Agilent MassHunter Easy Access Software

Quick Start Guide

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The procedures in this guide are for use with the Agilent 6100 Series Single Quad LC/MS or the Agilent 6200 Series Time-of-Flight LC/MS, with Easy-Access software.

What is Easy-Access Software?

Easy-Access Software provides walk-up access to LC and LC/MS systems for lab users who lack experience with mass-spectrometry instrumentation and data systems. The software allows lab managers, analysts and operators in chromatography labs of pharmaceutical enterprises to do drug discovery and drug development under non-regulated conditions. It can also be used in chemical analysis labs in petrochemical, environmental, food, and other industries.

MS users such as medicinal and synthetic organic chemists can conveniently and easily submit samples. System administrators have a flexible way to manage the security and user access for the system. The system can be configured to e-mail reports and data to users.

Agilent Technologies

What's New in Easy-Access B.02.01?

- Support for Agilent 1290 Infinity LC System.
- Support for both the Classic and standard view for ChemStation users.
- Support for 40-vial 2-mL tray and 15-vial 6-mL tray in any configuration.
- Support for CTC sampler on the TOF LC/MS.
- Ability to change the tray shown in the status window when using the CTC.

What's New in Easy-Access B.02.00?

- Support for Agilent MassHunter B.02.00 (or higher) Data Acquisition for TOF/Q-TOF and Qualitative Analysis programs as the reporting application.
- Support for generating Analytical Studio Reviewer (ASR) result files.
- Analyst QS 1.1 and TOF Software A.02.02 obsoleted.
- Recalibration now possible in all modes, both automatically on wakeup and via the Event Scheduler.

Where to Find More Information

You can access more information about Agilent Easy-Access Software as follows.

Easy-Access Online Help

Consult the Easy-Access online Help for in-depth information about administering, configuring, and using Easy-Access software.

To access online Help, click **Help** in the Administration or System Configuration dialog boxes.

The online Help is also available as a PDF book on the installation disk.

Agilent Web Site

To view support information for Easy-Access and other Agilent products, see:

http://www.chem.agilent.com

Software Status Bulletin

A list of known problems and issues for Easy-Access software, with possible solutions, is described in the Software Status Bulletin. You can find the Software Status Bulletin and the Software Release Bulletin in the support folder on the installation disk.

Installation

Use these instructions to install Easy-Access software on your computer.

Step 1. Prepare to install

The tasks below must be completed before installing Easy-Access software.

1. Install the following hardware:
   - Agilent 1100 or 1200 Series Liquid Chromatograph with ALS
   - Agilent 1290 Infinity LC System
   - Agilent CTC PAL Sample Injector
   - Agilent 6100 Series Single Quad LC/MS or Agilent 6200 Series Time-of-Flight LC/MS
2. Make all necessary electrical connections.
3. Install the computer and verify that your computer hardware meets the minimum requirements to install and operate, as described in the installation instructions for those products:
   - G2170BA LC ChemStation software (B.04.01 or higher)
   - G2710BA LC/MSD ChemStation software (B.04.01 or higher)
   - Agilent MassHunter Workstation (B.02.00 or higher) software
4. Install the workstation software, as described in the installation instruction. Verify that the software is operational.
5. (*optional*) Install MassHunter Analytical Studio Reviewer program if you want to create and browse ChemStation or MassHunter results. Also, install MassHunter Analytical Studio Reviewer on each client computer that will receive results by e-mail in ASR format. Check the ASR user guide for software compatibility.

Step 2. If you are upgrading from a previous version, back up your databases

If you are upgrading Easy-Access from a previous version, do these steps.

1. If you want to use your current databases with the new version, you need to back up your databases as follows. Otherwise, skip to step 2 below.
   a. Run the program **ezdbbackup.exe** in Database Backup Tool folder on the Easy-Access installation disk.
   b. If you are upgrading from Easy-Access A.02.00, note the folder where the databases are backed up. You will need this later (see "Step 4. Update databases" on page 7).
2. Remove Easy-Access using the **Add/Remove Programs** icon in the Windows Control Panel.
3. Continue with "Step 3. Install the software".

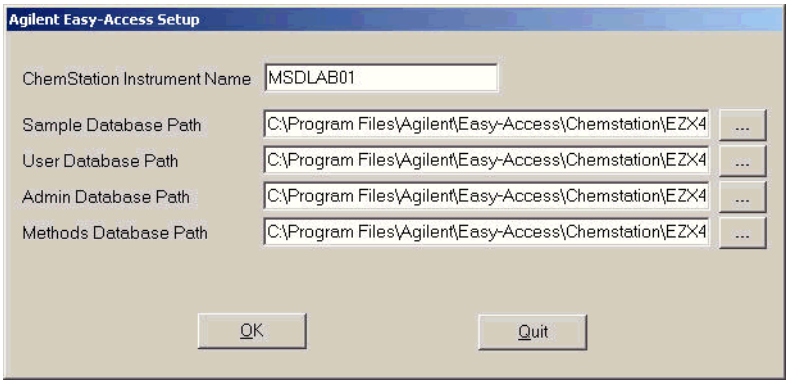
Step 3. Install the software

1. Start Windows. Log in to an account that has administrator privileges. Be sure that ChemStation or MassHunter Data Acquisition program is *not* running.
2. Insert the Easy-Access setup disk into the disk drive.
3. Using Windows Explorer, double-click **setup.exe** on the installation disk to start the installation program. Select the **setup.exe** file in the folder that is appropriate for your MS hardware: **SQ & LC** (for ChemStation) or **TOF** (for MassHunter Data Acquisition).
4. If a previous version of Easy-Access is installed:
   a. Click **Yes** when you are asked to remove the existing Easy-Access program.
   b. Run **setup.exe** again.
5. When the Agilent MassHunter Easy-Access Software Setup dialog box appears, click **Next** to continue.
6. Read the license agreement. Click **Yes** to accept its terms and continue the setup program.
7. When the Choose Destination Location dialog box appears, click **Next** to accept the default folder or click **Browse** to select a different location. The default installation directories are:
   C:\Program Files\Agilent\Easy-Access\ChemStation or
   C:\Program Files\Agilent\Easy-Access\TOF, depending on your LC/MS instrument.

