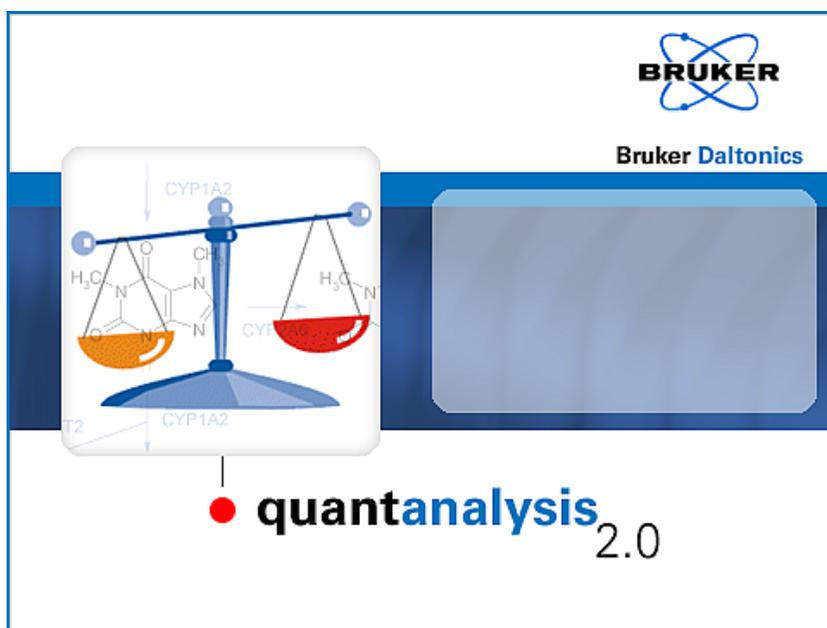

quantanalysis 2.0

User Manual



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

2 GETTING STARTED

2.1 Installing and Uninstalling QuantAnalysis

The QuantAnalysis 2.0 application installs automatically when the *Bruker Compass DataAnalysis* 4.0 application is installed on your system. The QuantAnalysis application is uninstalled automatically when you uninstall the DataAnalysis application from your system.

To work with QuantAnalysis, a valid 'ESI Compass 1.3' license must be present.

2.2 Compliance Mode and UserManagement

2.2.1 Running QuantAnalysis in Compliance or Non-Compliance Mode

QuantAnalysis can be run in 'Compliance' or 'Non-Compliance' mode. Working in Compliance mode can support you to meet *FDA 21 CFR Part 11* (FDA's rule on electronic signatures and records) requirements.

To run QuantAnalysis in Compliance mode, the *Bruker Daltonics Compass Security Pack* application providing *Bruker Daltonics UserManagement* needs to be installed either on this computer or, preferably, on a central server. When the 'Compass Security Pack' license is present, QuantAnalysis runs in Compliance mode automatically. Otherwise, QuantAnalysis runs in Non-Compliance mode.

Note: Compliance mode in the context of Compass Security Pack exclusively means the availability of Compass Security Pack tools and functionalities, which can be used to support the user to meet 21 CFR Part 11 requirements. Neither Compliance mode nor Compass Security Pack can assure full compliance with 21 CFR Part 11 requirements.

Compliance mode

The Compliance mode for QuantAnalysis offers the following features:

- Only operators created by the customer's UserManagement administrator can log into QuantAnalysis after identification by operator ID and password.

- The UserManagement administrator can administer access to QuantAnalysis by assigning individual rights to the operators he creates. These rights determine the actions the operator is allowed to perform in QuantAnalysis.
- Electronic signatures for signing electronic records are possible. Multiple signing of results is allowed.
- All Bruker Daltonics applications installed on the operator's computer can be locked and unlocked by the operator.

Note: Most of the features above apply to any application supported by the *Bruker Daltonics UserManagement*.

Non-Compliance mode

When QuantAnalysis is running in Non-Compliance mode:

- Anybody can log into QuantAnalysis because no identification by operator ID and password is needed.
- Operators who have different QuantAnalysis rights do not exist.
- QuantAnalysis and other Bruker Daltonics applications cannot be locked or unlocked.

2.2.2 Bruker Daltonics UserManagement

QuantAnalysis uses the *Bruker Daltonics UserManagement* application to run in Compliance mode.

UserManagement enables you to administer access to Bruker Daltonics applications and manage individual action rights based on operator's ID and password. Operators are created and assigned rights using the *Bruker Daltonics UserManagement Administration Tool* application. The customer's UserManagement default administrator and perhaps further UserManagement administrators (if they have the 'UserManagement Administration Tool: Administrate Operators' right) have the right to determine who can use QuantAnalysis and assign individual rights to them determining the actions these operators are allowed to perform in QuantAnalysis.

Before anybody apart from the UserManagement default administrator can log into QuantAnalysis when in Compliance mode, the UserManagement administrator has to create (an) desired operator(s) identified by operator ID and password. To become effective an operator must be assigned to an operator group that has specific rights. The UserManagement administrator can use the auto-generated operator groups or define new groups to be able to customize the assignments of rights based on specific requirements. All members within a group will have the same rights. The UserManagement administrator can also modify the default password policy and timeout settings as desired.

Note: For detailed information on how to create operators and assign rights, please refer to the UserManagement help tools.

UserManagement is client-server based. On the server PC the database defining operators and their rights is installed, on the client PC the Bruker Daltonics applications are installed.

2.2.2.1 QuantAnalysis Operating Rights in UserManagement

Specific rights for performing actions in QuantAnalysis are recorded in UserManagement. These rights can be assigned to an operator group and, therefore, to an operator. If an operator tries to perform an action without having the respective right, an error message appears.

The rights existing in QuantAnalysis are listed below. In most cases, several actions are associated with a single right, which an operator having this right is allowed to perform in QuantAnalysis. An operator must at least have the **Load/edit batches** right to be able to load and edit batch files in QuantAnalysis.

Right:	Actions permitted concerning the following subjects:
• Change parameter	Changing quantitation method parameters and calibration curve parameters.
• Delete result	Deleting a result.
• Load method	Loading quantitation methods.
• Load/edit batches	Opening and editing batch files.
• Process batch	Processing batch files using defined routines. (Includes e.g. Process, Clear Areas, Delete Peak)
• Process batch manually	Processing batch files manually. (Includes manually integrating and deleting compound peaks)
• Save batch	Saving processed batch files.
• Save method	Saving quantitation methods.

2.2.2.2 Auto-Generated Operator Groups and Their Right Assignments in QuantAnalysis

In UserManagement various auto-generated operator groups are predefined and each includes specific rights for performing actions in QuantAnalysis. The UserManagement administrator can assign a new operator to one of these auto-generated groups if he

does not want to define own groups. The administrator cannot change the group's right assignment.

The following operator groups are predefined in UserManagement:

- Administrators (auto-generated)
- Operators (auto-generated)
- Project Managers (auto-generated)
- Scientists (auto-generated)
- Service (auto-generated)

The QuantAnalysis rights assigned to the auto-generated operator groups are shown below (the figures show the respective sections in the UserManagement Administration Tool).

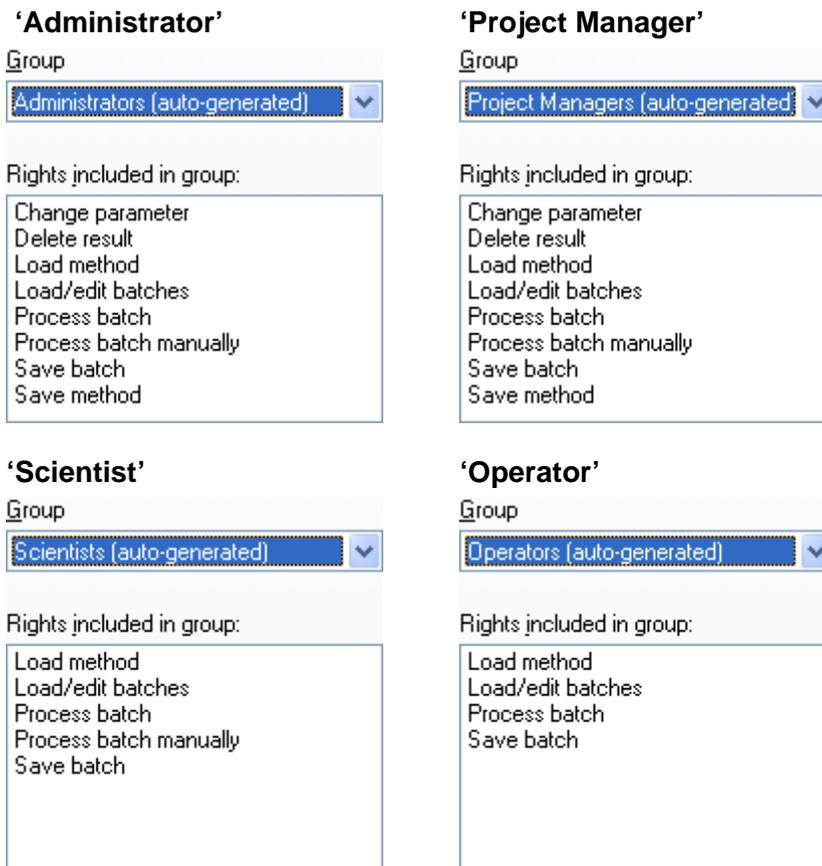


Figure 2-1 QuantAnalysis right assignments of predefined operator groups

No difference exists between an operator of the 'Administrators (auto-generated)' and the 'Project Managers (auto-generated)' group; both have all rights that are available

for this application. An operator of the ‘Scientists (auto-generated)’ group lacks the **Change parameter**, **Delete result** and **Load method** rights. An operator of the ‘Operators (auto-generated)’ group also lacks the **Process batch manually** right. The ‘Service’ group is used for service purposes of the manufacturer.

2.2.3 Electronic Records and Electronic Signatures

When QuantAnalysis is running in Compliance mode, an electronic record (= result of a batch file with corresponding method) can be signed electronically by operators who have the right to sign. An electronic signature consists of operator ID and password. Optionally, the meaning of signing can be given, and multiple signing of results is allowed.

Signing a result is done using the **History** command found in the Work Table window. You can see whether the results of a batch have already been signed by seeing the batch’s result history displayed in the **Result History** or the **Open** dialog.

2.3 Audit Trailing

A corresponding audit trail is recorded for each batch file that is set up. The audit trail lists all changes that were made to the loaded batch file with corresponding date and time, name of the operator who made the change and what was the change. This includes all changes saved during previous processing operations performed on this batch file and changes made during the current processing of this batch file, even if these changes have not been saved yet. When the batch file is closed only changes actually saved during the processing are stored in the audit trail.

You can view the audit trail of the loaded batch file using the **Show Audit** command found in the Work Table window.

2.4 Starting QuantAnalysis

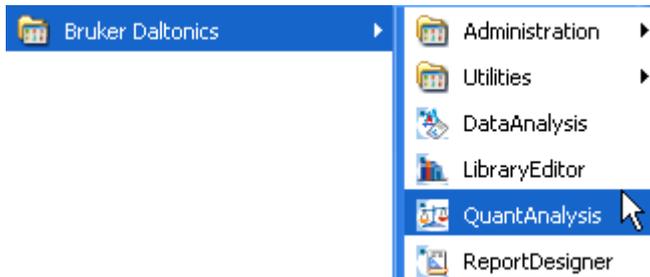
You can start QuantAnalysis from the Windows **Start** menu. During installation of the Bruker Daltonics applications package, a **Bruker Daltonics** folder was created automatically in the **Start** menu’s **Programs** folder. This folder contains the respective applications. You can also start QuantAnalysis via Windows Explorer by double-clicking an existing batch file (*.btc). This automatically starts QuantAnalysis and opens the selected batch file.

On starting QuantAnalysis, a dialog appears that requests you to log in unless you are already logged in another Bruker Daltonics application (for both Compliance and Non-Compliance mode) or the corresponding option for skipping this dialog is set (for Non-Compliance mode only).

After logging in, QuantAnalysis starts and the user interface displayed depends on the settings stored for the current user logged into Windows.

To start QuantAnalysis via the Windows Start menu:

1. Click .
2. Click **Programs**.
3. Click Bruker Daltonics.
4. Click QuantAnalysis. This starts QuantAnalysis and opens the **QuantAnalysis** dialog.



5. Log in if requested.

To start QuantAnalysis via Windows Explorer with opening the selected batch file:

1. Start Windows **Explorer**.
2. Navigate to the batch file you want to open.
3. Double-click the batch file. This starts QuantAnalysis and opens the **QuantAnalysis** dialog.
4. Log in if requested.

2.5 Logging an Operator into QuantAnalysis

When QuantAnalysis is running in Compliance mode, only operators created by the UserManagement administrator can log into QuantAnalysis (after being identified by their operator ID and password). UserManagement can lock an operator who enters the wrong password successively. The UserManagement administrator defines the maximum number of allowed false attempts.

When QuantAnalysis is running in Non-Compliance mode, any operator can log in after entering the operator ID. Identification by password is not required.

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

You must log in after starting QuantAnalysis unless you are currently logged in another Bruker Daltonics application (for both Non-Compliance and Compliance mode). When QuantAnalysis is running in Non-Compliance mode an option for automatic log in of the specified operator can be set.

In Compliance mode, if QuantAnalysis is the first Bruker Daltonics application into which you want to log after the UserManagement administrator has defined you as a new operator, you will be required to change your password.

The operator currently logged in is identified in the status bar when QuantAnalysis is running.

To log into QuantAnalysis:

1. Start QuantAnalysis or when in a running session select **Operator** from the **Help** menu. This opens the **QuantAnalysis** dialog that corresponds to the current mode in which QuantAnalysis is running.
2. In **Operator**, enter your operator ID. The operator ID is not case-sensitive.
3. In Non-Compliance mode, check **Always log in using this operator** if you want to log in automatically the next time without showing the login dialog again.
4. In Compliance mode, enter your password in **Password**.
Note: Passwords are case-sensitive. (Be careful, entering the wrong password successively will cause locking.)
5. Click **Log On**. In Compliance mode, log in will be successful only if operator ID and password are correct.
6. If you are required to change your password, change it using the **Change Password** dialog and then repeat steps 4 and 5.

2.6 Changing the Operator's Password

When QuantAnalysis is running in Compliance mode, any operator who wants to log in has to identify by password. The program requires you to change your password when you first log into a Bruker Daltonics application supporting UserManagement after the UserManagement administrator has defined you as new operator. You must also change your password after the administrator has changed your password or forced a password change on you. Apart from this, you can change your password as desired either during login or while running a QuantAnalysis session.

A new password must conform to the password policy settings defined by the UserManagement administrator; or the password will not be changed.

To change an operator's password:

1. Start QuantAnalysis or when in a running session, select **Operator** from the **Help** menu. This opens the **QuantAnalysis** dialog.
2. In **Operator**, enter your operator ID.
3. Click **Change Password**. This opens the **Change Password** dialog.
4. In **Operator**, the ID of the operator whose password can be changed is given. If the password for another operator should be changed, click **Cancel** to return to the **QuantAnalysis** dialog and repeat steps 2 and 3.
5. In **Old password**, enter your current password. The password is not displayed as you type it.
Note: Passwords are case-sensitive.
6. In **New password**, enter the new password. The new password must conform to the password policy settings.
7. In **Confirm new password**, enter your new password again.
8. Close the message confirming a successful password change. If an error message appears, repeat the corresponding steps.

2.7 Locking and Unlocking an Operator

An operator can be locked by UserManagement after too many wrong passwords are entered in succession. The UserManagement administrator defines how many wrong inputs are allowed. An operator can also be locked by direct UserManagement administrator action. The operator will get information about being locked after locking has occurred.

A locked operator cannot log into any Bruker Daltonics application supporting UserManagement. Only the UserManagement administrator can unlock a locked operator.

