

Biologics Explorer 2.0 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 facilitates successful installation and use of the Biologics Explorer software.

The Biologics Explorer software supports the characterization of proteins from:

- Intact molecule measurements
- Enzymatic digestion followed by information dependent acquisition (IDA) experiments

The software can interpret data 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 collision-induced dissociation (CID) 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* provide suggestions and best practices for the workflows, based on 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 access these topics.

New Features in Version 2.0

Peptide Mapping

- Isomeric amino acid residues, for example leucine/isoleucine and aspartic/isoaspartic acid can be differentiated in the Biologics Explorer software, based on the presence of signature fragment ions that result from EAD of peptides. The default EAD instrument configuration is updated to include these signature ions, and data with these ions will be annotated. The software automatically labels isomerizations as modifications, where appropriate.

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- Peptides with multiple N- and O-glycosylation events can be mapped. Detailed guidance on use of the new feature is available in the document: *Peptide Mapping: Biologics Explorer 2.0 Quick Guide*.

Intact Mass Analysis

- Intact sequence clips resulting from intact protein degradation can be mapped using the Intact Mass Analysis workflow templates. This feature helps to annotate species that have lost a portion of a chain, resulting in a mass that is smaller than the expected mass. The feature is intended for targeted mapping of a specific feature in the dataset. Guidance on the feature is available in more detail in the document: *Intact Mass Analysis: Biologics Explorer 2.0 Quick Guide*.
- New functionality is available for protein fragments in Protein Mapping. Protein fragments can be generated by enzymatic cleavage of the target amino acid sequence at one or more specific consensus sequences.

Known Issues

- If glycan libraries are used to characterize O-glycosylation, then the suggested modification sites are based on the location of serine (S) and threonine (T) in the peptide sequence. Fragment ion information that confirms the exact glycosylation site need not be present. This behavior is linked to the use of glycan tables in the mapping activities. If more precision is required, then use the variable modifications feature in the Peptide Mapping workflow. The software will more rigorously evaluate fragment ion coverage before assigning the location of glycans.
- The relative percentages in the Modifications table will sum to more than 100% if peptides have redundant annotations, that is, more than one possible answer, for example, glycosylated peptides with many isobaric possibilities. In these cases, the quantitative contribution of a peptide is counted more than once. The user must review the annotations and select a single annotation, rejecting all other possibilities. After this is done, the values in the peptide modification table total less than or equal to 100%.
- The Fragment Spectra Viewer shows the glycan structures of glycosolated peptides. Singly-glycosylated peptides show one glycan structure. Multi-glycosylated peptides show all of the relevant glycan structures. If a multi-glycosylated peptide is made up of identical glycans, then only one glycan is shown. To view all of the glycans, including identical glycans, refer to the peptide identification table.

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 degraded 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 potential installation issues, save the file to a location other than the computer desktop and then disconnect any external USB storage devices before starting 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-2.0.2.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 prompted for the installation path, use the default value, C:\.

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

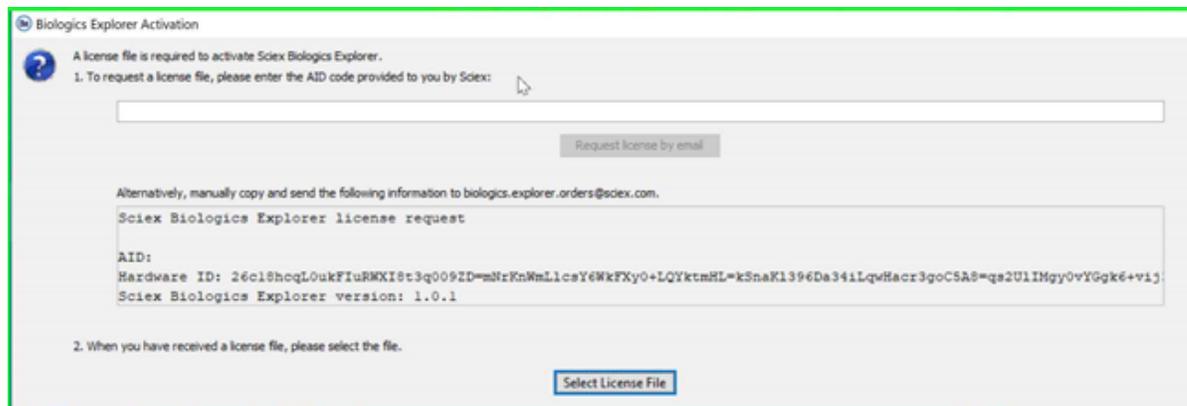
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The installation wizard opens the Biologics Explorer software. The Biologics Explorer Activation dialog opens. Continue with the section: [Activate the Software](#).

