OneOmics™ Suite 3.1 Release Notes

Introduction

The OneOmics™ Suite Powered by SCIEX Cloud is a set of web applications that allow 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. SCIEX Cloud is a platform developed to provide secure storage and fast processing capabilities, within a cloud-computing environment.

Requirements

Note: Customers using the beta version of OneOmics™ Suite must reconnect their Illumina account with their OneOmics™ account.

- CloudConnect App version 1.6
- Google Chrome
  Google Chrome is available at https://www.google.com/chrome. Chrome must be configured as the default browser on the computer. Refer to instructions for configuring the default browser.

New in this Version

New Features and Enhancements

Version 3.1

- **ZenoTOF™ 7600 LC-MS/MS System:** Support for the ZenoTOF™ 7600 LC-MS/MS 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 Cloud storage solution.

Fixed Issues

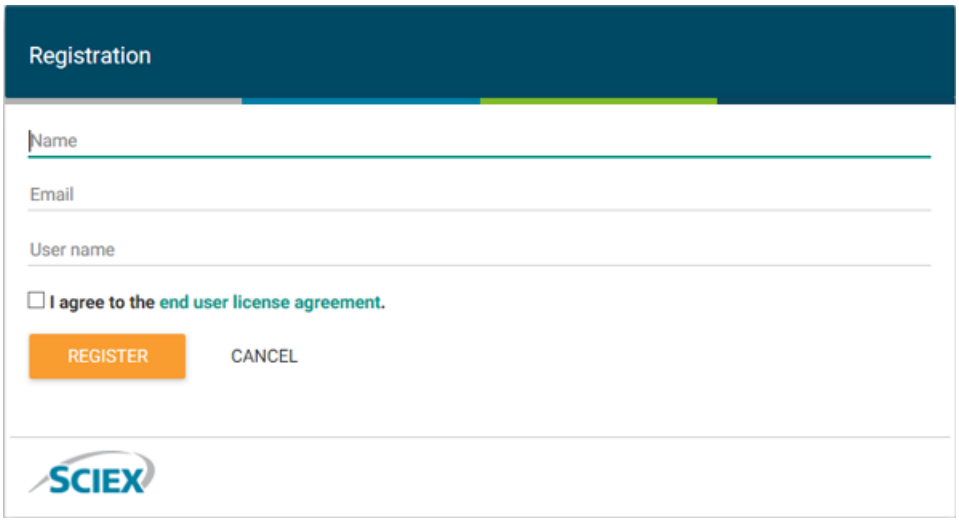
Version 3.1

- 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)

Register for a User Account on the OneOmics™ Suite Powered by SCIEX Cloud

1. In Google Chrome, go to https://oneomics.sciexcloud.com.
2. Click **Register**.

Figure 1 Registration Dialog



3. Complete the registration form, select **I agree to the end user license agreement**, and then click **Register**.

Note: To view the end user license agreement (EULA), click the link.

A confirmation e-mail is sent, with a link to set the account password.

4. Click the link in the confirmation e-mail and set a password for the OneOmics™ Suite account.

Activate the OneOmics™ Suite Account

After registering a OneOmics™ Suite account, the account administrator must perform this procedure to license the required features.

Note: If the user logs on to an account that is not activated, then the message, "You don't have a license", is shown.

1. Contact a SCIEX representative to purchase the required licenses. In the request, include the following information:
   - Group account or organization name representing the team
   - User name and e-mail address associated with the OneOmics™ Suite account

   Note: Multiple users can be added to a group account. A single request can specify all of the users to be included in the group. Ideally, user accounts are added at the time of initial registration, but they can be added later.

   The SCIEX representative notifies the user when the account is licensed. Do not log in to OneOmics™ Suite until after the receiving the notification.
2. After the notification is received, log on to OneOmics™ Suite.

Storage Options

The OneOmics™ Suite offers the following storage options:

- SCIEX Cloud (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, refer to Register an Illumina Account. To link a BaseSpace Sequence Hub account to OneOmics™ Suite, refer to Link an Illumina Account to the OneOmics™ Suite.