8 If you are updating the Easy-Access program, click **No** when you are asked to overwrite the existing database files.

9 Review the settings when presented and click **Next** to continue.

10 In the Easy-Access Setup dialog box, type the instrument name and location of the database files, as shown in the example below. If you are sharing databases between different computers, see "Sharing Configurations with Multiple Instruments" on page 10 before you fill out this dialog box. Click **OK**.



Instrument Name Must be set to at least three characters. If your organization has networked or is planning to network several Agilent 1100/1200/1290 LC systems with the Easy-Access software, then the last two characters of each instrument name must be unique. These characters can be used to name data subdirectories, as configured on the Data File Name tab of the System Configuration dialog box. See online Help for more information on options to name the folder path and data files.

Easy-Access Databases Use the default locations, or enter new ones.

Database	Path	Description
Sample	EZX4Smpls.mdb	Easy-Access saves all information, such as the sample queue, in a Microsoft Access database. The Sample database is specific to the associated instrument that is being controlled. If more than one instrument is running Easy-Access, each instrument must have its own Sample database file. *The Sample database cannot be shared by multiple instruments.*

Database	Path	Description
User	EZX4Users.mdb	The User database contains a list of all users and user groups registered in Easy-Access. By maintaining the users list in a separate database on a single network, multiple Easy-Access installations can have access to and use a common user list. The user list may be updated from any Easy-Access installation.
Admin	EZX4Admin.mdb	The Administrative database saves the configuration of the Easy-Access instances (that is, each instrument with an Easy-Access installation). In a multiple-instrument installation, this database file must be shared if the System Administrator wants newly installed instruments to be autoconfigured by applying the default Easy-Access configuration.
Methods	EZX4Mthds.mdb	The Methods database contains references to all of the ChemStation or MassHunter methods that may be used in Easy-Access. The database can be shared across a network between multiple instruments, but the System Administrator is responsible for ensuring that the ChemStation or TOF methods are available and updated locally on each instrument. The Methods database cannot be shared between a ChemStation Easy-Access installation and a TOF Easy-Access installation.

If you want to use existing databases with the new version of Easy-Access and you are upgrading from Easy-Access 2.0, see "Step 4. Update databases" below.

11 If you want to configure Easy-Access to use the SMTP option:

a Click **Yes** when prompted.

The SMTP installation begins if you choose Yes.

b Click **Close** when the installation is completed.

12 Click **Finish** when the Easy-Access installation is complete.

13 Reboot the computer only if you are prompted to do so.

Step 4. Update databases

If you are updating from Easy-Access version A.02.00, convert the databases as follows.

1 Be sure that the new Easy-Access software has already been installed as described in "Step 3. Install the software" on page 5.

2 Run the **setup.exe** file in the **Migration Tool** folder on the Easy-Access on the installation disk.

3 Run the **EZX Database Migration Tool.exe** file in the **C:\Program Files\Agilent\Easy-Access\Data Migration Tool** folder. Follow the prompts described below.

4 Select the Source Folder for the existing databases. Unless you specified a different location when you backed up the databases, the files are in **C:\Backup_Easy_Access_Database\ChemStation** or **C:\Backup_Easy_Access_Database\TOF**.

5 Select the Destination Folder that contains the newly installed databases, **C:\Program Files\Agilent\Easy-Access\ChemStation** for example. The information in these databases will be overwritten with the information in the old databases for use with the new Easy-Access software.

6 Select the database types that you want to migrate (**Users/Groups, Methods**, or Admin).

7 Click **Migrate Databases** to start the migration process. A message is displayed when the process is completed.

   The databases installed with the new Easy-Access software are copied and stored in **C:\Temp\dbBackup**. If a problem occurs with the conversion process, the backup copies are restored to their original location.

8 Click **Exit** to close the EZX Database Migration Tool dialog box.

Step 5. Install the Unpack Utility on other computers

Install the Easy-Access Unpack Utility on all computers that will be used to receive e-mail from the instrument computer running Agilent Easy-Access software.

You can configure Agilent Easy-Access software to send sample results to users by e-mail. The results are compressed into a .ZNE file.

1. Insert the Agilent Easy-Access installation disk into the disk drive.
2. Double-click the file **d:\EZXUNPCK\EZXUnpack_Install.exe** (where **d:** is the drive letter corresponding to the disk drive).
3. Follow the instructions displayed in the dialog box to install the Unpack Utility.

