "[printer name]" which is specified by the **Name** "New Value #1", the **Type** "REG_DWORD" and the **Data** "0x00000000 (0)". Overwrite the default name with "UseBitmaps".
8. Right-click the name "UseBitmaps" and from the CSM select **Modify**. In the **Edit DWORD Value** dialog change the current **Value data** value from "0" to "1" and click **OK**. This changes the "UseBitmaps" value accordingly and thus switches the key on.
9. Close the Registry Editor.

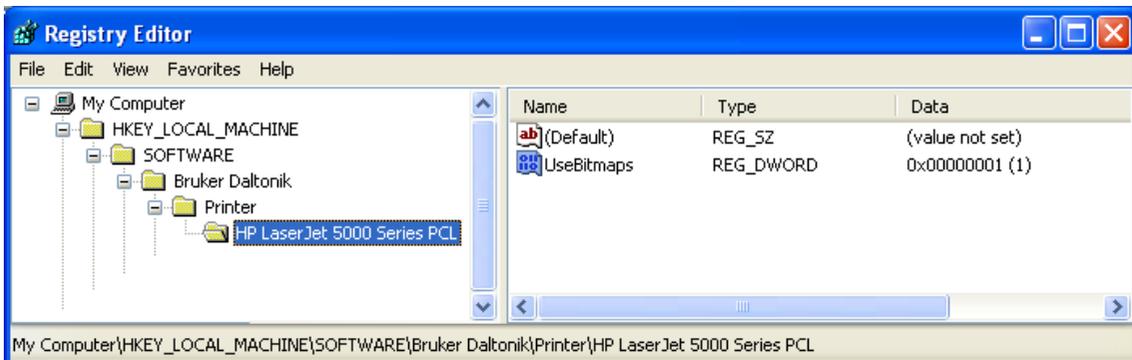


Figure 8-2 Example registry key for faster printing on the named printer

8.3 History Command (Work Table window)

The **History** command is used to show the result history of the open batch file and to load or delete a certain result of it. When QuantAnalysis is running in Compliance mode, it is also possible to sign a certain result.

Clicking  History in the Work Table window opens the **Result History** dialog. Depending on whether QuantAnalysis is running in Compliance or Non-Compliance mode, the dialog displays different information and allows for different operations. Generally, all results currently available for the open batch file are listed along with corresponding information about saving date and time, operator who saved as well as whether or not a result was deleted. When in Compliance mode, also information on already signed results is displayed.

(Result history list)

Lists all results saved since batch file setup, which also includes already deleted results. An arrow in front indicates the currently loaded result. Following information is given:

No

Running number of result referring to the chronology of saving.

Date

Date and time a result was saved.

Saved by

Operator who saved a result.

Signed

Shows whether a result is signed. Signing is indicated by a 'yes'; otherwise no entry is present. Additional information about signing a result is displayed after selecting the respective result.

Note: The **Signed** column is only available when QuantAnalysis is running in Compliance mode.

Deleted

Shows whether a result was deleted. Deletion is indicated by a 'yes'; otherwise no entry is present. Additional information about deleting a result is displayed after selecting the respective result.