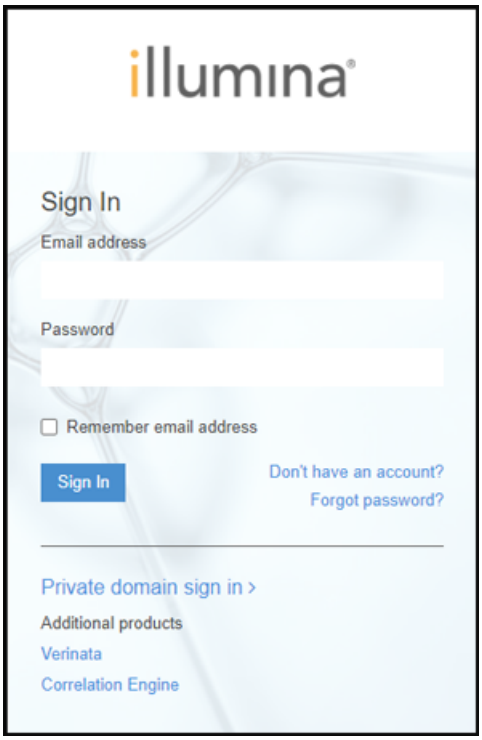
Illumina BaseSpace Sequence Hub

Optionally, if the Illumina BaseSpace Sequence Hub is being used for storage, perform the procedures in this section to link OneOmics™ to an Illumina account.

Register an Illumina Account

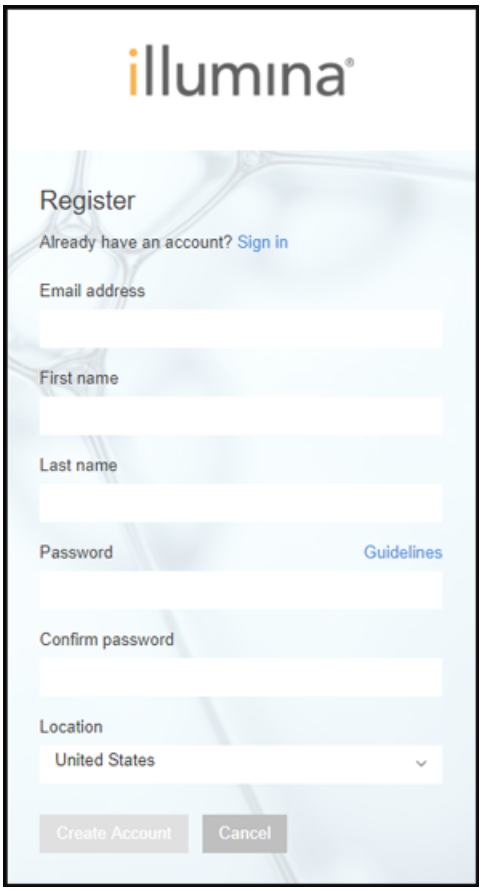
1. Go to https://basespace.illumina.com.

Figure 2 illumina Logon Dialog



2. Click **Don't have an account?**.

Figure 3 Register Dialog



3. Complete the registration form and then click **Create Account**.

   A confirmation e-mail will be sent.

4. Click the link in the confirmation e-mail to confirm registration.

   An e-mail will be sent to confirm the activation of the illumina account.

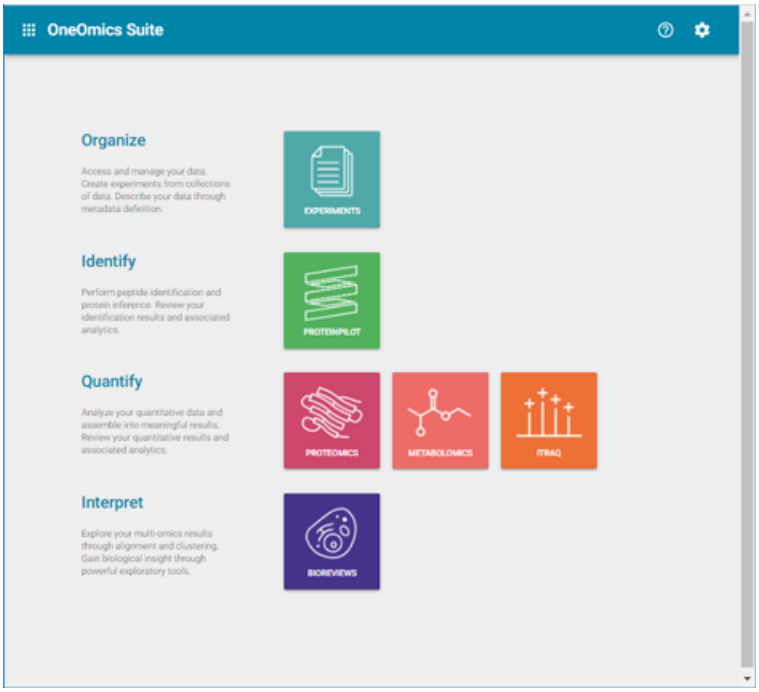
Link an Illumina Account to the OneOmics™ Suite

Note: For Illumina BaseSpace Sequence Hub storage, register for an Illumina account. Refer to Register an Illumina Account.

