ProSightPD 4.2 Release Notes

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

Contents

For additional information on ProSightPD, refer to the *ProSightPD 4.2 User Guide*.

New features

This release incorporates these new or enhanced features:

- Proteoform-specific database creation.
- Improved subsequence searching to handle off-by-one deconvolution errors.
- ProForma annotated results.
- Users can build a top-down database from exported FASTA database from Proteome Discoverer.
- Support for UniMod, RESID, and ProForma annotation in single proteoform search.

Enhanced features

- Results from subsequence search indicate sites of truncation.
- Custom mass modifications can be specified by molecular formula.
- Quan Experiments can be restricted by time or scan ranges.
- Users can specify the number of modifications per proteoform when searching.
- Enhanced range features editing.
- ProSight Annotator supports proteoform-specific searching.
- Delta M mode redundant hits removed.

Proteoform specific database creation	Isoforms can now be expanded into a collection of all possible proteoforms. These proteoforms can be further edited to create a fully customized database.
Improved searching to handle off by one error	Precursors that are +/-1 Da or 2 Da away from the deconvoluted masses are added to account for potential deconvolution artifacts. Supplemental search windows are added to account for off-by-one deconvolution errors. Additional search windows can be added to account for errors greater than one as well.
Proforma annotated results	Proteoform results now include a ProForma column.
Database export	You can import and edit databases directly in the Proteome Discoverer application using the FASTA tools utility and export in a top-down format, which is fully compatible with ProSightPD Database Manager.
Support ProForma and UniMod	You can now use popular modification databases to annotate single proteoform searches.
Truncation Sites	Results from Subsequence search indicate sites of truncation and the local amino acid motif at the truncation sites.
Specify modifications by molecular formula	You can enter the molecular formula and the ProSight Annotator applies the correct mass.
Restrict Quan Function with retention time and scan number	A new parameter in the Feature Detector nodes allows you to specify a scan or time range to quantify.
Max mods per proteoform at search time	You can specify the number of PTMs per proteoform to avoid long search times or consider non-viable candidates.
Range features	The range features dialog has been enhanced with its own user interface.
ProSight Annotator	Enhancements have been implemented to support proteoform specific searching.
Delta M mode redundant hits removed	Results which add and remove the same modification are ignored.

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
	• 16 GB RAM
	• 75 GB available on C drive
	• NTFS format
	• Microsoft .NET 5.0
	• Microsoft .NET Core Runtime 2.1
Operating system	Microsoft™ Windows 10

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 4.2 installer and the compatible Proteome Discoverer 3.0 installer. The standalone installer installs only the required software. If the ProSightPD installer detects that the correct version of Proteome Discover 3.0 is already installed on your system, then only the ProSightPD 4.2 installer will be used.

The version of Proteome Discoverer 3.0 included with the ProSightPD standalone installer only supports the ProSightPD 4.2 nodes (Proteome Discoverer 3.0 viewer without any Proteome Discoverer nodes). Additional Proteome Discover 3.0 features are available separately. If you already have Proteome Discoverer 3.0, 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 4.2 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
Database Searching	Medium	N15 enriched data will have large precursor mass error	Low
Workflow Management	Medium	FDR cannot be calculated for workflows containing both Med/High and Hi/Hi data types. Split into two workflows.	Low
Workflow Template	Minor	Workflow template(s) may be missing, please download directly from https://thermo.flexnetoperations.com/	Low
Fragment Match View	Medium	For larger proteoforms the fragment match view may load slowly.	Medium
Installer	Medium	If during installation the demo license has an issue, please install Proteome Discoverer 3.0 first, open the Proteome Discoverer 3.0 application, and then proceed with installing ProSightPD 4.2. If issues continue, uninstall and reinstall the Proteome Discoverer and ProSightPD applications.	Medium

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