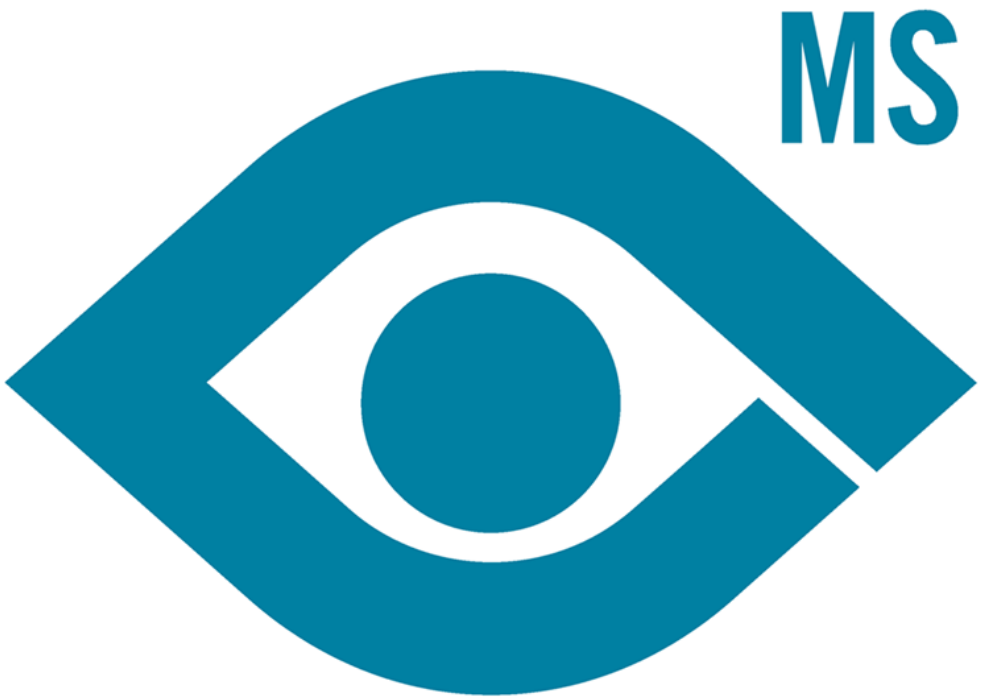
SCIEX
The Power of Precision

Accurate Mass E&L Open Access HR-MS/MS Spectral Library

High Resolution Accurate Mass Libraries

Release Notes



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Introduction 1

Features

The Accurate Mass E&L (Extractables and Leachables) Open Access Library is a free library for customers that can be download from sciex.com. It consists of 724 MS/MS spectra acquired from a TripleTOF 6600 or a X500 QTOF mass spectrometer.

These libraries are compatible with:

- Data acquired using a combination of the MasterView 1.1 software and the PeakView 2.2 software, on a TripleTOF accurate mass system or a QTRAP system.
- Data acquired using the SCIEX OS software version 2.0 or later on a X500 QTOF accurate mass system.

In the MasterView 1.1 software and SCIEX OS software, these libraries do this:

- Help accurately identify compounds and increase confidence in the reported results.
- Enable rapid compound searches for targeted and non-targeted screening.
- Leverage the accurate mass, retention time, and peak area reporting functionality in both the MasterView software and SCIEX OS.
- Compare a sample to a control for qualitative review using the comparative profiling option available in both the MasterView software and SCIEX OS.

Requirements

SCIEX OS	MasterView Software
An English (US) version of: • Windows 7 (64-bit) operating system with SP1. • Windows 10 (64-bit) operating system.	An English (US) version of: • Windows 7 (64-bit) operating system with SP1. • Windows 10 (64-bit) operating system.
A user with an Administrator privileges is required to log on to the computer.	The user must be logged on to the computer as a user with Administrator privileges.
An internet access is required to obtain a license file for each installed High Resolution Accurate Mass (HRAM) library.	Internet access is required to obtain a license file for each installed High Resolution Accurate Mass (HRAM) Library.