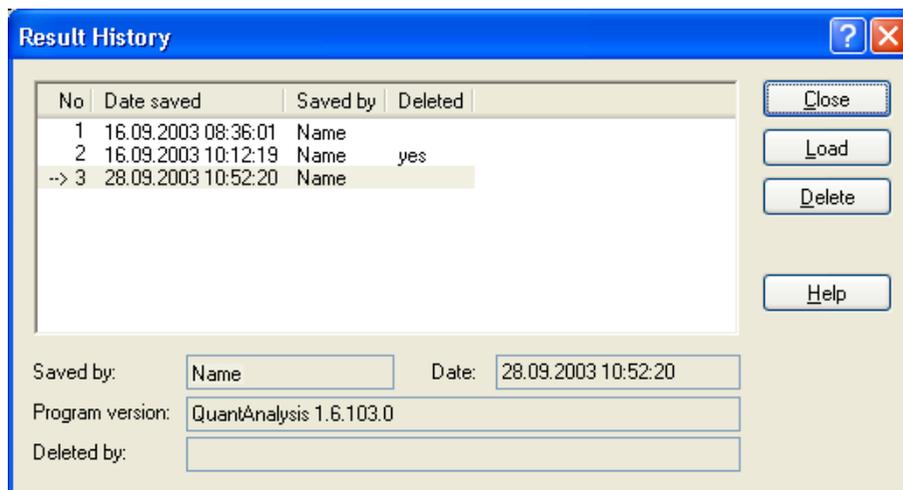


Figure 8-3 Result History dialog for a batch file when in Non-Compliance mode

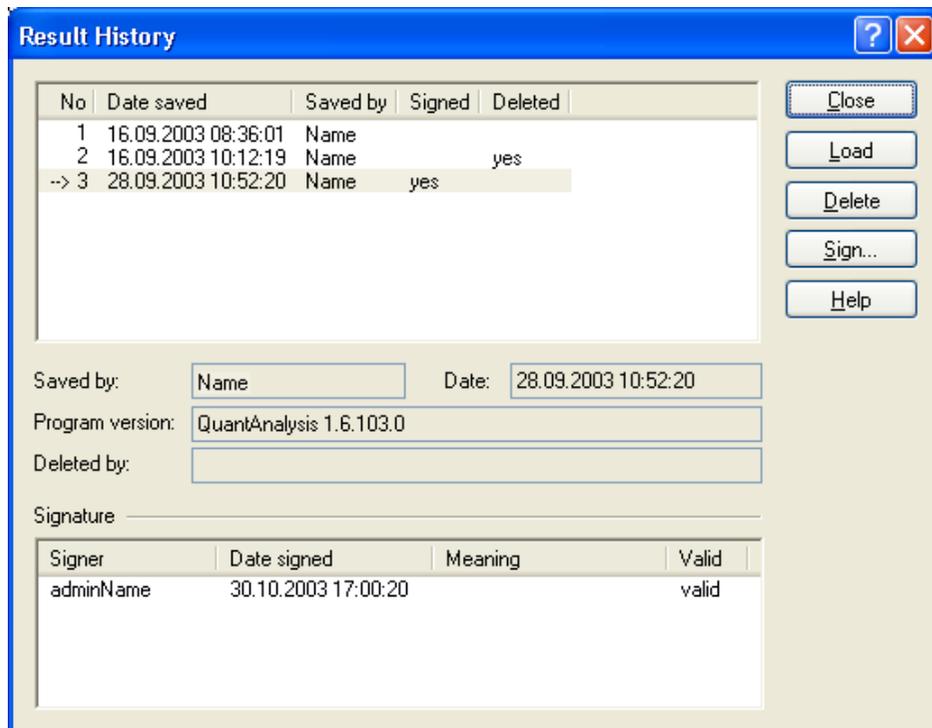


Figure 8-4 Result History dialog for a batch file when in Compliance mode

When a result is selected in the result history list, additional information is displayed below the list concerning the following parameters:

Saved by

Operator who saved the result.

Date

Date and time the result was saved.

Program version

Program version used for saving the result.

Deleted by

Operator who deleted the result.

In the **Signature** table, information about signing the selected result is shown.

Note: The **Signature** table is only available when QuantAnalysis is running in Compliance mode.

Signer

Lists the operator(s) who signed the selected result.

Date

Date and time the selected result was signed by the named signer.

Meaning

Meaning of signing the selected result by the named signer.

Validity

Result of signature check for the named signer.

Load

Loads the selected result of the open batch file. If changes made to the currently loaded result have not been saved yet, first a confirmation request on saving changed state will appear which you have to answer.

Delete

Deletes the selected result from the open batch file after you have affirmed the corresponding confirmation request. Deletion is indicated by a 'yes' being entered for this result under **Deleted**.

Note: When QuantAnalysis is running in Compliance mode, only operators who have the respective right can perform deleting a result.

Sign

Allows you to sign the selected result of the open batch file. Opens the **Sign Electronic Record** dialog (see below).

Note: The **Sign** button is available only in Compliance mode.

Note: Only operators who have the right to sign electronic records can sign a result. If the currently logged in operator does not have this right, an operator having this right can sign immediately. There is no need to change the logged in operator previously.

Sign Electronic Record dialog

The **Sign Electronic Record** dialog is used to sign electronically the electronic record (= result of a batch with corresponding method) that corresponds to the result currently selected in the **Result History** dialog. An electronic signature consists of operator ID and password. Optionally, the meaning of signing can be given. Multiple signing of results is allowed.

Note: Signing electronic records is possible only in Compliance mode.

Note: Only operators who have the right to sign electronic records can sign a result. If the currently logged in operator does not have this right, an operator having this right can sign immediately. There is no need to change the logged in operator previously.