Note: OneOmics™ beta users must re-link their Illumina accounts.

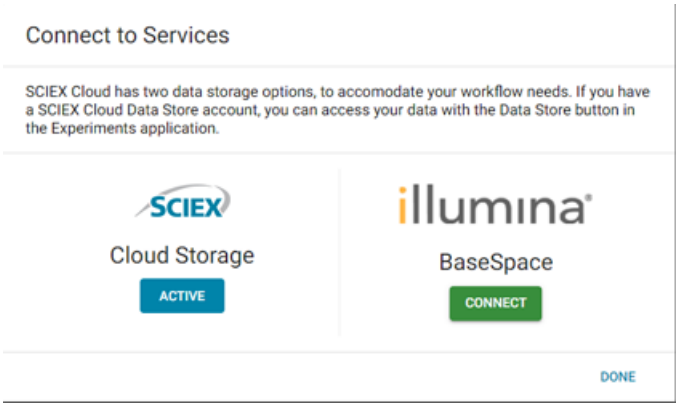
1. Log off of Illumina BaseSpace Sequence Hub.
2. Log on to the OneOmics™ Suite.

Figure 4 OneOmics™ Suite Dashboard



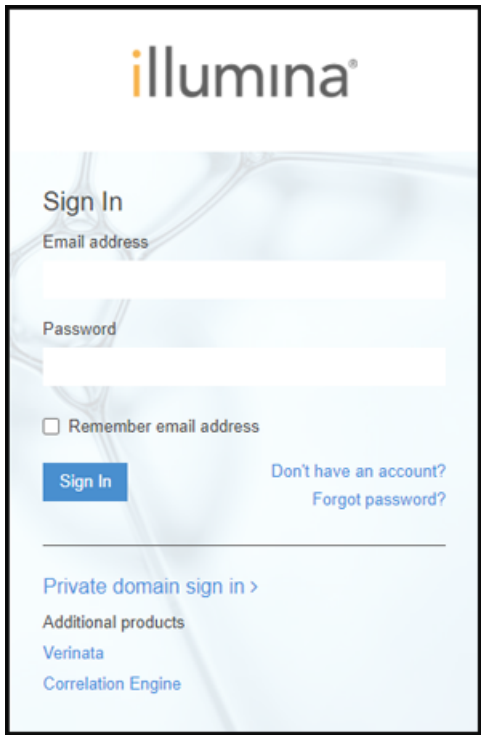
3. Click the Settings icon in the top right corner and then click **Connect Services**.

Figure 5 Connect Services Dialog



4. Click **Connect** under **BaseSpace**.

Figure 6 illumina Logon Dialog



5. Type the logon credentials and then click **Sign In**.
6. Read and accept the end user license agreement.

   The Connect to Services dialog is shown. The BaseSpace account is now connected (Active).
7. Click **Done**.

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 in to the BaseSpace Sequence Hub and create the project. Then return to the OneOmics™ Suite. (OOM-564)
- 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 apps 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)
- 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)
- When SCIEX iTRAQ reagents are being used, we recommend that all channels be used during sample preparation. If the number of experimental conditions is less than the number of iTRAQ channels, then use the additional channels for experimental group replicates. The reporter ion calibration step is optimized for samples where all reporter ions are present. (OOM-2091)
- Make sure that the accession numbers in fasta files used in the ProteinPilot™ App or the iTRAQ app do not contain special characters ("&<>). (OOM-2094)
- When theoretical fragments are viewed in the Browser in the ProteinPilot™ App or the 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.
  Work-around: Use the filters in the MarkerView™ App to show selected confident data. (OOM-2334)
- Files and folders containing special characters, such as the number sign (#), asterisk (*), and plus sign (+) might not be found in searches. (OOM-2387)
- When users try to import results in folders that contain the plus sign (+) and ampersand (&) characters, the workspace might not be created in the Bioreviews app. (OOM-2441)
- The presence of meta data groups not used to define samples within an RNA experiment might result in a partially functional Bioreviews workspace.
  Workaround: When assigning meta data, 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™ App 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™ App 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™ App 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)

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 7-1 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 University™
- 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.

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