

Biologics Explorer 3.1

Software Release Notes



Introduction

Thank you for using the Biologics Explorer software.

Read this document carefully for information about changes, new features, and resolved and known issues. The information in this document makes installation and use of the Biologics Explorer software easier.

The Biologics Explorer software supports the characterization of therapeutic protein candidates from these analysis approaches:

- Protein mapping that uses intact molecule measurements (TOF MS)
- Peptide mapping that uses data-dependent acquisition (DDA) measurements of enzymatically digested proteins (TOF MS/MS)
- Top-down/Middle-down protein sequencing by tandem mass spectrometric analysis of intact proteins that are fragmented in the mass spectrometer (TOF MS/MS)

The software can interpret data that is collected with both the Analyst TF and the SCIEX OS software.

The Biologics Explorer software can annotate data from the ZenoTOF 7600 system, from MS/MS measurements of both collisionally-activated dissociation (CAD) and electron-activated dissociation (EAD) fragmentation.

The Biologics Explorer software is also compatible with data from TripleTOF 6600 and X500B QTOF systems.

Related Documentation

Workflow guides are available in the software. These *Quick Guides* give suggestions and best practices for the workflows for a variety of supported applications.

In addition, contextual help is available throughout the software. To open contextual help topics in a web browser, click the ? icon.

Note: An internet connection is required to get access to these topics.

New Features in Version 3.1

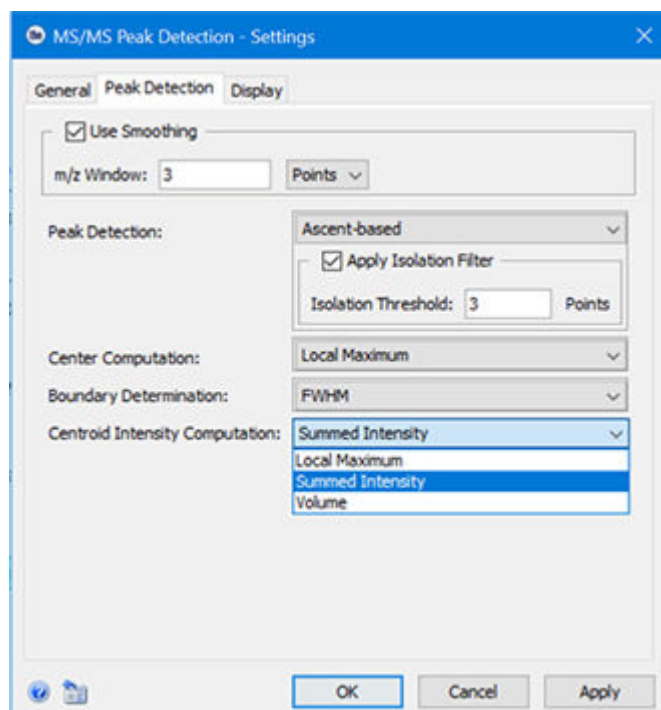
- **Intact Protein and Peptide Mapping: Sequential One-at-a-Time Processing:** To give a result for each data file, the software can process a batch of data files in a sequential one-at-a-time queue. All data files can use the same FASTA format sequence file, or each data file

Biologics Explorer 3.1 Software Release Notes

can use a different FASTA format sequence file. New template workflows are supplied for intact protein and peptide mapping analysis. For intact protein analysis, we recommend a batch size of up to 100 data files. For peptide mapping analysis, we recommend a batch size of up to 12 data files.

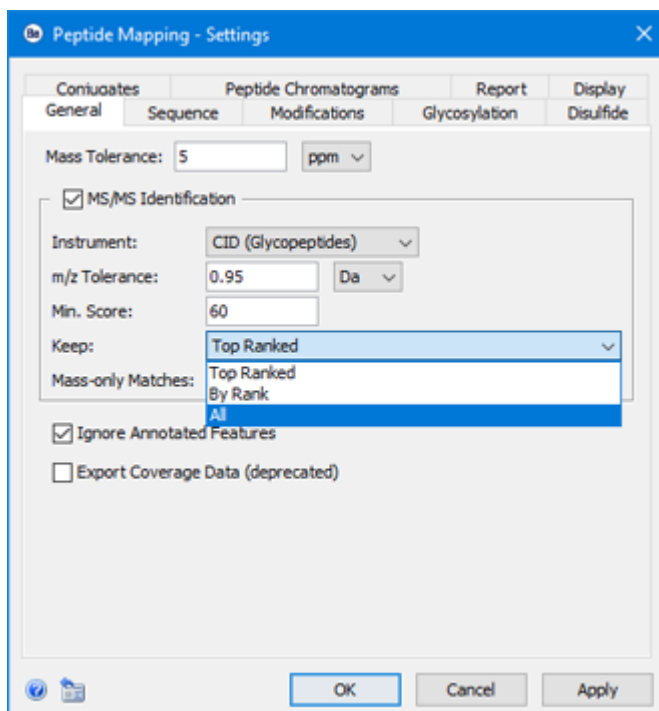
- **Peptide Mapping: Peak Detection:** In the peptide mapping workflow, a new option is available for the **Centroid Intensity Computation** field in the MS/MS Peak Detection - Settings dialog. The new option supplies another method to calculate the centroid mass intensity value.