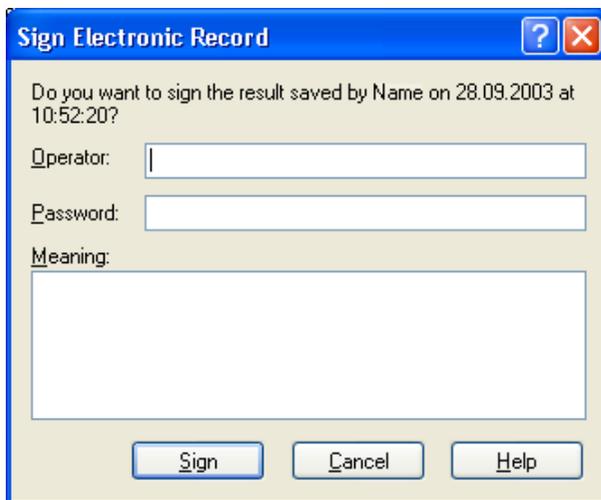


Figure 8-5 Sign Electronic Record dialog

Operator

Enter your operator ID.

Password

Enter your password.

Meaning

Enter the meaning of signing the selected result if desired.

Sign

If operator ID and password meet and if the respective operator has the right to sign electronic records the selected result is signed. This is indicated in the **Result History** dialog by a 'yes' being entered for the selected result under **Signed**. Also, additional signing information is shown.

If operator ID and password do not meet or the operator does not have the right to sign electronic records a corresponding error message will appear.

8.4 Import Command (Work Table Window)

The **Import** command is used to import a sample table into QuantAnalysis in order to create a batch file from it. You can import a sample table set up in Agilent ChemStation and stored in Comma Separated Values Files format (*.csv) or a sample table set up in Bruker Compass HyStar and stored in HyStar Sample Table Extract format (*.seq)

You can set up a new batch file from a sample table by importing it. Alternatively, you open an existing batch file that already contains a sample table and append the imported sample table to the present one or replace the present by the imported one.

Note: If you want to import a sample table into an existing batch file, this batch file must still be unprocessed.

When importing a sample table, that sample data contained in this file that is needed by QuantAnalysis is automatically entered in the Work Table of the newly created or existing batch file.

If you want to import a sample table into an existing batch file, the respective batch file must be opened before selecting the **Import** command.

Clicking  in the Work Table window opens the **Import Sample Table** dialog, which allows you to specify the name and location of the sample table you wish to import. In case of an import into a batch file already containing a sample table, define how to proceed with the imported sample table.

Look in and folder list

Navigate to the drive and folder that contains the sample table you wish to import. Double-click the sample table or select it and click **Open**.

File name

Enter the file name of the sample table or select it from the folder list.

Files of type

Select the type of sample table files to be displayed in the folder list:

Comma Separated Values File (*.csv). Lists Agilent ChemStation sample table

files.
HyStar Tample Table Extract (*.seq). Lists HyStar sample table extract files.

