

Xcalibur

Thermo QuickQuan

Version 2.4

Installation Guide

XCALI-97252 Revision A

July 2009

DOCUMENTATION
SURVEY

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Release history:

Revision A—July 2009

Software requirements:

QuickQuan 2.4, Foundation 1.0, Xcalibur 2.1, TSQ Series 2.1.1 or later, LC Devices 2.2.1 or later (includes Thermo PAL), Microsoft Windows XP Service Pack 3, Microsoft Office, and compatible autosampler drivers

For Research Use Only. Not for use in diagnostic procedures.

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Preface

About This Guide

This guide describes how to install the **QuickQuan™ 2.4** rapid optimization and acquisition solution and register the database. You can use this application to perform high-throughput optimization and quantitative analysis of your compounds.

For details on how to use the QuickQuan application, refer to the *QuickQuan User Guide* and Help available from the QuickQuan Help menu.

❖ **To suggest changes to documentation or to Help**

Complete a brief survey about this document by clicking the link below.
Thank you in advance for your help.



Related Documentation

The following QuickQuan manuals are available on the QuickQuan CD as PDF files:

- *QuickQuan Installation Guide* describes how to install the QuickQuan application and register the database.
- *QuickQuan User Guide* describes how to use the QuickQuan application to perform high-throughput optimization and quantitative analysis of your compounds.
- *QuickQuan Quick Start* describes how to use the main features of the QuickQuan application.
- *QuickQuan and Aria Quick Start* describes how to use the QuickQuan application with the Aria™ OS system.

❖ **To view QuickQuan manuals**

From the Windows™ taskbar, choose **Start > All Programs > Thermo Xcalibur > Manuals > QuickQuan**.

❖ **To open QuickQuan Help**

- From the QuickQuan window, choose **Help > QuickQuan Help**. To locate a particular topic, use the Help Contents, Index, or Search panes.
- If available for a specific window or dialog box, click **Help** or press F1 for information about setting parameters.

Special Notices

This guide includes the following types of special notices:

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

❖ **To contact Technical Support**

Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at mssupport.thermo.com.

❖ **To contact Customer Service for ordering information**

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
Web site	www.thermo.com/ms

❖ **To copy manuals from the Internet**

Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

❖ **To suggest changes to documentation or to Help**

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

QuickQuan Overview

The QuickQuan application can perform compound optimization, acquisition, processing, and reporting of quantitative sequences using standard methods.

You can use this application to perform an entire acquisition of an assay or as a stand-alone tool to perform compound optimization. You can configure any number of compounds in any arrangement in a tuning plate. This application can then optimize all the compounds for maximum analysis.

When you use the QuickQuan application to optimize compounds, you can lay out the configuration graphically on a tuning plate and specify the contents of each compound. After you initiate a run, this application sends a request to the mass spectrometer to optimize each compound specified in the tuning plate. Following optimization of each compound, the mass spectrometer generates the data in corresponding raw and XML files. The QuickQuan application retrieves and stores the data in a database, which can be on the local computer or on a remote computer. This application processes the entire tuning plate in this way until it completes the analysis of all the compounds.

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About the QuickQuan Database

The QuickQuan application stores all compound information for both the tuning and data acquisition in a database. The database contains information such as compound name, polarity, selective reaction monitoring (SRM) transitions of the parent-to-product ion, charge state, Q1 and Q3 factors, collision energy, skimmer offset setting, and tune file. This application also enforces the use of drug sets, which are groups of compounds under a common name.

You can create more than one QuickQuan database (giving each database a unique name), and you can store the databases on a local QuickQuan computer or on a remote system.

The QuickQuan application uses the Open Database Connectivity (ODBC) call-level interface to access the data. ODBC is the database portion of the Microsoft™ Windows™ Open Services Architecture (WOSA). You must register the database that you intend to use prior to the first time you start the application. See [“Registering the QuickQuan Database”](#) on [page 12](#) for more details.

IMPORTANT The size limit for a Microsoft Access database is approximately 2 GB. You cannot update your database when its size exceeds this limit.

Supported Instruments and Data Systems

QuickQuan version 2.4 supports the Thermo Scientific TSQ Quantum™ or TSQ Vantage™ mass spectrometers, CTC PAL autosampler, Phytronix LDTD™ autosampler, and Thermo Scientific LC devices.