Figure 1 MS/MS Peak Detection - Settings Dialog



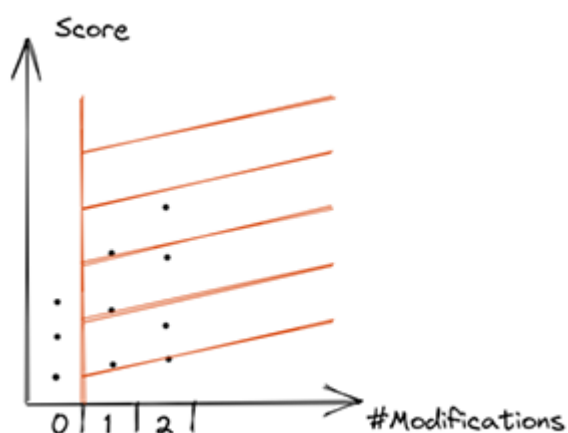
- **Peptide Mapping: All Option for the Keep Filter for MS/MS Identification:** When the **Keep All** filter is applied to peptide mapping MS/MS identifications, complex annotations are not ignored.

Figure 2 Keep Filter



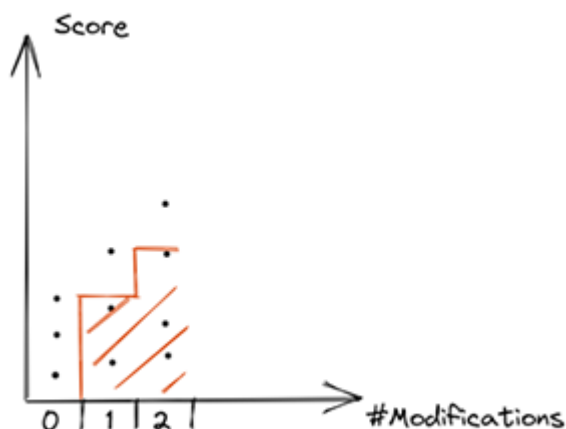
In earlier versions of the software, the filter showed only the annotations with the lowest complexity, even if a more complex annotation would have been identified with a better score. The following figure shows this behavior. Only annotations to the left of the line are kept. Annotations in the region with hash marks are ignored.