SCIEX OS	MasterView Software
At least one of the following applications is required to install a library: • A licensed version of SCIEX OS, version 2.0 or higher. • A licensed version of the LibraryView software, version 1.4 or higher.	At least one of the following software applications is required to install a library: • A licensed version of the PeakView software, version 2.2 or higher and a licensed version of the MasterView software, version 1.1 or higher. • A licensed version of the LibraryView software, version 1.0.3 or higher
A licensed version of the LibraryView software, version 1.4 or higher, is required to edit the library.	A licensed version of the LibraryView software, version 1.0.2 or higher, is required to edit the library.

Supported Equipment

- A TripleTOF accurate mass system
- A QTRAP system
- An X500 QTOF accurate mass system
- A Dell Precision T3600 computer, or later model, provided by SCIEX, with a minimum of 32 GB of RAM

Notes on Use, Known Issues, and Limitations 2

Accurate Mass E&L Open Access Library

The library includes polymer degradants covering nylon oligomers or degradants, polypropylene glycol (PPG) species, polyethylene glycol (PEG) species, piperidines, polyethylene terephthalate (PET) species, poly (tetramethylene glycol) (PTMG) species, and hydroxy terminated polyethylene polyols. The library also contains other polymer components, preservatives, stabilizers, antioxidants, light stabilizers or UV absorbers, and fatty acids. A new class of siloxane related compounds is added into the library.

The library data includes compound name, CAS, formula, molecular weight, and structure, for both positive and negative ionization spectra.

In the LibraryView software, each compound is assigned a score, which is shown in the **Comments** field. The score might be one of the following:

- **Score 2**: Compound names or classes are predicted based on the TOF MS and in-silico MS/MS scan of the unknown sample.
- **Score 3**: Compound names or classes are predicted based on the sample background information, mass accuracy of the TOF MS data, structural elucidation, or external library references of the unknown sample.
- **Score 4**: Actual compound names or classes are obtained from the reference standard material.

Isobaric compounds with the same MS/MS pattern have similar product ion spectra, they must be differentiated by the retention time.

The LibraryViewServiceHost stops responding intermittently

On the Windows 7 (64-bit) operating system, when the MasterView software is opened from the PeakView software menu bar, the LibraryViewServiceHost service occasionally stops responding. To resolve this issue, do the following:

1. In Windows Explorer, right-click **Computer** and then click **Manage**.

   The Computer Management dialog opens.
2. Double-click **Services and Applications** and then double-click **Services**.
3. Right-click **LibraryViewServiceHost**, and then click **Start**.

The LibraryViewServiceHost service starts again.

The LibraryView Software occasionally stops responding while it is loading the library, or results are not found during searches of the library

To resolve these issues, do the following:

1. Make sure that the computer has 32 GB RAM available.
2. Start the computer again.
3. If the issue persists, then contact SCIEX Technical Support at sciex.com/request-support and request that the SQL databases be cleared and that the libraries be installed again.

SCIEX OS and the MasterView software occasionally stop responding when the Import compounds from LibraryView software database feature is used

The Import compounds from LibraryView software database feature is used to import compound names and formulas from the library into SCIEX OS and the MasterView software.

Installation 3

Install a Licensed High Resolution Accurate Mass Library

A licensed library can be installed from a zip file downloaded from the SCIEX website. The zip file can include compound names, compound transition information, and compound library spectra.

Note: Internet access is required to obtain the license.

If the Accurate Mass E&L Open Access Library 1.0 is installed, then download the Accurate Mass E&L Open Access Library 2.0, and then overwrite the old license key with the new one.

1. Log on to the computer as a Windows user with administrator privileges.
2. Download the required zip file from the SCIEX website.

   Tip! To prevent potential installation issues, save the file to a location other than the computer desktop.
3. After the download is complete, right-click the downloaded file and then click **Extract All**.
4. Go to https://sciex.com/support/activate-software and then log on using a SCIEX username and password.

   Note: If an account does not exist, then follow the on-screen instructions to create an account.

   The Activate Software page opens.
5. Select the appropriate instrument in the **Select Your Instrument** field.

   Tip! If the instrument is not listed, then go to the SCIEX Now profile for the logged-on user and add the instrument information.
6. In the Windows search field, type `ipconfig /all` to obtain the physical addresses, that is, the MAC addresses of the computer.
   A physical address, in the format `34-02-86-06-8A-05`, is shown for each active adapter.
7. Type all of the physical addresses in the **Computer ID** field.