2.8 Locking and Unlocking QuantAnalysis and Other Bruker Daltonics Applications

When QuantAnalysis is running in Compliance mode, you can lock QuantAnalysis and all other Bruker Daltonics applications supporting UserManagement installed on your system. Only the previous operator or someone with the special right to unlock applications is permitted to unlock a locked application.

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

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.

To lock all Bruker Daltonics applications:

1. Click  or press the Ctrl+Alt+K keys. Or from the **Help** menu, select **Lock All Applications**. This opens the **QuantAnalysis** dialog that informs you that QuantAnalysis is currently locked and how it can be unlocked.

To unlock all Bruker Daltonics applications:

1. In the **QuantAnalysis** dialog, enter in **Operator** your operator ID. The dialog displays the name of the previous operator who has locked Bruker Daltonics applications. The respective ID will automatically be entered if the UserManagement administrator has set the corresponding option.
Anyone other than the previous operator who wants to unlock the applications must enter their operator ID.
Note: To do this, the operator must have the right to unlock applications.
2. If you want to change the password before logging in, click **Change Password** and change it as instructed.
3. In **Password**, enter the password for the operator named in **Operator**.
Note: Passwords are case-sensitive. (Be careful, entering the wrong password successively will cause locking).
4. Click **Log On**. If operator ID and password are correct and if the respective operator is allowed to unlock applications, QuantAnalysis is unlocked and the respective operator is logged in.

2.9 Closing QuantAnalysis

You can close QuantAnalysis when you have finished your current session. On closing, the current user interface settings are stored automatically for the current user logged into Windows.

To close QuantAnalysis:

1. Click the application's **Close**  or select **Exit** from the **File** menu.
2. If required, answer the appearing confirmation request on saving the current processing state of the open file.

3 QUANTANALYSIS USER INTERFACE

The QuantAnalysis graphical user interface consists of the title bar, the menu bar, the toolbar, the status bar and three display windows; the Work Table window, the Chromatogram/Spectrum window and the Calibration window. These elements are used for displaying and processing the quantitation data and results currently available for the open batch file. When QuantAnalysis is running in Compliance mode, the status bar displays the full name of the current operator.

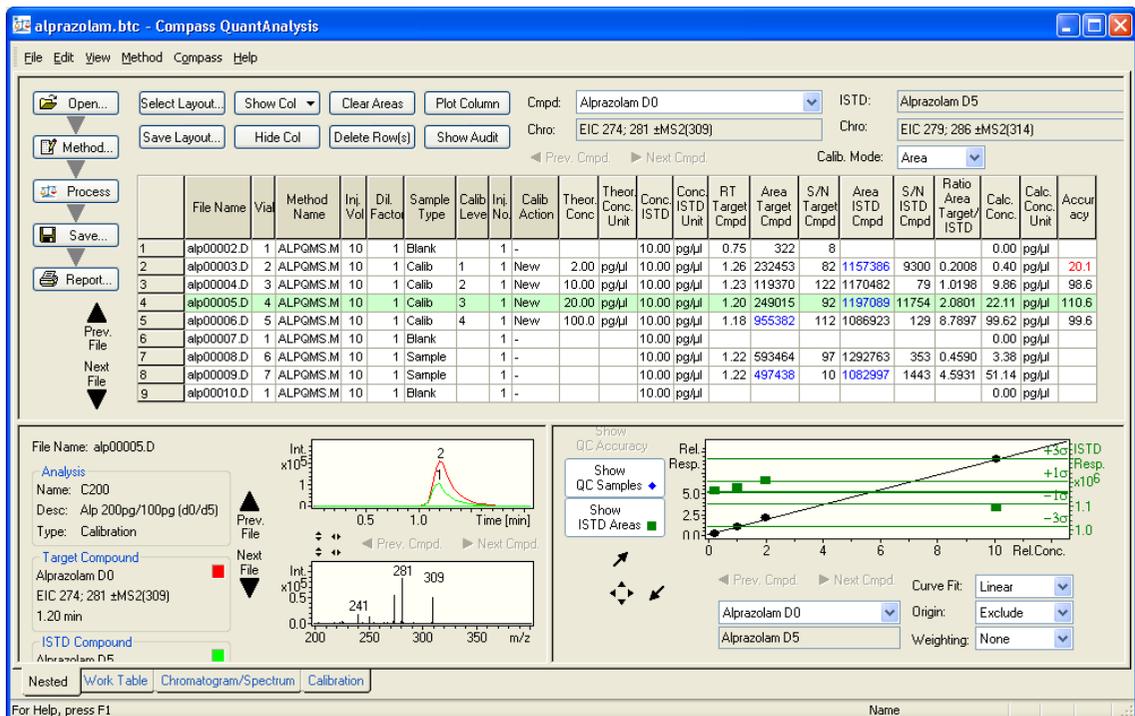


Figure 3-1 QuantAnalysis user interface in Nested display mode showing the quantitation results of the loaded, processed batch file in the Work Table window, Chromatogram/ Spectrum window and Calibration window

You can display the three windows individually or nested together to provide four different display modes that you can toggle among by clicking the corresponding **Nested**, **Work Table**, **Chromatogram/Spectrum** or **Calibration** tabs in the lower left corner of the QuantAnalysis window.

The contents of the three windows are linked dynamically. Changes made in one window are instantly updated in the other windows. For example: if you select another type

of calibration curve in the Calibration window, then that calibration curve is recalculated and redisplayed as well as all corresponding quantitation results listed in the Work Table window. This allows you to adjust parameters, or corrections like manual integration of single peaks, quickly and easily.

3.1 Work Table Window

The Work Table window displays the current Work Table and information on the target and ISTD compounds used in quantitating the open batch file. It contains buttons for customizing the Work Table layout and for processing the current Work Table contents. It also provides buttons for performing the quantitation.

	File Name	Via	Method Name	Inj. Vol	Dil. Factor	Sample Type	Calib Level	Inj. No	Calib Action	Theor. Conc.	Theor. Conc. Unit	Conc. ISTD	Conc. ISTD Unit	RT Target Cmpd	Area Target Cmpd	S/N Target Cmpd	Area ISTD Cmpd	S/N ISTD Cmpd	Ratio Area Target/ISTD	Calc. Conc.	Calc. Conc. Unit	Accuracy
1	alp00002.D	1	ALPGMS.M	10	1	Blank		1	-			10.00	pg/µl	0.75	322	8				0.00	pg/µl	
2	alp00003.D	2	ALPGMS.M	10	1	Calib	1	1	New	2.00	pg/µl	10.00	pg/µl	1.26	232453	82	1157366	9300	0.2008	0.40	pg/µl	20.1
3	alp00004.D	3	ALPGMS.M	10	1	Calib	2	1	New	10.00	pg/µl	10.00	pg/µl	1.23	119370	122	1170482	79	1.0198	9.86	pg/µl	98.6
4	alp00005.D	4	ALPGMS.M	10	1	Calib	3	1	New	20.00	pg/µl	10.00	pg/µl	1.20	249015	92	1197089	11754	2.0801	22.11	pg/µl	110.6
5	alp00006.D	5	ALPGMS.M	10	1	Calib	4	1	New	100.0	pg/µl	10.00	pg/µl	1.18	955382	112	1086923	129	8.7897	99.62	pg/µl	99.6
6	alp00007.D	1	ALPGMS.M	10	1	Blank		1	-			10.00	pg/µl							0.00	pg/µl	
7	alp00008.D	6	ALPGMS.M	10	1	Samp		1	-			10.00	pg/µl	1.22	593464	97	1292763	353	0.4590	3.38	pg/µl	
8	alp00009.D	7	ALPGMS.M	10	1	Samp		1	-			10.00	pg/µl	1.22	497438	10	1082997	1443	4.5931	51.14	pg/µl	
9	alp00010.D	1	ALPGMS.M	10	1	Blank		1	-			10.00	pg/µl							0.00	pg/µl	

Figure 3-2 Work Table window displaying data from a processed batch file

Work Table

The Work Table contains all the information that is associated with quantitating a batch of samples. By defining and saving this table you create the batch file (*.btc) that provides easy access to the complete series of files you may later use to review the results or to reprocess them.

The Work Table has two major areas indicated by either dark gray or light gray column headers. You can adjust the Work Table layout to specific quantitation tasks. Thus, the columns that are displayed depend on the loaded Work Table layout and/or the current user settings.

Sample-specific columns

The dark gray-headed columns are used to enter sample-specific data.

File Name. File name of the analysis acquired for the respective sample.

Sample Name. Name of the sample.

Sample Info. Information on the sample.

Vial. Number of the vial the sample was placed in.

Method Name. Name of the quantitation method to be used for the file. It must be given for each file and it must be the same for all files within a batch of files.

Inj. Vol. Injected volume of the sample. The value cannot be zero.

Dil. Factor. Dilution factor used for the sample. The value cannot be zero (e.g. just use "1" for all samples).

Sample Type. Type of the sample. Each sample must be defined by selecting the desired sample type from the corresponding drop-down list:

Sample. (Default) Sample to be quantified.

Calib. Sample to be used for setting up a calibration curve.

QC. Sample to be used in quality control for validation of a calibration curve.

Blank. Blank sample.

Calib. Level. Calibration level of the sample. This must be defined only for 'Calib' and 'QC' samples. 'Sample' and 'Blank' samples do not get a calibration level. QuantAnalysis uses this level to read the corresponding concentration from the table defined in the quantitation method used. The calibration level can be given in arbitrary numbers (e.g. 1, 2, 3, ...) or as text in the case of 'QC' samples (e.g. low, medium, high).

Inj. No. Injection number. This value cannot be zero.

Calib. Action. Calibration action to be carried out. This must be defined for each 'Calib' sample by selecting the desired action from the corresponding drop-down list. For all other sample types enter a hyphen, '-', which is the default setting.

New. Adds an additional calibration point to the calibration curve.

Replace. Deletes an already existing calibration point of the respective calibration level and replaces it. This applies to multiple injections of a sample.

Acq. Date. Acquisition date.

Operator. Name of the operator.

Compound- and sample-specific columns

The light gray-headed columns are used to enter compound- and sample-specific data needed for performing the quantitation as well as to display the quantitation results. In the case of a multi-component calibration, each of these columns exists multiple times, one time for each compound. The target compound whose data are currently displayed is indicated in the **Cmpd** list box found above the table.

Theor. Conc. Theoretical concentration of the target compound in the sample if it is a 'Calib' or 'QC' sample. If this column is left blank, the QuantAnalysis software enters the corresponding values defined in the quantitation method used during processing of the batch file.

Theor. Conc. Unit. Unit of the theoretical concentration of the target compound in the sample if it is a 'Calib' or 'QC' sample. If this column is left blank, the QuantAnalysis software enters the corresponding values defined in the quantitation method used during processing of the batch file.

Conc. ISTD. Concentration of the internal standard in the sample.

Conc. ISTD Unit. Unit of the internal standard in the sample.

RT Target Cmpd. Retention time of the target compound in the sample.

Area Target Cmpd (or Height Target Cmpd). Calculated peak area (or height) of the target compound in the sample. Whether peak area or peak height is calculated depends on the selected calibration mode ('Area' or 'Height').

S/N Target Cmpd. Signal-to-noise ratio of the target compound.

Area ISTD Cmpd (or Height ISTD Cmpd). Calculated peak area (or peak height) of the internal standard in the sample. Whether peak area or peak height is calculated depends on the selected calibration mode ('Area' or 'Height').

S/N ISTD Cmpd. Signal-to-noise ratio of the ISTD compound.

Ratio Area Target/ISTD (or Ratio Height Target/ISTD). Ratio between the peak area (or peak height) of the target compound and the peak area (or peak height) of the internal standard in the sample. Whether the ratio between peak areas or peak heights is calculated depends on the selected calibration mode ('Area' or 'Height').

Calc. Conc. Calculated concentration of the target compound in the sample.

Note: An 'n/c' (= not calculated) will be entered if no concentration value could be assigned to the calculated peak area (or height) because there is not data point in the calibration curve that fits this area or height value. This may happen with quadratic calibration curves only.

Calc. Conc. Unit. Unit of the calculated concentration of the indicated target compound in the respective sample.

Accuracy. Calculated accuracy determined as the ratio between the calculated concentration (evaluation of the peak area against the current calibration curve) of the indicated target compound and its (known) theoretical concentration. It will be calculated only for 'Calib' and 'QC' samples. This value allows you to assess easily the quality of the integration results and calibration curve.

Target and ISTD compound fields

Cmpd. Displays the active target compound whose corresponding data is currently shown in the Work Table. In the case of a multi-component calibration, you can click  to display the complete list of target compounds used and switch to another compound by selecting it from this list.

Chro. Displays the chromatogram trace to be used for the active compound in peak integration.

ISTD. Displays the ISTD compound used. If no internal standard is used in the respective batch file, '<None>' is displayed.

Chro. Displays the chromatogram trace to be used for the ISTD compound in peak integration.

Calib. Mode. Displays the currently active calibration mode. Two modes are available:

Area. This uses the calculated area of a target or ISTD compound peak.

Height. This uses the calculated height of a target or ISTD compound peak.

'Work Table layout' buttons



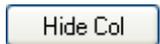
Opens the **Select Work Table Layout** dialog to select a layout.



Opens the **Save Work Table Layout** dialog to save the current layout.

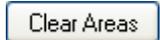


Lists the currently hidden Work Table columns and redisplay the selected column.



Hides the selected column(s).

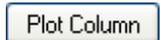
'Work Table contents processing' buttons



Resets the Work Table to the situation that existed before processing the batch. This allows all Work Table fields to be editable again. This allows you to remove incorrect entries from fields that otherwise cannot be edited after batch processing was performed.

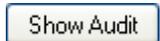


Deletes the selected row(s).

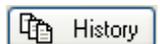


Plots the data contained in the selected column. This function is only available for certain columns.

'Showing batch information' buttons



Opens the **Audit Trail** dialog for the open batch file.

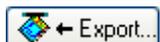


Opens the **Result History** dialog for the open batch file.

'Importing and exporting' buttons

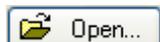


Opens the **Import Sample Table** dialog to import a sample table.

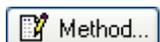


Opens the **Save Sample Table** dialog to export the batch file to a Comma Separated Values (*.csv) file. For a processed batch file its results table will be exported; otherwise, the respective sample table file will be exported.

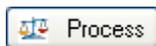
'Quantitation task flow' buttons:



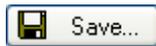
Opens the **Open Batch** dialog to open a batch file.



Starts the Method Editor to create the quantitation method to be used with opening the **General** dialog.



Processes the open batch file.



Saves the open batch file. If the respective batch has not been saved before the **Save Batch** dialog is opened.



Opens the **Print** dialog to select the desired report layout and to set up and print the selected report.

'Toggling between files' buttons



Toggles to the previous or to the next data file contained in the open batch file and displays the results corresponding to the currently selected target compound.

'Toggling between target compounds' buttons



Toggles in the case of a multi-component calibration to the previous or to the next target compound in the compound list of the currently selected data file and displays the corresponding data.

3.2 Chromatogram/Spectrum Window

After you have performed a quantitation, the Chromatogram/Spectrum window displays the individual compound peaks and the corresponding averaged mass spectra calculated for the target and ISTD compounds contained in the processed data files. Chromatogram traces display in the Chromatogram view (above) and mass spectra display in the Spectrum view (below).

You can browse through the results for all files and compounds. If compound peaks are not recognized during the quantitation process or are not properly integrated, then the integration can be corrected by means of the manual integration mode. This mode allows you to reintegrate easily and individually each compound peak without having to reprocess the entire batch of files.

Chromatogram view

The Chromatogram view displays the chromatogram trace edited from the active data file for the active target compound. If an ISTD compound is contained, its corresponding trace will be displayed. If during the automatic integration process the corresponding compound peak(s) has/have been recognized, this/these become(s) labeled with an index. You can adjust the display range of the Chromatogram view.

