

OneOmics Suite 3.4

Release Notes



The OneOmics suite is a unified platform that enables processing and analysis of data files acquired on a SCIEX ZenoTOF 7600 or TripleTOF 5600, 5600+, 6600, or 6600+ system. It enables visualization of large and complex data sets for proteomics, metabolomics, and multi-omics applications. The web-based and cloud-powered suite also enables easy access, fast processing, and collaborative sharing.

Google Chrome is required for use with the OneOmics apps, which are available at <https://oneomics.sciexcloud.com>. The two supported cloud storage solutions include the Data Store, a SCIEX storage solution, and the Illumina BaseSpace Sequence Hub.

Requirements

- CloudConnect version 1.8
- Google Chrome

Google Chrome is available at <https://www.google.com/chrome>. Chrome must be configured as the default browser on the computer. Go to the web page: [Instructions for configuring the default browser](#).

New in Version 3.4

New Features and Enhancements

Version 3.4

- **New Metabolomics Libraries:** New NIST20-based ion libraries are now available for use in the Metabolomics app Extractor.
- **Browser App Improvements:** The p-values in the Browser app have been changed to $-\log_{10}(p)$ for easier recognition of significant fold changes.

Version 3.3

- **Support for CloudConnect 1.8:** OneOmics suite 3.3 requires CloudConnect 1.8. CloudConnect 1.8 can be downloaded from sciex.com/software-support/software-downloads.
- **Ion Library App:** A new app that helps users to easily create ion libraries for downstream use in OneOmics suite and DIA-NN compatible formats.
- **DIA Results App:** A new app that has tools for transforming, assembling, and visualizing DIA-NN-based reports.
- **Data Store App:** Access to the Data Store from the dashboard.

OneOmics Suite 3.4 Release Notes

- **Account Management:** The ability for group administrators to add users to and remove them from the Group account.
- **ProteinPilot App Improvements:** Support for Rapid search and searching with Special Factors. The app also includes a new results summary page and new filters on the Proteins Detected page.
- **Licensing Transparency:** The ability to download the usage report for the group in comma-separated value (csv) format.
- **UX Enhancements:** The ability to launch processing from an experiment.

Version 3.2

- **CloudConnect Support:** Support for CloudConnect 1.7 for PeakView software 2.2.
- **MGF Support:** Support for Mascot generic format (MGF) data in the ProteinPilot and iTRAQ apps.
- **iTRAQ:** Improved iTRAQ quantitation when only a subset of the reagent labels are used.
- **UI Improvements:** User interface re-design and small usability fixes.

Version 3.1

- **ZenoTOF 7600 System:** Support for the ZenoTOF 7600 system for discovery and next-generation proteomics and metabolomics workflows.
- **Pathways Support:** Upgrade of Pathways to version 75.
- **CloudConnect Support:** Support for CloudConnect 1.6 for PeakView software 2.2.

Version 3.0

- **ProteinPilot App for Protein Identification:** Processing of IDA data for proteomics samples using the Paragon™ algorithm and Pro Group™ algorithm. Intuitive visualization tools facilitate data quality analysis and protein identification. Processing of iTRAQ reagent-labeled data is included.
- **SWATH Acquisition for Proteomics:**
 - Processing of SWATH acquisition data for proteomics samples, using ion library-driven extraction. Integrated normalization and false discovery rate analysis, with intuitive visualization tools for data quality and protein expression analysis.
 - Support for the UniProt proteome database, including reviewed entries for all species and unreviewed entries for human, mouse, *escherichia coli* (*E. coli*), yeast, and Chinese hamster cells. The following versions are supported:
 - All reviewed (SwissProt) protein accessions, regardless of species: December 2018

- Unreviewed (Trembl) protein accessions of species human, mouse, *E. coli*, Chinese hamster ovarian cells: July 2020
- Remaining unreviewed protein accessions: Current version of UniProt
- **SWATH Acquisition for Metabolomics:**
 - Processing of SWATH acquisition data for metabolomics samples, using the Accurate Mass Metabolomics Spectral Library. Integrated normalization and false discovery rate analysis, with intuitive visualization tools for data quality and metabolite changes across samples.
 - Support for version of 3.0 of the Human Metabolome Database (HMDB).
- **MarkerView App for Multivariate Statistics:** Align and perform multivariate analysis on proteomics, metabolomics, and genomics data using PCA and K-means clustering. Explore differences between sample groups with powerful visualization tools.
- **Tools for Interpretation in Biological Context:** Visualize quantitative results using gene ontology enrichment analysis and pathway analysis, powered by Reactome.
- **Group-based Product Licensing:** Simplified licensing that allows one or more licensed packages to be assigned to all members of the group. All group members have their own account, but share the same licensed features, such as processing applications, compute capacity, and storage space. The supported storage space is on the Data Store, a new SCIEX storage solution.