This application works with the following versions of Thermo Scientific data system and device software:

- Foundation™ version 1.0
- or—
- (Optional) Foundation version 1.0.1 (for loop injection optimization)
- Xcalibur™ version 2.1
- TSQ Series version 2.1.1 or later
- LC Devices version 2.2.1 or later (includes Thermo PAL)
- (Optional) Aria OS version 1.6.2 or later (for the Aria system)
- (Optional) Phytronix LDTD for Xcalibur driver version 1.1 or later (for LDTD autosampler)

Hardware and Software Requirements

The QuickQuan application runs in conjunction with the Xcalibur mass spectrometry data system on the Microsoft Windows operating system.

To operate the QuickQuan application, you must meet these requirements:

System	Requirements
PC	<ul style="list-style-type: none"> • 2 GHz processor with 1 GB RAM • CD-ROM drive • Resolution display 1280x1024 (XGA) • 75 GB or greater available on the C: drive • NTFS format
Autosampler	<ul style="list-style-type: none"> • CTC PAL • Phytronix LDTD
Mass spectrometer	<ul style="list-style-type: none"> • TSQ Quantum • TSQ Vantage
Software	<ul style="list-style-type: none"> • Microsoft Windows XP with Service Pack 3 • Microsoft Office

You can download Microsoft Windows XP Service Pack 3 from this Web address:

<http://www.microsoft.com/windows/products/windowsxp/sp3/default.msp>

Thermo Fisher Scientific recommends a clean installation of Windows XP rather than an upgrade from Windows 2000 to Windows XP.

Installing and Integrating QuickQuan Version 2.4

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- [Installing the QuickQuan Application](#)
- [Integrating with the Aria System](#)

Installing the QuickQuan Application

Before installing QuickQuan version 2.4, first remove your older versions of LC devices and TSQ series applications. Then verify that you have the following applications installed on your system, in this order:

1. Foundation version 1.0 or later

IMPORTANT If you are running loop injection optimization, you must install Foundation version 1.0.1 or later, which requires that you first have the Microsoft .NET Framework version 3.5 installed. In addition, if you are upgrading from Xcalibur version 2.1/Foundation version 1.0 or Xcalibur version 2.0.7 to Foundation version 1.0.1, you must reinstall the following applications in the indicated order after performing the Foundation upgrade.

2. Xcalibur version 2.1

To use either the Aria system or the LDTD autosampler, verify that you also have the Xcalibur XDK application installed.

3. TSQ series version 2.1.1 or later

4. If you do not plan to use the Aria system,

- And you are using the Thermo PAL autosampler, verify that you also have the LC devices 2.2.1 application or later and the pump's driver installed.
- And you are using another non-LDTD autosampler, verify that you also have the drivers for the autosampler and pump installed.
- And you are using the LDTD autosampler, verify that you also have the LDTD driver version 1.1 or later installed.

Install QuickQuan version 2.4 last, after all of the previous applications are on your system.

IMPORTANT If you have an existing QuickQuan database, do the following:

1. Make sure you give your database a name other than QuickQuanCompounds, which is the default database name upon installation. Otherwise, the new installation can overwrite your existing database. The default QuickQuan database folder is:

C:\Xcalibur\QuickQuan\QuickQuanDatabase\

2. After the QuickQuan installation, create a new file data source to register the database whose name you have changed. For details, see [“Registering the QuickQuan Database”](#) on [page 12](#).

If you are upgrading from a previous QuickQuan version to QuickQuan version 2.4, the installer does the following:

- Overwrites files shared by other Xcalibur-related applications with newer versions of those files included with the installer, under this folder:

C:\Xcalibur\system\programs\

- Overwrites files installed by earlier QuickQuan versions with newer versions of those files included with the installer, under these folders:

C:\Xcalibur\system\programs\

C:\Xcalibur\QuickQuan\Templates\

C:\Xcalibur\QuickQuan\QuickQuanDataBase\

C:\Xcalibur\QuickQuan\ImportFiles\

- Updates the registry entries.
- Removes the following .dll files from the C:\Xcalibur\system\programs\data\ folder:

1valarms.dll, 1vdaq.dll, 1vuste.dll, and LVWUt1132.dll

Aria version 1.6.2 automatically installs a newer version of these files to your default Aria installation folder, for example, the C:\Program Files\Thermo\Aria OS 1.6\ folder.

- Removes the following files from the C:\Xcalibur\system\programs\ folder:

ThermoFisher.Foundation.ClientMessage.dll and
ThermoFisher.Foundation.ClientMessage.tlb

Foundation version 1.0 or later automatically installs a newer version of these files to your Foundation installation folder, for example, the C:\Program Files\Thermo\Foundation\ folder. The QuickQuan application detects these files in their installation location and registers them.