If a compound peak has not been recognized during automatic integration, you can switch to the manual integration mode to manually integrate the respective peak in the Chromatogram view.

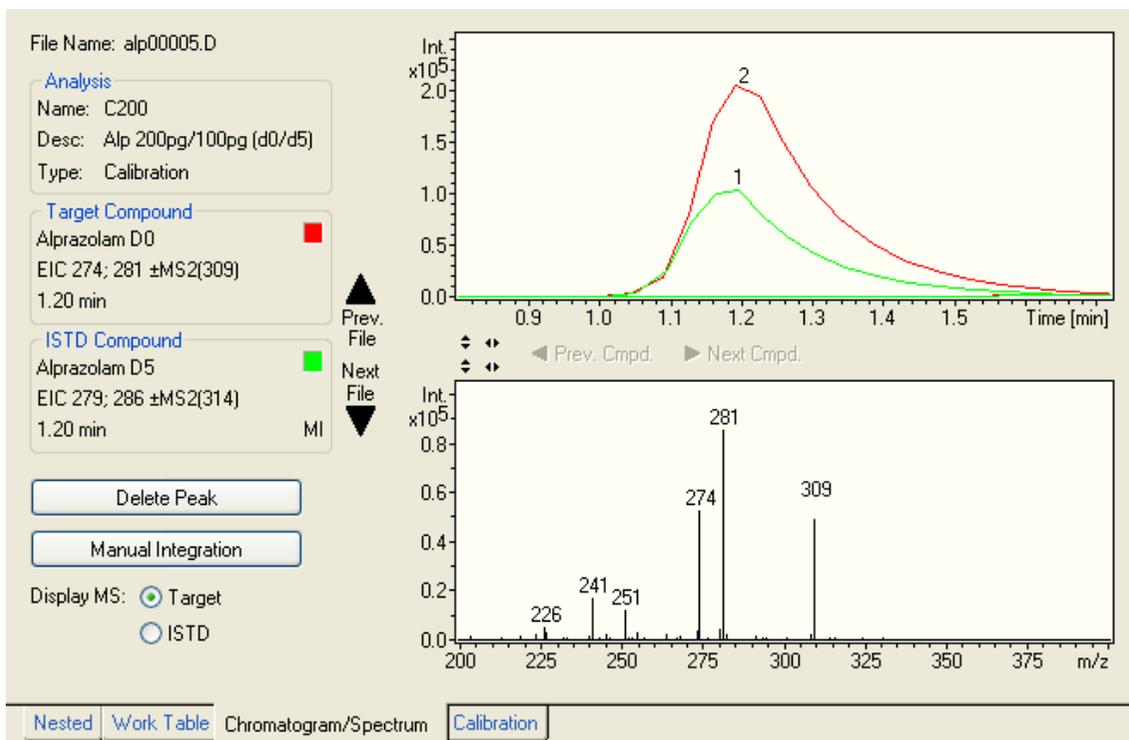


Figure 3-3 Chromatogram/Spectrum window after performing a quantitation: The Chromatogram view displays a recognized target compound peak, the Spectrum view the corresponding averaged mass spectrum

Spectrum view

The Spectrum view displays the averaged mass spectrum calculated for that peak that has been detected for the selected target compound or the ISTD compound. Which mass spectrum currently is displayed depends on the selected option (**Target** or **ISTD**). You can adjust the display range of the Spectrum view.

File Name

Displays the name of the currently active data file whose chromatogram and mass spectrum data are displayed in the Chromatogram and Spectrum views. This file is highlighted in dark green in the Work Table. You can toggle between the different data files of a batch using the **Prev. File** and **Next File** buttons.

Analysis

Displays analysis data corresponding to the active data file.

Name. Sample Name as entered in the **Sample Name** column of the Work Table.

Desc. Sample description as entered in the **Sample Info** column of the Work Table.

Type. Sample type as selected in the **Sample Type** column of the Work Table.

Target Compound

Displays the active target compound, the chromatogram trace to be edited for its quantitation and the retention time of the corresponding compound peak recognized from the active data file. In addition, it shows the color used for displaying the chromatogram trace in the Chromatogram view. In the case of a multi-component quantitation, you can toggle between the various target compounds using the **Prev. Cmpd** and **Next Cmpd** buttons.

ISTD Compound

Displays the ISTD compound assigned to the active target compound, the chromatogram trace to be edited for its quantitation and the retention time of the ISTD compound peak recognized from the active data file. In addition, it shows the color used for displaying the respective chromatogram trace in the Chromatogram view.

Display MS

Note: This parameter is displayed instead of **Integrate** when the manual integration mode is not active.

Target. Displays the averaged mass spectrum calculated for the compound peak of the selected target compound.

ISTD. Displays the averaged mass spectrum calculated for the compound peak of the selected ISTD compound.

Integrate

Note: This parameter is displayed instead of **Display MS** when the manual integration mode is active.

Target. Hides the chromatogram trace edited for the ISTD compound and displays the Manual Integration cursor for defining the target compound peak to be integrated.

ISTD. Hides the chromatogram trace edited for the target compound and displays the Manual Integration cursor for defining the ISTD compound peak to be integrated.

'Deleting peak' button



Deletes the currently displayed target or ISTD compound peak.

'Starting and stopping manual integration mode' buttons



Activates or deactivates the manual integration mode. This mode allows you to manually integrate compound peaks that were not recognized in the automatic integration process.

'Toggling between files' buttons



Toggles to the previous or to the next data file contained in the open batch file and displays the results corresponding to the currently selected target compound.

'Toggling between target compounds' buttons



Toggles, in the case of a multi-component calibration, to the previous or to the next target compound contained in the target compound list and displays its corresponding data.

'Toggling between auto-scaling and non auto-scaling' buttons

-  Toggles between auto-scaling and non-auto-scaling of the ordinate in the Chromatogram view (upper button) or Spectrum view (lower button).
-  Toggles between auto-scaling and non-auto-scaling of the abscissa in the Chromatogram view (upper button) or Spectrum view (lower button).

3.3 Calibration Window

After you have performed a quantitation, the Calibration window displays, the calibration curve for the active target compound that was calculated from the active calibration points obtained for this compound. You can change the type of calibration curve to be calculated or deactivate particular calibration points to exclude them from being used in calibration curve calculation. In addition, you can change other parameters used to set up the calibration curve.

Note: If you have made any changes in the parameter settings used for calculating the calibration curve, the corresponding data is instantly recalculated, and the new data is displayed both here and in the Work Table.

In addition, if you have performed a quantitation using an ISTD compound, you can display the corresponding ISTD response data.

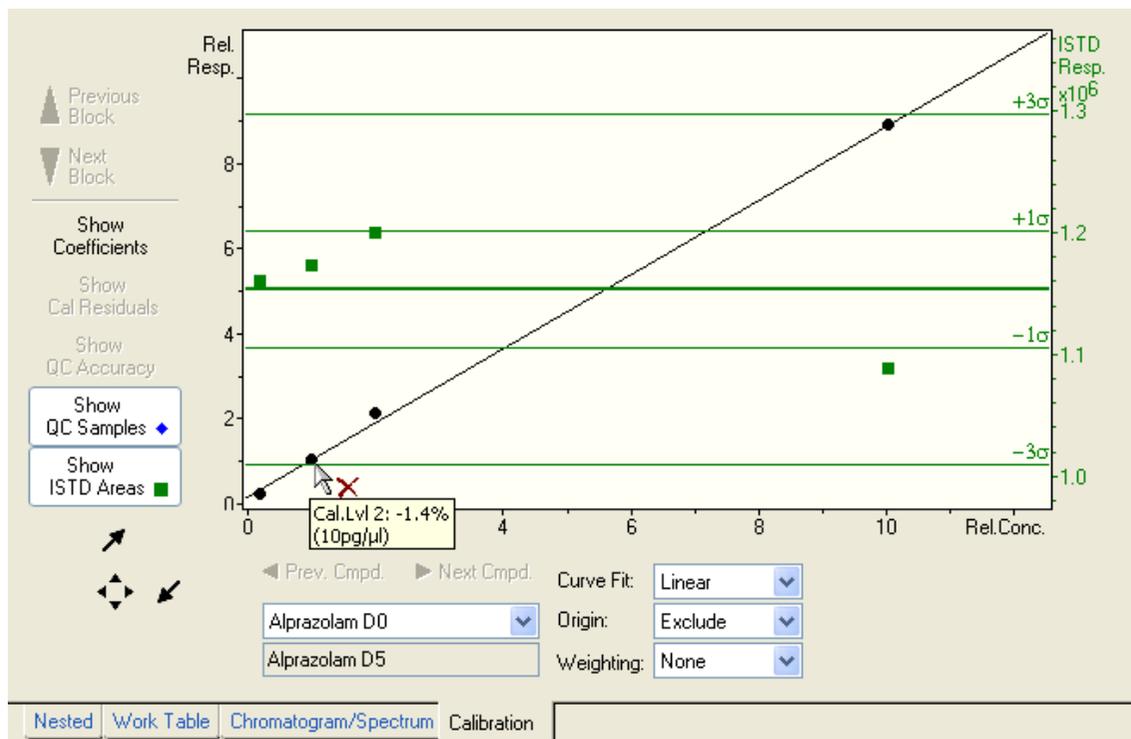


Figure 3-4 Calibration window after performing a quantitation: Display of calibration curve and ISTD data

Calibration view

Displays the individual calibration points for the active target compound and the resulting calibration curve that is calculated according to the parameters set up for the current curve. The curve is automatically recalculated if you change one of these parameters.

The calibration points are displayed as filled black points (●) or as filled green points (●) if there were multiple injections of a sample and QuantAnalysis calculates averaged calibration points. You can exclude a calibration point from being used in the calibration curve calculation by disabling it. Disabled points are indicated by an open circle (○) instead of the filled point. If necessary, you can re-enable a disabled calibration point and include it back in the calibration curve set up.

When you move the mouse cursor near a calibration point, it changes either to  or to  depending on whether the point is currently enabled or disabled. Additionally, a data tip will appear for a few seconds displaying information about the respective calibration point (calibration level, accuracy, theoretical concentration).

Depending on the current settings in the Calibration window, further data may be displayed in the Calibration view if the corresponding buttons (see below) are activated:

- The current calibration coefficients are shown when the **Show Coefficients** button is active.
- If you have performed a quantitation with an internal standard, the integration results for the ISTD compound are displayed as green squares (■) when the **Show ISTD Areas** button is active. A green line in the middle of the view marks the averaged integration result. Additional green lines above and below denote the limits of single ($+1\sigma$, -1σ) and triple ($+3\sigma$, -3σ) standard deviation from the value.
Note: It may happen that a standard deviation line is not shown since it is outside the view.
- If you have defined QC samples, the corresponding results are displayed as blue rhombs (◆) when the **Show QC Samples** button is active.
- If a QC sample is located in the batch file between the data files of calibration samples, the calibration files are separated into two blocks and QuantAnalysis calculates a separate calibration curve for each block separately. You can toggle between the different calibration curves for a target compound using the **Next Block** and **Previous Block** buttons, which in this case will be active.

You can adjust the display range of the Calibration view.

(Target compound list)

Displays the selected target compound whose calibration data is displayed in the Calibration view. In the case of a multi-component quantitation, click  to select the target compound whose calibration curve you wish to display from this list or use



(ISTD compound)

Displays the ISTD compound assigned to the selected target compound. The calibration points calculated for this ISTD are displayed in the Calibration view as dark green squares.

Curve Fit

This parameter sets the type of calibration curve to be calculated. To change the curve fit, select another one from this list.

Average RF. Mean "Response Factor" (RF).

Linear. Linear equation.

Quadratic. Quadratic equation.

Cubic. Cubic equation.

Origin

This parameter sets how the point of origin (data point 0;0) will be included in the calculation of the calibration curve. To change the mode of origin, select another option

from this list.

Exclude. Calculates the calibration curve only from the data points.

Include. Calculates the calibration curve from the data points and the point of origin.

Force. Calculates the calibration curve from the data points and forces it through the point of origin.

Weighting

This parameter sets how the data points will be weighted in calibration curve calculation. To change the weighting of calibration points, select another option from this list. The following weightings are possible: **None** (Default), **1/X**, **1/X²**, **1/Y**, **1/Y²**, **In-In**, **log-log**.

'Toggling between target compounds' buttons



Toggles in the case of a multi-component calibration to the previous or to the next target compound in the compound list of the currently selected data file and displays the corresponding data.

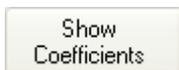
'Toggling between blocks' buttons



Toggles in case of a multiple calibration curve setup between the calibration curves calculated for the previous and the next block of calibration samples for the selected target compound.

'Showing specific data' buttons

Activating one of these buttons (button becomes highlighted) results in the corresponding data being displayed in the Calibration view.



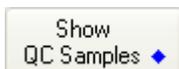
Toggles between displaying and not displaying the current calibration coefficients.



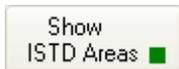
This tool is not yet implemented.



This tool is not yet implemented.



Toggles between displaying and not displaying QC sample data.



Toggles between displaying and not displaying the ISTD data and areas.

'Changing scaling' buttons



Increases the Calibration view's ordinate and abscissa scaling by a factor of 5 each time you click this button (e.g. if abscissa and ordinate each display a range from 0 to 10, then clicking this button once results in abscissa and ordinate becoming re-scaled to only display a range from 0 to 2).



Decreases the Calibration view's ordinate and abscissa scaling by a factor of 5 each time you click this button.



Resets a changed Calibration view's ordinate and/or abscissa scaling to full display of all data.

3.4 Nested Display of Windows

In the Nested display mode, the Work Table, Chromatogram/Spectrum and Calibration windows are nested together and displayed simultaneously. You can adjust the Nested display, and therefore the data currently shown, by dragging the corresponding window borderlines.

Note: After the first start of QuantAnalysis, the Nested display may seem to show only one of these three windows. In this case, rearrange the borderlines to an appropriate view.

3.5 Customizing the User Interface

3.5.1 Modifying the Work Table Layout

The layout of the Work Table can be adjusted for the kind of quantitation you wish to do. For example, if you want to do an external calibration you can hide all Work Table columns which define parameters of an internal standard. When you have optimized a Work Table layout for a specific kind of quantitation, you can save the modified layout and reload it anytime you are going to do this kind of quantitation.

3.5.1.1 Hiding a Work Table Column

You can hide a Work Table column which you currently do not need for the quantitation you wish to perform. Using multiple selections, you can hide several columns at once.

Note: Make sure that the columns **Sample Type** and **Calib Level** are always displayed.

To hide a single column:

1. Click on the header of the desired column.
2. Click .

To hide a series of neighboring columns:

1. Hold down the Shift key and click the headers of the first and last columns in the desired series. Or position the mouse cursor on the header of the first column in the desired series and drag it, with the left mouse button held down, to the header of the last column.
2. Click .

To hide multiple individual columns:

1. Hold down the Ctrl key and click the headers of each desired column.
2. Click .

3.5.1.2 Showing a Hidden Work Table Column

You can show a currently hidden Work Table column again.

To show a hidden column:

1. Click . A drop-down field appears listing all currently hidden Work Table columns.
2. Click the desired column name. This displays the respective column

3.5.1.3 Changing the Width of a Work Table Column

You can change the current width of a Work Table column e.g., if an entry is not shown in full length.

To change the width of a column:

1. Position the mouse cursor on the left or right border of the desired column head to

display the Column Width cursor .

2. Drag the border with the left mouse button held down until the desired width is reached.

3.5.1.4 Saving a Work Table Layout

The current layout of the Work Table can be saved, e.g. after you have optimized it for a particular kind of quantitation. This allows you to select this Work Table layout whenever you want to perform this type of quantitation. Work Table layout files are saved in the QuantAnalysis Layout File format *.qal.