See Also "To display reports that have been sent in a compressed format" on page 24

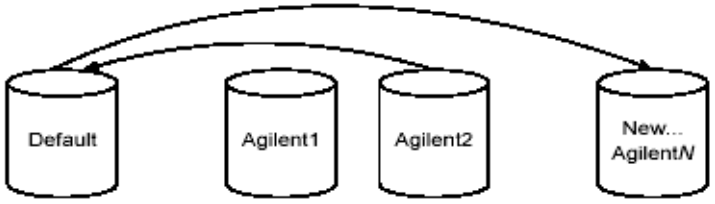
Sharing Configurations with Multiple Instruments

In laboratories where more than one Easy-Access system is used to submit samples, the administrator can use the shared configuration feature to simplify the initial configuration of new systems. Configuration is shared when the database files are placed on a shared network drive, and the Easy-Access program points to that database file. Easy Access has four associated databases that are described in "Easy-Access Databases" on page 6.

Administrative Database

Easy-Access saves a default configuration in the Administrative database. When you save an Easy-Access configuration, you have the option to save it as the new default configuration. When a new instrument is added to the network, and its Administrative database path points to the shared Administrative database, the default configuration on the shared Administrative database is used to configure the new instrument.

The following figure shows the conceptual layout of multiple instrument configurations in the Easy-Access Administrative database (EZX4Admin.MDB). The default configuration record is automatically copied as the initial configuration for any new instrument that is added to the networked system. Afterwards, the configuration can be modified, if necessary, for the individual instrument.



Installed Files

The Easy-Access Setup program installs in the location specified in "Step 3. Install the software" on page 5.

The files marked with a * are only part of the ChemStation installation. The files marked with ** are only part of the TOF installation. All of the other files are part of both installations.

File	Description
EZAccess.exe	The main Easy-Access executable program
EZXsetup.exe	The program that sets the instrument name and the paths for the Easy-Access databases
Database files	See "Easy-Access Databases" on page 6.
EXTERNAL.mdb	An example database for linking Easy-Access to another system
***EZXMMAIN.mac**	The main macro that ChemStation calls to load all Easy-Access features
***EZXM_DA.mac**	ChemStation Data analysis/report macros, copied to **c:\chem 32\core**
Easy-Access.chm	The help file for Easy-Access
EZXTEMPLATE.htm	Template file for HTML status page
***EZWPSctrl.ocx**	Control used by Easy-Access to display the sampler and fraction collector
PopupStopper.dll	DLL used by Easy-Access to close ChemStation message boxes
watch.list	Test list of message boxes to be closed automatically
Logo.BMP	Bitmap logo used in the HTML status page
****ESATofCom.exe**	Program to help with communication between TOF and Easy-Access
****TOFEasyAccess.ico**	Icon displayed when TOF Easy-Access is minimized

Using Easy-Access Software

The following sections introduce the Easy-Access software. Full operating instructions are given in the Easy-Access online Help.

To start the Easy-Access software

1. Log in to a Windows account that has Windows administrator privileges.
2. Start ChemStation or TOF software.
3. Start Easy-Access as follows:
   - For ChemStation, click **Easy-Access > Start Software**.
   - For Agilent TOF, click the TOF Easy-Access desktop icon.

   The Easy-Access STATUS dialog box appears.

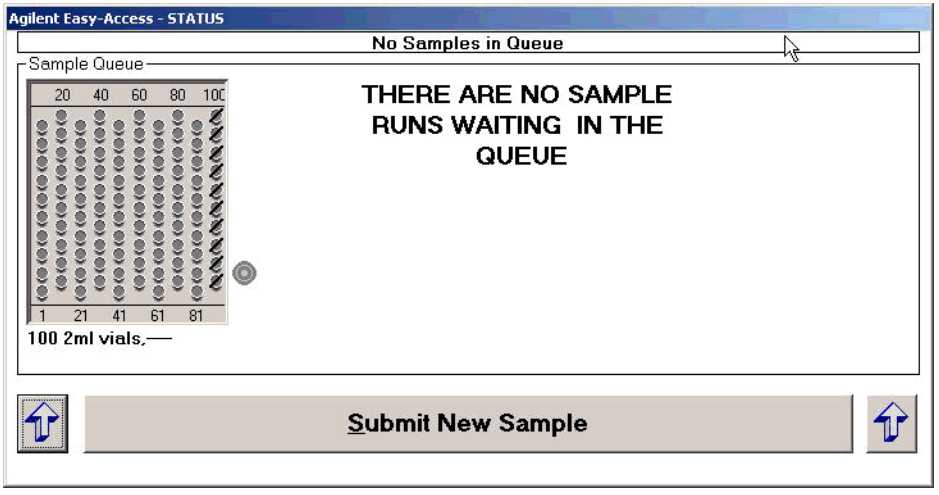


Figure 1 Status dialog box

To open the Administration dialog box

1 Click **Submit New Sample** in the Easy-Access Status dialog box. The Main Login dialog box appears.

2 Select a **User Name** that has administrator privileges, such as **sysadmin**. The **Admin** button appears at the bottom of the dialog box.