- Removes the following files from the C:\Xcalibur\system\programs\ folder if you have not removed a previous QuickQuan version:

AriaXtern.dll, AriaXtern.ini, AriaAddSup.11b, and AriaXtern.aliaes

Aria version 1.6.2 automatically installs a newer version of these files (except for AriaXtern.aliaes) to the C:\WINDOWS\system32\ folder.

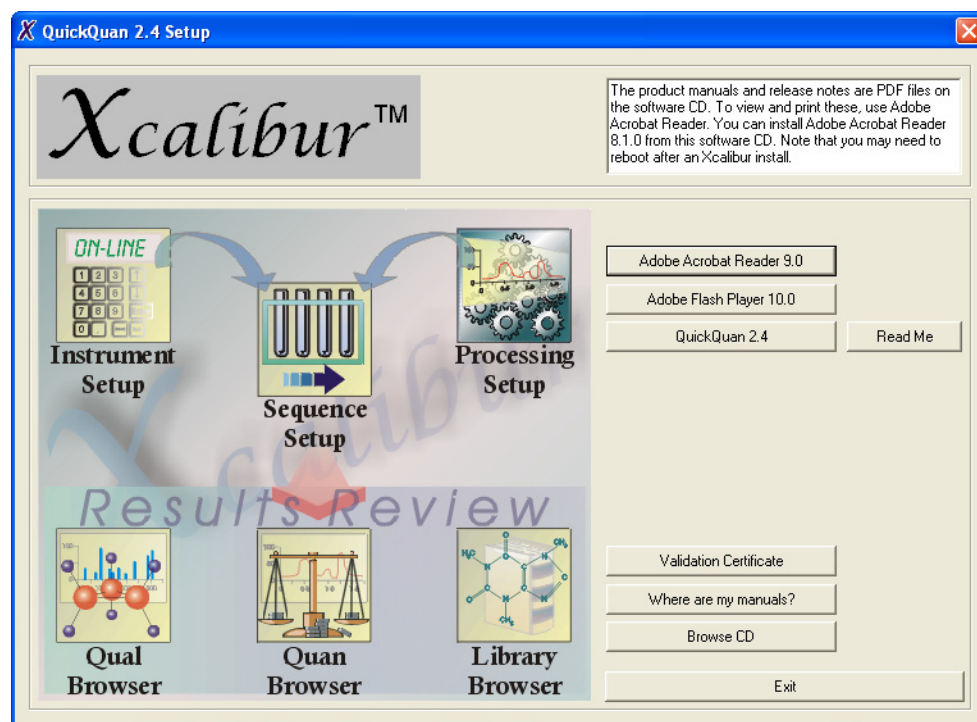
- Removes the C:\Xcalibur\system\programs\data\ folder if it is empty.
- Logs the file and/or folder removals in the Installation Qualification (IQ) report and log files, located in the C:\Program Files\Thermo\IQ Reports\ folder.

❖ To install the QuickQuan application

1. Insert the QuickQuan CD in the CD-ROM drive of your computer. The installer starts automatically and displays the Xcalibur Setup window (see Figure 1).

If the installer does not start automatically, choose **Run** from the Windows Start menu. In the Run dialog box, type **D:\XInstall.exe**, where D is the letter of your CD drive. Then click **OK**.