To save the current Work Table layout:

1. Click . This opens the **Save Work Table Layout** dialog for saving a layout file.
2. In **Save in** and the folder list, navigate to that drive and folder in which you want to store the layout file.
3. Depending on whether you want to save the layout under a new or an existing file name, do one of the following:
 - If you want to save the layout file under a new name, enter the new name in **File name**.
 - If you want to save the layout file under an existing name, select this name from the folder list.
4. Click **Save**.

3.5.1.5 Selecting a Work Table Layout

You can select a Work Table layout suitable for the kind of quantitation you want to perform. This can be one of the standard layouts available for external or internal standard quantitation tasks or a self-created layout. Loading another layout changes 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).

To select a Work Table layout:

1. Click . This opens the **Select Work Table Layout** dialog for loading a *.qal format file.
2. In **Look in** and the folder list, navigate to the folder that contains the layout file you want to load.
3. Double-click the desired layout file. Or select it and click **Open**.

3.5.2 Changing Data Display Ranges

You can adjust the display range of the Chromatogram and Spectrum views of the Chromatogram/Spectrum window and the Calibration view of the Calibration window.

3.5.2.1 Changing the Display Range of the Chromatogram and Spectrum Views

You can adjust the display range of the Chromatogram or Spectrum view in the Chromatogram/Spectrum window to the optimal display of the data you are interested in.

You can toggle the ordinate and abscissa between auto-scaling and non auto-scaling: auto-scaling means that the display range of an axis is automatically adjusted to display the maximum measured values. If auto-scaling is disabled, the first displayed data or the scaling that was used at the moment of auto-scaling deactivation specifies the display range for the subsequently displayed data. Whether auto-scaling of an axis is enabled or not, you can see from the status (highlighted or not) of the corresponding auto-scaling button.

In addition, you can displace, increase or decrease the display range of ordinate or abscissa and, if desired, reset a changed scaling to full display of data.

To toggle between auto-scaling and non auto-scaling of ordinate or abscissa:

1. Click  or  that corresponds to the axis you wish to toggle to auto-scaling or non auto-scaling.

To displace the display range of ordinate or abscissa:

1. Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor.
2. Drag the cursor with the left mouse button held down either right, left, up, or down until the respective axis is displaced as desired. Then release left mouse button. During dragging, the scaling and the values displayed are continuously updated to show the effect of displacement.

To increase or decrease the display range of ordinate or abscissa:

1. Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor.
2. Drag the cursor with the right mouse button held down either downwards, to the left (for increasing), upwards or to the right (for decreasing), until the desired display range is reached. Then release the right mouse button. During dragging, the scaling and the values displayed are continuously updated to show the effect of the changes.

To reset a changed ordinate or abscissa scaling to full display of data:

- ▶ Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor and double-click the left mouse button. This resets the axis.

3.5.2.2 Changing the Display Range of the Calibration View

You can adjust the display range of the Calibration view in the Calibration window to the optimal display of the data you are interested in. You can change the ordinate and abscissa scaling either continuously by using the mouse or by predefined steps using the appropriate buttons. By using the mouse, you can independently adjust the display range of the ordinate and abscissa.

To displace the display range of the ordinate or abscissa:

1. Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor.
2. Drag the cursor with the left mouse button held down either to the right, left, up, or down until the axis is displaced as desired. Then release the left mouse button. During dragging, the scaling and the values displayed are continuously updated to show the effect of displacement.

To continuously increase or decrease the display range of ordinate or abscissa:

1. Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor.
2. Drag the cursor with the right mouse button held down either downwards, to the left (for increasing), upwards or to the right (for decreasing), until the desired display range is reached. Then release the right mouse button. During dragging, the scaling and the values displayed are continuously updated to show the effect of the changes.

To increase or decrease the display range of ordinate and abscissa in defined steps:

1. Click  to increase the display range of ordinate and abscissa by a factor of 5.
-or-
Click  to decrease the display range of ordinate and abscissa by a factor of 5.

To reset a changed axis scaling to full display of data:

- 1 Position the mouse cursor left of the ordinate or below the abscissa to display the Vertical  or Horizontal  scaling cursor and double-click the left mouse button. This resets the axis.

-or-

Click . This resets both ordinate and abscissa.

4 CREATING AND MANAGING BATCH FILES

4.1 Creating a New Batch File

To perform a quantitation, first you have to create a Batch Files format file (*.btc) file, which must contain all the data files that have been acquired from the various calibration and "unknown" sample solutions. Optionally, a batch file can contain further data files from quality control and/or blank samples. Additionally, the batch file must contain specific information about the data files including their sample type, calibration level, and calibration action.

How you create a batch file depends on how the data files to be used in quantitation were acquired. Data acquisition can be done within a sample table set up in either the Bruker Compass HyStar or the Agilent ChemStation application. In this case, you can import the respective sample table with automatically entering some of the data required for batch creation in the QuantAnalysis Work Table. Alternatively, you can use a series of individually acquired data files; in this case, you have to enter all data required manually.

QuantAnalysis can handle data files obtained by multiple injections of the same sample. The program identifies such samples by having the same calibration level but different injection numbers.

Furthermore, QuantAnalysis allows set up of separate calibration curves for different sample series with e.g. different matrices but the same target compound in one batch sequence. This requires the respective data files to be entered in the batch file as separate blocks.

Once a batch file has been set up, you can create or open a quantitation method suitable for processing the respective batch file and then process the batch file.

4.1.1 Creating a Batch File from a Sample Table

A batch file can be created from an Agilent ChemStation sample table stored in Comma Separated Values Files format (*.csv) or a HyStar sample table extract stored in HyStar Sample Table Extract format (*.seq). You can import the respective sample table into QuantAnalysis, enter additional information required to perform a quantitation, and save the data as a batch file (*.btc).

You can import the sample table into a new (untitled) batch file or an existing batch file that already contains a sample table. In the latter case, you have the choice between

appending the new sample table to the existing one, and replacing the existing by the new one.

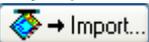
Note: To import a sample table in an existing batch file the respective batch file must be open and unprocessed.

On importing a sample table, specific information is automatically entered in the Work Table. This includes the names of the data files in the sample table, corresponding sample names, vial positions, and injection volumes. The resulting batch file automatically gets a name, which depends on how the sample table is imported. If the sample table is imported in an existing batch file with the **Append** option set, the name of the batch file is not changed. If it is imported with the **Replace** option set, the batch file gets the name of the imported sample table with the extension changed to *.btc. The same applies to a sample table that is imported in a new (untitled) batch file. You can change this name, if desired.

To perform a quantitation QuantAnalysis needs additional information, which you have to enter manually, e.g., the sample type and calibration level for each data file used. After entering all necessary and any additional information in the Work Table, review the Work Table. Check that the entries in the **File Name**, **Sample Name**, **Sample Info**, **Vial**, **Method Name**, **Inj. Vol.**, and **Sample Type** columns are complete. After processing the batch file these columns cannot be edited again so that changes you try to make in these fields will be ignored. If you notice a mistake in one of these particular fields after batch processing, you can reset the Work Table to the situation before processing.

To create a batch file from a sample table:

1. Click the **Work Table** tab to switch to full-screen display for the Work Table.
2. Depending on whether you want to import the sample table into a new (untitled) or an existing batch file, do one of the following:
 - If you want to import it into a new batch file and a batch file is already open, select **New** from the **File** menu and, if needed, answer the pop-up confirmation request on saving the open batch file. This closes the respective file and clears the Work Table.
 - If you want to import it into an existing batch file, open the desired batch file if not already open.

3. Click  to select and import the sample table from which you want to create a batch file.

This automatically enters specific information stored in the sample table into the **File Name**, **Sample Name**, **Sample Info**, **Vial**, **Method Name**, **Inj. Vol**, **Dil Factor**, **Sample Type**, **Calib Level**, **Inj. No.** and **Calib Action** columns. You have to check these entries and, if necessary, change them.

4. Click  to load a Work Table layout suitable for the type of quantitation

you want to perform. Alternatively, adjust the current Work Table layout accordingly.

Tip: You can save an optimized layout using  to use it for further quantitations.

5. In the **Method Name** column, check that a method is assigned to each data file. Within a batch of files, this method name must be the same for all. Change any differing method names.
6. In the **Inj. Vol.** column, check that an injection volume is given for each sample that must differ from zero. Change incorrect values.
7. In the **Dil. Factor** column, check that the given dilution factors differ from zero. Change incorrect values.
8. In the **Sample Type** column, for each sample define its sample type.
9. In the **Calib Level** column, for each 'Calib' or 'QC' sample define its calibration level.

In case of multiple injections of the same sample, you must assign the same calibration level to these samples

Note: In the actual software version, the concentrations belonging to the different calibration levels have to be defined later during creating the quantitation method.

10. In the **Inj. No.** column, check that the given numbers differ from zero and change incorrect values.

In case of multiple injections of the same sample QuantAnalysis, on importing a sample table, only reads the total number of injections for the same sample and therefore sets all **Inj. No.** fields belonging to the same sample to this total number, e.g. '3'. You have to change these fields manually to '1', '2', and '3' for the corresponding data files having the same **Calib Level**.

11. In the **Calib Action** column, for each 'Calib' sample define its calibration action to be performed. Choosing **New** will add an additional calibration point to the calibration curve whereas choosing **Replace** will delete an already existing calibration point from the calibration curve and replace it by a new one. This latter action can be used in the case of multiple injections of a sample.
12. After entering all necessary and any additional information in the Work Table, review the Work Table. Check that the entries in the **File Name**, **Sample Name**, **Sample Info**, **Vial**, **Method Name**, **Inj. Vol.**, and **Sample Type** columns are complete. After processing the batch file these columns cannot be edited anymore so that changes you try to make in these fields will be ignored.

Note: If you notice a mistake in one of these particular fields after batch processing, you can reset the Work Table to the situation before processing and repeat the respective entries.

13. Check that all data files belonging to 'Calib' type samples are placed together within the sequence of the batch, as it is needed for the calibration curve setup you

wish to perform.

Please consider to the following fact: The program will calculate separate calibration curves if more than one block of 'Calib' type samples exist, separated within the sample by a 'Sample', 'QC' or 'Blank' type sample. This means:

- If the calibration points from all 'Calib' type samples contained in a batch should be entered into one calibration curve, then all 'Calib' type samples must be entered as one block (e.g. see the example below: all 'Calib' samples have been entered as one block consisting of the rows 2 to 5). This means e.g., if you want to do an external calibration and you have done alternating runs of unknown and calibration samples you cannot enter the files in the same order as you have run them. Therefore, after importing the sample table you must sort all 'Calib' type samples within one block.
- If more than one calibration curve should be setup for a batch, the respective 'Calib' type samples must be placed into different blocks which must be separated by at least one 'Sample', 'QC' or 'Blank' type sample. This will be necessary e.g. if you want to quantitate different sample series with e.g. different matrices but the same target compound in one sample.

You can rearrange the data files within the sample, if necessary, by moving the Work Table rows accordingly.

14. Check that within the Work Table there are no rows left blank since QuantAnalysis considers the first row that contains no **File Name** entry to be the end of the batch. If there are blank rows, delete them.
15. Save the batch file using either the **Save** or the **Save As** command from the **File menu**.

Note: Batch file saving can be performed even earlier within this procedure. In this case, afterwards continue filling the Work Table and save the modified batch file again.

The following example shows an Agilent ChemStation sample table imported into QuantAnalysis. In the upper figure, you can see the Work Table entries automatically made on importing the sample table. The lower figure shows the Work Table as finally set up. The respective sample consists of four standard solutions containing the target compound, Alprazolam d0, at concentrations of 2, 10, 20, and 100 pg/μl, and the ISTD compound, Alprazolam d5 (penta-deuterated derivative), at a constant concentration of 10 pg/μl. Two solutions containing 5 or 50 pg/μl d0 and 10 pg/μl d5 function as "unknown" samples. Additionally, three injections of a blank solution were used.

	File Name	Sample Name	Sample Info	Vial	Method Name	Inj. Vol	Dil. Factor	Sample Type	Calib Level	Inj. No.	Calib Action	Acq. Date
1	alp00002.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	0	1	-	
2	alp00003.D	C20	Alp 20pg/100pg (d0/d5)	2	ALPQMS.M	10	0.05	Calib	1	1	Replace	
3	alp00004.D	C100	Alp 100pg/100pg (d0/d5)	3	ALPQMS.M	10	0.01	Calib	2	1	Replace	
4	alp00005.D	C200	Alp 200pg/100pg (d0/d5)	4	ALPQMS.M	10	0.005	Calib	3	1	Replace	
5	alp00006.D	C1000	Alp 1000pg/100pg (d0/d5)	5	ALPQMS.M	10	0.001	Calib	4	1	Replace	
6	alp00007.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	4	1	-	
7	alp00008.D	S50	Alp 50pg/100pg (d0/d5)	6	ALPQMS.M	10	1	Sample	4	1	-	
8	alp00009.D	S500	Alp 500pg/100pg (d0/d5)	7	ALPQMS.M	10	1	Sample	4	1	-	
9	alp00010.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	4	1	-	
10								Sample			-	
11								Sample			-	
12								Sample			-	

Figure 4-1 Work Table entries automatically filled in by importing an Agilent ChemStation sample table

	File Name	Sample Name	Sample Info	Vial	Method Name	Inj. Vol	Dil. Factor	Sample Type	Calib Level	Inj. No.	Calib Action	Theor. Cc
1	alp00002.D	Blank	Blank	1	ALPQMS.M	10	1	Blank		1	-	
2	alp00003.D	C20	Alp 20pg/100pg (d0/d5)	2	ALPQMS.M	10	1	Calib	1	1	New	
3	alp00004.D	C100	Alp 100pg/100pg (d0/d5)	3	ALPQMS.M	10	1	Calib	2	1	New	
4	alp00005.D	C200	Alp 200pg/100pg (d0/d5)	4	ALPQMS.M	10	1	Calib	3	1	New	
5	alp00006.D	C1000	Alp 1000pg/100pg (d0/d5)	5	ALPQMS.M	10	1	Calib	4	1	New	
6	alp00007.D	Blank	Blank	1	ALPQMS.M	10	1	Blank		1	-	
7	alp00008.D	S50	Alp 50pg/100pg (d0/d5)	6	ALPQMS.M	10	1	Sample		1	-	
8	alp00009.D	S500	Alp 500pg/100pg (d0/d5)	7	ALPQMS.M	10	1	Sample		1	-	
9	alp00010.D	Blank	Blank	1	ALPQMS.M	10	1	Blank		1	-	
10								Sample			-	
11								Sample			-	
12								Sample			-	

Figure 4-2 Finally set up Work Table as needed for processing the batch file created from the imported Agilent ChemStation sample table

4.1.1.1 Importing a Sample Table

You can import an Agilent ChemStation sample table stored in Comma Separated Values Files format (*.csv) or a HyStar sample table extract stored in HyStar Sample Table Extract format (*.seq) into QuantAnalysis in order to create a batch file for this sample.

Note: To import a sample table into an existing batch file the respective batch file must be open and still unprocessed.

To import a sample table:

1. Depending on whether you want to import the sample table into a new (untitled) or an existing batch file, do one of the following:

- If you want to import it into a new batch file and a batch file is already open, select **New** from the **File** menu and, if needed, answer the pop-up confirmation request on saving the open batch file. This closes the respective file and clears the Work Table.
 - If you want to import it into an existing batch file, open the desired batch file if not already open.
2. Click  → Import... This opens the **Import Sample Table** dialog.
 3. In **Files of type**, select the type of sample tables to be shown in the folder list.
 4. In **Look in** and the folder list, navigate to that folder that contains the sample table you want to import.
 5. If a batch file is open, select how to proceed with the sample table when importing it. This setting is of no importance if the sample table should be imported into a new batch file.
 - Select **Append**, if the imported sample table should be appended to the present one.
 - Select **Replace**, if the imported sample table should replace the present one.
 6. Double-click the desired sample table or select it and click **Open**.
 7. Save the resulting batch file under a desired file name.