   Tip! A maximum of three physical addresses can be typed. Separate the addresses with a space. For example, 34-02-86-06-8A-05 34-02-86-06-8A-01 34-02-86-06-8A-09.

8. In the the **License Key** field, type the license key.
   The license key might be distributed through an e-mail from SCIEX Now. If the license key is missing, then contact a SCIEX sales representative.

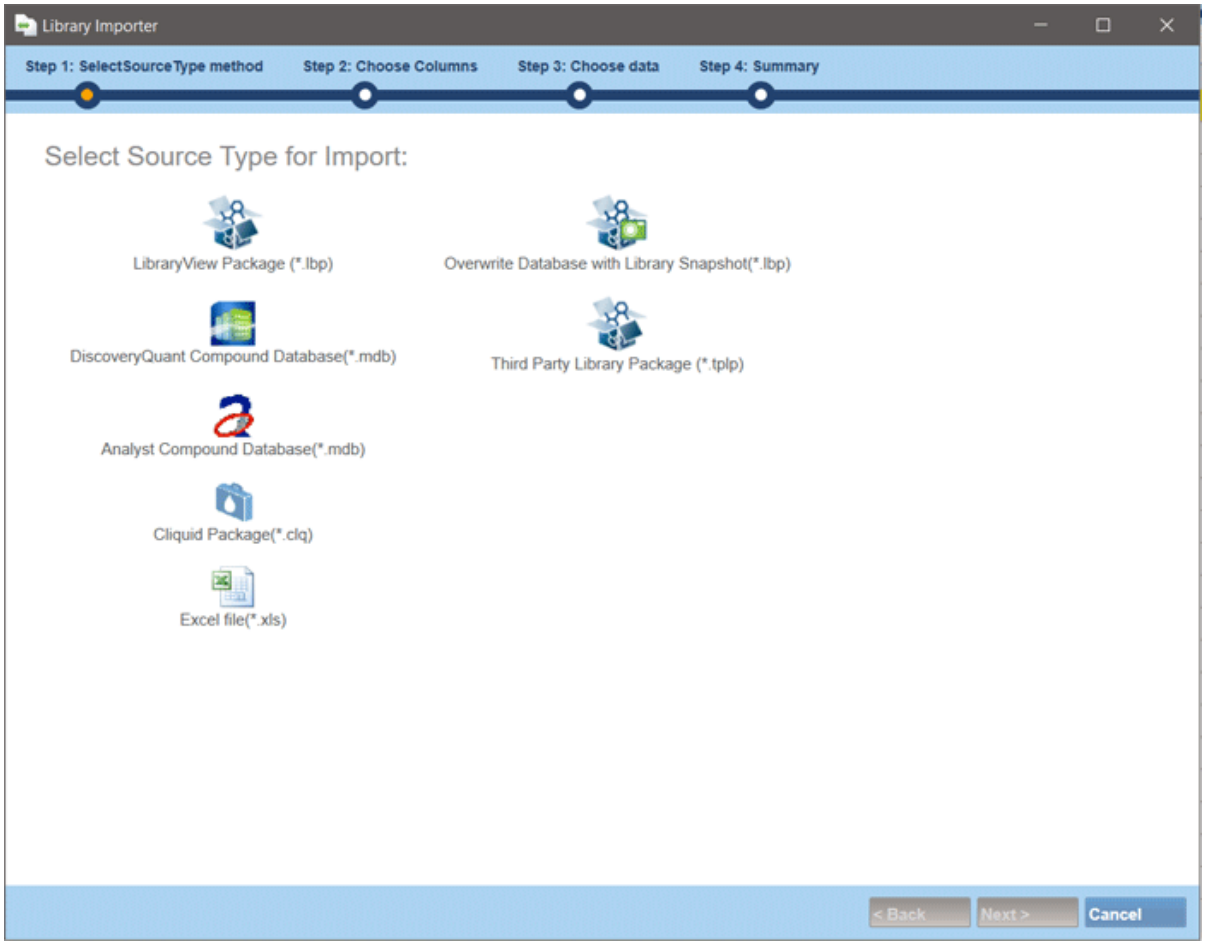
   Note: The key begins with the letters AID. If a license key is not available, then contact sciex.com/request-support.