Figure 1. Thermo Xcalibur Setup window

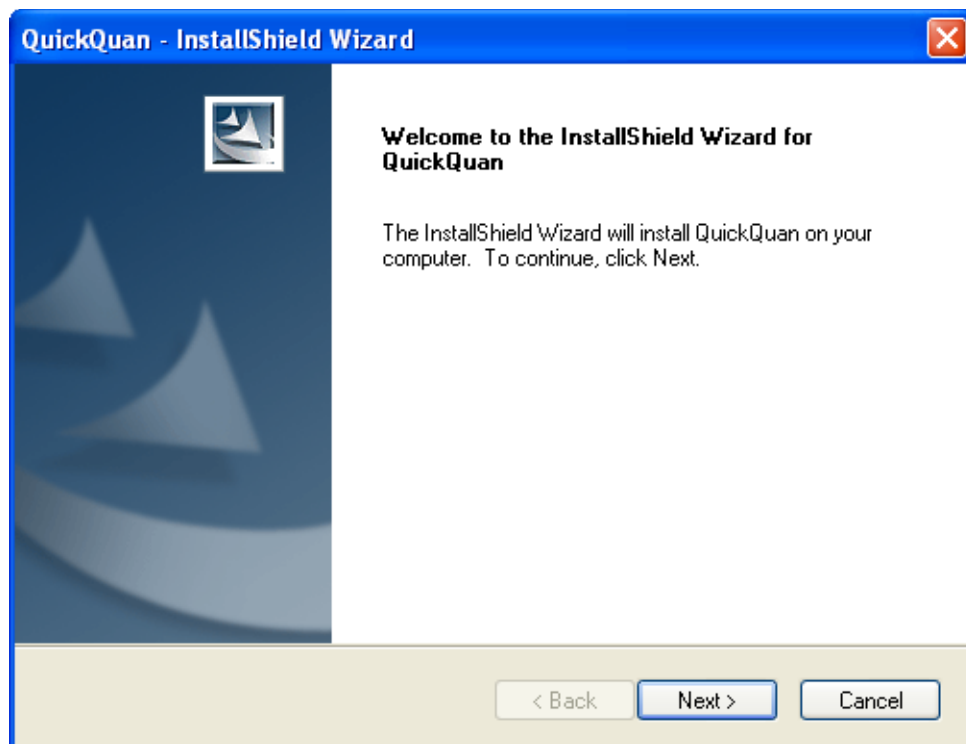


2 Installing and Integrating QuickQuan Version 2.4

Installing the QuickQuan Application

2. In the Setup window, click **QuickQuan 2.4**. The Welcome page of the InstallShield Wizard appears (see [Figure 2](#)).

Figure 2. QuickQuan InstallShield Wizard – Welcome page



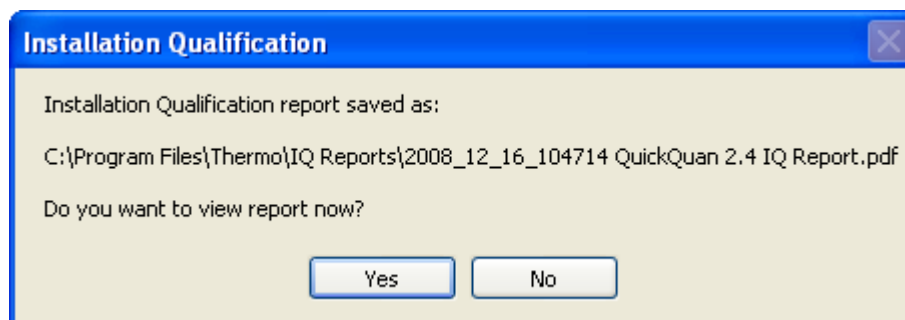
3. Click **Next** to continue the installation.
4. Follow the prompts that appear in the InstallShield Wizard.

The Setup Status box appears and displays the progress of the installation.

Note QuickQuan files and folders are installed in the C:\Xcalibur\QuickQuan and C:\Xcalibur\system\programs folders.

5. When the Installation Qualification dialog box appears (see [Figure 3](#)), click **Yes** to view the Installation Qualification report.

Figure 3. Installation Qualification dialog box



The Installation Qualification report indicates whether the installation qualification passed or not. The report is a time-and-date stamped PDF file located in the C:\Program Files\Thermo\IQ Reports\ folder.

6. On the Complete page of the InstallShield Wizard, click **Finish**.

Integrating with the Aria System

If you plan to use the Aria system, follow these steps:

1. Install Aria OS version 1.6.2. Refer to *Aria Version 1.6.2 Installation Instructions* on the Aria OS CD.
2. For details on the valve connections to the Aria system, see [“Plumbing Connections for Aria System”](#) on [page 19](#).