4.1.2 Creating a Batch File for a Set of Individually Acquired Data Files

You can also create a batch file for a set of individually acquired data files, which must be contained in the same directory.

In contrast to creating a batch file from a sample table, it is not possible to import data in the Work Table. Thus, you have to enter all necessary information manually. However, you can make your work easier e.g. by copying Work Table entries multiple times using either copy and paste or performing an 'Excel-like fill' of columns.

After entering all necessary and any additional information in the Work Table, review the Work Table. Check that the entries in the **File Name**, **Sample Name**, **Sample Info**, **Vial**, **Method Name**, **Inj. Vol.**, and **Sample Type** columns are complete. After processing the batch file, these columns cannot be edited anymore so that entries you try to make in these fields will be ignored. If you notice a mistake in one of these particular fields after batch processing, you can reset the Work Table to the situation before processing.

To create a new batch file:

1. Click the **Work Table** tab to switch to full-screen display for the Work Table.

2. If a batch file is already open, select **New** from the **File** menu and, if needed, answer the pop-up confirmation request on saving the open file. This closes the respective file and clears the Work Table.
3. Click  to load a Work Table layout suitable for the type of quantitation you want to perform. Alternatively, adjust the current Work Table layout accordingly.

Tip: You can save an optimized layout using  to use it for further quantitations.

4. In the **File Name** column, enter the names of the individual data files. Make sure that all data files needed are copied into the same directory.

Note: The file names must be entered together with the file extension.

In placing 'Calib' type samples within the sequence of a batch, please consider the following fact: the program will calculate separate calibration curves if more than one block of 'Calib' type samples exist, separated within the sequence by a 'Sample', 'QC' or 'Blank' type sample. This means:

- If the calibration points from all 'Calib' type samples contained in a batch be entered into one calibration curve, then all 'Calib' type samples must be entered as one block (e.g. see the example below: all 'Calib' samples have been entered as one block consisting of the rows 1 to).

This means e.g., if you want to do an external calibration and you have done alternating runs of unknown and calibration samples you cannot enter the files in the same order as you have run them. You must sort them accordingly.

- If more than one calibration curve should be setup for a batch, the respective 'Calib' type samples must be placed into different blocks which must be separated by at least one 'Sample', 'QC' or 'Blank' type sample.

This will be necessary e.g. if you want to quantitate different sample series with e.g. different matrices but the same target compound in one sample.

You can rearrange the data files within the sample, if required, by moving the Work Table rows accordingly.

5. In the **Sample Info** column, enter that sample information that corresponds to the respective data file.
6. In the **Method name** column, check that a method is assigned to each data file. Within a batch of files, this method name must be the same for all. Change any differing method names.
7. In the **Inj. Vol.** column, enter the injection volumes. They must differ from zero.
8. In the **Dil. Factor** column, enter the dilution factors. They must differ from zero.
9. In the **Sample Type** column, select for each sample its sample type.
10. In the **Calib Level** column, select for each 'Calib' or 'QC' sample its calibration level. In case of multiple injections of the same sample, you must assign the same calibration level to these samples

Note: In the actual software version, the concentrations that belong to the different calibration levels have to be defined later during creating the quantitation method.

11. In the **Inj. No.** column, enter the corresponding injection numbers.
12. In the **Calib Action** column, select for each 'Calib' sample its calibration action to be performed.
13. After entering all information that is necessary, or that you want to see additionally in the Work Table, review the Work Table. Check that the entries in the **File Name**, **Sample Name**, **Sample Info**, **Method Name**, **Inj. Vol.**, and **Sample Type** columns are complete. After processing the batch file these columns may not be edited anymore so that changes you try to make in these fields will be ignored.

Note: If you notice a mistake in one of these fields after batch processing, you can reset the Work Table to the situation before processing and alter the respective entries.
14. Check that within the Work Table there are no rows left blank since QuantAnalysis considers the first row that contains no **File Name** entry to be the end of the batch. Delete blank rows if existing.
15. From the **File** menu, select **Save As** and save the entries in a new batch file.

Note: You can save and, therefore, create the batch file even earlier within this procedure. In this case, afterwards continue filling the Work Table and save the modified batch file using the **Save** command from the **File** menu.

	File Name	Sample Info	Method Name	Inj. Vol.	Dil. Factor	Sample Type	Calib Level	Inj. No.	Calib Action	Theor. Conc.	Theor. Conc. Unit	R
1	CARB0016.D	10 pg/µl, 100 pg abs.	Carbamate.M	10	1	Calib	5	1	New			
2	CARB0017.D	1 pg/µl, 10 pg abs.	Carbamate.M	10	1	Calib	3	1	New			
3	CARB0018.D	0,1 pg/µl, 100 pg abs.	Carbamate.M	10	1	Calib	1	1	New			
4	CARB0020.D	1 pg/µl, 5 pg abs.	Carbamate.M	5	1	Calib	2	1	New			
5	CARB0021.D	10 pg/µl, 50 pg abs.	Carbamate.M	5	1	Calib	4	1	New			
6	CARB0022.D	100 pg/µl, 500 pg abs.	Carbamate.M	5	1	Calib	6	1	New			
7	CARB0023.D	100 pg/µl, 100 pg abs	Carbamate.M	10	1	Calib	7	1	New			
8	CARB0024.D	"unknown" 100pg/µl	Carbamate.M	3	1	Sample		1	-			
9						Sample			-			

Figure 4-3 Batch file for a set of individually acquired data files created by manually entering data

4.2 Filling and Manipulating the Work Table for a Batch File

Before processing a batch file, the Work Table must be filled with all data that is needed for performing the respective quantitation. Which data actually has to be entered depends on the type of quantitation to be performed e.g. whether internal standards are used.

Some data can be entered automatically when importing a sample table but all other data needed for quantitation must be entered manually either by typing in or selecting the respective data. You can manipulate the Work Table by moving or deleting rows. When a batch file has already been processed, you can reset the Work Table to its state before processing.

4.2.1 Filling the Work Table Automatically

When a sample table is imported, the program makes particular Work Table entries automatically. The corresponding data is stored in the respective sample table, which includes the names of the data files as well as the corresponding sample names, vial positions, and injection volumes.

To perform a quantitation, QuantAnalysis needs additional information, which has to be entered manually, e.g. the sample type and calibration level, for each data file used.

4.2.2 Filling the Work Table Manually

Depending on whether you create a batch file from a sample table or for a set of individually acquired data files you have to enter manually some data needed for quantitation into the Work Table.

Entering data manually is done by first clicking the desired Work Table field and then either typing in the respective data (e.g. file name, sample name, etc.) or selecting the desired option from the corresponding list box (in the case of sample type or calibration action). You can make your work easier by copying Work Table entries multiple times.

4.2.3 Copying Work Table Entries Multiple Times

You can copy a Work Table entry multiple times by performing an 'Excel-like fill' of a Work Table column or by using copy and paste.

Note: This 'Excel-like fill' is only active before the batch file is processed.

To perform an 'Excel-like fill' of a Work Table column:

1. Click the field you want to copy multiple times.
2. Position the mouse cursor on the square in the lower right corner of the field so that it changes to **+**.
3. Drag the cursor with left mouse button held down downwards until the desired number of fields is reached.
4. Release the left mouse button. The marked fields are filled according to the entry shown in the selected field even if the respective fields already contain entries. In case of the **Vial** column, the vial numbers will be incremented automatically. This is also the same for the **File Name** column when the selected file name contains a number.

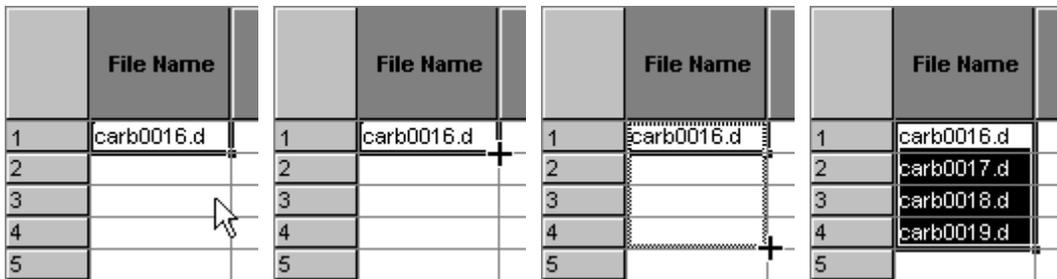


Figure 4-4 'Excel-like fill' of the File Name column

To perform copy and paste:

1. Click the field whose contents you want to copy. This selects the respective entry.
2. Click . Or from the **Edit** menu, select **Copy**. This copies the selection and puts it on the Clipboard.
3. Click the field in which you want to paste the copied entry.
4. Click . Or from the **Edit** menu, select **Paste**. This inserts the current Clipboard contents in the selected field.

4.2.4 Moving a Row within the Work Table

You can move a row in the Work Table up or down in order to sort the Work Table.

To move a Work Table row:

1. Position the mouse cursor in the number field of the row you want to move so that the Select Row cursor  appears and click the left mouse button. This selects the respective row.
2. Position the mouse cursor on the number field and with the left mouse button held down drag the cursor up or down to the desired new position. During dragging, the current insertion position that the selected row will be moved to is indicated by a red line. On releasing mouse button, the row is moved to the selected new position.

1	alp00002.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	0	1	-
2	alp00003.D	C20	Alp 20pg/100	2	ALPQMS.M	10	0.05	Calib	1	1	Replace
3	alp00004.D	C100	Alp 100pg/10	3	ALPQMS.M	10	0.01	Calib	2	1	Replace
4	alp00005.D	C200	Alp 200pg/10	4	ALPQMS.M	10	0.005	Calib	3	1	Replace
5	alp00006.D	C1000	Alp 1000pg/1	5	ALPQMS.M	10	0.001	Calib	4	1	Replace

1	alp00002.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	0	1	-
2	alp00003.D	C20	Alp 20pg/100	2	ALPQMS.M	10	0.05	Calib	1	1	Replace
3	alp00004.D	C100	Alp 100pg/10	3	ALPQMS.M	10	0.01	Calib	2	1	Replace
4	alp00005.D	C200	Alp 200pg/10	4	ALPQMS.M	10	0.005	Calib	3	1	Replace
5	alp00006.D	C1000	Alp 1000pg/1	5	ALPQMS.M	10	0.001	Calib	4	1	Replace

1	alp00002.D	Blank	Blank	1	ALPQMS.M	10	1	Sample	0	1	-
2	alp00003.D	C20	Alp 20pg/100	2	ALPQMS.M	10	0.05	Calib	1	1	Replace
3	alp00005.D	C200	Alp 200pg/10	4	ALPQMS.M	10	0.005	Calib	3	1	Replace
4	alp00004.D	C100	Alp 100pg/10	3	ALPQMS.M	10	0.01	Calib	2	1	Replace
5	alp00006.D	C1000	Alp 1000pg/1	5	ALPQMS.M	10	0.001	Calib	4	1	Replace

Figure 4-5 Moving a Work Table row upwards by one position

4.2.5 Deleting a Row from the Work Table

You can delete a row from the Work Table. This must be done e.g. in case 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 by mistake which should not be contained in a batch file to be created. Using multiple selections, you can delete several rows at once. All entries currently contained in the selected row(s) are removed from the Work Table.

To delete a single row:

1. In the Work Table, click the number field of the row you wish to delete. This selects the respective row.
2. Click .

To delete a series of neighboring rows:

1. Hold down the Shift key and, in the Work Table, click the number fields of the first and last row in the desired series.
-or-
Position the mouse cursor on the number field of the first row in the series and drag it with the left mouse button held down to the number field of the last row.
2. Click .

To delete multiple individual rows:

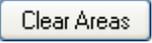
1. Hold down the Ctrl key and, in the Work Table, click the number fields of each desired row.
2. Click .

4.2.6 Resetting the Work Table

The Work Table of an already processed batch file can be returned to its state before processing. This allows you to correct a mistake in the Work Table after processing the respective batch file and then repeat processing.

When resetting the Work Table, all data entered during batch processing is cleared from the table and those columns that after batch processing cannot be edited any more are released for being edited again.

To reset the Work Table:

1. Click .

4.2.7 Defining Sample Parameters

For performing a quantitation, you have to define specific sample parameters for the data files (samples) involved. First you must define the sample type, i.e. you have to select whether a respective data file should serve either as a sample to be quantified, as calibration sample, as a quality control sample or as a blank sample. Depending on the sample type you have assigned to a data file, you may further define the corresponding calibration level and calibration action.

4.2.7.1 Defining the Type of a Sample

QuantAnalysis can handle four different sample types:

- **'Sample'** "Unknown" sample that is to be quantified.
- **'Calib'** Sample of known concentration that is used to set up a calibration curve.
- **'QC'** Quality control sample that is used to validate the calibration curve.
- **'Blank'** Blank sample that is used for system control.

By default, the sample type is set to **Sample**. When you wish to assign another type to a sample, select it from the corresponding list.

To select the type of a sample:

1. In the Work Table's **Sample Type** column, click the field that corresponds to the sample whose sample type you want to define. A drop-down button appears.
2. Click the drop-down button to open the sample type list.



3. Click the desired sample type.

4.2.7.2 Defining the Calibration Level of a Calibration or Quality Control Sample

For a calibration ('Calib') or quality control ('QC') sample, you have to define the corresponding calibration level. The program uses this level to read the corresponding concentrations from the table defined in the quantitation method in the Method Editor's **Target Compounds** dialog. The calibration level can be given in arbitrary units (e.g. 1, 2, 3, ...) or in the case of quality control sample as text (e.g. low, medium, high). In case of multiple injections of a same sample, QuantAnalysis identifies such samples from the entries in the **Calib Level** and **Inj. No.** columns.

To define the calibration level of a sample:

1. In the Work Table's **Calib Level** column, click that field that corresponds to the calibration or quality control sample whose calibration level you want to define
2. Enter the desired calibration level as either arbitrary unit (1, 2, 3 ...) or text (for quality control samples, only).

4.2.7.3 Defining the Calibration Action of a Calibration Sample

For a calibration sample ('Calib') you have to define the corresponding calibration action. Different types of action exist:

- **'New'** Adds an additional calibration point to the calibration curve.
- **'Replace'** Deletes an already existing calibration point from the calibration curve and replaces it by a new one. This action can be used in the case of multiple injections of a sample.
- **'-'** Performs no calibration action. This action has to be set for all non-calibration samples.

To define the calibration action:

1. In the Work Table's **Calib Action** column, click the field that corresponds to the calibration sample whose calibration action you want to define. A drop-down button appears.
2. Click the drop-down button to open the calibration action list.



3. Click the desired calibration action.

4.3 Saving a Batch File

You can save a not yet processed or an already processed batch file to the Batch Files format (*.btc). For an unprocessed batch file, the corresponding Work Table is saved whereas for an already processed batch file the quantitation method used and the quantitation results obtained are also saved in the batch file.

When creating a new batch file you have to save the new file. Use the **Save As** command from the **File** menu and select an already existing or a new file name. Later changes made to this batch file can be saved using the **Save** command from the **File** menu.

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

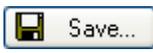
Saving a batch file under a new file name will result in a subfolder with the specified batch file name being set up in the chosen target folder and a corresponding result file being saved to this batch folder. In the following, each saving operation you perform on this batch file will result in a new, additional result being stored to this batch file folder. Existing result files are not overwritten. The batch file folder contains all result files currently available for the respective batch file as well as further corresponding files.