Fixed Issues

Version 3.4

- The UniProt ontologies lookup did not work for some accessions. (OOM-3814)

Version 3.3

- The %CV plot and table exclude features that are not detected across all replicates in a group. (OOM-3126)
- The results and workspaces expire in 30 days instead of 7 days. (OOM-3581)

Version 3.2

- For samples acquired by TOF instruments, the ranking of peptides within groups that contain competing hypotheses has been improved in the ProteinPilot and iTRAQ apps. As a result, peptide IDs have increased. Protein IDs are unaffected. (OOM-2759)
- The ProteinPilot app now supports the new system name format in data files created when processing samples acquired by the ZenoTOF 7600 system with the SCIEX OS 2.1 software. (OOM-2737)

OneOmics Suite 3.4 Release Notes

- The iTRAQ app now supports the processing of samples labeled using a subset of SCIEX iTRAQ reagents, that is, where the number of experimental conditions is less than the number of iTRAQ channels. (OOM-2091)
- In the ProteinPilot and iTRAQ apps, an error was shown for some results in the Analytics app. This issue typically occurred for results from samples such as fractions with low peptide and protein identifications or samples with zero yields at critical FDR values. The results are now shown on Analytics app. (OOM-2673, OOM-2665, OOM-2750)

Version 3.1

- Merging of libraries sometimes failed in an Extractor run that merged more than 100 ion libraries. (OOM-2471)
- If processing was started quickly after the Process page opened, then the Select an Experiment page sometimes included invalid experiment types. (OOM-2495)

Storage Options

The OneOmics suite offers the following storage options:

- Data Store: The licensed package includes space allocation on the Data Store in the OneOmics suite. The amount of space available is dependent on the license purchased.
- Illumina BaseSpace Sequence Hub: To register for an Illumina account and link a BaseSpace Sequence Hub account to OneOmics suite, refer to the document: *User Account Setup Guide*.

Known Issues and Limitations

Known Issues

Note: The numbers in brackets are reference numbers to each issue or feature in the SCIEX internal tracking system.

- The implementation of fixed column headers in the protein and peptide heat maps has resulted in the removal of the svg export icons (orange buttons in the top right corner of the plot windows).

Workaround: For protein results, users can export the heat maps as csv files, open the files in Microsoft Excel, and then apply conditional formatting to achieve the required results. (OOM-316)

- BaseSpace: A new BaseSpace project cannot be created in the OneOmics suite.

Workaround: Log on to the BaseSpace Sequence Hub and create the project. Then return to the OneOmics suite. (OOM-564)

- If more than 50 experiments are added to a study in the Experiments app, then only 50 experiments are shown in the Select an Experiment dialog during the setup of a processing job in the ProteinPilot, iTRAQ, Proteomics, or Metabolomics apps and during creation of a workspace in the Bioreviews app.

Workaround: Limit the number of experiments in a study to 50. For studies with more than 50 experiments, to view the first 50 experiments in the study, click the name of the study in the Select an Experiment dialog. To view the 50 most recent experiments, click **Recent** in the Select an Experiment dialog. (OOM-1073)

- The protein, peptide, and transition summary shown in the Browser in the Proteomics app might differ from the corresponding summary in the MarkerView app in Bioreviews. This occurs because decoy proteins, if present in results, are excluded from downstream processing applications such as the MarkerView app. (OOM-1234)
- Ion libraries in the Metabolomics app cannot be merged. Only select one installed library or one custom library, when running Extractor in the Metabolomics app. (OOM-1423)
- In the MarkerView app, a failure to report group data might be reported during reprocessing of PCA-PCVG results.