Figure 3 Before Version 3.1



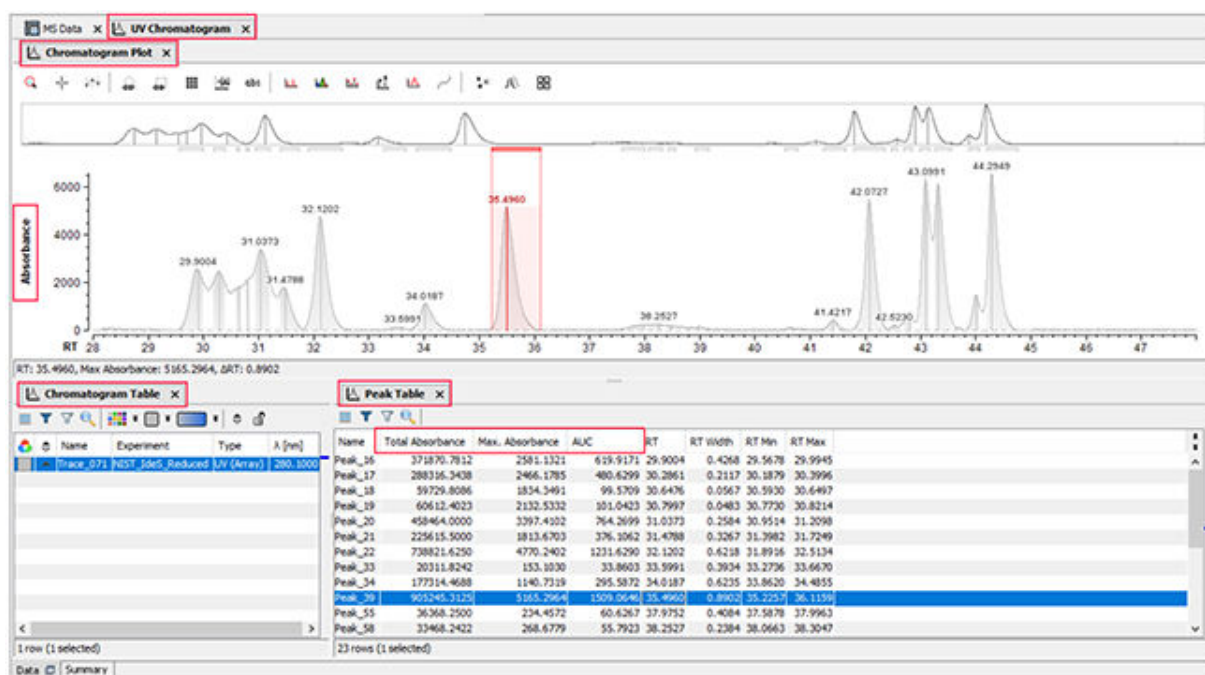
This issue is now corrected, and the algorithm keeps more complex annotations with a higher score. The following figure shows the new behavior. Annotations above and to the left of the stepped line are kept. Annotations in the region with hash marks are ignored.

Figure 4 Version 3.1



- **Standardization of Terminology:** Terms in the software have been changed to terms that are used in the industry:
 - The y-axis of UV chromatograms has been changed to **Absorbance**.
 - The **Intensity** for UV peaks has been changed to **Total Absorbance**.
 - The **Max. Intensity** for UV peaks has been changed to **Max. Absorbance**.
 - The **Intensity** for MS peaks has been changed to **Total Intensity**.
 - The **Volume** for MS and UV peaks has been changed to **AUC** (area-under-curve).
 - The UV chromatogram panes and tabs have been changed as shown in the following figure.

Figure 5 Pane Names




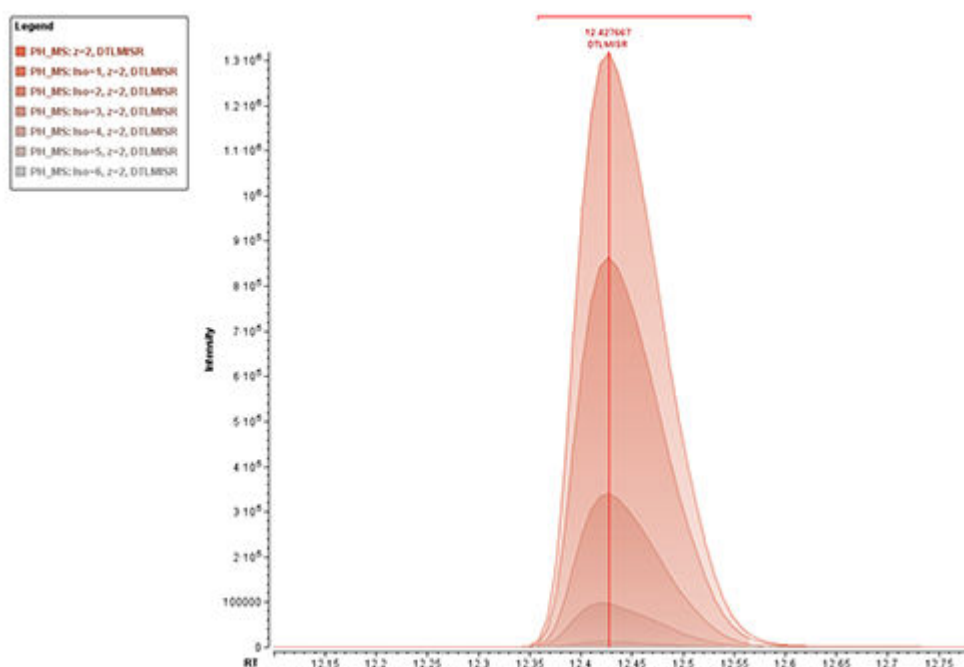
- **Peak Shading:** To more easily identify overlaid features in visualizations, such as chromatograms and mass spectra, users can click  to apply shading to the peaks.