Starting the QuickQuan Application and Registering the Database

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Starting the QuickQuan Application

❖ To start the application

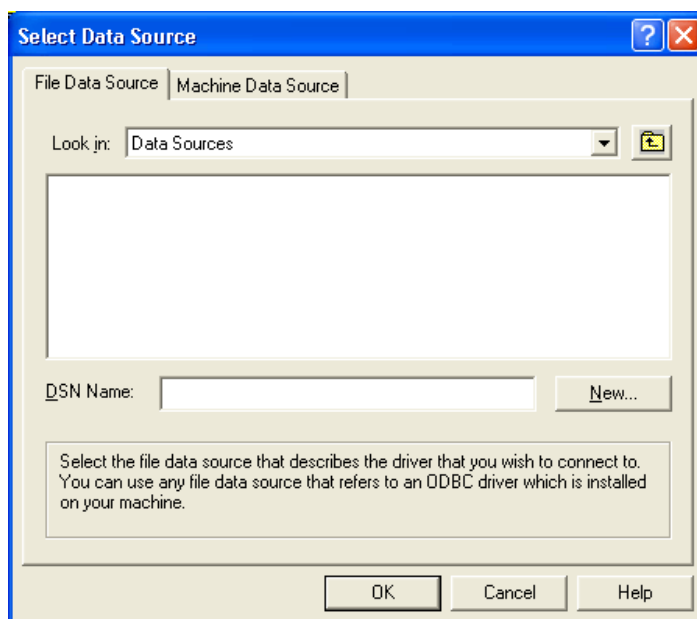
From the Windows taskbar, choose **Start > All Programs > Thermo Xcalibur > QuickQuan**, or on your desktop, double-click the QuickQuan icon, . The QuickQuan window appears.

When you start the application the first time, you must register and select the database. The QuickQuan application uses the selected database whenever you start the software unless you choose a different database. If you have not registered a database before, when you start the application, the Select Data Source dialog box automatically appears showing the File Data Source page.

3 Starting the QuickQuan Application and Registering the Database

Registering the QuickQuan Database

Figure 4. Select Data Source dialog box

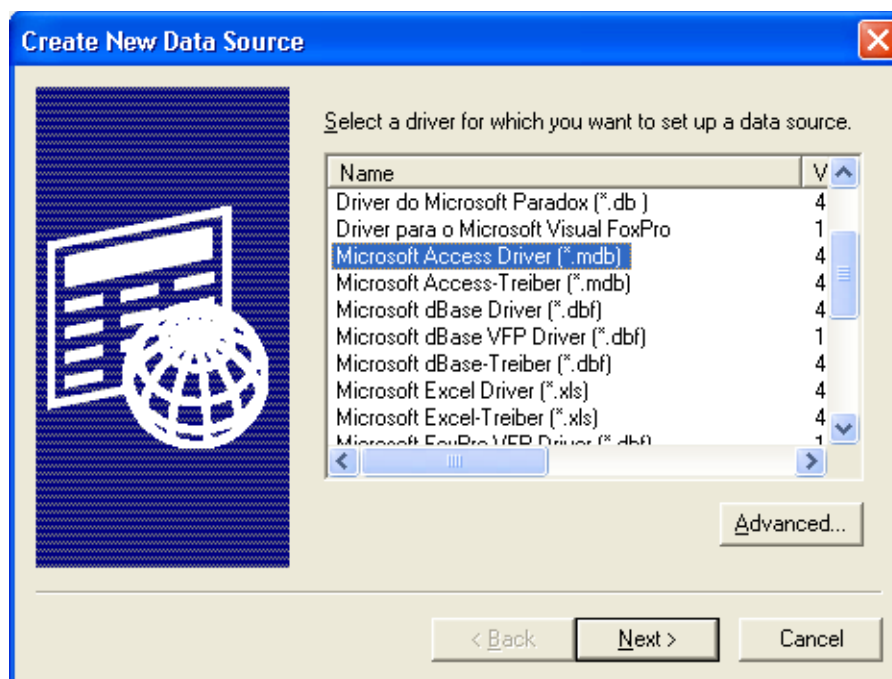


Registering the QuickQuan Database

You can register the QuickQuan database through an ODBC connection on the computer that has the QuickQuan application installed. Each time you start this application, you can use the last opened database or connect to a different ODBC database. The databases reside either on the local computer running the QuickQuan application or on a network computer. You create a separate file data source for each database that you want to connect to.

❖ To create a file data source connection and register the database

1. If the Select Data Source dialog box is not already open, then in the QuickQuan window, choose **File > Open Database**. The Select Data Source dialog box appears (Figure 4).
2. On the File Data Source page (Figure 4), click **New**. The Create New Data Source Wizard appears (Figure 5).

