# Biologics Explorer Software 5.0.1 Release Notes



## Introduction

Thank you for using the Biologics Explorer software.

Read this document carefully for information about changes, new features, and corrected 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/middle-down protein sequencing by tandem mass spectrometric analysis of intact proteins or subunits of proteins (TOF MS/MS)

The software can interpret data that is collected with both the Analyst TF and 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**

Quick guides and workflow guidelines are available in the software. These documents 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 5.0.1**

• Top/middle-down workflow:

- Results from multiple MS measurements for the same molecule can be put together to give a combined bond coverage. The combined and individual results are shown on the coverage map and in the tabulated results. The workflow supports experiments with a combination of EAD measurements at different energies and with a combination of CAD and EAD measurements.
- To make it easier to review bond evidence for confirmation of protein sequences, the bond coverage map, fragments table, and fragment spectrum are synchronized in the user interface.
- To make it easier to compare different measurements, mirror plots of fragment spectra are available in the user interface. To make these comparisons more useful, labels can be added to both the top and bottom of the mirror plot.
- To supply a summary of the work and any findings, reports can be created in PDF format.
- · Protein crosslinking:
  - A new De Novo mode is available in the *Peptide Mapping* activity, on the Crosslinks tab. This mode finds unexpected protein crosslinks, such as scrambled disulphides, trisulphides, and thioethers. This mode also finds crosslinking events that are related to amino acids.

**Note:** We do not recommend the use of the older Scrambled Disulphide and De Novo modes.

- The difference between expected and unexpected or scrambled crosslinks is highlighted by the Automated Review activity. This activity is available in all peptide mapping templates.
- · Package Manager:
  - Workflow templates continue to be available for download from the Package Manager.
  - An update in this release makes the Package Manager available for users in China.
- Intact template workflows:
  - The name of the Intact\_AutomatedDeconvolution template has been changed to Intact SpectralDeconvolution, to agree with the following changes:
    - RT condensing for deconvolution has been moved to a new activity node.
    - A new differential analysis capability supports comparative sample analysis in spectral deconvolution workflows.

## **Known Issues**

 Batch processing for peptide mapping is resource-intensive and makes temporary files on the C:\ drive. To make disk space available, 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, but they have not been tested and might result in decreased performance.

## **Operating System Requirements**

Windows 10 and Windows 11, 64 bit, operating system

### **Internet Requirements**

- Internet access: Port 443 of the workstation must be open, so that the Package Manager can connect to the package server for access to the template workflows.
- · Google Chrome browser.

## Install the Biologics Explorer Software

### **Prerequisites**

- A Biologics Explorer license key is available. The license key, also known as an activation ID (AID), is sent 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 https://sciex.com/support/software-support/software-downloads.

**Tip!** To prevent 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**.

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By default, the files are extracted to the location where the zip file was saved.

- 4. Double-click biologics\_explorer-5.0.1.exe. The SCIEX Biologics Explorer Setup window opens.
- Obey 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:\.

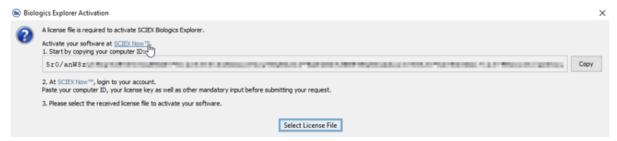
6. After the installation is completed, click **Finish**.

The installation wizard opens the Biologics Explorer software. The Biologics Explorer Activation dialog opens. Continue with the section: Activate the Software.

### **Activate the Software**

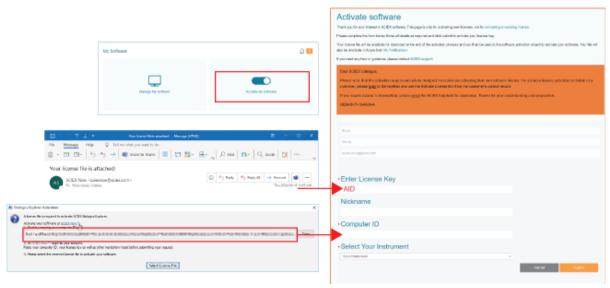
1. If required, then open Biologics Explorer.

### **Figure 1 Biologics Explorer Activation Dialog**



- 2. To copy the computer ID to the clipboard, click **Copy**.
- Click the SCIEX Now link.
   The SCIEX Now activation page opens in a web browser.
- 4. Log on to SCIEX Now.
- 5. Obey the instructions to get a software license.

Figure 2 Activate the Software



- Open the Biologics Explorer software, and then click Select License File.
- 7. 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.
- Click Tools > Package Manager.
   The list of available workflow packages is shown.

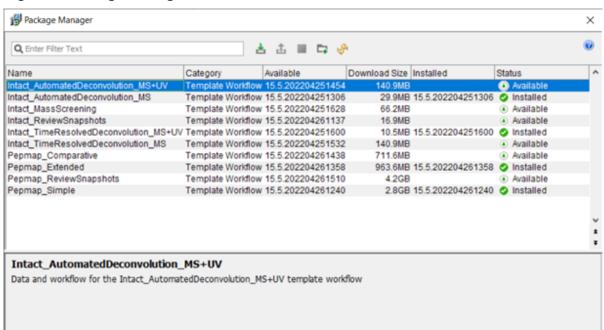


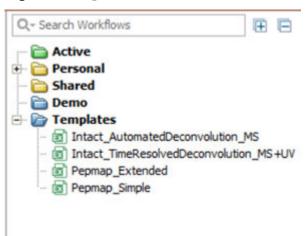
Figure 3 Package Manager Window

# 3. Click (Install Package).

1 out of 10 items selected

The downloaded workflow is now available in the Templates folder.

Figure 4 Templates Folder



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

## Remove the Biologics Explorer Software

### **Prerequisites**

- Remove any Biologics Explorer 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, click software.



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## **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 kept in the  $C:\$  home folder. During processing, data is kept 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 adjusts to 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 related 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 much time does the installation usually require?

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

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

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

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**

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- sciex.com/contact-us
- sciex.com/request-support

## Cybersecurity

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### **Documentation**

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

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