Figure 6 Peak Shading



Known Issues

- Peptide mapping batch processing is resource-intensive and makes temporary files on the C:\ drive. To free up disk space, close the software and then open it again between batches.

Installation

Requirements

Workstation Requirements

- SCIEX Workstation Plus computer with:
 - Xeon 8 core processor
 - 32 GB RAM
 - 2 × 2 TB SSD storage disks, C:\ for Biologics Explorer software installation path, and D:\ for disk cache

Note: Newer systems might become available. For more information, contact the local sales representative. Older computer models might be compatible. However, they have not been tested and might result in decreased performance.

Operating System Requirements

- Windows 10, 64-bit, operating system

Internet Requirements

- Internet access
- Google Chrome browser

Install the Biologics Explorer Software

Prerequisites
<ul style="list-style-type: none">• A Biologics Explorer license key is available. The license key, also known as an activation ID (AID), might be distributed on a printed activation certificate, or in an e-mail from SCIEX Now. If the license key is missing, then contact a SCIEX sales representative.

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Download the required `zip` file from sciex.com/software-support/software-downloads.

Tip! To prevent possible installation issues, save the file to a location other than the computer desktop and then disconnect any external USB storage devices before the start of the installation.

3. After the download is complete, right-click the downloaded file and then click **Extract All**. By default, the files are extracted to the location where the `zip` file was saved.
4. Double-click `biologics_explorer-3.1.1.exe`. The SCIEX Biologics Explorer Setup window opens.
5. Follow the on-screen instructions to complete the installation. The installation wizard installs the Biologics Explorer software.

Note: When a prompt for the installation path is shown, use the default value, `C:\`.

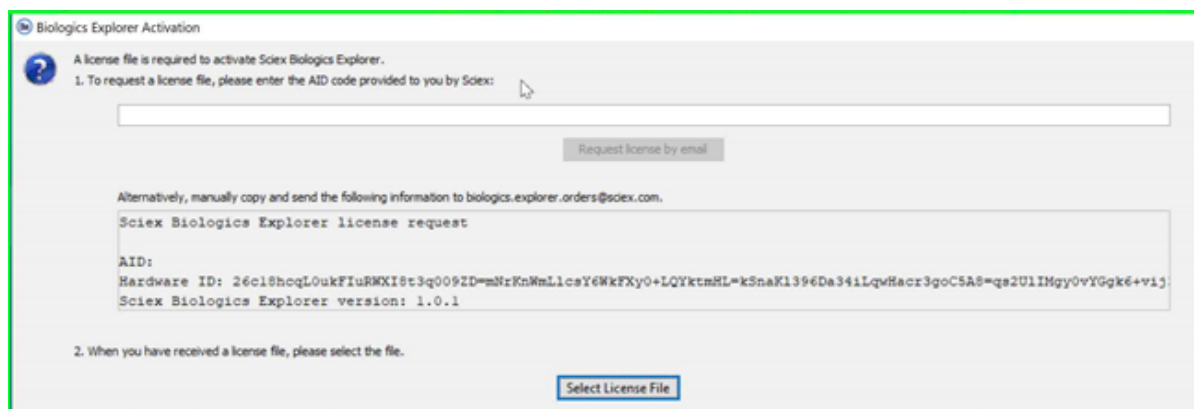
6. After the installation is completed, click **Finish**. The installation wizard opens the Biologics Explorer software. The Biologics Explorer Activation dialog opens. Continue with the section: [Activate the Software](#).

Activate the Software

1. If required, then open Biologics Explorer.

Biologics Explorer 3.1 Software Release Notes

Figure 7 Biologics Explorer Activation Dialog



2. Type the license key in the appropriate field.
3. Click **Request license by email**.

Note: As an alternative, copy the contents of the text box into an e-mail, type `Biologics Explorer License Request` in the subject line, and then send the e-mail to `biologics.explorer.orders@sciex.com`.

The license file will be sent by e-mail in approximately one day.