9. Click **Submit**.
   After the required information is submitted, a license file is sent to the e-mail address registered to the SCIEX Now account.
10. Save the license file to the appropriate location:
    - On a computer with version 1.0.2 or 1.0.3 of the LibraryView software installed, save the license file in the `C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Server` folder.
    - On a computer with version 1.4 of the LibraryView (SCIEX OS) software installed, save the license file in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server` folder.
11. In the Windows search field, type `libraryviewpackager.exe` and then run the file.

    Note: The `libraryviewpackager.exe` can also be accessed from one of the following locations, depending on the version of the LibraryView software that is installed.
    - On a computer with version 1.0.2 or 1.0.3 of the LibraryView software installed, the `libraryviewpackager.exe` file is located in the `C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Packager` folder.
    - On a computer with version 1.3 or 1.4 of the LibraryView software installed, the `libraryviewpackager.exe` file is located in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager` folder.

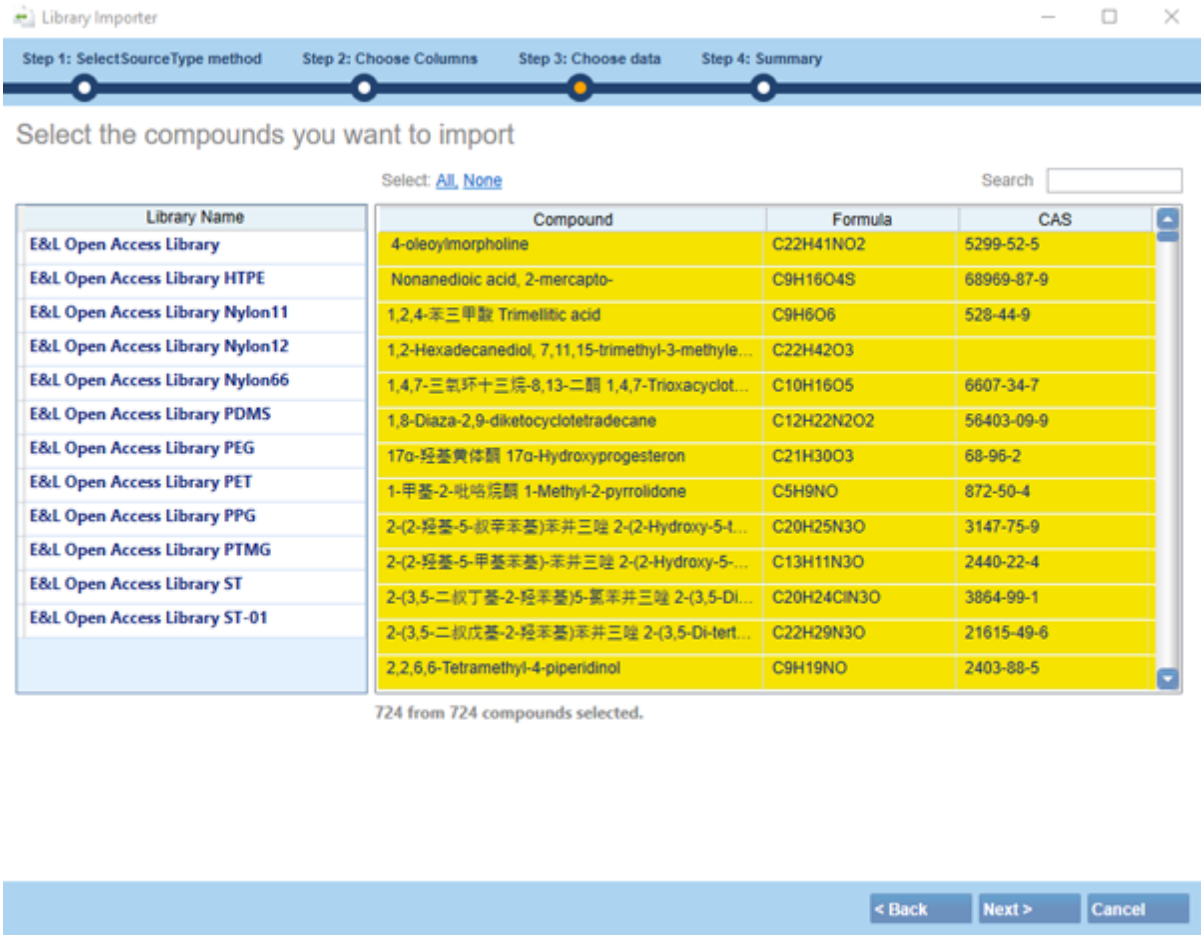
    The Library Importer dialog opens.
12. Click the **LibraryView Package (*lbp)** option on the Library Importer dialog.