Automatic batch saving will be performed only before the process operation really starts. In case of a still unprocessed batch file, the **Save Batch** dialog will appear automatically to select a file name for saving the batch. This allows you to save the processed batch file under another file name while keeping the original batch file unprocessed. If you process an already processed batch file again, the batch file will automatically be saved under the same file name. Moreover, if you want to close QuantAnalysis or open another or a new batch file, the program will ask you about saving yet unsaved changes made to the currently open batch file.

To save a batch file using a new or an already existing name:

1. From the **File** menu, select **Save As**.
2. In **Look in** and the folder list, navigate to that folder that contains the data files to be quantified.
3. Depending on how you want to save the batch file, do one of the following to specify its file name:
 - To save under a new name, enter the desired name in **File name**.
 - To save under an existing name, enter the name in **File name** or select it from the folder list.
4. Click **Save**
5. If you have selected an already existing file name, affirm the appearing confirmation request on overwriting the existing file.
6. Completing the **Save As** dialog results in saving the batch file under the specified name. In case this dialog has appeared automatically after starting batch processing, the respective batch file is first processed and then saved.

To save a batch file using the same name:

1. Click  or . Or from the **File** menu, select **Save**.

4.4 Opening a Batch File

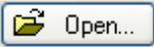
QuantAnalysis uses Windows conventions for opening batch files. You can open a batch file from either within QuantAnalysis or Windows Explorer. QuantAnalysis supports the drag-and-drop functionality, i.e. you can open a batch file by dragging its file name from Windows Explorer into the QuantAnalysis window.

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. Loading a previous result is only possible with the **Open** command from the **File** menu. When opening a batch file from Explorer or using the **File** menu's Recent File List always its last saved result is loaded.

If you open an unprocessed batch file, its current processing state displays in the Work Table window while the Chromatogram/Spectrum window and the Calibration window are empty. If you open an already processed batch file, all windows automatically show the respective corresponding data saved in the batch file.

Only one batch file can be open at a time.

To open a batch file from within QuantAnalysis:

1. Start QuantAnalysis.
2. Click  or . Or from the **File** menu, select **Open**. This opens the **Open Batch** dialog.
3. In **Look in** and the folder list, navigate to that folder that contains the batch file you want to open.
4. Select the desired batch file from the folder list or enter its name in **File name**.
5. If more than one result is available in the chosen batch file's **Result History**, and if you do not want to load the last but a previous result, select the desired result from this list. Otherwise, the last result will be loaded.
6. Double-click the desired batch file or click **Open**.

Tip: You can quickly open a batch file you have recently worked with by clicking the respective recent file name at the bottom of the **File** menu. This loads the last saved result of the selected batch file.

Tip: If you want to open another result of the currently open batch file you can also use the **History** button in the Work Table window to load it.

To open a batch file from Windows Explorer using drag and drop:

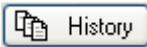
1. Start QuantAnalysis.
2. Start Windows **Explorer**.
3. Navigate to the folder that contains the batch file you want to open.
4. Click the desired batch file and drag it with the left mouse button held down in the QuantAnalysis window. Then release the mouse button. This loads the last saved result of the selected batch file.

4.5 Showing the Result History of a Batch File

You can show the result history for the open batch file. Depending on whether QuantAnalysis is running in Compliance or Non-Compliance mode, the **Result History** dialog displays different information and allows for different operations. Generally, all results that have been saved since batch file creation 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 about already signed results is displayed. An arrow indicates the currently loaded result.

From the **Result History** dialog, you can load or delete a certain result. When QuantAnalysis is running in Compliance mode, you can also sign a certain result.

To show a batch file's result history:

1. In the Work Table window, click . This opens the **Result History** dialog.
2. To return to the Work Table window, click **Close**.

4.6 Signing a Result of a Batch File

When QuantAnalysis is running in Compliance mode, an electronic record (= result of a batch with corresponding method) of the open batch file can be signed electronically. Electronic signatures consist of operator ID and operator password. Only operators who have received from their UserManagement administrator the right to sign electronic records can sign. Multiple signing of a result is allowed.

To sign a result there is no need for the signing operator to be logged into QuantAnalysis. Thus, even if currently an operator who does not have the right to sign is logged in, signing can be performed without previous change of operator.

Already signed results are indicated in the batch file's result history by a 'yes' under

Signed. This applies to the **Result History** dialog as well as to the result history list displayed in the **Open** dialog if QuantAnalysis is currently running in Compliance mode.

To sign a result of a batch file:

1. In the Work Table window, click . This opens the **Result History** dialog.
2. From the result list, select the result you want to sign.
3. Click **Sign**. This opens the **Sign Electronic Record** dialog.
4. In **Operator**, enter the operator ID.
5. In **Password**, enter the corresponding password.
6. In **Meaning**, enter the meaning of this signing, if desired.
7. Click **Sign**. If operator ID and password meet, and the respective operator has the right to sign, the selected result is signed. The **Result History** dialog returns with a 'yes' being entered for this result under **Signed** and additional information being shown by the **Signature** parameters.
8. To return to the Work Table window, click **Close**.

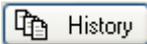
4.7 Deleting a Result from a Batch File

Since QuantAnalysis creates and stores a new, additional result file on each saving operation you perform on a batch file, several results can be available for one batch file probably representing different states of the same batch file. Results that are not needed any longer can be deleted again.

Deleted results will be listed further on in the batch files **Result History** dialog indicated by a 'yes' under **Deleted** but will not appear any longer in the **Open** dialog.

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

To delete a result from a batch file:

1. In the Work Table window, click . This opens the **Result History** dialog.
2. From the result list, select the result you want to delete.
3. Click **Delete**.
4. Affirm the appearing confirmation request. This deletes the selected result and enters a 'yes' for this result under **Deleted**.
5. To return to the Work Table window, click **Close**.

4.8 Showing the Audit Trail of a Batch File

For each batch file the corresponding audit trail is recorded which could be shown when the batch file is open.

The audit trail lists all changes made to the batch file with corresponding date and time, who (operator name) made the change and what happened. This includes all changes that were 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 are stored in the audit trail.

To show the audit trail for the open batch file:

1. In the Work Table window, click . This opens the **Audit Trail** dialog.
2. To return to the Work Table window, click **Close**.

4.9 Closing a Batch File

You can close an open batch file. Depending on what you intend to do hereafter there are several ways to close a batch file.

To close an open batch file:

1. To close the open batch file, you can do one of the following:
 - Click  or from the **File** menu, select **Open** if you want to open another batch file.
 - Click  or from the **File** menu, select **New** if you want to create a new batch file.
 - Click  if you want to import a sample table for creating a new batch file.
 - From the **File** menu, select **Exit** if you want to close the current QuantAnalysis session.
2. In each case, answer the appearing confirmation request on saving the current processing state of the batch file to be closed.

5 CREATING QUANTITATION METHODS

Batch files are processed by using a defined quantitation method which is stored in the QuantAnalysis part of the method embedded in the batch file.

Methods consist of application-specific method parts. Each method contains at least one method part and each method part can be contained in a method only once. Often, methods contain several method parts e.g., for data acquisition (e.g. the esquireControl part) and data processing (e.g. the DataAnalysis and QuantAnalysis parts).

To process a batch file the quantitation method needs to contain all information required to detect the respective target and ISTD compound peaks on the various data files of the batch and to calculate the corresponding quantitation results. The method defines the chromatogram trace(s) to be used in peak detection, the target and ISTD compounds present in the samples, corresponding chromatographic and concentration data, as well as the integration parameters to be used in peak detection and mass spectrum calculation.

After editing a quantitation method, you can save the parameter settings into a new or an existing method. As long as you do not save the settings into a method, the settings will be saved only in the batch file when this is saved. Thus, saving quantitation parameter settings into a method allows using them for future quantitations making results comparable. When saving into an existing method, the previous QuantAnalysis part of the method will be overwritten with the new one. When saving into a new method, the new created method will contain the QuantAnalysis part only.

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. All operators who are allowed to load methods can load SOP methods but only operators with a special right can load non-SOP methods, too. The UserManagement administrator can define a default SOP method folder for saving/loading methods; in this case operators need a special right to use non-default method folders, too.

5.1 Creating a Quantitation Method

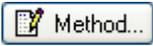
You can create a quantitation method to be used in processing the open batch file. After setting up the method, you can save it as QuantAnalysis processing part into a method, which allows you to use these settings in future quantitations.

In Compliance mode, methods can be saved as SOP or non-SOP methods if SOP method handling is turned on. Only operators who have the special right can mark

methods with the SOP flag.

A method wizard will guide you through the set up of the quantitation method. During set up, you have to define general quantitation parameters, the chromatogram trace(s) to be edited, the target and ISTD compound(s) present, corresponding chromatographic and concentration data, and the integration parameters to be used for peak detection and mass spectrum calculation.

To create a quantitation method:

1. Click  or . Or from the **Method** menu, select **Edit**. This starts the Method Editor.
2. In the **General** dialog, define general settings. Do the following steps:
 - (a) In **Default Injection Volume** and **Accuracy Limit [%]**, enter the desired values.
 - (b) Check **Apply dilution factor to ISTD compounds**, if the dilution factor set in the Work Table's **Dil. Factor** column should be applied to ISTD compounds, too.
 - (c) Check **Load calibration from DataAnalysis results** if the mass spectra in an analysis being loaded in QuantAnalysis should automatically be calibrated using the calibration coefficients stored in the last DataAnalysis result of the respective analysis.
3. Click **Next**.
4. In the **Chromatograms** dialog, define the chromatogram trace(s) for the compound(s) to be quantified. Do the following steps:
 - (a) Define a chromatogram trace by making the corresponding entries in the **Type, Filter, of, Masses, Width, Polarity, Color, Smth Width (Gauss[sec])** and **Cycles** boxes.
 - (b) Click **Add**. This enters the respective trace in **Traces**.
 - (c) Repeat (a) and (b) for each chromatogram trace you want to use in peak detection.
5. Click **Next**.
6. In the **ISTD Compounds** dialog, define the ISTD compound(s) you want to use in the respective quantitation. Do the following steps:

Note: If no ISTD compound is to be used, skip this dialog and continue with step 8.

 - (a) Define an ISTD compound by making the corresponding entries in **Name, CAS No.** (optionally), **Chrom., Retention time [min], Window [min], Default concentration**, and **Concentration units**.
 - (b) Click **Add**. This enters the respective compound in **ISTD Compounds**.
 - (c) Repeat (a) and (b) for each ISTD compound you want to use.
7. Click **Next**.

8. In the **Target Compounds** dialog, define the target compound(s) you want to use in the respective quantitation.
 - (a) Define a target compound by making the corresponding entries in **Name**, **CAS No.** (optionally), **Chrom.**, **ISTD**, **Retention time [min]**, **Window [min]**, and **Concentration units**. In **Standard conc.** enter the calibration levels and corresponding concentrations for this target compound in the calibration samples.
 - (b) Click **Add**. This enters the respective compound in **Target Compounds**.
 - (c) Repeat (a) and (b) for each target compound you want to use.
9. Click **Next**.
10. In the **Integration Parameters** dialog, define the parameter settings to be used in detecting and integrating the respective target and ISTD compound peaks on the defined chromatogram traces as well as in calculating the corresponding mass spectra. Do the following steps:

Note: Normally, the default values already allow good integration results, but if necessary, the parameters can be given independently for each individual chromatogram trace. In case there are peaks within the same chromatogram that differ a lot in width or intensity, it is quite often not possible to integrate all peaks in a correct way when using only one set of integration parameters. Optimizing the integration parameters then will minimize the need for manual integration of peaks after batch processing.

 - (a) In **Chromatogram**, select the chromatogram trace for which you want to define the integration parameter settings.
 - (b) Make the desired entries for the **Peak detection** and **Mass spectrum calculation** parameters.
 - (c) Repeat (a) and (b) for each chromatogram trace defined.
11. Click **Finish**. This closes the method editor.
12. Save the quantitation method if you want to use its parameter settings for further quantitations.

5.2 Saving a Quantitation Method

You can save a new or modified quantitation method as QuantAnalysis processing part into a new or existing method. When saved into an existing method, the previous QuantAnalysis part of the method will be overwritten by the new one. Saving into a new method will create a new method with only the QuantAnalysis part contained. Saving a quantitation method into a method allows using its parameter settings in future quantitation operations.

In Compliance mode, methods can be saved as SOP or non-SOP methods if SOP method handling is turned on. Only operators who have the special right can mark methods with the SOP flag. SOP methods cannot be modified. If a default SOP method

folder has been defined, the method must be saved to that default folder except the operator has the right to use non-default method folders.

To save a quantitation method:

1. From the **Method** menu, select **Save As**. This opens the **Save QuantAnalysis Method Part As** dialog.
2. Navigate to the folder where the method should be saved. When in Compliance mode with SOP method handling being turned on and an SOP method folder being defined this must be the default folder if you do not have the right to use non-default method folders.
3. Depending on how you want to save the quantitation method, do one of the following to specify its file name:
 - To save it into the method attached to the open batch file or another existing method, select the respective method from the folder list or enter its name in **Method name**. This does not apply to SOP methods.
 - To save it into a new method, enter the desired new name in **Method name**.
4. In **Method part name**, if desired, enter a name for the QuantAnalysis part. This can be entered in a sense of a comment. If you do not enter a name, the QuantAnalysis part will be saved with a part name same as the method name specified.
5. In **Comment**, if desired, enter a comment for the method. This comment applies to the entire method, not only to the QuantAnalysis part.
6. When in Compliance mode with SOP method handling being turned on: Check the **SOP method** box if you want to save the method with the SOP flag. This is only allowed if you have the right to mark methods as SOP.
7. Click **Save**.
8. If you have chosen an existing file name, confirm the appearing request to overwrite the QuantAnalysis part of the original method.

5.3 Opening a Quantitation Method

You can open a quantitation method and attach it to the loaded batch file. This overwrites the QuantAnalysis processing part of the method currently embedded in the batch file.

When in Compliance mode with SOP method handling being turned on, all operators can load SOP methods but only operators who have a special right can load non-SOP methods, too. If a default SOP method folder has been defined, only methods placed in that default folder can be loaded except the operator has the right to use non-default method paths, too.

You can view the parameters settings of the open quantitation method after starting the

method editor.

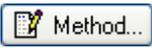
To open a quantitation method:

1. Click . Or from the **Method** menu, select **Open**.
2. Navigate to the folder that contains the method with the desired QuantAnalysis part. When in Compliance mode with SOP method handling being turned on and an SOP method folder being defined, you can only load a method placed in that default folder if you do not have the right to use non-default method folders.
3. Select the method or enter its name in **Method name**.
4. Click **Open**.

5.4 Viewing a Quantitation Method

The current parameter settings of the open quantitation method can be viewed in the Method Editor.

To view a quantitation method:

1. Open the quantitation method you want to view.
2. Click  or . Or from the **Method** menu, select **Edit**.
3. Click **Next** or **Back** to browse through the method editor's dialogs and view the current parameter settings.
4. Click **Finish** to close the method editor.

5.5 Modifying a Quantitation Method

You can modify a quantitation method according to your needs by changing its current settings. When finished, the modified method can be saved as QuantAnalysis part into a new or an existing method.

When in Compliance mode with SOP method handling being turned on you cannot modify methods for which the SOP flag is set. Modification is only possible after the SOP flag has been cleared. This can be done by saving the method without the **SOP method** option being set using the same file name.

To modify a quantitation method:

1. Open the quantitation method you want to modify.

2. Click  or . Or from the **Method** menu, select **Edit**. This starts the method editor and opens the **General** dialog.
3. Click **Next** (and/or **Back**) to reach the dialog whose current settings you want to change.
4. Change the current settings as required.
Note: Take care, that changes you have made in the **Chromatograms**, **ISTD Compounds**, or **Target Compounds** dialogs must be entered by clicking the appropriate button (**Change** or **Add**) before leaving the respective dialog by clicking **Next** or **Back**. Otherwise, these changes will be lost.
5. Click **Finish** when you have finished modifying the respective method.
6. Save the modified quantitation method.

