ProSightPD 4.1 Release Notes

These release notes briefly list changes in the Thermo ProSightPD™ nodes for Proteome Discoverer™, fixes for reported issues, and known issues still existing in the ProSightPD nodes.

Contents

For additional information on ProSightPD, refer to the *ProSightPD 4.1 User Guide*.

New features

This release incorporates these new or enhanced features:

- Standalone installer for ProSightPD.
- Support for data with MS3 fragmentation.
- Support for spectral calibration shifts in cRAWler.
- Support for labile modification mass shifts in search nodes.
- Support for custom modifications in database.
- Support for heavy isotope labeling experiments.
- Proteoform Repository Annotation node for annotating and grouping PrSMs into shared proteoforms.
- Users can build a ProSightPD database using bottom-up PD results in mzIdentML format.
- Example data included, see the topic Working with Example Data in the user guide.
- Disulfide bond toggle to overcome incorrect disulfide bond annotations.

Enhanced features

- Delta M Mode now displays tabular and visual results.
- TDValidator Lite is fully integrated into ProSightPD and has new features such as fragment ion FDR.
- Databases can now be selected by a dropdown menu in the search nodes.
- Protein Annotator supports user-defined Custom Mass Modifications and "locked" modifications.
- Disulfide bond consideration in search can be deactivated with a search node parameter.

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System requirements

The following tables list the minimum and recommended hardware and software configurations for the ProSightPD operation.

Table 1. Minimum system requirements

System	Requirements
Data system computer	• 2 GHz processor • 8 GB RAM • 75 GB available on C drive • NTFS format • Microsoft .NET 4.7.2 • Microsoft .NET Core Runtime 2.1
Operating system	Microsoft™ Windows 10 with latest service pack

Table 2. Recommended system requirements

System	Requirements
Data system computer	• 2.5 GHz or higher with multiple cores • 64 GB RAM • 1 GB boot and data SSD drives • NTFS format
Operating system	Microsoft Windows 10 with latest service pack

Installation

This section provides installation information.

General installation

The new standalone ProSightPD installer includes both the ProSightPD 4.1 installer and the compatible Proteome Discoverer 2.5 installer. The standalone installer installs only the required software. If the ProSightPD installer detects that the correct version of Proteome Discover 2.5 is already installed on your system, then only the ProSightPD 4.1 installer will be used.

The version of Proteome Discoverer 2.5 included with the ProSightPD standalone installer only supports the ProSightPD 4.1 nodes (Proteome Discoverer 2.5 viewer without any Proteome Discoverer nodes). Additional Proteome Discover 2.5 features are available separately for an upgrade. If you already have Proteome Discoverer 2.5, then you will still have access to existing licenses and features. For additional information about licensing, refer to the *Software installation and activation* section in the *ProSightPD 4.1 User Guide*.

Known issues

Suggested recovery actions

If you encounter an unexpected error, reboot the application.

If the error persists, create a bug report (**Tools > Create Bug Report**) and email to prosightpdsupport@thermofisher.com

Risk	Interpretation
High	Occurrence is likely to happen and can compromise operation.
Medium	Occurrence is uncommon, but if it occurs, can compromise operation.
Low	Issue is minor; however, the software might operate differently from a user's expectations. A workaround is often available.
No Risk	This issue causes no problems, but is commonly an inconsistency or a cosmetic issue.

Known defects

Table 3 contains known defects in the software, categorized by software section, with a brief abstract and information related to each defect's severity and risk. Product management assesses risk, which can differ significantly from the reported severity.

Table 3. Known defects

Software section	Severity	Abstract	Risk
Export	Low	ProSightPD cannot export all annotated spectra. However, you can copy and paste individual spectra from the MS/MS spectrum view.	High
LFQ	Low	The feature detector node quantifies features across the entire file. There is no way to select a retention time window at this time.	High
Annotated Spectrum	Low	In cases where fragments are reported but not seen in the MS/MS annotated spectrum, open the fragment view options and set the annotation threshold to 0% relative abundance.	High
Database annotation	Low	In some cases it might be unclear how to remove a modification. To remove modifications from a residue, hold down the CTRL key and click *the modification name*.	High
Installer	Low	In some cases PDF files such as release notes and installation reports do not automatically open. Thermo Fisher Scientific recommends to have Adobe™ Acrobat™ Reader™ installed and set as the default program to view PDF files. The release notes can also be found on Flexera and the ProSightPD application. IQ reports can also be found at: C:\Program Files\Thermo\IQ Reports	Medium
TDViewer	Low	There are known issues related to displaying Delta M results and results with Custom Mass Modifications in TDViewer. Issues related to displaying Delta M results will be resolved in the next release of TDViewer. Issues related to results with Custom Mass Modifications will be resolved in ProSightPD 4.2.	Medium
Report Item Distribution	Medium	Most top-down results tables are incompatible with the Venn Diagram chart feature. Additionally, the Proteins results are not available in the Histogram or Scatter Plot charts.	High
Database	High	In some cases the database dropdown is empty. Restart the application to resolve this issue.	Medium
Search Parameters	High	In some cases there are incorrectly annotated disulfide bonds in UniProt. These annotations might cause a search to crash. You can toggle the Remove Disulfide Bonds option to TRUE in order to resolve this issue.	Low

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