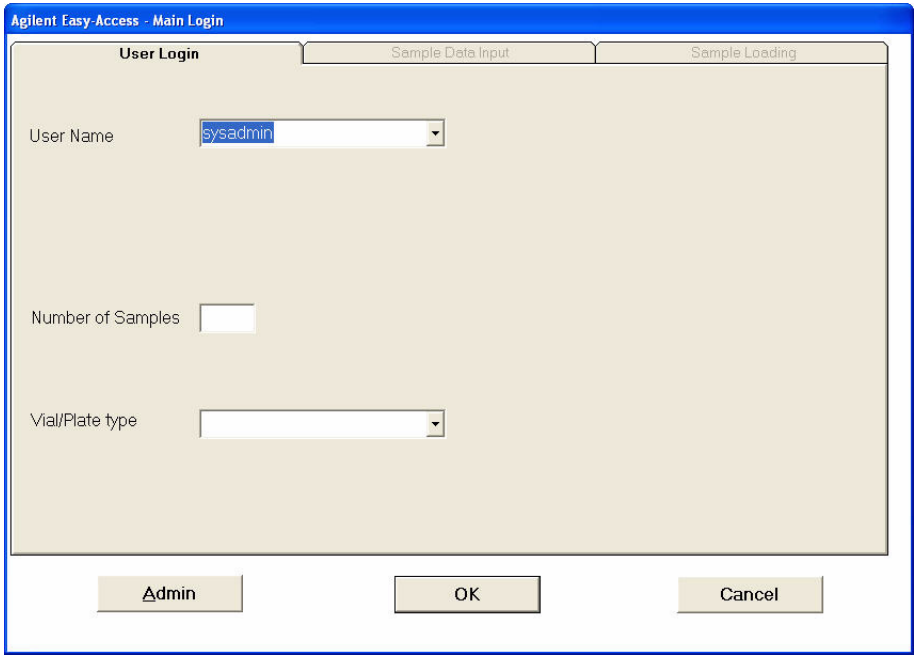


Figure 2 Main Login dialog box

3 Click **Admin**.

4 Enter your password when prompted (`3000hanover` when shipped).

The Administration dialog box appears.