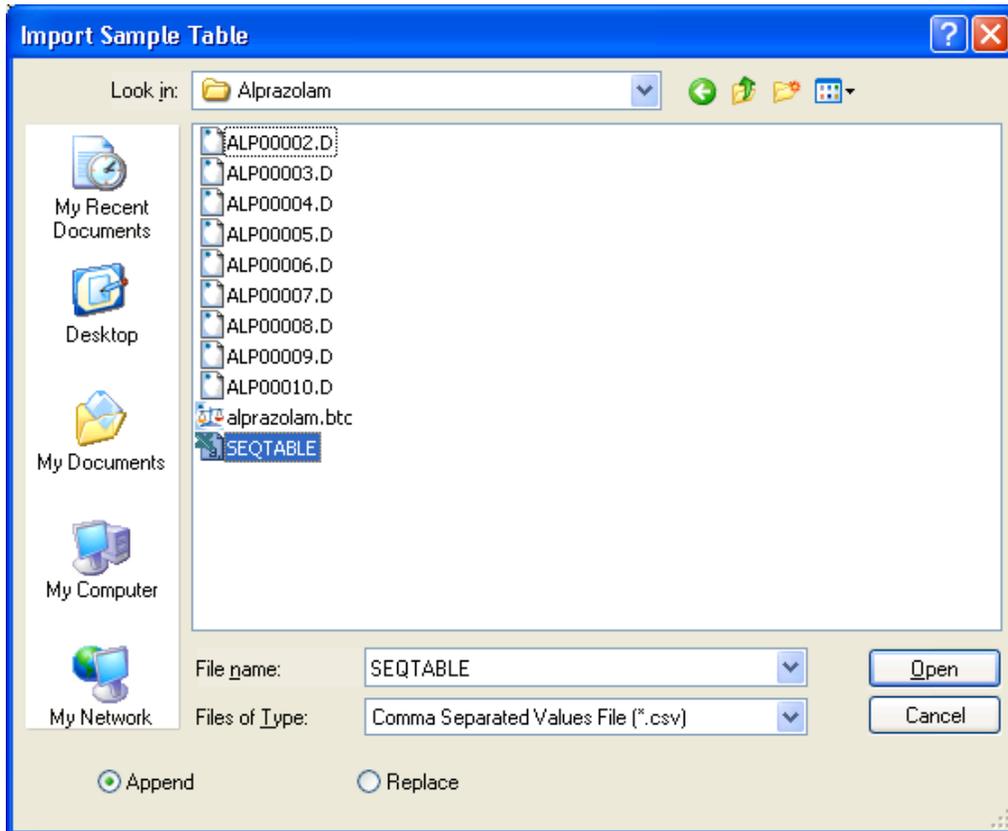


Figure 8-6 Import Sample Table dialog

Append

Select this option if the sample table to be imported should be appended to a present sample table. This setting is only relevant if on importing the sample table a batch file is currently open that contains an already imported sample table. In this case, the new sample table will be appended. Default setting.

Replace

Select this option if the sample table to be imported should replace a present sample table. This setting is only relevant if on importing the sample table a batch file is open that contains an already imported sample table. In this case, the new sample table will replace the current one.

Open

If a folder is selected, opens the folder and displays its contents in the folder list.

If a sample table file is selected, imports the respective sample table in QuantAnalysis, and enters all data files this sample table consists of and corresponding sample data already contained in the sample table in the Work Table. The name of the resulting batch file depends on how the sample table is imported. If it is imported in an existing batch file with **Append** set, the name of the batch file is not changed. If it is imported with **Replace** set, the batch file gets the name of the imported sample table file with the extension being changed to *.btc. The same applies to a sample table that is imported in a new (untitled) batch file regardless of whether **Append** or **Replace** is set.

8.5 Export Command (Work Table Window)

The **Export** command is used to export the open batch file to a Comma Separated Values Files format (*.csv) e.g. for loading this respective file in *Excel*. The data actually exported depends on whether the respective batch file is already processed. Processed batches are exported as a results table while unprocessed batches are exported as sample table in *.csv file format.

Clicking  in the Work Table window opens the **Export Sample Table** dialog which allows you to specify the name of the *.csv file to be exported and the target folder.

Save in and folder list

Navigate to the drive and folder where the exported file should be saved.

File name

Enter a new file name or select an existing name from the folder list.

Save as type

Select the type of files to be displayed in the folder list:

Comma Separated Values File (*.csv). Lists files of the Comma Separated Values Files format.

Save

If a new file name is entered, exports the open batch file to the Comma Separated Values File format and saves the resulting *.csv file in the chosen target folder.

If an already existing file name is selected, a confirmation request appears, informing you that this file already exists and asks if you really wish to overwrite it. Clicking **Yes** results in the existing file being overwritten, clicking **No** allows you to enter a new file name.