Figure 5. Create New Data Source Wizard – select driver list

3. Select **Microsoft Access Driver (*.mdb)** from the list of drivers, and click **Next**.

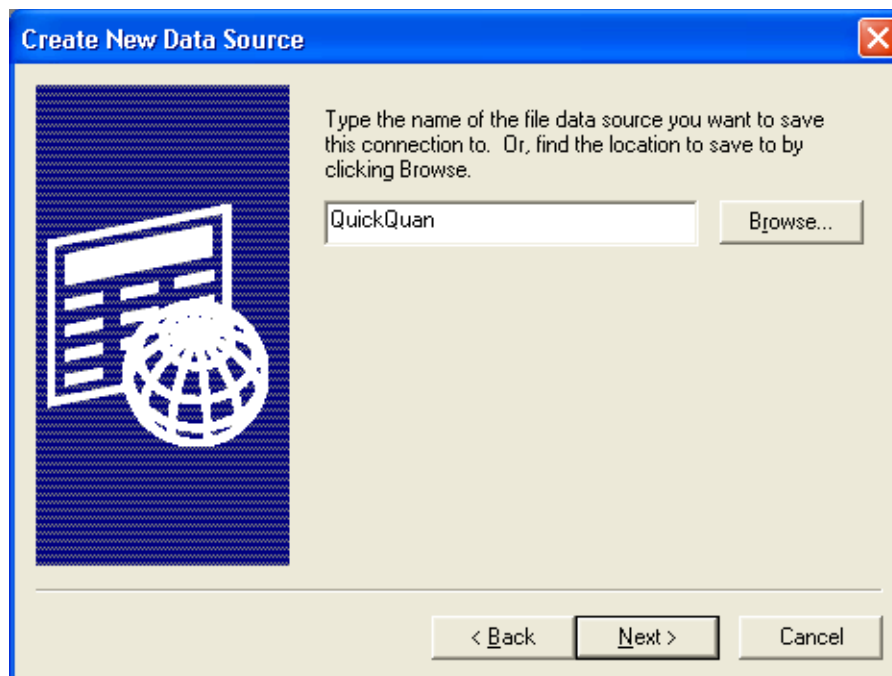
Note If your site uses an Oracle™ database, select an appropriate Oracle driver. Contact your local Oracle administrator for details on how to configure the QuickQuan application for an Oracle database.

3 Starting the QuickQuan Application and Registering the Database

Registering the QuickQuan Database

4. In the name box (Figure 6), type your data source name, for example, **QuickQuan**. Click **Next**.

Figure 6. Create New Data Source Wizard – data source name box



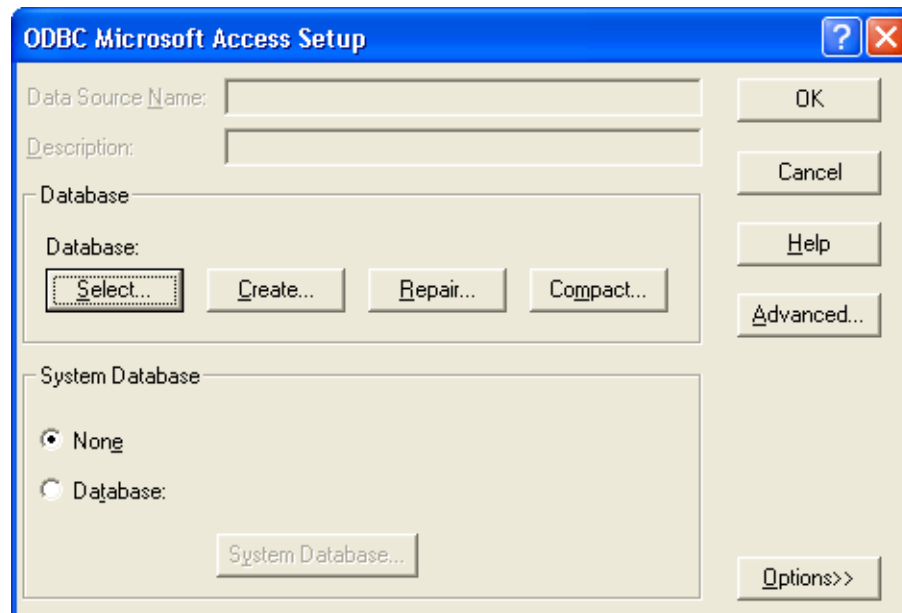
5. Verify that the file name of the new data source appears in the file data source box (Figure 7).