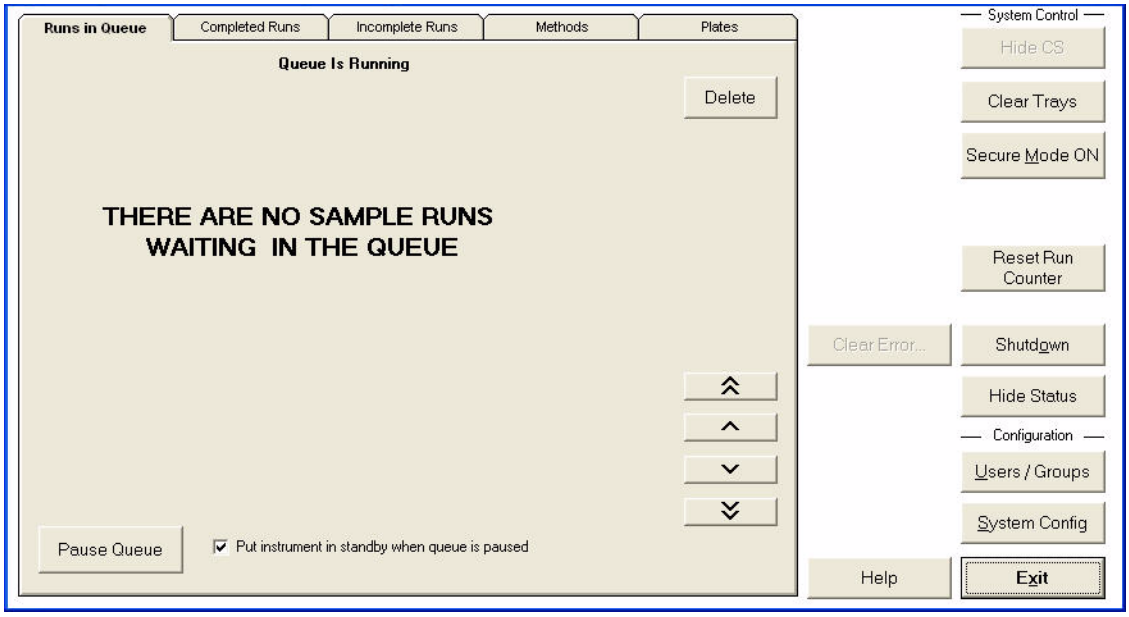


Figure 3 Administration dialog box

5 Click the appropriate tab or button to do the desired administration activity.

6 Click **Exit** to close the Administration dialog box and return to the Status dialog box.

To configure the system

1 Open the Administration dialog box. See "To open the Administration dialog box" on page 13.

2 Click **System Config** in the Administration dialog box. The System Configuration dialog box appears.

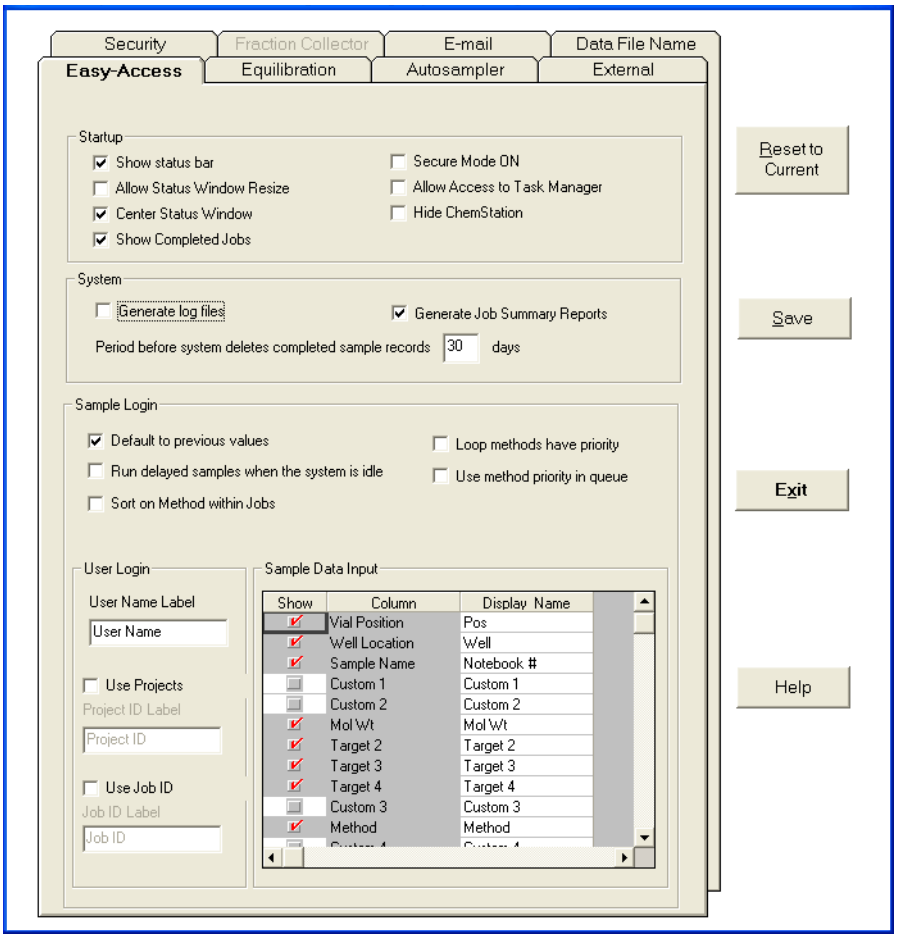


Figure 4 System Configuration dialog box

3 Set the features that you need in the System Configuration dialog box, then click **Save**. See "Setup Tips" on page 25.

4 Click **Exit** to close the dialog box.

5 Close Easy-Access and restart it to invoke the new settings. See "To close the Easy-Access software" on page 23.

To enable overlapped injection

1 Click the **Autosampler** tab in the System Configuration dialog box.

2 Mark the **Enable overlapped injections** check box.

3 If Easy-Access is configured to run multiple methods, then

   a Click the **Easy-Access** tab in the System Configuration dialog box.

   b Mark the **Sort on Method within Jobs** check box.