6 PROCESSING BATCH FILES

After creating a batch file and defining the quantitation method to be used with this batch file you can process the respective batch files. Processing a batch file means that the data files (analyses) contained in this batch are processed according to the parameter settings defined in the selected quantitation method and that the concentrations of the specified target compounds are calculated from the calibration curves set up.

- When processing starts, QuantAnalysis first evaluates the information and gives an error message if important information is missing.
- After evaluation, the data files are loaded and analyzed. If the **Load calibration from DataAnalysis results** option is set in the method used, the mass spectra in the loaded analyses will be calibrated using the calibration coefficients stored in the respective last DataAnalysis result.
- The chromatogram traces specified in the Method Editor's **Chromatograms** dialog are created for each data file.
- Compound peaks are detected and integrated according to the settings in the Method Editor's **Target Compounds**, **ISTD Compounds** and **Integration Parameters** dialogs.
- Calibration curves are calculated using the calibration levels set in the Work Table and the corresponding target compound standard concentrations defined in the **Target Compounds** dialog.
- From these calibration curves, the target compound concentrations of the unknown 'Sample' samples are calculated and entered in the Work Table.

A blue bar at the bottom of the screen shows the progress of this process. The entire process usually takes only a few seconds.

The quantitation results are automatically saved during data analysis. You can review the quantitation results and, if required, alter them e.g., by modifying calibration curves or manually integrating compound peaks. You can plot particular quantitation data, print specific quantitation reports and export quantitation data to use them in other applications.

6.1 Processing a Batch File

You can process the open batch file according to the current parameter settings defined in the selected quantitation method and save the quantitation results and the method used with the respective processed batch file.

When starting batch processing, the respective batch file is automatically saved before

processing starts. For a yet not processed batch file, the **Save As** dialog will appear which allows you to save the processed batch file under a new file name and, thus, keep the original batch file unprocessed for performing further processing operations on it, e.g. by using another quantitation method. For an already processed batch file no saving dialog will appear.

Processing a batch file usually 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 can review the quantitation results obtained.

To process a not yet processed batch file:

1. Open the unprocessed batch file you want to process.
2. Open the quantitation method you want to use or create a new method.
3. Click  Process.
4. In the appearing **Save As** dialog, select or enter the file name the processed batch file should be saved with
Note: The batch file must be saved in that folder that contains the data files to be quantitated.
Note: This dialog will appear only on processing a not yet processed batch file.
5. Click **Save**. This starts batch processing.
6. Save the processed batch file.

To reprocess an already processed batch file:

1. Open the processed batch file you want to reprocess.
2. Open the quantitation method you want to use or create a new method.
3. Click  Process. This starts batch processing.
4. Save the processed batch file.

6.2 Calculation of Calibration Curves

Calibration curves will be calculated using the following formulas:

Calculation of the theoretical concentration

The theoretical concentration is calculated using the following formula:

$$Conc_{theor} = Conc_{Level} \cdot \frac{1}{DilFactor} \cdot \frac{InjVol}{DefInjVol}$$

with:

$Conc_{theor}$: theoretical concentration, calculated and displayed in the Work Table.

$Conc_{Level}$: standard concentration for this level of the target compound entered in the quantitation method.

$DilFactor$: dilution factor entered in the Work Table.

$InjVol$: injection volume for this analysis entered in the Work Table.

$DefInjVol$: default injection volume entered in the quantitation method.

Calculation of the internal standard concentration

The concentration of the internal standard is calculated in the same way. The dilution factor is applied only if it is enabled in the quantitation method. This will result in the following X, Y pairs shown in the calibration plot:

$(Conc_{theor}, Area)$ resp. $\left(\frac{Conc_{theor}}{Conc_{ISTD}}, \frac{Area_{Target}}{Area_{ISTD}} \right)$ with internal standard calculation.

For calibration mode *height* (instead of *area*) the calibration is performed equivalently.

Calculation of the calibration curve

The calibration curve is calculated using these X, Y pairs, resp. the average value for the same.

Weighting is applied in the calculation of the calibration curve by applying the inverse of the weight factor as standard deviation at each individual point.

Calculation of the concentration of an unknown sample

The concentration of an unknown sample is calculated by solving the calibration curve with the area, respectively the height, of the peak. Then the dilution factor and injection volume is applied using the above equation.

7 REVIEWING CALIBRATION AND QUANTITATION RESULTS

For reviewing calibration and quantitation results, we recommend that you switch to the Nested display. This shows all results simultaneously displayed in the Work Table window, Chromatogram/Spectrum window and Calibration window.

Note: If necessary, adjust the relative size of the windows by dragging the respective window borders.

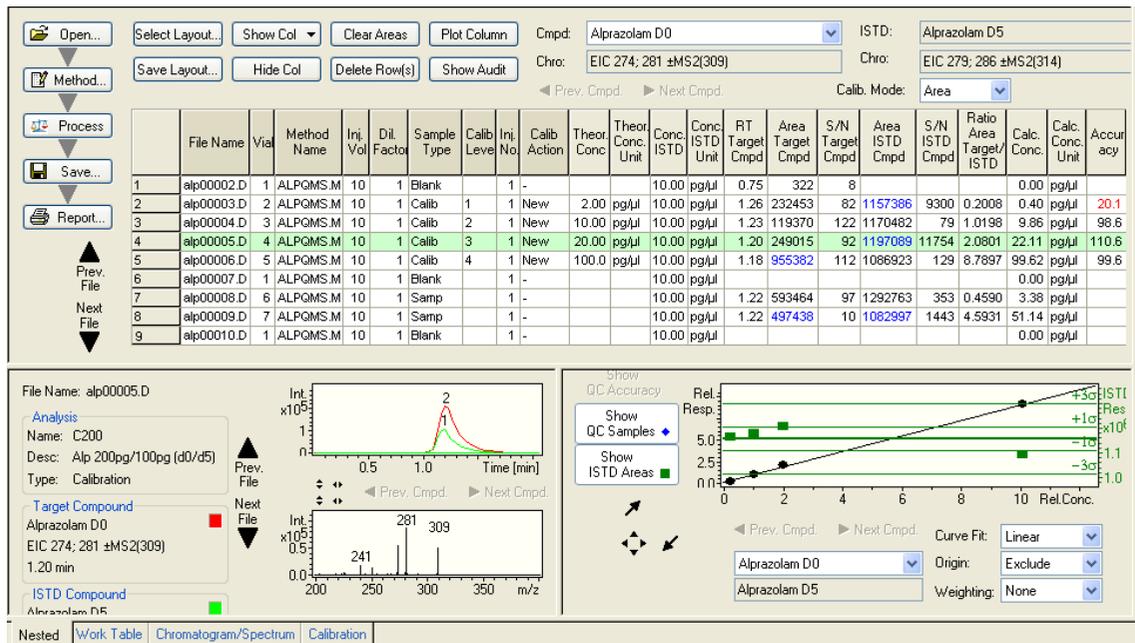


Figure 7-1 Quantitation results obtained for a batch file created from an Agilent ChemStation sample table

7.1 Determining Which File or Target Compound is Currently Active

One of the lines in the Work Table is highlighted in green to indicate that the respective data file is the "active" (selected) one. The respective **Data File** name is also displayed at the top of the Chromatogram/Spectrum window.

The active target compound is shown in  found in the Work Table as well as under **Target Compound** in the Chromatogram/Spectrum window and in the corresponding list box of the Calibration window.

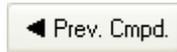
The Chromatogram/Spectrum window will display the chromatogram peak and mass spectrum that corresponds to the currently selected ("active") target compound of the "active" data file. It also displays the respective ISTD compound peak if an internal standard was assigned to this target compound. The Calibration window shows the calibration curve that was calculated for the selected target compound along with corresponding ISTD and quality control data provided such data are present and their display is activated.

7.2 Toggling Between Different Files and Target Compounds

You can toggle between different data files or different target compounds. The one currently selected is the "active" one whose corresponding data is displayed.



Use  and  from either the Work Table window or the Chromatogram/Spectrum window to toggle between different data files.

Use  and  from either the Work Table window, Chromatogram/Spectrum window or Calibration window to toggle between different target compounds.

Alternatively, you can use  from the Work Table window to select the desired target compound directly. This is helpful in cases where the quantitation contains many compounds.

7.3 Viewing the Quantitation Data for a Target Compound

The quantitation data obtained for a target compound is listed in the corresponding columns of the Work Table window. This includes the retention times and areas of the target compound peaks, and the calculated concentrations and the accuracy values for the calibration samples. In case of a quantitation with an internal standard, the areas of the ISTD compound peaks and the area ratios of target and ISTD compound peaks are also given.

In some instances, no entries are made in one of the data file rows for the calculated area, concentration and accuracy for a selected target compound. This indicates that the respective target compound or corresponding ISTD compound was not found in the peak integration operation, and the corresponding values could not be calculated. If this occurs, try to integrate the respective compound manually.

Area values for manually integrated compounds display in blue, accuracy values, which lie outside the specified accuracy limit, display in red.

The quantitation data displayed in the Work Table are automatically recalculated when the corresponding calibration curve is altered or a target or ISTD compound peak is manually integrated. You can plot specific quantitation data obtained for the data files of a batch.

7.4 Viewing the Peak Integration Results for a Target Compound

The peak integration results for the selected target compound of the active data file and the calculated corresponding mass spectrum are displayed in the Chromatogram/Spectrum window.

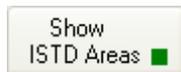
If an internal standard was assigned to the target compound, its corresponding peak is also shown in the Chromatogram view. For viewing the corresponding mass spectrum, you have to select the **ISTD** for **Display MS**.

Note: We recommend that you check the peak integration results for improperly integrated peaks. Give special attention to chromatogram traces of the 'Sample' type. If necessary, correct the integration of a target or ISTD compound peak in the manual integration mode.

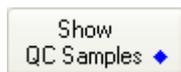
7.5 Viewing the Calibration Curve for a Target Compound and Corresponding ISTD and Quality Control Data

The calibration curve for the selected target compound is displayed in the Calibration window.

You can display additional information by activating the following buttons:



Shows the ISTD areas if an internal standard was assigned to the selected target compound.



Shows quality control samples provided such samples have been defined.



Shows the curve coefficients for the calculated calibration curve.



When setting up multiple calibration curves, use  and  to toggle between the calibration curves that were calculated for the previous block and the next block of calibration samples for the selected target compound.

You can alter the calculated calibration curve for a target compound by disabling calibration points as well as with respect to its curve fit, mode of origin and/or weighting of calibration points. Each of these changes will result in recalculating the calibration curve immediately and redisplaying it. The corresponding quantitation data listed in the Work Table are recalculated accordingly.

7.6 Plotting Quantitation Data

You can plot specific quantitation data obtained for the individual data files of a batch file by plotting the contents of the corresponding Work Table column. This function is restricted to specific columns.

To plot the contents of a Work Table column:

1. Click the header of the desired Work Table column (e.g. **Cal. Conc.**).
2. Click . The Plot Column window appears displaying the respective plot.
3. To change the current plot type, click the desired option **Bar**, **Line** or **Area**.

4. Click **Close** to close the current plot.

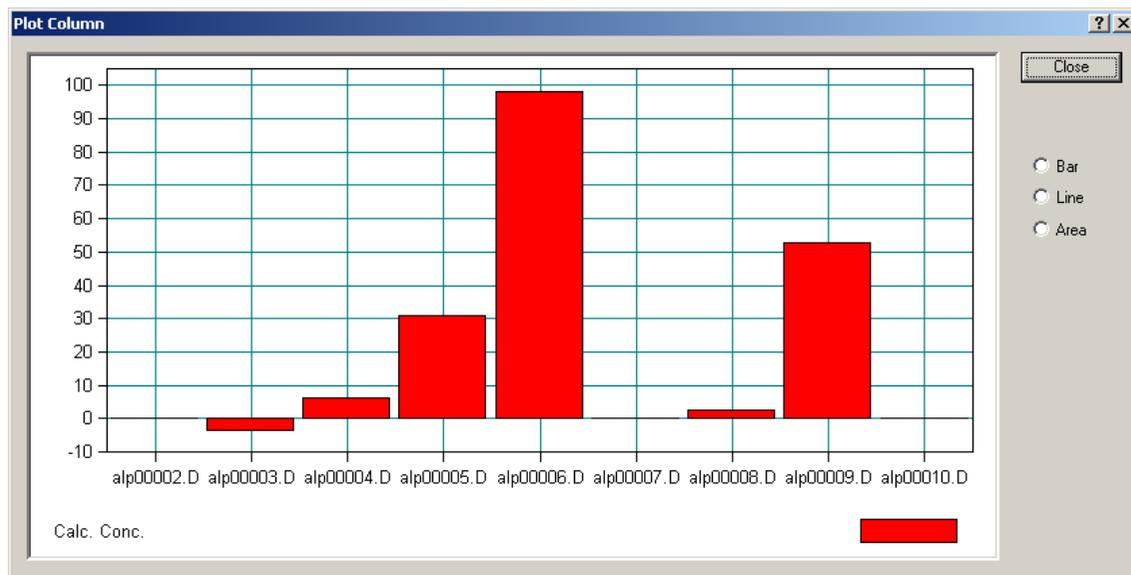


Figure 7-2 Plot of target compound concentrations calculated for the data files investigated with the concentrations displayed as bars

8 ALTERING QUANTITATION RESULTS

You can alter the quantitation results obtained after a batch file was processed. This can be done by manually integrating or deleting target or ISTD compound peaks. This can be done also by altering calculated calibration curves e.g. by deactivating calibration points, or by changing their weighting, changing the curve fit, or mode of origin. Each of these changes will result in recalculating the corresponding quantitation results listed in the Work Table. Furthermore, you can reprocess an already processed batch file e.g. with using another quantitation method.

8.1 Integrating a Compound Peak Manually

You can manually integrate a target or an ISTD compound peak which has not been recognized during the automatic integration process performed on the corresponding chromatogram or which has been improperly integrated. A compound peak that has not been recognized during automatic integration is indicated in the Work Table by its corresponding **Area (or Height) Target (or ISTD) Cmpd** field being left empty.

When the Manual Integration mode is active, manual integration can be performed in the chromatogram view of the of Chromatogram/Spectrum window. The corresponding quantitation results are immediately updated in the other windows. Compound peak areas that were obtained through manual integration are displayed in blue in the Work Table.

To manually integrate a compound peak:

1. Click the **Chromatogram/Spectrum** tab to switch to full-screen display for the Chromatogram/Spectrum window.
2. Click  to activate 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 not displayed. If you wish to integrate this hidden chromatogram, click the corresponding option to display it and hide the other one.
 - For an already integrated peak, its current start and end positions are indicated by two handles.
3. Select the data file containing the compound peak to be integrated by clicking



or

. The currently active data file is shown right beside **File name**.

4. Select the compound whose peak you wish to integrate by clicking or if there is more than one target compound. The currently active target compound is shown in **Target Compound**, the corresponding **ISTD compound**, if available, in **ISTD Compound**. This displays the corresponding chromatogram trace(s) edited for this/these compound(s) in the chromatogram view.
5. Adjust the display range of the chromatogram view to display the peak you are interested in.
6. Depending on whether or not the peak you wish to integrate has already been integrated proceed as follows:
 - In the case of an already integrated peak, position the mouse cursor near (3 pixel) to the handle whose position you want to change so that it changes to . Then drag the respective handle with the left mouse button held down to the desired position (data point) and release the mouse button. If desired change the position of the second handle, too.