Figure 7. Create New Data Source Wizard – finish page



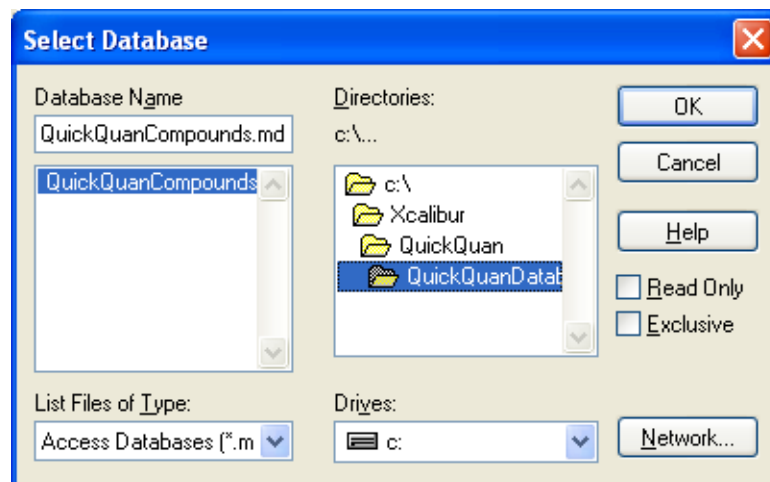
6. Click **Finish**. The wizard creates the file data source and then displays the ODBC Microsoft Access Setup dialog box (Figure 8).

Figure 8. ODBC Microsoft Access Setup dialog box



7. Click **Select**. The Select Database dialog box appears (Figure 9).

Figure 9. Select Database dialog box



8. If you are using the QuickQuan application for the first time, in the Directories list, browse to and select the following folder:

C:\Xcalibur\QuickQuan\QuickQuanDatabase\

Otherwise, to use an existing QuickQuan database, in the Directories list, browse to the folder where your database is stored.

3 Starting the QuickQuan Application and Registering the Database

Registering the QuickQuan Database

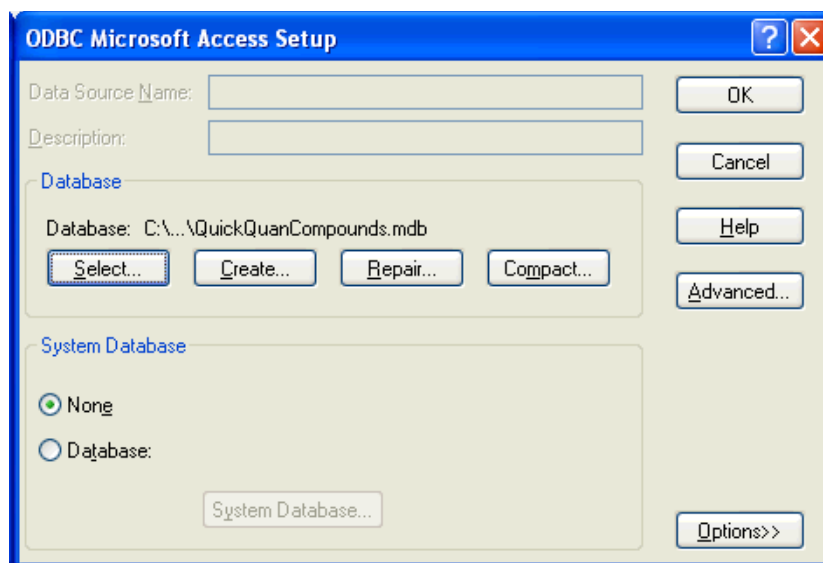
9. If you are using the QuickQuan application for the first time, in the Database Name list, select **QuickQuanCompounds.mdb**. The installation program places this default “QuickQuanCompounds.mdb” database in the QuickQuanDatabase folder.

Otherwise, if you have an existing QuickQuan database that you have renamed, then in the Database Name list, select that database.

The file data source that you created connects to the selected database.

