Compound Discoverer 3.1 Release Notes

These release notes briefly list new features in the Thermo Compound Discoverer™ 3.1 application, a qualitative data-processing application for small molecule research. Also included are known issues in the 3.1 release of the application.

Contents

For information on installing the Compound Discoverer software, refer to the instruction card in the full-version box. For information on licensing, configuring, and using the Compound Discoverer 3.1 application, refer to the manuals available as PDF files or the Help.

Features

The Compound Discoverer 3.1 release contains the following new features and enhancements.

New Features

- Molecular Networks (beta) to interactively explore relationships between compounds based on transformations and spectral similarity
- Scripting node to embed scripts—for example, Python or R scripts—in workflows
- Mass Defect Plot for Compounds and Expected Compounds
- Calculate Mass Defect node with support for up to 5 Kendrick formulas
- Peak area scaling using values from a numerical study factor that you specify as the scaling factor in the Normalize Areas node
- Search mzCloud node:
  - Supports automatic searches of multiple spectral libraries
  - Supports the new “Autoprocessed” mzCloud library
  - Supports using both DIA and DDA scans as the query scans to search against the mzCloud library
  - Highlights matching and non-matching spectral peaks in green and red, respectively
  - Displays the fragment structure for matching peaks
- Apply Spectral Distance node to score the observed isotopic pattern versus the simulated isotopic pattern of a candidate from, for example, ChemSpider
- Manual export of detected compounds in a result file to a mass list file
- Installation of the mzVault 2.2 application for creating and editing mass spectral libraries

Note The mzVault 2.2 application supports importing NIST MSP and MassBank MB files.

XCALI-98078, Rev A

thermoscientific

Enhancements

- Improved performance of ChemSpider searches
- Chromatographic peak areas are now calculated on a seconds timescale (was minutes before, so results are now scaled by a factor of 60)
- Extended retention time search window for the assignment of MSn spectra to a compound
- Changes in the Expected Compounds database are now immediately reflected in the Generate Expected Compounds node
- New parameter for Compound Class Scoring node to use entire MSn tree
- New version of the HighChem Fragmentation Library
- New licensing mechanism

System Requirements

The Compound Discoverer 3.1 application can process data files produced by high-resolution accurate-mass (HRAM) Thermo Scientific™ instruments, such as the Orbitrap ID-X™, Orbitrap Fusion™, Orbitrap™ hybrids, Q Exactive™, and Exactive™ mass spectrometers.

Table 1 lists system requirements for the data processing computer.

Table 1. System requirements for the data processing computer

System	Requirements
Hardware	• 3.4 GHz dual-core processor • 16 GB RAM • 500 GB hard drive • DVD-ROM and USB drive • Display monitor resolution of 1920×1080
Software	• Microsoft™ Windows™ 7 Pro SP1 (64-bit) or Windows 10 (64-bit) operating system • Microsoft .NET Framework 4.7.2 • Microsoft Office 2013 or higher • Adobe™ Reader™ 11 • Adobe Flash™ Player 15

Table 2 lists the recommended hardware configurations for enhanced performance using the Compound Discoverer application.

Table 2. Recommended hardware configurations

System	Requirements
Hardware	• Dual 8-core processor (for example, 2x Intel™ Xeon™ Gold 6134 CPU @ 3.20 GHz) • 64 GB RAM • 1 TB SSD (solid-state disk) hard drive for operating system • 2nd 3 TB (conventional disk) hard drive for data storage • DVD-ROM and USB drive • Two 27 in. UHD monitors: Display monitor resolution of 3840 × 2160

Important Information

Supported Local Language and Date/Time Format for the Data System Computer

The Compound Discoverer 3.1 application was tested and supported for US-English Only locale settings. To change the format on your computer, go to **Control Panel > Region and Language**.

Upgrading from Compound Discoverer 1.0, 2.0, 2.1, or 3.0

To install Compound Discoverer 3.1 software on a processing computer that has version 1.0, 2.0, 2.1, or 3.0 you do **not** need to uninstall the earlier version. Compound Discoverer 1.0, 2.0, 2.1, 3.0, and 3.1 can coexist on the same computer. For detailed installation instructions, refer to the Installation Instructions located on the software media.

Using the Search mzVault Node

The Search mzVault node does **not** require the mzVault application, so installing the mzVault 2.2 software is optional. However, Thermo Fisher Scientific recommends installing the software to do any of the following:

- Create your own spectral libraries.
- Edit existing spectral libraries (in Library Manager format or mzVault format).
- Convert existing spectral libraries (in Library Manager format or mzVault 1.0 format) for use in the Compound Discoverer application.
- Import spectral libraries in the NIST MSP format (.msp) or MassBank records (.mb).

To use your own mzVault spectral libraries in the Compound Discoverer application, add it to the Lists & Libraries editor in the application. Refer to the User Guide or Help for additional information on using your own spectral libraries.

Compound Discoverer 3.1 ships with two mzVault spectral libraries: mzVault Reference May 2019.db and mzVault Autoprocessed May 2019.db. These files are local copies of the mzCloud library (MS2 only) as of May 2019. Approximately every 6 months, Thermo Fisher Scientific provides an updated local mzCloud library as an mzVault database file, which you can download from the Flexera™ software download site (thermo.flexnetoperations.com). This local version of mzCloud is only compatible with mzVault 2.2 or later.

Multiple Monitor Support

Compound Discoverer data review supports multiple monitors. To connect the data system computer to two monitors, use the two display ports on the back of most computers.

