Biologics Explorer Software 8.0 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 the installation and use of the Biologics Explorer software easier.

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

- Protein mapping that uses measurements of intact molecules, partially cleaved intact molecules, and reduced intact molecules (TOF MS)
- Intact mass mapping of nucleotide molecules (TOF MS) and nucleotide sequencing (TOF MS/MS) and mapping
- Peptide mapping that uses data-dependent acquisition (DDA) measurements of enzymatically digested proteins (TOF MS/MS)
- Top/middle-down protein sequencing with tandem mass spectrometric analysis of intact proteins or subunits of proteins (TOF MS/MS)

The Biologics Explorer software can analyze data that is collected with the Analyst TF software and SCIEX OS software.

The Biologics Explorer software can annotate data from ZenoTOF 7600 systems, ZenoTOF 7600+ systems, and ZenoTOF 8600 systems, from MS/MS measurements of collisionally activated dissociation (CAD) and electron-activated dissociation (EAD) fragmentation.

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

Software Versions

The software is available with a subscription license. New versions of the Biologics Explorer software are released regularly. During the license period, users with active subscriptions can upgrade to the next version of the software. When new versions of the software become available, e-mails are sent with information about new features and the location to download the software on the SCIEX website.

To get access to the latest features, optimized settings, and workflows, we recommend that users upgrade the software when possible.

Related Documentation

A *Quick Guide* and workflow guidelines are supplied with the software. These documents give suggestions and best practices for the workflows for different supported applications.

To see the guidelines for a workflow, click the link shown at the top of the workflow.

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

Note: To get access to these topics, an Internet connection is required.

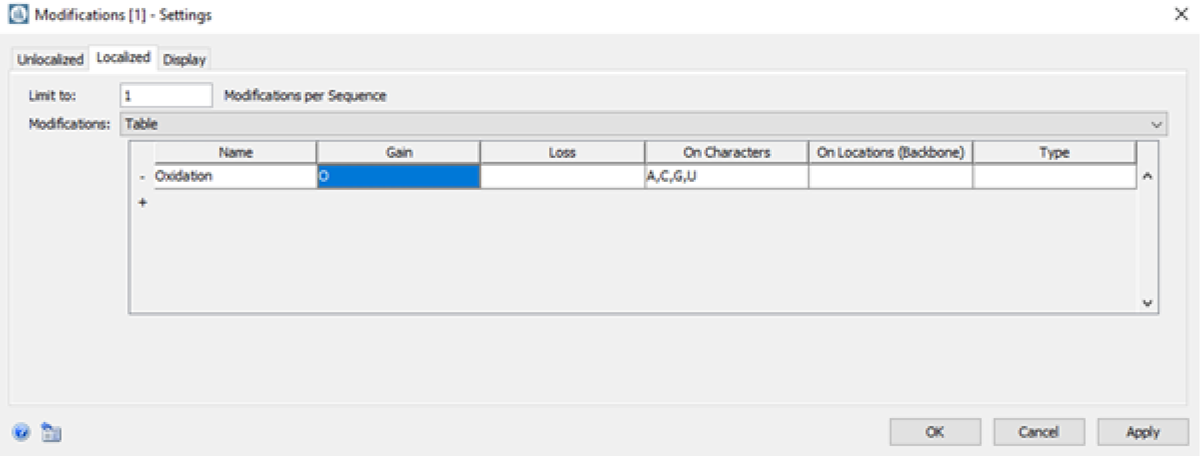
New Features in Version 8.0

- Nucleotide mapping workflow: A new workflow is available for the analysis of large oligonucleotides. This workflow does digestion with nucleases followed by the confirmation of MS/MS sequences and mapping.
- Nucleotide sequencing workflow: The Nucleotide_NoDeconvolution workflow was renamed and has been updated to use MS/MS data for the confirmation of sequences.
- All nucleotide workflows: The isotope clustering algorithm for TOF MS was made better and supplies better results for co-eluting species.
- A new viewer for oligonucleotide coverage supplies an overview of identified candidates.
- The software can use the Nucleotide editor to create custom oligonucleotide linkers and related MS/MS fragments.
- A new Amino Acid editor lets users create custom amino acids.
- A new Crosslinker editor lets users examine and manage the database of crosslinkers.
- Users can create a report of annotated base peak chromatograms (BPCs) or total ion chromatograms (TICs).
- Users can customize the number format for some fields.

Known Issues and Limitations

- Batch processing for peptide mapping is resource intensive. It creates temporary files on the `C:\` drive. To make disk space available, between batches, close the software, and then open it again.
- The nucleotide workflows process one sample at a time. Multi-sample analysis is not supported.
- Before MS/MS data is used to assign modifications, the modifications must be added on the Localized tab in the Modifications node.