To configure users and groups

1 Open the Administration dialog box. See "To open the Administration dialog box" on page 13.

2 Click **Users/Groups**.

3 To add or edit group information, click a group from the left side of the dialog box to display the Group dialog box.

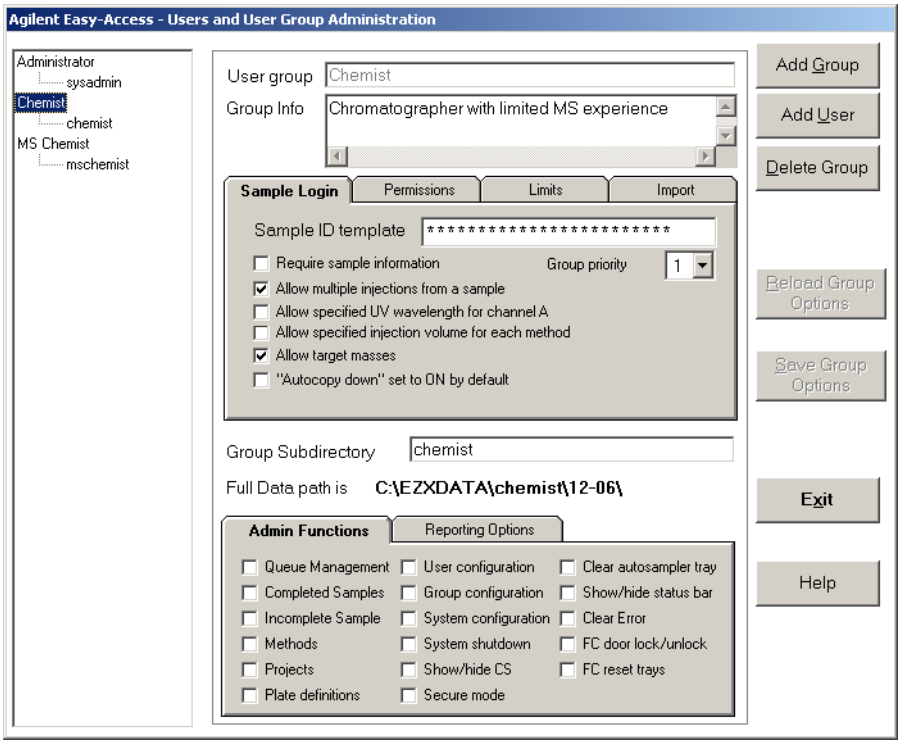


Figure 5 Users and User Group Administration dialog box

4 Make the desired changes to the group information, then click **Save Group Options**.

5 To add or edit user information, click a user from the left side of the dialog box to display the User dialog box.

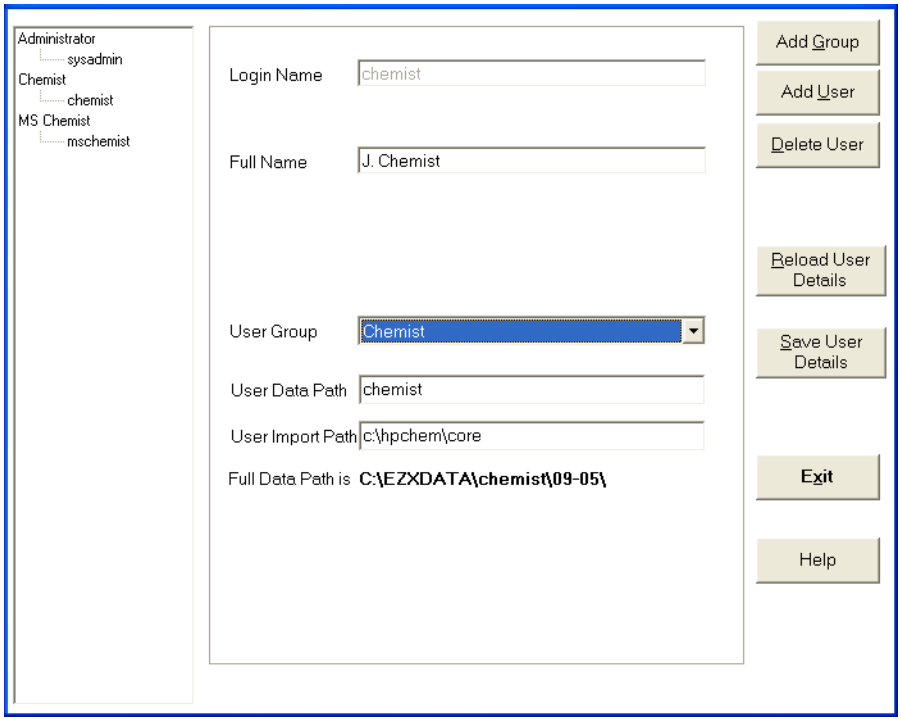


Figure 6 User and Group Administration dialog box

6 Make the desired changes to the user information, then click **Save User Details**.

7 Click **Exit** to close the dialog box.

To use Easy-Access with MassHunter Workstation

When you use Easy-Access with MassHunter Workstation:

- Pause the Easy-Access queue before you change the MassHunter context to Tune. You are not be able to change context while Easy-Access is running samples.
- If a MassHunter worklist is in progress, do not start Easy-Access.
- If after Easy-Access completes a sample run and you close Easy-Access, if worklist is still open, do not use that worklist to start a new run. Create a new worklist.

To configure MassHunter Workstation software for Easy Access

The MassHunter Workstation system administrator must set up methods in the MassHunter Qualitative Analysis program to work with Easy Access.

1. In the MassHunter Data Acquisition program, for all methods that will be used with Easy Access, make sure all the values on the **Instrument State** tab — including Fast Polarity Switching — are the same.
2. In the MassHunter Qualitative Analysis program, update all methods that were created in a release prior to B.02.00 and with which you want to use Easy Access.

   See “Update methods for use with the Easy Access program” in the Qualitative Analysis online Help.

3. Set up each method so that:
   - Result files (either reports or exported files) are located with the data files.
   - Automated processing steps are included in the method.

   See “Update methods for use with the Easy Access program” in the Qualitative Analysis online Help for more information.

   You may want to use the DA Reprocessor program with an existing data file to check that an automated report is generated.

4. If you are running the MassHunter BioConfirm program, for each method, set the **Match source** option in the Match Sequence pane to **Worklist**.

   See “Set match sequence method parameters” in the Qualitative Analysis online Help.

To use Analytical Studio Reviewer with Easy-Access

Analytical Studio Reviewer lets you view, print, and export your ChemStation or TOF data without having to purchase and run full analytical software on every desktop. To use Analytical Studio Reviewer, the ChemStation results or the TOF results file is converted to ASR format. With Easy-Access, ASR files can be e-mailed to users who can review the results on client computers where Analytical Studio Reviewer software is installed.

1 Set up MassHunter Workstation to generate ASR data.

   See “Procedure to generate ASR files from TOF data in the MassHunter Workstation” in the *Agilent G3772AA MassHunter Analytical Studio Reviewer Quick Start Guide* to generate ASR files in MassHunter Workstation.

2 In Easy-Access software, enable e-mail notification and mark the **ASR** check box on the E-mail tab in the System Configuration dialog box. See the Easy-Access online Help for more information.