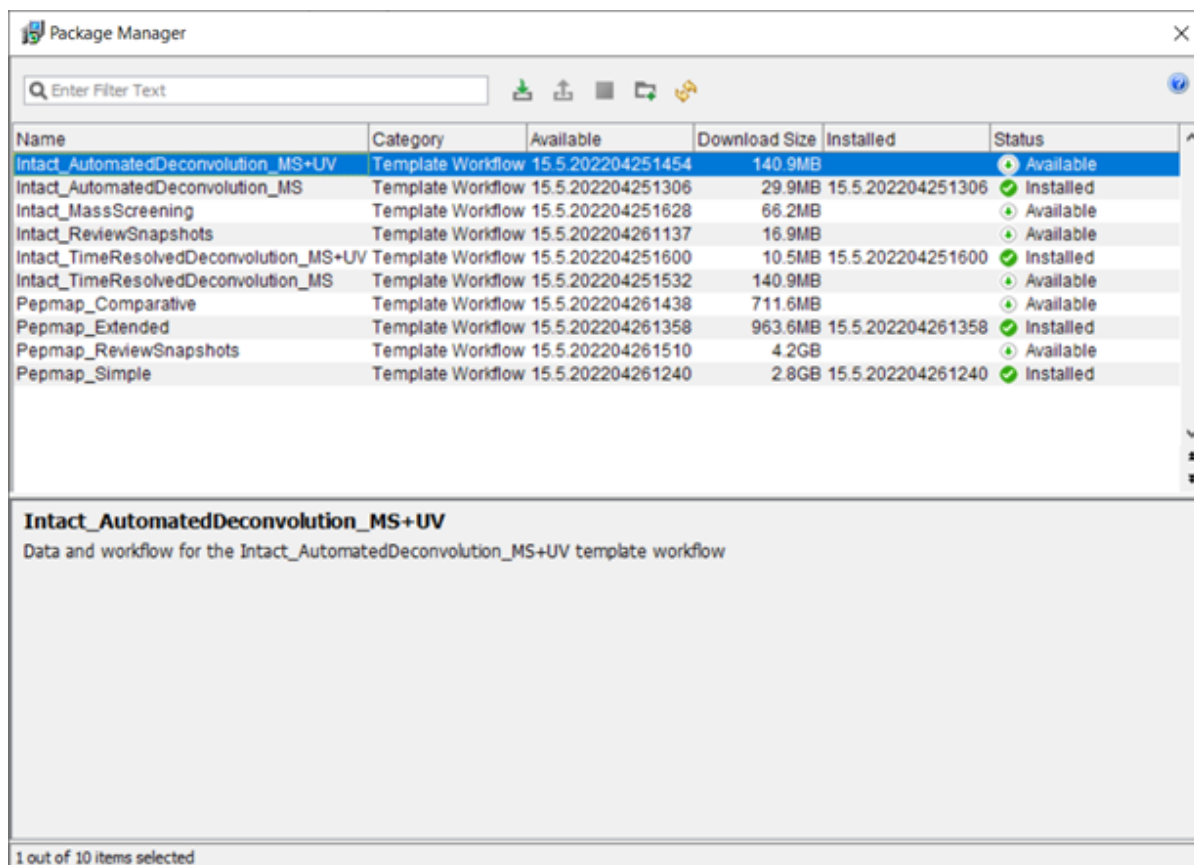
4. Copy the license file to the computer.
5. Open Biologics Explorer and then click **Select License File**.
6. Browse to and select the license file and then click **Load license**.
The software is activated.

Install the Workflow Package

Note: Workflow templates are updated regularly. We recommend the use of the latest available version of a template, which is available through the Package Manager.

1. Open the Biologics Explorer software.
2. Click **Tools > Package Manager**.
The list of available workflow packages is shown.

Figure 8 Package Manager Window




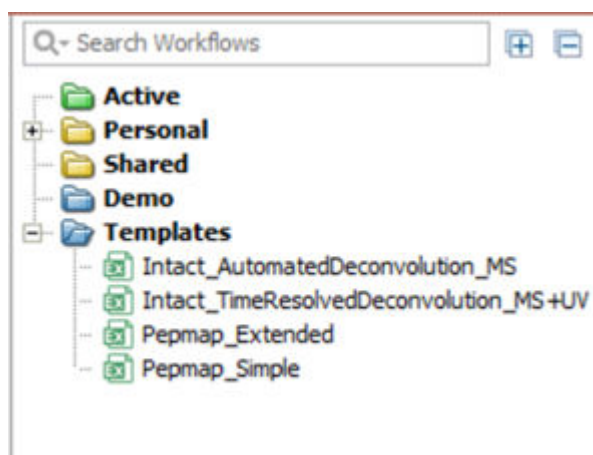
- Click  (install package).
The downloaded workflow is now available in the Templates folder.

Figure 9 Templates Folder



Tip! To make and run customized workflows, refer to the *Quick Start Guide*.

Remove the Biologics Explorer Software

Prerequisites
<ul style="list-style-type: none">Remove any HotFixes.


1. Log on to the computer as a user with Administrator privileges.
2. Click **Start > Control Panel > Programs and Features**.