Figure 1 Modifications on the Localized Tab



Limit to: 1 Modifications per Sequence

Modifications: Table

Name	Gain	Loss	On Characters	On Locations (Backbone)	Type
Oxidation	O		A,C,G,U		

Installation

Requirements

Computer Requirements

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

Operating System Requirements

One of these operating systems is required:

- Windows 10, 64 bit
- Window 11, 64 bit

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 license key for the Biologics Explorer software 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 Windows user with Administrator privileges.
2. Go to sciex.com/software-downloads, and then download the required `zip` file.

   Tip! To prevent installation issues, save the file to the local computer, in a different location than the desktop.

3. After the download is completed, right-click the downloaded file, and then click **Extract All**, browse to the destination folder, and then click **Extract**.

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

4. Double-click `biologics_explorer-8.0.exe`.
   The SCIEX Biologics Explorer Setup window opens.
5. Obey the on-screen instructions to complete the installation.

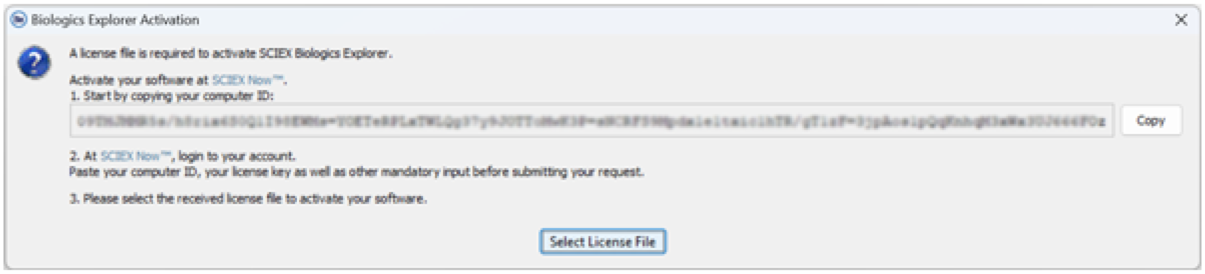
   Note: When a prompt for the installation path is shown, use `C:\` (default) or a different local drive. If a different local drive is used, then set the **Cache Location** to `C:\SCIEX\BiologicsExplorer\var\cache`.

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 the Biologics Explorer software.

Figure 2 Biologics Explorer Activation Dialog



A license file is required to activate SCIEX Biologics Explorer.

Activate your software at SCIEX Now™.
1. Start by copying your computer ID:

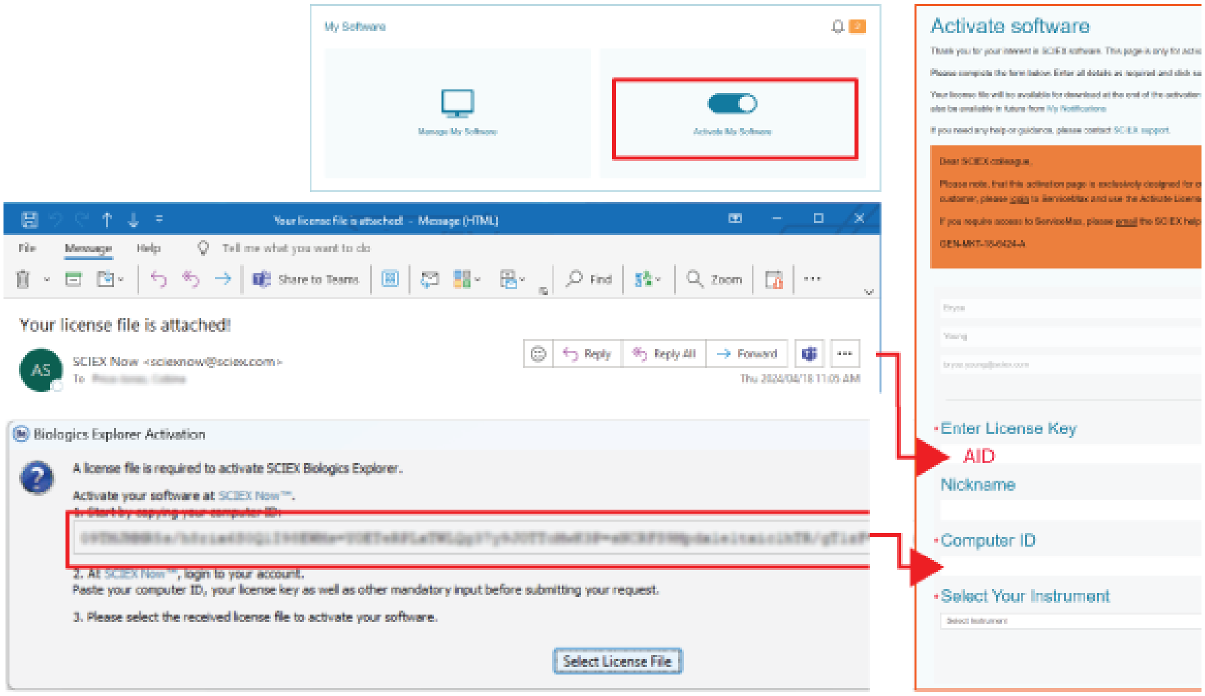
[redacted]

2. At SCIEX Now™, login to your account.
Paste your computer ID, your license key as well as other mandatory input before submitting your request.