To log in and submit samples

1 Click **Submit New Sample** in the Easy-Access Status dialog box. The Main Login dialog box appears.

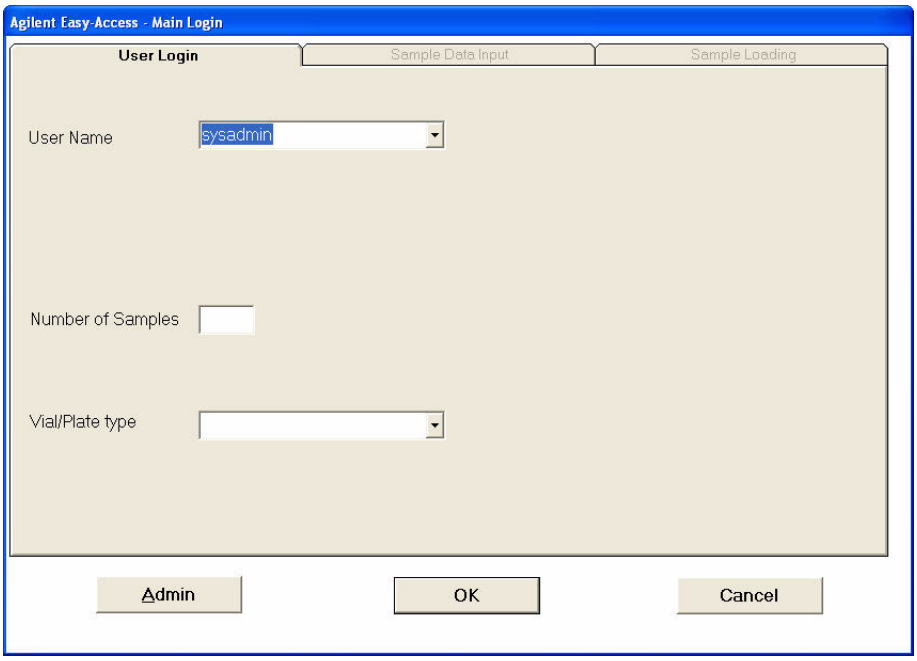


Figure 7 Admin Login dialog box

2 Type the required information on the User Login tab, then click **OK**. You may be required to enter a password as well.

The Sample Data Input tab appears.

3 Type the sample information on the Sample Data Input tab. Assign a method for each sample from the list of available methods.

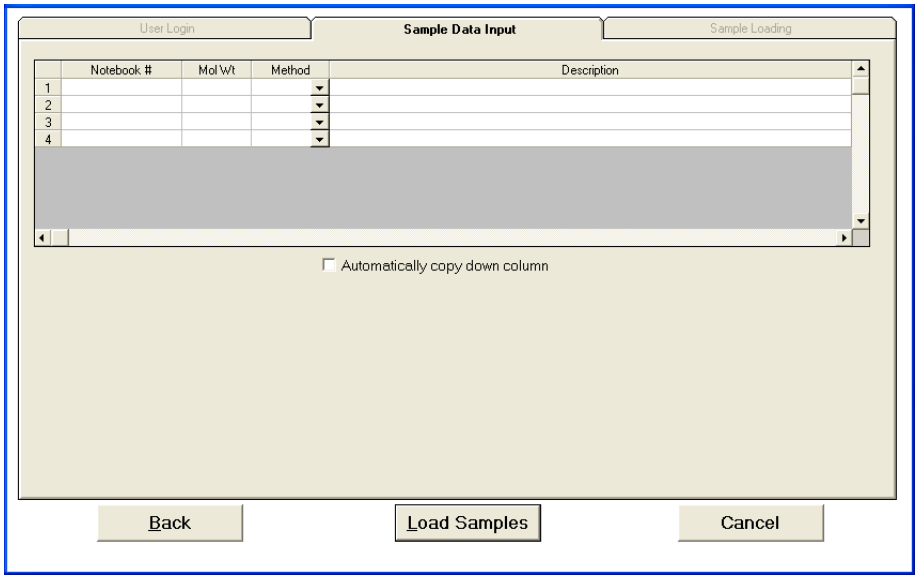


Figure 8

4 When you have finished entering the sample information, click **Load Samples**.

The Sample Loading tab appears. A message is displayed in blue, indicating the starting position for the samples in the tray.

5 Place the samples in the indicated positions in the sampler.

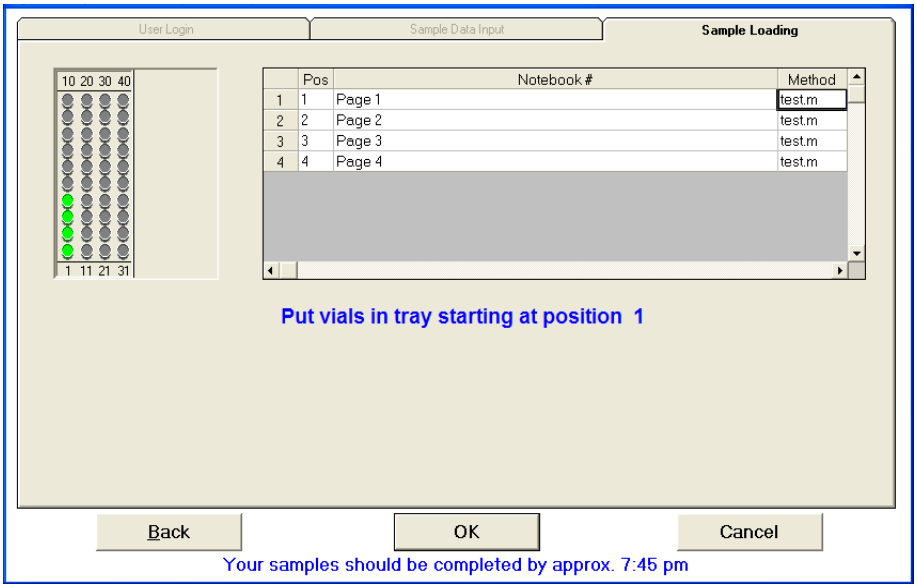


Figure 9 Sample Data Input dialog box - Sample Loading tab

6 Click **OK** to submit the samples. The new samples are listed in the queue in the Status dialog box, following samples submitted previously. When sample analysis is completed, the reports are created and e-mailed to you if that option is configured and selected.

To close the Easy-Access software

1 Open the Administration dialog box. See "To open the Administration dialog box" on page 13.

2 Click **Shutdown**. *Do not shut down Easy-Access while samples are running.*

To display reports that have been sent in a compressed format

Use the Easy-Access Unpack Utility on client computers to display reports that have been e-mailed in a compressed format. Before you begin, check that the Easy-Access Unpack Utility is installed on your computer; see "Step 5. Install the Unpack Utility on other computers" on page 9.