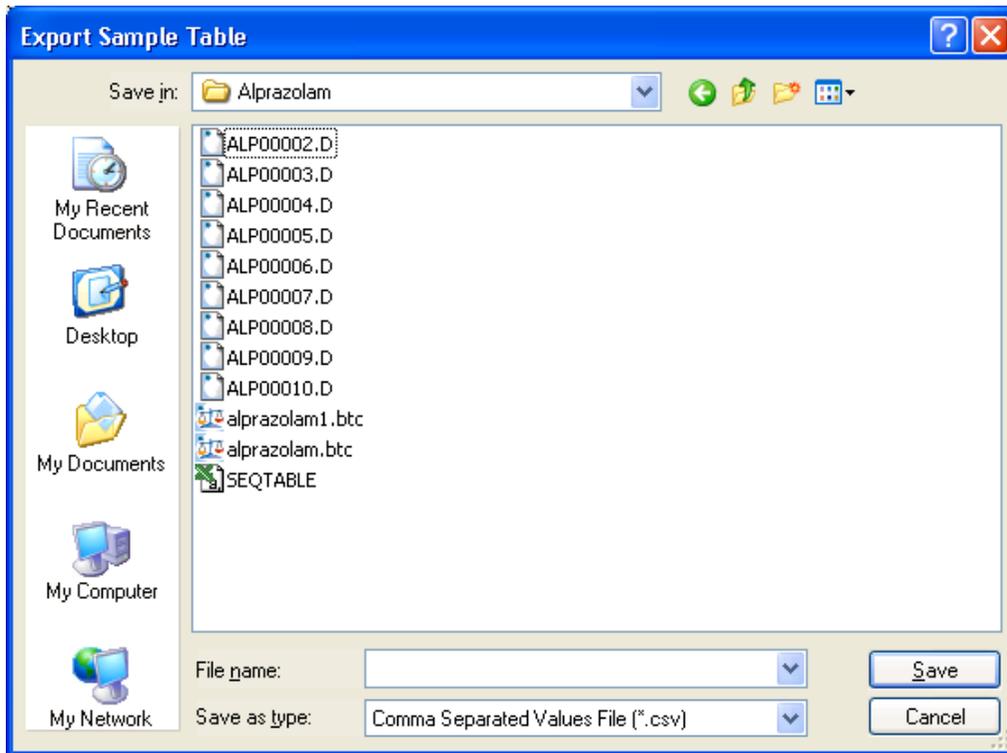


Figure 8-7 Export Sample Table dialog

8.6 Select Layout Command (Work Table Window)

The **Select Layout** command is used to select a Work Table layout suitable for that kind of quantitation you currently want to perform. This can be one of the standard layouts delivered with your system or a layout you created. Loading another layout will change the current Work Table layout according to the settings of the new layout. Work Table layout files are saved in the QuantAnalysis Layout Files format *.qal.

Clicking [Select Layout...](#) in the Work Table window opens the **Select Work Table Layout** dialog, which allows you to select a Work Table layout.

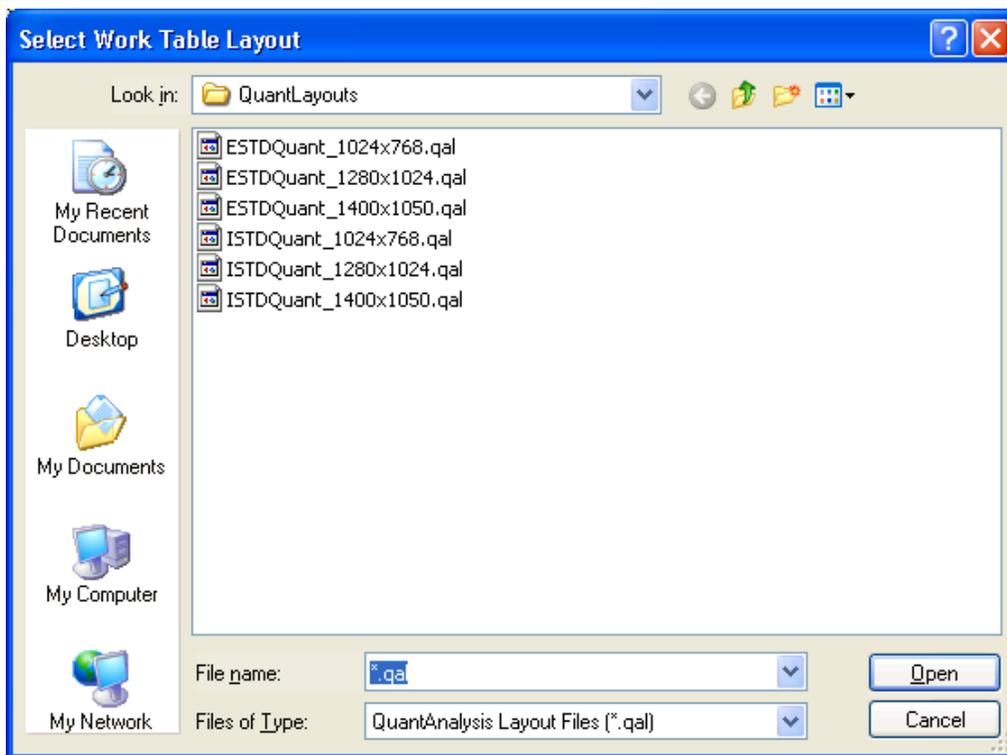


Figure 8-8 Select Work Table Layout dialog

Look in and folder list

Navigate to the drive and folder that contains the layout file you want to select. Double-click it or select it and click **Open**.

File name

Enter the file name of the layout file or select a layout file from the folder list.

Files of type

Select the type of files to be displayed in the folder list:

QuantAnalysis Layout Files (*.qal). Lists *.qal files.

All Files (*.*). Lists all data file types.

Open

When a folder is selected, opens the folder and displays its contents in the folder list.

When a layout file is selected, loads the respective layout and changes the current Work Table layout according to the settings of the new layout.

8.7 Save Layout Command (Work Table Window)

The **Save Layout** command is used to save the current the Work Table layout. Work Table layout files are saved in the QuantAnalysis Layout File format *.qal.

Clicking **Save Layout...** in the Work Table window opens the **Save Work Table Layout** dialog which allows you to specify the name of the Layout and the folder it should be saved in.