3. Please select the received license file to activate your software.

2. To copy the computer ID to the clipboard, click **Copy**.
3. Click SCIEX Now.
   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 3 Activate the Software



Your license file is attached!

SCIEX Now <sciexnow@sciex.com>

A license file is required to activate SCIEX Biologics Explorer.

Activate your software at SCIEX Now™.

2. At SCIEX Now™, login to your account.
Paste your computer ID, your license key as well as other mandatory input before submitting your request.

3. Please select the received license file to activate your software.

Note: The **Computer ID** is not the MAC address. To find the **Computer ID**, see the Biologics Explorer Activation dialog.

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6. 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 version of a template, which is available through the Package Manager.

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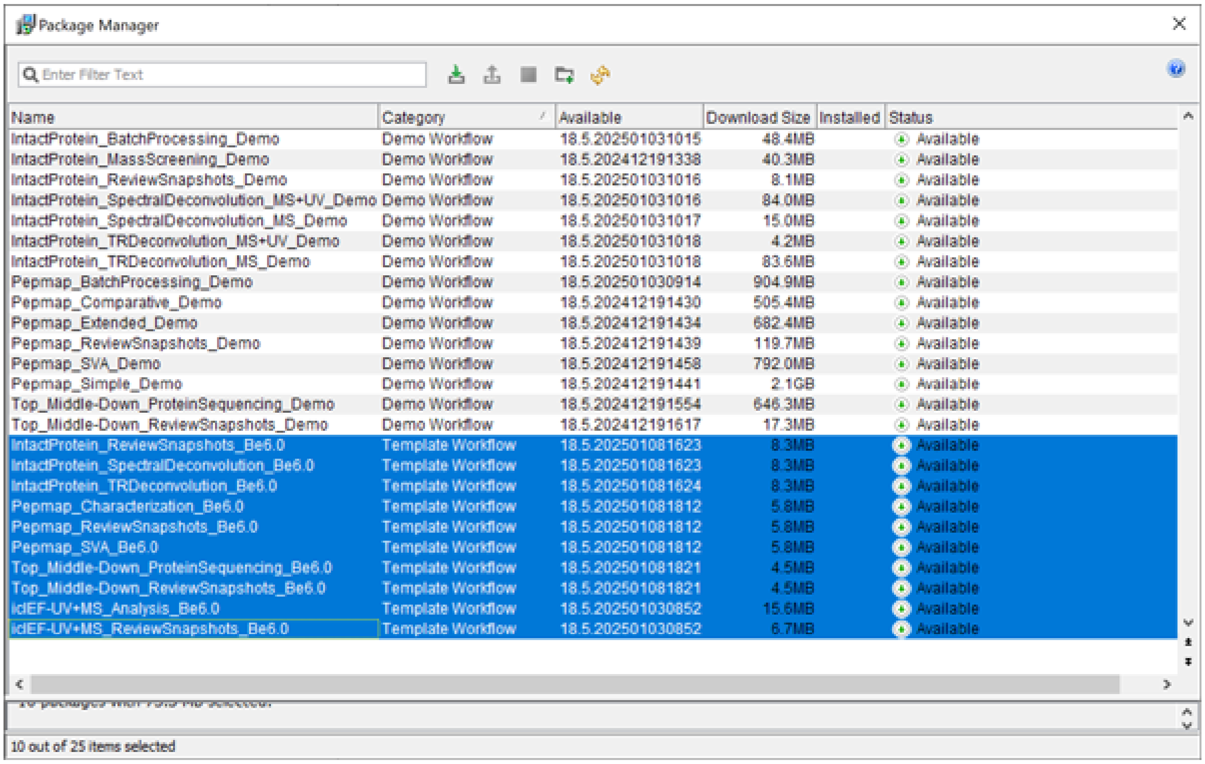
1. Open the Biologics Explorer software.
2. Click **Tools** > **Package Manager**.
   The list of available workflow packages is shown.