Workaround: Wait until processing is complete. (OOM-1539)

- The OneOmics suite logs the user off after a period of inactivity. When assigning meta data on the Sample Editor page in the Experiments app, make sure to save the changes. (OOM-1923)
- Subsequent results analysis based on a MarkerView app session is limited to using the original PCA-PCVG clustering analysis rather than reprocessed results. (OOM-2040)
- Make sure that the accession numbers in fasta files used in the ProteinPilot or iTRAQ app do not contain special characters ("&<>"). (OOM-2094)
- When theoretical fragments are viewed in the Browser in the ProteinPilot or iTRAQ app, only theoretical forms in the experimental *m/z* range are shown. (OOM-2208)
- In the Experiments app, when users search for files within a folder containing their files, the filtered list shown in the File Selection dialog might not contain all of the files that meet the search criteria.

Workaround: Scroll to the end of all the page before searching. (OOM-2273)

- When more than 1,000 files are present in a Data Store folder, only up to 1,000 files are shown in the File Selection dialog.

Workaround: Limit the number of files saved to a folder. (OOM-2273)

- Users cannot search for files and folders in the `SHARED` folder in the Data Store. (OOM-2283)
- The Pathway app might not be able to generate results for very large analyses.

Workaround: Use the filters in the MarkerView app to show selected confident data. (OOM-2334)

OneOmics Suite 3.4 Release Notes

- Files and folders containing special characters, such as the number sign (#), asterisk (*), and plus sign (+) might not be found in searches. (OOM-2387)
- The presence of metadata groups not used to define samples within an RNA experiment might result in a partially functional Bioreviews workspace.

Workaround: When assigning metadata, remove any groups that are not used to define the samples. (OOM-2458)

- If the proteins in the ion library do not include UniProt identifiers, then ontology results might not be generated. (OOM-2474)
- ProteinPilot and iTRAQ app identifications might differ slightly depending on the order of the wiff files.

Workaround: To get the same identification result, either use the same experiment, or make sure to add samples in the same order in new experiments. (OOM-2476)

- If a new job is created in the ProteinPilot or iTRAQ app with the same results file analysis name as an existing job, then results are imported into the existing results, resulting in duplication of entries.

Workaround: When processing data in the ProteinPilot or iTRAQ app, use a unique analysis name for each job. (OOM-2484)

- If a custom ion library includes modified peptides and unmodified peptides on different proteins that share the same base sequence, then the Extractor in the Proteomics app appends the modified and unmodified peptides to all of the proteins with overlapping peptides. (OOM-2498)
- PCA-PCVG results might not be shown for an area-based session created with multiple experiment sets.

Workaround: Use fold-change sessions when analyzing multiple experiment sets. (OOM-2522)

- An area-based session created with multiple experiment sets, and in a vertical matrix format, might have differing order of samples in the Area plot.

Workaround: Use fold-change sessions when analyzing multiple experiment sets. (OOM-2524)

- Protein and metabolomics SWATH acquisition experiments are marked as valid if one of the experimental groups has a single replicate. This causes a processing error in the Assembler in the Proteomics and Metabolomics apps. Each experiment group must contain at least two replicates, either biological or technical, for processing in the Proteomics and Metabolomics apps. (OOM-2577)
- On the QUANT tab of results in the iTRAQ app, only the reporter ions are shown, not the zoomed in region around the reporter ions. (OOM-3117)

Workaround: Use the zooming graph control on the SPECTRUM tab to view the reporter ions region of the spectrum.

- In the Proteomics, Metabolomics, and DIA Results apps, the **Show Percentage** option on the Protein Areas tab persists when the user clicks a different compound in the heat map. (OOM-3598)

Workaround: After selecting a different compound, click **Update** on the Protein Areas tabs to update the information shown on the graph.

- If the last or first name of the user is changed on the Update Profile page, then the page is not updated until after the user logs off and then on. (OOM-3599)
- Custom libraries that contain both negative and positive polarity spectra are not filtered with the **Compound DB Polarity** filter in the Extractor in the Metabolomics app. (OOM-3774)

Workaround: Use custom libraries that contain a single polarity, positive or negative.