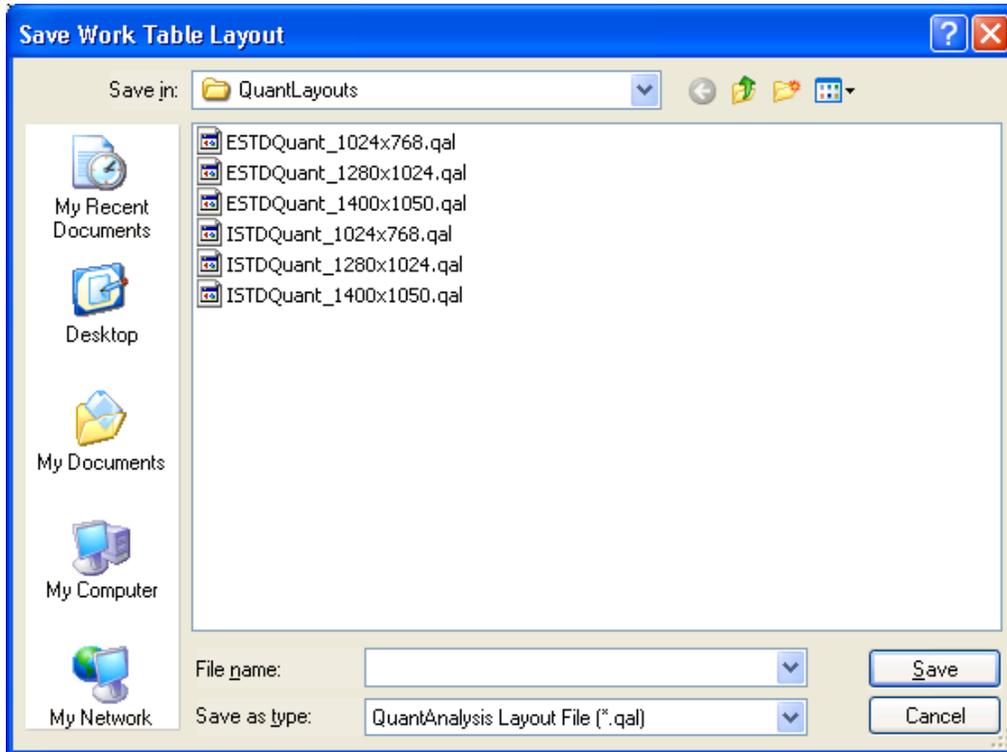


Figure 8-9 Save Work Table Layout dialog

Save in and folder list

Navigate to the drive and folder where the layout file should be saved.

File name

Enter a new file name or select an existing name from the folder list.

Save as type

Select the type of files to be displayed in the folder list:

QuantAnalysis Layout Files (*.qal). Lists *.qal files.

Save

If a new file name is entered, saves the current layout in the chosen target folder. If an already existing file name is selected, a confirmation request appears, informing you that this file already exists and asks if you really wish to overwrite it. Clicking **Yes** results in the existing file being overwritten, clicking **No** allows you to enter a new file name.

8.8 Delete Row(s) Command (Work Table Window)

The **Delete Row(s)** command is used to delete a row from the Work Table. This must be done in cases such as when you have left a row blank within a batch (because the first row that contains no entry in the **File Name** field is considered to be the end of the batch), or if you have entered a sample in a batch file by mistake. Using multiple selections, you can delete several rows at once.

Clicking  in the Work Table window removes all entries currently contained in the selected row(s) from the Work Table.

8.9 Show Column Command (Work Table Window)

The **Show Column** command is used to show a hidden Work Table column.

Clicking  in the Work Table window opens a drop-down list of all currently hidden Work Table columns. Click a column in this list to show the corresponding column in the Work Table again.



Figure 8-10 List of currently hidden Work Table columns

8.10 Hide Column Command (Work Table Window)

The **Hide Column** command is used to hide a Work Table column. Using multiple selections, you can hide several columns at once.

Clicking  in the Work Table window hides the selected Work Table column(s).

Note: Never hide the **Sample Type** and **Calib Level** columns.

8.11 Clear Areas Command (Work Table Window)

The **Clear Areas** command is used to reset the Work Table of an already processed batch file to its state before processing. This allows you to correct a mistake in the Work Table after processing has occurred, then reprocess.

Clicking  in the Work Table window clears all data entered during batch processing from the Work Table. This also releases columns that could not be edited after batch processing to be available for editing again.

8.12 Plot Column Command (Work Table Window)

The **Plot Column** command is used to plot specific quantitation data obtained for a batch file's individual data files by plotting the contents of the corresponding Work Table column. This function is restricted to specific columns.

Clicking  in the Work Table window opens the Plot Column window which displays the plot for the selected Work Table column. The plot type can be toggled between **Bar** (default), **Line** and **Area**.