1 Double-click a .ZNE file that is attached to an e-mail or a .ZNE file that has been saved to disk. This automatically starts the Unpack Utility and opens the .ZNE file.

2 Mark the **View Report** check box, as shown in the example below.

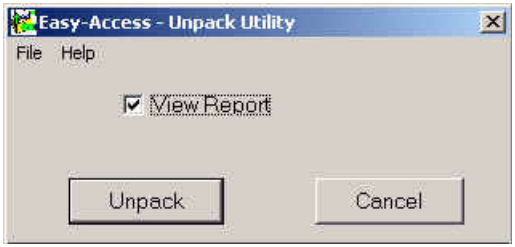


Figure 10 Unpack Utility dialog box

3 Click **Unpack**.

The ChemStation report files are extracted and displayed in an internet browser window.

A .ZNE file that has been saved to disk can also be opened with WinZip or PKZip decompression software. In this case, the report is *not* automatically displayed in a browser window.

To generate and send a .ZNE file by e-mail

- Configure the Easy-Access software on the instrument computer for e-mail capabilities as described in the Easy-Access online Help.
- Mark the **HTML report (as .zne file)** check box on the E-mail tab in the System Configuration dialog box in Easy-Access.
- The .ZNE file will only be sent if ChemStation creates an HTML report for the run. To configure this, click the **Destination File** option and **File Type .HTM** option in the Specify Report dialog box in ChemStation.

Setup Tips

To optimize standby settings

The optimum settings for standby time depend on the operating conditions of the instrument.

1 In the System Configuration dialog box, click the **Equilibration** tab.

2 Adjust the standby setting:

- For prep systems with high flow rates, reduce the standby time to minimize the consumption of solvent when no samples are being run.
- For analytical systems with low flow rates, increase the standby time so that the system is ready to run when samples are submitted.

To configure e-mail to send reports and error notifications

You can configure Easy-Access to send reports and error notifications via e-mail.

- To use this feature, see these topics in online Help:
  - "To set up e-mail for the SMTP option"
  - "To set up e-mail for the Outlook Express/MAPI option"
  - "To configure e-mail in Outlook Express"
- If you use Outlook Express/MAPI, make sure that the **Account Name** used in "To configure e-mail in Outlook Express" is identical to **Sender Account** used in "To set up e-mail for the Outlook Express/MAPI option".

To configure e-mail to allow zip file attachments

1 In the System Configuration dialog box, click the **E-mail** tab.

2 Mark the **Send attachments in a ZIPPED file** check box.

To prevent pop-up messages from interfering with automatic operations

Do these steps if you use Outlook Express.

1. Click **Tools > Options**.
2. On the Security tab, clear the **Warn me when other applications try to send mail as me** check box.
3. On the Send tab, clear the **Automatically complete e-mail addresses when composing** check box.

To optimize the format of the Easy-Access Loop Qualitative report

- Set the **Chromatogram Output Size Response** parameter in the Specify Report dialog box in ChemStation to `20%` or `25%`.

  This setting allows two chromatograms and two spectra to fit on a single page.

When Easy-Access is present on a system, a section is added to the end of the Loop Qualitative Report and the LCMS Qualitative Report that shows the full calculations for the estimated sample purity. See Easy-Access online Help for more information on setting up these reports.

To change the behavior of the Easy-Access software when a vial is missing

When the Easy-Access software encounters a Missing Vial error, the system can either stop until the system administrator clears the error, or it can continue to run samples. To set how the Easy-Access software behaves when it encounters this error:

1 Open the **Autosampler** tab in the System Configuration dialog box.

2 Mark the **Stop on missing vial** check box for the desired behavior as follows:

- When selected, the system will pause until the system administrator clears the error
- When cleared, the system will continue to run the remaining samples (this is the default setting).

To determine the desired behavior for your system, consider the following possible scenarios that result in a missing vial error:

- If a user loads a vial incorrectly into the ALS tray, all subsequent samples are located in a different position than expected by Easy-Access. The incorrect location leads to incorrect sample information in the report and possibly to the wrong instrument methods being run for subsequent samples.
- If a user removes a vial before it is analyzed, continuing to run samples has no effect on the analysis of the remaining samples.

To format the custom values display in reports

Custom values are appended to the sample description field in ChemStation and the sample comment field in MassHunter Software. You can change the Easy-Access initialization file to set how or whether custom values are displayed. The values are formatted by default as

<custom value name>: <custom value>

1 Click **Start > Run**.
2 Type or select the name of the initialization file, then click **OK**. The initialization files are in your Windows system folder.
   - **eztof.ini** for MassHunter Software
   - **chemstation.ini** for ChemStation
3 Edit the initialization file as needed, then save and close the file.

You can change these options:

- IncludeCustomFieldsInReports

  1 (default) – activate reporting of custom fields
  0 – deactivate reporting of custom fields

  If this feature is deactivated, no custom field information is appended to the sample description/comment field.

- CustomFieldsReportSeparator

  Type the character that you want to use to separate custom fields. The default separator, "|", causes the ChemStation program to report each value on a separate line. Use a different separator if you want to keep the values on the same line for ChemStation reports.

- QuoteCustomFields

  0 (default) – do not put quotes around the value of custom fields
  1 – put quotes around all custom field values

- ReportCustomFieldName

  1 (default) – format the value by `<custom value name>:` before the custom field
  0 – do not include the <custom value name> when formatting the custom values

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In this Book

The *Quick Start Guide* presents first steps to use the Easy Access Software.

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