10. Click **OK**. The ODBC Microsoft Access Setup dialog box appears (Figure 10).

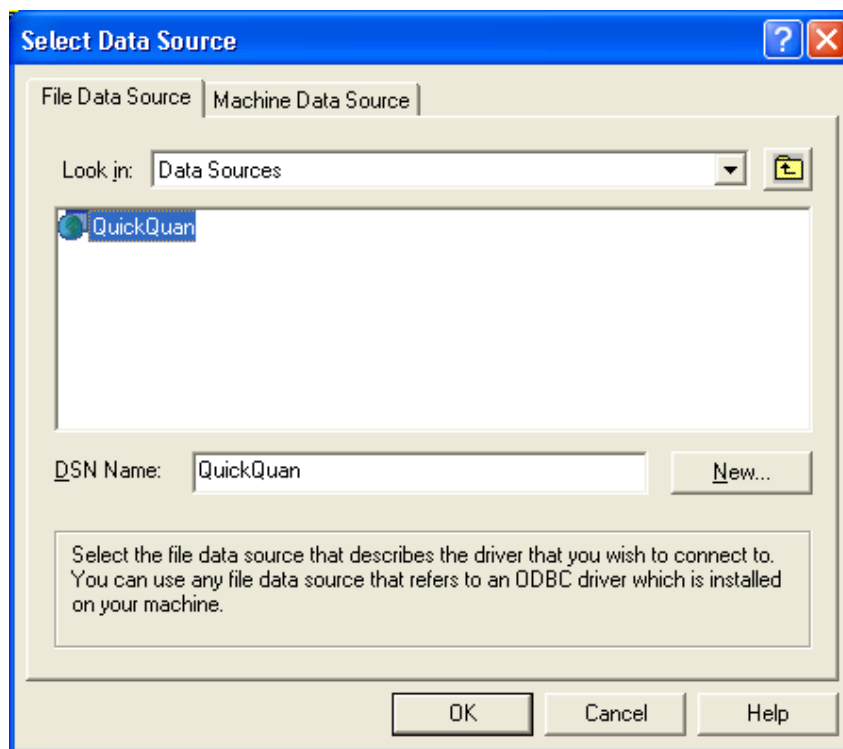
Figure 10. ODBC Microsoft Access Setup dialog box



11. In the Database area, verify that the name of your selected database appears.

12. Click **OK** to close the ODBC Microsoft Access Setup dialog box. The new file data source, for example QuickQuan, appears in the Select Data Source dialog box (Figure 11).

Figure 11. New file data source



13. Click **OK** to close the Select Data Source dialog box.
14. Click **OK** to close the ODBC Microsoft Access Setup dialog box.

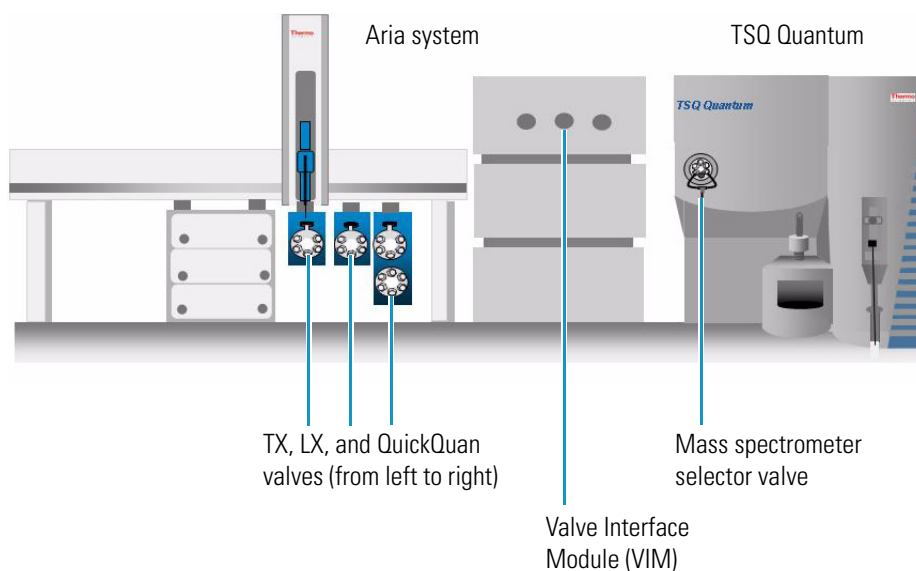
After you create and then select a file data source connection for the QuickQuan application to use, it stores the name of the file data source in the registry. The next time you start the application, it checks the registry for a known file data source connection and automatically opens the last database used. You can choose to use a different database for your QuickQuan session if you wish. For details, refer to the *QuickQuan User Guide* or the QuickQuan Help.

Plumbing Connections for Aria System

Use the following diagrams to verify the system plumbing connections between the Aria system and the mass spectrometer, when necessary.

Figure 12 shows the valve placement on the Aria system and the TSQ Quantum mass spectrometer as an example.

Figure 12. Valve placement



Note The valve placement on the Aria system might vary depending on your system hardware configuration.

Figure 13 shows the plumbing diagram of the TX and LX injector valves, the QuickQuan valve unit, and the mass spectrometer selector valve.

Figure 13. Plumbing diagram