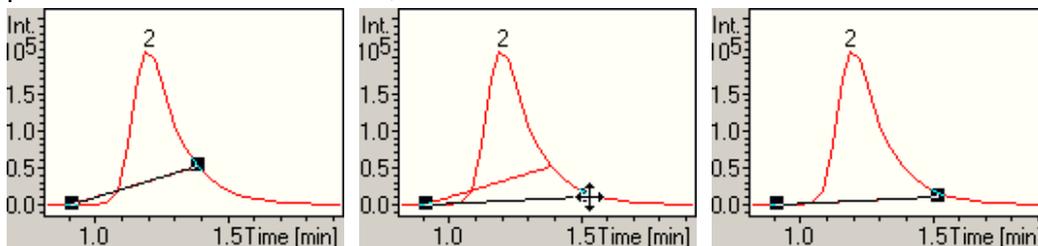


Figure 8-1 Integrating a compound peak manually

- In the case of an unintegrated peak, position the mouse cursor at the beginning of the peak and click the left mouse button. This causes two peak handles to be displayed. Then drag these handles to desired positions as described above. The (new) calculated peak area is automatically entered in the corresponding Work Table field.
7. Repeat steps 3 to 6 for all peaks you want to integrate manually.
 8. Click to deactivate the Manual Integration mode. The peak handles will disappear and a hidden chromatogram trace is redisplayed.
 9. Save the processed batch file that you have changed, if desired.

8.2 Deleting a Compound Peak

You can delete a target or ISTD compound peak from the open batch file. This removes the corresponding data from the Work Table and, therefore, from being used in quantitation. On deleting a peak, all corresponding quantitation results are immediately updated in the other windows.

Tip: If you have deleted a compound peak from a batch file, you can include it again in quantitation by integrating it manually. This will add the peak again.

To delete a compound peak:

1. Click the **Chromatogram/Spectrum** tab to switch to full-screen display for the Chromatogram/Spectrum window.
2. Select the compound peak you want to delete by displaying it in the chromatogram

view. For this, use , ,  or .

3. Click . This opens the **Confirm Delete** dialog.
4. In the case of a quantitation with internal standard, select which peak, the **Target Peak** or the **ISTD Peak**, you want to delete.
5. Click **OK**.
6. Repeat steps 2 to 5 for all compound peaks you want to delete.

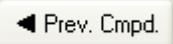
8.3 Altering a Calibration Curve

You can alter a compound's calibration curves in several ways. Altering the calibration curve, such as by disabling single calibration points or changing its origin, automatically results in recalculating and redisplaying the curve. The corresponding quantitation results are displayed immediately in the Work Table, which is updated accordingly.

8.3.1 Disabling a Calibration Point

You can disable individual calibration points on the calibration curve to exclude them from the calibration curve calculation. An enabled calibration point is displayed as a black point (●) or in case of an average value from multiple injections as a green point (●). In the latter case you must disable all calibration points of the respective level individually.

To disable a calibration point:

1. In the Calibration window, display the calibration curve you want to alter. To do this, select the respective target using  and . In case of a multiple injection quantitation, additionally select the respective calibration block using  and .

2. Move the mouse cursor near to the calibration point (● or ●) you want to disable so that it changes to .
3. Click the left mouse button. The black point will turn into an open circle (○).
4. Save the changed processed batch file, if desired.

8.3.2 Enabling a Calibration Point

You can re-enable a disabled calibration point and include it again in the calibration curve calculation. A disabled calibration point is indicated by an open circle (○).

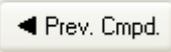
To enable a disabled calibration point:

1. In the Calibration window, display the calibration curve you want to alter. To do this, select the respective target using  and . In case of a multiple injection quantitation additionally select the respective calibration block using  and .
2. Move the mouse cursor near the desired disabled calibration point (○) so that it changes to .
3. Click the left mouse button. The open circle will turn into a filled black point (●).
4. Save the changed processed batch file, if required.

8.3.3 Changing the Curve Fit of a Calibration Curve

You can alter the calibration curve for the selected target compound by changing the **Curve Fit** currently selected. You can choose between **Linear**, **Average RF**, **Quadratic** or **Cubic** curve fit.

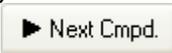
To change the curve fit of a calibration curve:

1. In the Calibration window, display the calibration curve you want to alter. To do this, select the respective target using  and . In case of a multiple injection quantitation, additionally select the respective calibration block using  and .
2. From the **Curve Fit** list box, select the desired fit.
3. Save the changed processed batch file, if desired.

8.3.4 Changing the Mode of Origin of a Calibration Curve

You can alter the calibration curve for the selected target compound by changing the **Origin** currently selected. You can select between **Exclude**, **Include** or **Force**.

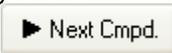
To change the mode of origin of a calibration curve:

1. In the Calibration window, display the calibration curve you want to alter. To do this, select the respective target using  and . In case of a multiple injection quantitation, additionally select the respective calibration block using  and .
2. From the **Origin** list box, select the desired mode of origin.
3. Save the changed processed batch file, if desired.

8.3.5 Changing the Weighting of Calibration Points

You can alter the calibration curve for the selected target compound by changing the **Weighting** currently selected. You can choose between different types of weighting.

To change the weighting of calibration points of a calibration curve:

1. In the Calibration window, display the calibration curve you want to alter. To do this, select the respective target using  and . In case of a multiple injection quantitation, additionally select the respective calibration block using  and .
2. From the **Weighting** list box, select the desired weighting.
3. Save the changed processed batch file, if desired.

9 PRINTING AND SENDING REPORTS

Several standard report layouts for printing specific quantitation data are available. They are installed on your system automatically when you install QuantAnalysis. You can use these default layouts or you can also create your own layouts using the *Bruker Compass ReportDesigner*. You can preview a report before printing it to allow you to decide whether to print it. In addition, you can send a report as an email to a recipient or save it as PDF document.

Support for printing on older printer models

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 printers with insufficient firmware performance.

9.1 Printing a Report w/o Previewing

You can print a quantitation report. Several standard report layouts for printing specific quantitation data are available. All layouts can be printed in portrait and landscape format. Before printing a report, you can preview it. This allows you to first look at the respective report and then to decide whether it should be printed.

To print a report w/o previewing it:

1. Click . This opens the **Print** dialog.
2. In **Name**, select the printer you want to use.
3. Click **Properties** and select in **Orientation** the format (**Portrait** or **Landscape**) you want to use for printing. If needed, change page set up options. Then click **OK**.
Note: The options available depend on the selected printer.
4. In **Instrument**, the instrument used is selected by default. If you want to select a report layout appropriate for another instrument, uncheck **Select automatically** and select the desired instrument.
5. In **Layout**, select the layout for the report you want to print.
6. If you wish to preview the report before printing it, click **Preview**.
7. To print the report, click **OK** in the **Print** dialog, or if in the preview, click the preview's . This prints the report on the selected printer.

9.2 Setting a Registry Switch for Faster 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 printer 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.

To set a registry key for faster printing:

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 "Printers".
6. Right-click the key "Printers" 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".
Note: The proper printer name is best taken from the QuantAnalysis **Print** dialog. Let's assume a network printer is listed thereof as "\\MyServer\My-Printer". The key name used in the registry then must be: "\\MyServer|My-Printer", replacing back slashes ('\') with vertical bars ('|').
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.

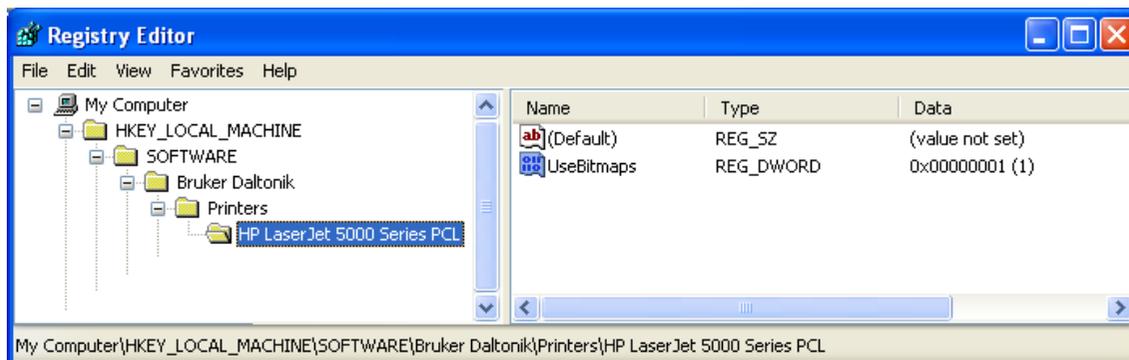


Figure 9-1 Example registry key for faster printing on the named printer

9.3 Sending a Report as an Email

You can print a selected report to a PDF file and send this automatically as an attachment of an email to a specified email address. If desired you can preview the report (Section 9.1) before sending it.

To send a report as email:

1. From the **File** menu, select **Send To** and then **Mail Recipient**. This opens the **Send To Mail Recipient** dialog.
2. In **Email Address**, enter the email address of the recipient to whom you want to send the report.
3. In **Name**, select the printer you want to use.
4. Click **Properties** and select in **Orientation** the format (**Portrait** or **Landscape**) you want to use for printing. If needed, change page set up options. Then click **OK**.
Note: The options available depend on the selected printer.
5. In **Instrument**, the instrument used is selected by default. If you want to select a report layout appropriate for another instrument, uncheck **Select automatically** and select the desired instrument.
6. In **Layout**, select the layout for the report you want to preview.
7. Click **Send**. This opens the **Choose Profile** dialog.
8. In **Profile Name**, select the profile you want to use. If desired, create a new profile and/or set advanced logon options.
9. Click **OK**. This creates the selected report and sends it to the specified email address. If no email address is specified, the email program will prompt for it.

9.4 Sending a Report to a PDF Document

You can print a selected report to a PDF file and save it to a chosen target folder. If desired you can preview the report (Section 9.1) before saving it as PDF document.

To save a report as PDF document:

1. From the **File** menu, select **Send To** and then **PDF Document**. This opens the **Send To PDF Document** dialog.
2. In **PDF file name**, enter path and name for the PDF document to be saved. To enter the path, you can click  and select the target folder using the appearing dialog.
3. In **Name**, select the printer you want to use.
4. Click **Properties** and select in **Orientation** the format (**Portrait** or **Landscape**) you want to use for printing. If needed, change page set up options. Then click **OK**.
Note: The options available depend on the selected printer.
5. In **Instrument**, the instrument used is selected by default. If you want to select a report layout appropriate for another instrument, uncheck **Select automatically** and select the desired instrument.
6. In **Layout**, select the layout for the report you want to preview.
7. Click **Save**. This saves the PDF document with the specified file name in the chosen target folder.

9.5 Creating a Custom Report Layout

The *Bruker Compass ReportDesigner* application allows you to create your own report layouts for printing specific reports. You can either modify an existing report layout available on your system or set up a completely new layout. For help on creating report layouts, please refer to the ReportDesigner Help.

Note: It is recommended not to modify the standard layout but to save the modified layout under a new file name. Otherwise, there is a risk that your changed standard layout version may be overwritten by a later system upgrade.

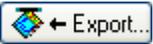
To start ReportDesigner:

1. Click . This opens the **Print** dialog.
2. In **Report Layout**, select the layout based on which you want to create a new layout. Alternatively, you can select the respective layout in ReportDesigner after it is started.
3. Click **ReportDesigner**. This starts ReportDesigner and loads the layout currently selected in **Layout**.

10 EXPORTING BATCH FILES

You can export the data in the open batch file in Comma Separated Values Files format (*.csv) to allow you to load the file in Microsoft *Excel*. The data actually exported depends on whether the respective batch file has already been processed. Processed batches are exported in the form of results tables while in unprocessed batches, the sample table is exported as *.csv file.

To export a batch file:

1. Click . This opens the **Export Sample Table** dialog for exporting a Comma Separated Values file (*.csv).
2. In **Save in** and the folder list, navigate to that folder the batch file should be exported to.
3. In **File name**, enter the name of the file you want to export.
4. Click **Save**.

A APPENDIX

A.1 QuantAnalysis 2.0 Toolbar

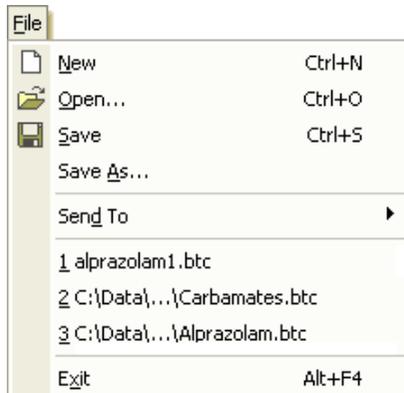
QuantAnalysis 2.0 provides the following tool buttons:

Button	Menu - Command	Shortcut	Used to...
	File – New	Ctrl+N	Create a new batch
	File – Open	Ctrl+O	Open an existing analysis.
	File – Save	Ctrl+S	Save active batch using the same file name.
	Edit – Cut	Ctrl+X	Cut the selection and put it on the Clipboard.
	Edit – Copy	Ctrl+C	Copy the selection and put it on the Clipboard.
	Edit – Paste	Ctrl+V	Insert the Clipboard contents.
	Method – Open		Open and attach quantification method.
	Help – Help Topics		Start QuantAnalysis help and list help topics.

A.2 QuantAnalysis 2.0 Menus and Commands

QuantAnalysis 2.0 provides the following menus and commands:

File menu



Commands

Commands	Used to...
New	Create a new batch.
Open	Open an existing batch.
Save	Save the active batch using the same file name.
Save As	Save the active batch using another file name.
Send To popup	Send report.
Recent files	List the last processed batches.
Exit	Close QuantAnalysis.

View menuCommands

Toolbar
Status Bar

Used to...

Show or hide toolbar.
Show or hide status bar.

Edit menuCommands

Undo
Cut

Used to...

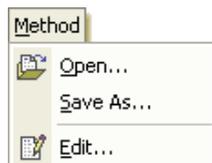
- not yet implemented -
Cut the selection and put it on the Clipboard.

Copy

Copy the selection and put it on the Clipboard.

Paste

Insert the Clipboard contents.

Method menuCommands

Open

Used to...

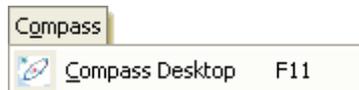
Open and attach a quantification method.

Save As

Save quantification method.

Edit

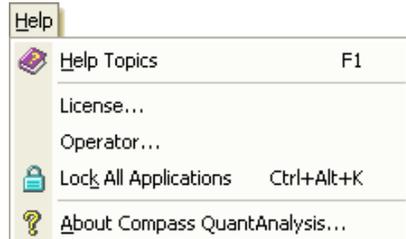
Edit parameters of open quantification method.

Compass menuCommands

Compass Desktop

Used to...

Launch Compass Desktop.

Help menuCommands

Help Topics

Used to...

Launch QuantAnalysis help.

License

Show license information.

Operator

Log in specified operator.

Lock All
Applications

Lock all Bruker Daltonics applications.

About Compass
QuantAnalysis

Show program information.

A.3 QuantAnalysis 2.0 Shortcuts

QuantAnalysis 2.0 provides the following shortcuts:

<u>Shortcut</u>	<u>Menu - Command</u>	<u>Used to...</u>
Alt+F4	File – Exit	Close QuantAnalysis.
Ctrl+Alt+K	Help – Lock All Applications	Lock all Bruker Daltonics applications.
Ctrl+C	Edit – Copy	Copy the selection and put it on the Clipboard.
Ctrl+N	File – New	Create a new batch.
Ctrl+O	File – Open	Open an existing batch.
Ctrl+S	File – Save	Save the active batch using same file name.
Ctrl+V	Edit – Paste	Insert the Clipboard contents.
Ctrl+X	Edit – Cut	Cut the selection and put it on the Clipboard.
Ctrl+Z	Edit – Undo	- not yet implemented -
F1	Help – Help Topics	Launch QuantAnalysis help.
F11	Compass – Compass Desktop	Launch Compass Desktop.

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