Activate the Software

1. If required, open Biologics Explorer.

Figure 1 Biologics Explorer Activation Dialog



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

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

The license file will be sent by e-mail in about 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

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

Figure 2 Package Manager Window

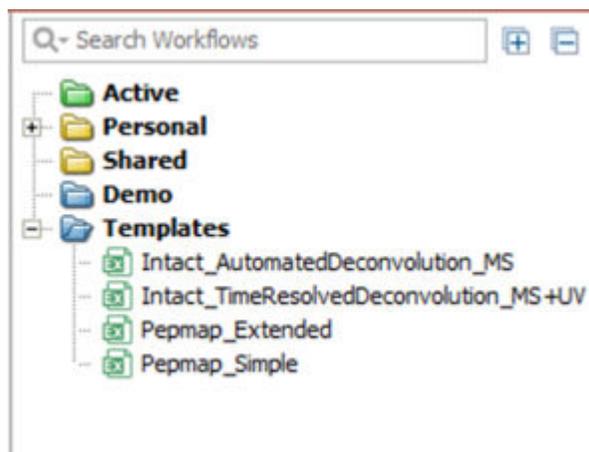
Name	Category	Available	Download Size	Installed	Status
Intact_AutomatedDeconvolution_MS+UV	Template Workflow	15.5.202204251454	140.9MB		Available
Intact_AutomatedDeconvolution_MS	Template Workflow	15.5.202204251306	29.9MB	15.5.202204251306	Installed
Intact_MassScreening	Template Workflow	15.5.202204251628	66.2MB		Available
Intact_ReviewSnapshots	Template Workflow	15.5.202204261137	16.9MB		Available
Intact_TimeResolvedDeconvolution_MS+UV	Template Workflow	15.5.202204251600	10.5MB	15.5.202204251600	Installed
Intact_TimeResolvedDeconvolution_MS	Template Workflow	15.5.202204251532	140.9MB		Available
Pepmap_Comparative	Template Workflow	15.5.202204261438	711.6MB		Available
Pepmap_Extended	Template Workflow	15.5.202204261358	963.6MB	15.5.202204261358	Installed
Pepmap_ReviewSnapshots	Template Workflow	15.5.202204261510	4.2GB		Available
Pepmap_Simple	Template Workflow	15.5.202204261240	2.8GB	15.5.202204261240	Installed

Intact_AutomatedDeconvolution_MS+UV
Data and workflow for the Intact_AutomatedDeconvolution_MS+UV template workflow

1 out of 10 items selected

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

Figure 3 Templates Folder



4. Drag workflows from the `Templates` folder into a `Personal` folder, as required, and then customize and save them.

Remove 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, with no user intervention required.

Note: If the product is licensed, then the license file is not removed and can be used if Biologics Explorer is installed again.

Note: Alternatively, use the biologics_explorer Administration application () to remove the software.

Frequently Asked Questions

Drive C:/ and D:/ contain folders for Biologics Explorer. What are these folders used for?

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

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

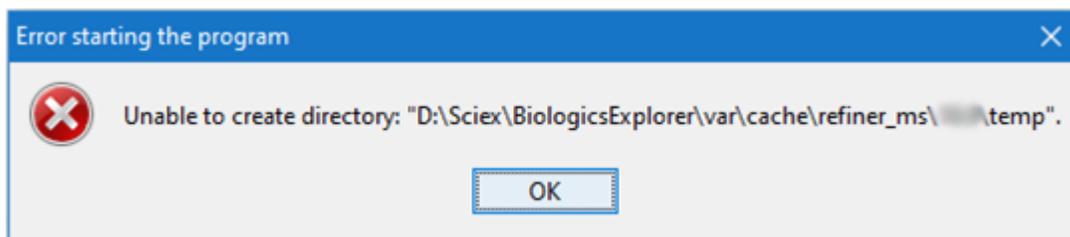
For optimal performance in routine use, SCIEX recommends the use of the SCIEX Workstation Plus. Refer to the section: [Workstation Requirements](#).

However, for the purposes of demonstration, training, and non-routine usage, the software can be installed on a laptop with a single hard drive. To do so, follow these steps:

1. Install the software. Refer to the section: [Install the Biologics Explorer Software](#).

After **Finish** is clicked, the following error message is shown.

Figure 4 Error starting the program Dialog



2. In the `Biologics_Explorer_2.0.2.zip` file, browse to the `app-extend.properties` file, and then copy `app-extend.properties` to the folder: `C:\Program Files\Sciex\BiologicsExplorer\runtime\16.0\refiner_ms\etc\`.
3. Open the Biologics Explorer software.
The software prompts for the license file.
4. Activate the software. Refer to the section: [Activate the Software](#).
The software opens as usual, but it uses the C:\ drive for the disk cache.

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.

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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 appropriate for the application, copy it into a `Personal` folder, open it, add data files and customize parameters, and then save the workflow with a different name.

Alternatively, 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?

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

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

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

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

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

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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>.

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

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