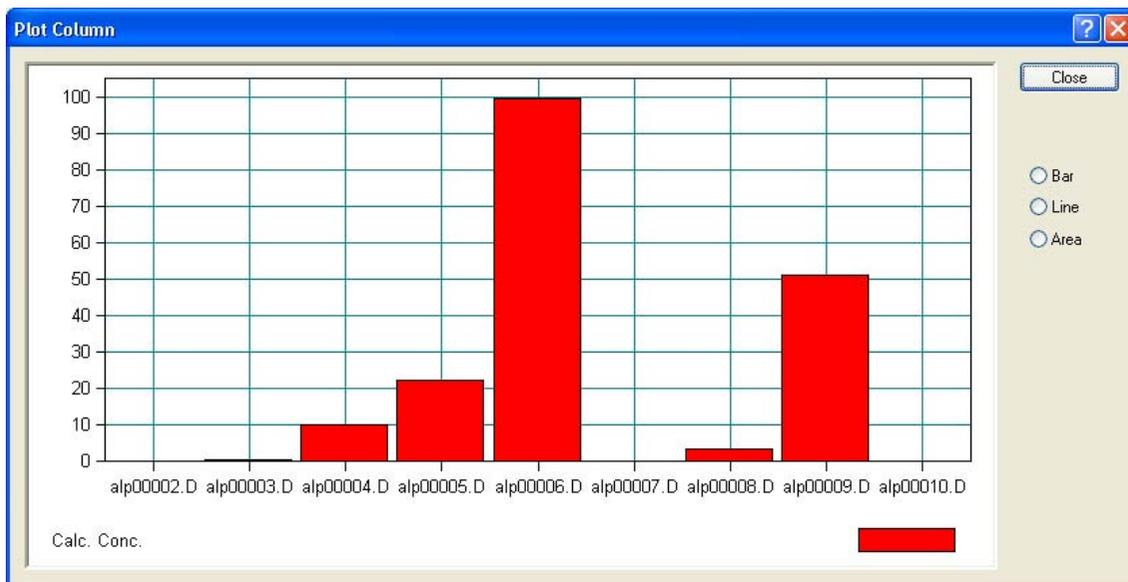


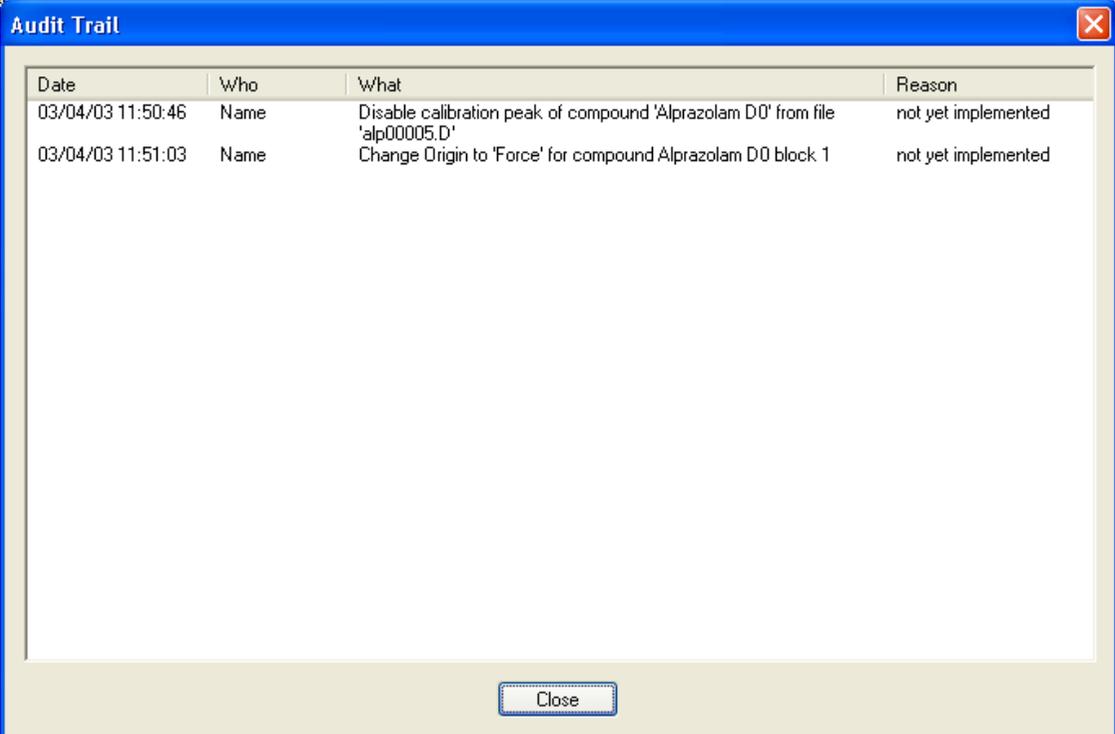
Figure 8-11 Plot of target compound concentrations calculated for the data files investigated with the concentrations displayed as bars

8.13 Show Audit Command (Work Table window)

The **Show Audit** command is used to show the audit trail for the open batch file. The audit trail lists all changes that were made to this batch file since its setup.