Figure 4 Package Manager Window

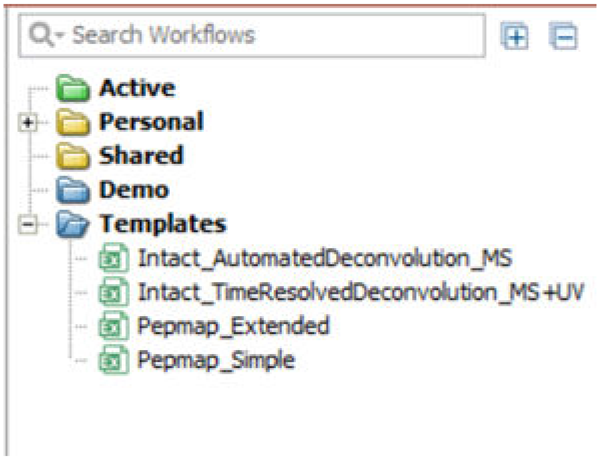


Name	Category	Available	Download Size	Installed	Status
IntactProtein_BatchProcessing_Demo	Demo Workflow	18.5.202501031015	48.4MB		Available
IntactProtein_MassScreening_Demo	Demo Workflow	18.5.202412191338	40.3MB		Available
IntactProtein_ReviewSnapshots_Demo	Demo Workflow	18.5.202501031016	8.1MB		Available
IntactProtein_SpectralDeconvolution_MS+UV_Demo	Demo Workflow	18.5.202501031016	84.0MB		Available
IntactProtein_SpectralDeconvolution_MS_Demo	Demo Workflow	18.5.202501031017	15.0MB		Available
IntactProtein_TRDeconvolution_MS+UV_Demo	Demo Workflow	18.5.202501031018	4.2MB		Available
IntactProtein_TRDeconvolution_MS_Demo	Demo Workflow	18.5.202501031018	83.6MB		Available
Pepmap_BatchProcessing_Demo	Demo Workflow	18.5.202501030914	904.9MB		Available
Pepmap_Comparative_Demo	Demo Workflow	18.5.202412191430	505.4MB		Available
Pepmap_Extended_Demo	Demo Workflow	18.5.202412191434	682.4MB		Available
Pepmap_ReviewSnapshots_Demo	Demo Workflow	18.5.202412191439	119.7MB		Available
Pepmap_SVA_Demo	Demo Workflow	18.5.202412191458	792.0MB		Available
Pepmap_Simple_Demo	Demo Workflow	18.5.202412191441	2.1GB		Available
Top_Middle-Down_ProteinSequencing_Demo	Demo Workflow	18.5.202412191554	646.3MB		Available
Top_Middle-Down_ReviewSnapshots_Demo	Demo Workflow	18.5.202412191617	17.3MB		Available
IntactProtein_ReviewSnapshots_Be6.0	Template Workflow	18.5.202501081623	8.3MB		Available
IntactProtein_SpectralDeconvolution_Be6.0	Template Workflow	18.5.202501081623	8.3MB		Available
IntactProtein_TRDeconvolution_Be6.0	Template Workflow	18.5.202501081624	8.3MB		Available
Pepmap_Characterization_Be6.0	Template Workflow	18.5.202501081812	5.8MB		Available
Pepmap_ReviewSnapshots_Be6.0	Template Workflow	18.5.202501081812	5.8MB		Available
Pepmap_SVA_Be6.0	Template Workflow	18.5.202501081812	5.8MB		Available
Top_Middle-Down_ProteinSequencing_Be6.0	Template Workflow	18.5.202501081821	4.5MB		Available
Top_Middle-Down_ReviewSnapshots_Be6.0	Template Workflow	18.5.202501081821	4.5MB		Available
icIEF-UV+MS_Analysis_Be6.0	Template Workflow	18.5.202501030852	15.6MB		Available
icIEF-UV+MS_ReviewSnapshots_Be6.0	Template Workflow	18.5.202501030852	6.7MB		Available

10 out of 25 items selected

3. Click **(Install Package)**.
   The downloaded workflow is available in the applicable folder: `Demo` or `Templates`.

Figure 5 `Demo` and `Templates` Folders



Tip! To create and use customized workflows, refer to the document: *Quick Guide*.

Remove the Biologics Explorer Software

Prerequisites
• Remove installed HotFixes for the Biologics Explorer software.

1. Log on to the computer as a Windows 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.

   Tip! As an alternative, click (**biologics_explorer Administration**) to remove the software.

Frequently Asked Questions

The C:\ and D:\ drives contain folders for the Biologics Explorer software. 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: Computer Requirements.

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. Prompts for the **Data Location** and **Cache Location** are shown during the installation.

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

Yes, but 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 completed. 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 download and installation of all of the 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?

For the most efficient data post-processing in the Biologics Explorer software, we recommend that a minimum of 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.

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