- For negative polarity data, on the Analytes page, the analytes are incorrectly annotated with a plus sign. For example, the correct charge is [-1], but [-1+] is shown. (OOM-3781)
- Results generated from negative polarity data with the NIST20 High-Resolution Library cannot be opened in CloudConnect for review. (OOM-3825)

Limitations

- The total number of transitions that the Proteomics Assembler app can handle in one processing job is approximately 250,000 after false discovery rate (FDR) filtering. In practical terms, this can be reached by exceeding the following scenarios:
 - Assembling 100 extracted result files (qresult files) that were processed using a ProteinPilot software ion library containing 6,000 proteins.
 - Assembling 30 extracted results files (qresult files) that were processed using an ion library with approximately 1 million transitions, for example, derived from the pan-human library.
- Multivariant grouping works well when most of the variance across samples can be explained by a small number of the principal components (PCs) identified in the principal component analysis (PCA) algorithm. When there are many experimental groups with very high variance across samples, it might take a large number of PCs to explain most of the variance. A negative consequence of this would be that a large number of groups can be formed, too many to be reviewed in the software. To fix this issue, we have limited the number of PCs that are used for grouping, even if this results in some PCs that explain a non-trivial amount of the variance being omitted. As a result, the number of groups formed will typically be in the interval [10,100], but minor differences in protein expression trends that ideally might be split into multiple groups are instead merged. If, after manual review, groups are found with member proteins that exhibit dissimilar expression trends within the same group, then it might be possible to further split the groups by selecting the groups of interest and selecting **Reprocess**.

- OneOmics suite supports alphanumeric characters in object names, as well as a limited set of special characters. The following table shows the supported special characters.

Table 1 Supported Special Characters

| Object | Supported Characters |
|---|----------------------------------|
| Analysis names | @ ^ () - _ |
| BaseSpace project | @ ^ () - _ [] ` ~ \$ % ; ' , ! |
| Experiment names | @ ^ () - _ |
| Data Store folder names | @ ^ () - _ [] ` ~ \$ % ; ' , ! |
| Session names | @ ^ () - _ |
| Study names | @ ^ () - _ |
| Workspace names | @ ^ () - _ |
| File names (for files uploaded from CloudConnect for PeakView software 2.2) | @ ^ . () - _ [] |

- Multi-sample SWATH acquisition wiff files are not supported in the OneOmics suite.

Contact Us

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- [SCIEX Now Learning Hub](#)
- [SCIEX OneOmics Suite User community](#)

SCIEX Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the SCIEX website at sciex.com or contact us in one of the following ways:

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

CyberSecurity

For the latest guidance on cybersecurity for SCIEX products, visit sciex.com/productsecurity.

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>.

Note: To request a free, printed version of this document, contact sciex.com/contact-us.

This document is provided to customers who have purchased SCIEX equipment to use in the operation of such SCIEX equipment. This document is copyright protected and any reproduction of this document or any part of this document is strictly prohibited, except as SCIEX may authorize in writing.

Software that may be described in this document is furnished under a license agreement. It is against the law to copy, modify, or distribute the software on any medium, except as specifically allowed in the license agreement. Furthermore, the license agreement may prohibit the software from being disassembled, reverse engineered, or decompiled for any purpose. Warranties are as stated therein.

Portions of this document may make reference to other manufacturers and/or their products, which may contain parts whose names are registered as trademarks and/or function as trademarks of their respective owners. Any such use is intended only to designate those manufacturers' products as supplied by SCIEX for incorporation into its equipment and does not imply any right and/or license to use or permit others to use such manufacturers' and/or their product names as trademarks.

SCIEX warranties are limited to those express warranties provided at the time of sale or license of its products and are the sole and exclusive representations, warranties, and obligations of SCIEX. SCIEX makes no other warranty of any kind whatsoever, expressed or implied, including without limitation, warranties of merchantability or fitness for a particular purpose, whether arising from a statute or otherwise in law or from a course of dealing or usage of trade, all of which are expressly disclaimed, and assumes no responsibility or contingent liability, including indirect or consequential damages, for any use by the purchaser or for any adverse circumstances arising therefrom.

(GEN-IDV-09-10816-D)

For Research Use Only. Not for use in Diagnostic Procedures.

Trademarks and/or registered trademarks mentioned herein, including associated logos, are the property of AB Sciex Pte. Ltd., or their respective owners, in the United States and/or certain other countries (see sciex.com/trademarks).

AB Sciex™ is being used under license.

© 2022 DH Tech. Dev. Pte. Ltd.



AB Sciex Pte. Ltd.
Blk33, #04-06 Marsiling Industrial Estate Road 3
Woodlands Central Industrial Estate, Singapore 739256