Clicking in the Work Table window opens the **Audit Trail** dialog, which displays the audit trail for the open batch file.

The audit trail records each change with its corresponding date and time (**Date**), name of the operator (**Who**) and what happened (**What**). It lists all changes that have been saved in previous processing of this batch file as well as all current changes already made during the running processing of this batch even if the changed state has not been saved yet. When the batch file is closed, only those changes that were saved during the running processing will be stored in the audit trail.



The screenshot shows a window titled "Audit Trail" with a close button in the top right corner. Inside the window is a table with four columns: "Date", "Who", "What", and "Reason". There are two rows of data in the table. Below the table is a "Close" button.

Date	Who	What	Reason
03/04/03 11:50:46	Name	Disable calibration peak of compound 'Alprazolam D0' from file 'alp00005.D'	not yet implemented
03/04/03 11:51:03	Name	Change Origin to 'Force' for compound Alprazolam D0 block 1	not yet implemented

Figure 8-12 Audit trail for a batch file (example)

8.14 Delete Peak Command (Chromatogram/Spectrum Window)

The **Delete Peak** command is used to delete a target or ISTD compound peak. Deleting a peak results in the corresponding data being removed from the Work Table and, therefore, from being used in quantitation of the open batch file. All corresponding quantitation results are immediately updated in the other windows.

Before selecting this command, you must display the target or ISTD compound peak you want to delete in the chromatogram view of the Chromatogram/Spectrum window.

Clicking  opens the **Confirm Delete** dialog. If quantitation was done with an internal standard you have to select whether the target or the ISTD compound peak is to be deleted by clicking **Target Peak** or **ISTD Peak**. If no internal standard was used **ISTD Peak** is disabled. On clicking **OK**, the selected peak is deleted and its peak number is removed from the chromatogram view. All corresponding entries in the Work Table are also removed.



Figure 8-13 Confirm Delete dialog (when an internal standard is used)

8.15 Manual Integration Command (Chromatogram/Spectrum Window)

The **Manual Integration** command is used to manually integrate a target or ISTD compound peak which was not recognized during the automatic integration process performed on the corresponding chromatogram or which was improperly integrated.

Manual integration is performed in the chromatogram view of the of Chromatogram/Spectrum window when the Manual Integration mode is active.

Clicking  in the Chromatogram/Spectrum window activates the Manual Integration mode. This can result in the following:

- In the case of a quantitation with internal standard, the chromatogram trace currently not selected in **Integrate (Target or ISTD)** is hidden from display. If you wish to integrate the currently hidden chromatogram, click the corresponding option to display it and hide the other chromatogram.
- For an already integrated peak, its start and end positions are indicated by two handles.

Depending on whether the peak you wish to integrate has already been integrated, proceed as follows:

Integrating an already integrated peak:

Decide which handle you would like to move, and position the mouse cursor near (3 pixel) the handle so that it changes to . Then drag the handle with the left mouse button held down to the desired position (data point) and release the mouse button. If desired, you can change the position of the second handle in the same way.

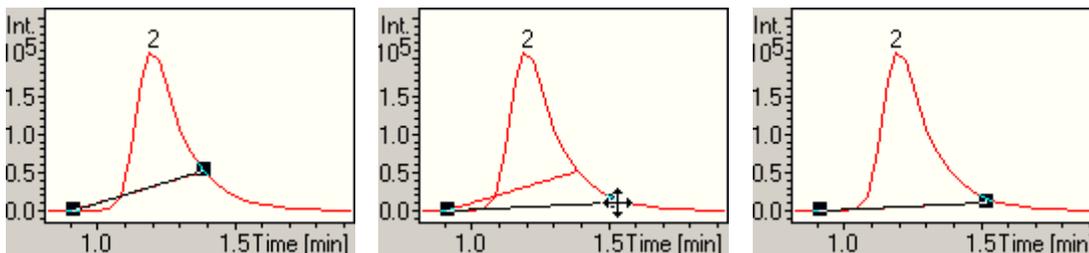


Figure 8-14 Integrating a compound peak manually

Integrating an unintegrated peak

Position the mouse cursor, for example to the start of the peak, and click the left mouse button to display the two peak handles. Then click and drag these handles to the desired positions as described above.

In both cases, the (new) calculated peak area is entered automatically in the corresponding Work Table field and the corresponding quantitation results are immediately updated in the other windows. Compound peak areas that were obtained by manual integration are colored blue in the Work Table.

Clicking deactivates the Manual Integration mode. The peak handles disappear and a hidden chromatogram trace is redisplayed.

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