Tip! If the control panel components are shown by **Category**, then click **Start > Control Panel > Programs > Programs and Features > Uninstall a program**.

3. Select **SCIEX Biologics Explorer**, and then click **Uninstall**.

The software is removed. User intervention is not required.

Note: The license file is not removed and can be used if the Biologics Explorer software is installed again.

Note: As an alternative, use the biologics_explorer Administration application () to remove the software.

Frequently Asked Questions

The C:\ and D:\ drives contain folders for Biologics Explorer. What are these folders used for?

By default, the software is installed on the C:\ drive, and processed data is stored in the C:\Home folder. During processing, data is stored in the D:\Cache folder. To monitor resource consumption during processing, click **Tools > Resource Status**.

Can I install the software on a laptop that only has a C:\ drive?

For optimal performance in routine use, we recommend the use of the SCIEX Workstation Plus. Refer to the section: [Workstation Requirements](#).

However, for the purposes of demonstration, training, and nonroutine usage, the software can be installed on a laptop with a single hard drive. The installation program automatically detects that the computer has a single hard drive and accommodates this configuration.

Can I install the software on a processing computer that does not meet the recommended requirements?

Yes. However, the software processing speed is best when the computer meets the specified requirements.

Do multiple users of the software require separate license files?

No. The license file is specific to the computer on which the software is installed.

My installation is now complete. How can I start my processing?

Select the workflow template that is applicable to the application, copy the template into a `Personal` folder, open the template, add data files and customize the parameters, and then save the workflow with a different name.

As an alternative, open the template in the `Templates` folder, add data files and customize the parameters, and then save the workflow with a different name.

How long does the installation usually take?

The installation and download of all workflow templates usually takes less than 30 minutes on the recommended computer.

We use the D:\ drive to store raw data files. Is there a minimum free disk space that we should keep on the D:\ drive?

We highly recommend that at least 250 GB of free disk space be available on the D:\ drive, to allow for efficient data post-processing in the Biologics Explorer software.

Can the software be installed on a drive other than the C:\ or D:\ drive?

No. We recommend that the software only be installed on these drives.

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
- sciex.com/request-support

CyberSecurity

For the latest guidance on cybersecurity for SCIEX products, visit sciex.com/productsecurity.

Documentation

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

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

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

Note: To request a free, printed version of this document, contact sciex.com/contact-us.

This document is provided to customers who have purchased SCIEX equipment to use in the operation of such SCIEX equipment. This document is copyright protected and any reproduction of this document or any part of this document is strictly prohibited, except as SCIEX may authorize in writing.

Software that may be described in this document is furnished under a license agreement. It is against the law to copy, modify, or distribute the software on any medium, except as specifically allowed in the license agreement. Furthermore, the license agreement may prohibit the software from being disassembled, reverse engineered, or decompiled for any purpose. Warranties are as stated therein.

Portions of this document may make reference to other manufacturers and/or their products, which may contain parts whose names are registered as trademarks and/or function as trademarks of their respective owners. Any such use is intended only to designate those manufacturers' products as supplied by SCIEX for incorporation into its equipment and does not imply any right and/or license to use or permit others to use such manufacturers' and/or their product names as trademarks.

SCIEX warranties are limited to those express warranties provided at the time of sale or license of its products and are the sole and exclusive representations, warranties, and obligations of SCIEX. SCIEX makes no other warranty of any kind whatsoever, expressed or implied, including without limitation, warranties of merchantability or fitness for a particular purpose, whether arising from a statute or otherwise in law or from a course of dealing or usage of trade, all of which are expressly disclaimed, and assumes no responsibility or contingent liability, including indirect or consequential damages, for any use by the purchaser or for any adverse circumstances arising therefrom.

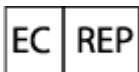
(GEN-IDV-09-10816-D)

For Research Use Only. Not for use in Diagnostic Procedures.

Trademarks and/or registered trademarks mentioned herein, including associated logos, are the property of AB Sciex Pte. Ltd., or their respective owners, in the United States and/or certain other countries (see sciex.com/trademarks).

AB Sciex™ is being used under license.

© 2023 DH Tech. Dev. Pte. Ltd.



Leica Microsystems CMS GmbH
Ernst-Leitz-Strasse 17-37
35578 Wetzlar
Germany



AB Sciex Pte. Ltd.
Blk33, #04-06 Marsiling Industrial Estate Road 3
Woodlands Central Industrial Estate, Singapore 739256