Figure 3-1 Library Importer Dialog—Select Source Type for Import



13. Browse to the files extracted in step 3 and then select the `Accurate Mass E&L Open Access Library 2.0.lbp` file.
14. Click **All** above the **Compound** column to import all of the compounds.

Figure 3-2 Library Importer Dialog—Select Compounds to Import



15. Click **Next**.

Note: If the user cancels the import before all of the compounds have been copied to the database, then any compounds that have already been imported stay in the database. The software will not revert the database to the pre-import state.

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16. (For users with Accurate Mass E&L Open Access Library 1.0) Click **Overwrite All** . Refer to the section: Compound Conflicts.
17. Click **Finish**.
18. If the LibraryView software is installed, then create a backup of all of the libraries using the **Export** > **Library as snapshot (lbp)** feature after installation.

Note: If issues occur with any of the libraries, then importing the entire library as a snapshot is faster than installing all of the libraries again using the lbp packages.

Compound Conflicts

When installing a library containing a group of compounds or installing individual compounds, the software searches the database for compounds with the same name or formula as a compound in the package. If compounds with the same name are found, then the software flags the compounds in the package and prompts the user for a decision.

Users have the option to:

- Merge the compound information. New spectra, transitions, and retention times from the compound in the package are added to the compound information stored in the database.
- Overwrite the compound information. Compound information from the package replaces the compound information stored in the database.
- Keep compound information. Compound information in the database is kept and the compound information from the package is discarded.

Conflict information is available to help the user make the correct choice.

View Compound Conflicts

1. Click **Resolve** beside the compound library importer dialog to view the details of the conflict.
2. Do one of the following
    - To keep the existing compound information and discard the new information, click **Keep Original**.
    - To replace the existing compound information with the new information, click **Use New** .
3. Repeat steps 1 and 2 for each compound.
4. After all of the conflicts are resolved, click **Finish**.

Merge Compounds

1. On the Library Importer dialog, do one of the following:
    - To merge new spectra, transitions, and retention times from individual compounds in the import package with the corresponding compound information stored in the database, click **Merge**
    - To merge new spectra, transitions, and retention times from all of the compounds in the import package with the corresponding compound information stored in the database, click **Merge All** .
2. After all of the conflicts are resolved, click **Finish**.

Overwrite Compounds

1. Do one of the following on the Library Importer dialog:
   - To overwrite all of the compound information stored in the database with the corresponding compound information from the import package, click **Overwrite All**.
   - To overwrite the compound information stored in the database with the corresponding compound information from the import package, click **Resolve** beside the appropriate compound and then click **Use New**.
2. Click **Finish** after all of the conflicts are resolved.

Keep Original Compounds

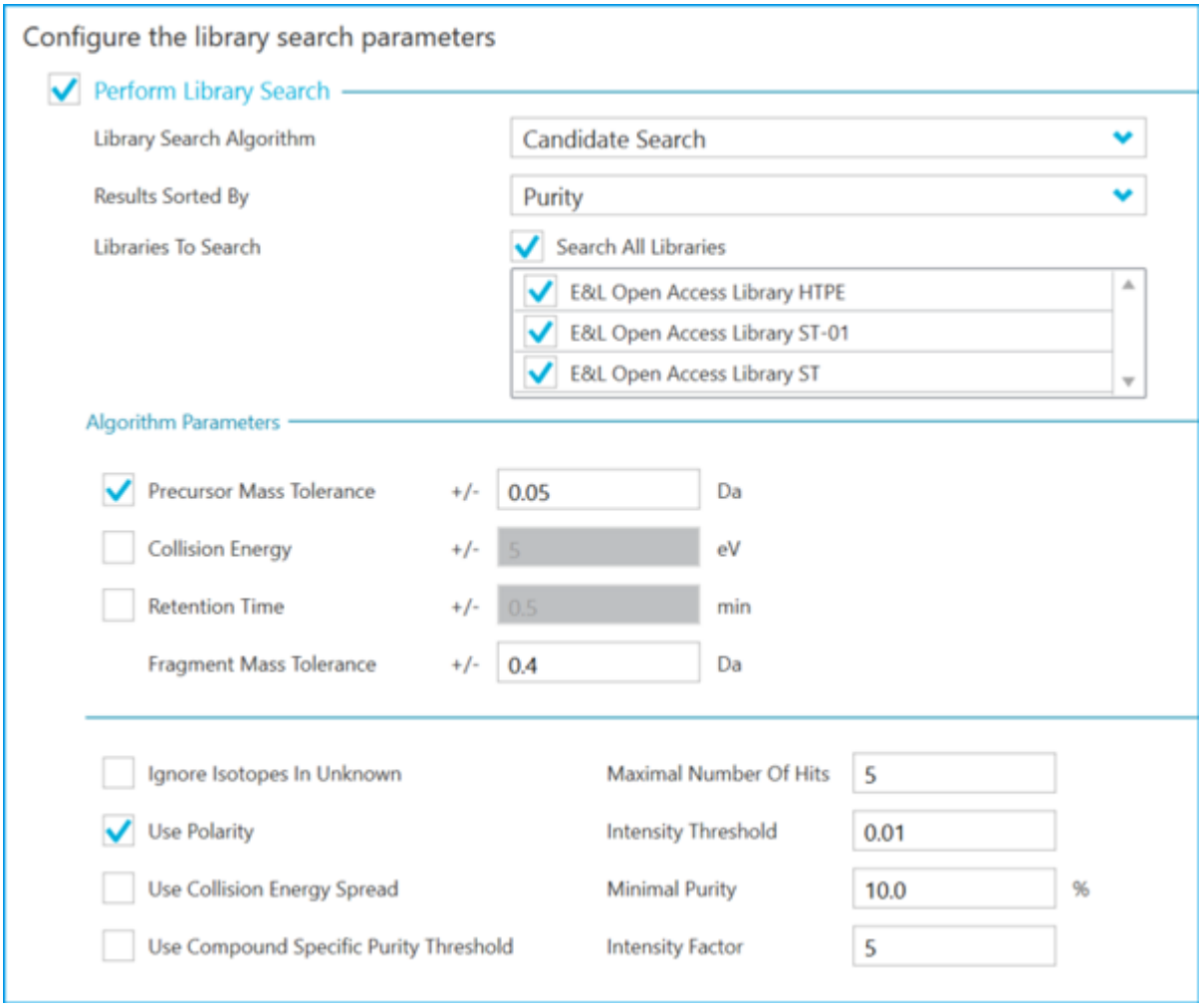
1. Do one of the following on the Library Importer dialog:
   - To keep all of the compound information stored in the database and discard the compound information from the import package, click **Keep All Original**.
   - To keep the individual compound information stored in the database and discard the compound information from the import package, click **Keep Original** beside the appropriate compound.
2. Click **Finish** after all of the conflicts are resolved.

Recommended Library Search Settings

The Accurate Mass E&L Open Access library contains spectra from multiple instrument platforms and spectra acquired at various collision energy (CE) settings. Therefore, the library search parameters must be carefully optimized to effectively search the library. For the recommended library search settings for SCIEX OS, refer to the figure: Figure 3-3. Complete the following settings:

- Deactivate the collision energy filtering to prevent false negatives.
- Set the **Precursor Mass** and **Fragment Mass Tolerance** to 0.05 Da to accelerate the processing time.
- Lower the **Intensity Factor** to 0.01 to improve the searching results of some lower intensity spectra.

Figure 3-3 Recommended Search Settings for the Accurate Mass E&L Open Access Library



For the MasterView software settings, refer to the document: *High Resolution Accurate Mass Libraries Release Notes*.

Contact Us

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- SCIEX Now Learning Hub

SCIEX Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the SCIEX website at sciex.com or contact us in one of the following ways:

- sciex.com/contact-us
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Documentation

This version of the document supercedes all previous versions of this document.

To view this document electronically, Adobe Acrobat Reader is required. To download the latest version, go to https://get.adobe.com/reader.

To find software product documentation, refer to the release notes or software installation guide that comes with the software.

To find hardware product documentation, refer to the documentation DVD for the system or component.

The latest versions of the documentation are available on the SCIEX website, at sciex.com/customer-documents.

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