Compound Discoverer Permanent Viewer

A licensed demonstration version of Compound Discoverer becomes a permanent viewer even after license expiration. With the Compound Discoverer viewer, you can open previously processed result files and generate reports. Nodes such as Input Files, Select Spectra, and Export Spectra are still available for use within the viewer, while other license-protected nodes will no longer be available for data processing.

Ensuring Access to the Online Databases

A typical Compound Discoverer analysis that identifies unknown compounds searches mass spectrum databases on the Internet. To run these searches, the application must have unblocked Internet access to these databases. To test the application's access to the online mass spectrum databases, follow this procedure.

❖ **To test and troubleshoot the application's access to the online databases**

1. Run the communication tests (see Running the Communication Tests).

   If the communication tests succeed, the application has access to the online databases.
2. If a communication test fails, do the following as needed:
   - If only the mzCloud communication test fails, check the Date and Time settings on the processing computer (see "Setting the Correct Time and Time Zone on the Processing Computer" on page 5).
   - If the Check Subscription test for the BioCyc database fails, check the subscription information in the BioCyc User Login view of the Configuration page.

     IMPORTANT You must create a BioCyc user account and then enter, test, and save your account credentials in the BioCyc User Login view (see "Setting Up a BioCyc Account or Subscription" on page 6).

- If any of the other communication tests also fail, check the access to the URLs for the online databases (see "Checking the URLs for the Online Databases in Your Browser" on page 5).

  If you can access the URLs for the online databases through your browser, but the communication tests still fail, the firewall or proxy setting for your company network is blocking the application's access to the online databases.

3. If the communication tests fail, but you can access the URLs for the online databases, do the following as needed:
   - If a firewall is blocking the application's access to the online databases, ask your IT department to make sure that the company firewall is not blocking "Compound Discoverer" or "Compound Discoverer Server" from accessing the URLs. The application uses the following protocol: http port 80 and https on port 443.
   - If a proxy setting is blocking access, see "Specifying the IP Address of the Proxy Server" on page 5.

See any of these topics as appropriate:

- Running the Communication Tests
- Checking the URLs for the Online Databases in Your Browser
- Specifying the IP Address of the Proxy Server
- Setting the Correct Time and Time Zone on the Processing Computer

Running the Communication Tests

Use the Communication Tests dialog box to test your processing computer's access to the online databases.

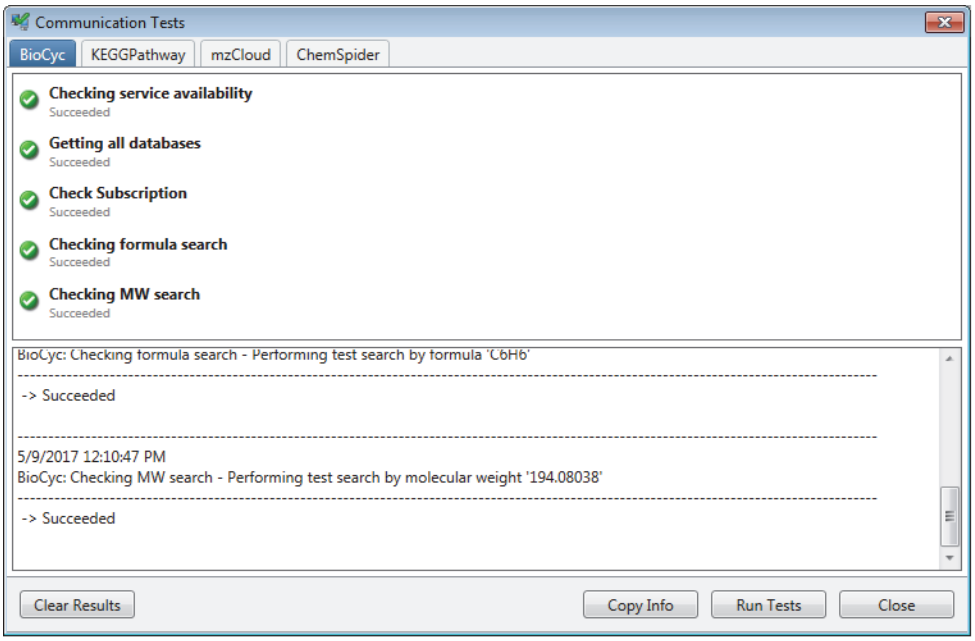
❖ To verify that your computer has access to the external databases

1. From the menu bar, choose **Help > Communication Tests**.

   The Communication Tests dialog box opens.
2. To open the page for the database that you want to access, click its tab.
3. Click **Run Tests**.

   Figure 1 shows the communication tests in progress.

   Figure 1. BioCyc communication tests



4. If the tests are successful, your computer has access to the required databases on the Internet. If only the mzCloud test fails, check the Date and Time settings for the processing computer (see "Setting the Correct Time and Time Zone on the Processing Computer" on page 5). If any of the other tests also fail, check the access to the URLs in your browser (see Checking the URLs for the Online Databases in Your Browser).

Checking the URLs for the Online Databases in Your Browser

Table 3 lists the URLs for the online mass spectrum databases. If a communication test fails, test the URL for the affected database.

Table 3. URLs of online mass spectrum databases

Database	URL
mzCloud Identity	https://identity.mzcloud.org/
	https://www.mzcloud.org/Services/MzCloudApiV1.svc
	https://www.mzcloud.org/Services/MzCloudApiLightService.svc
ChemSpider	http://www.chemspider.com
	http://chemspider.com/MassSpecAPI.asmx
	http://chemspider.com/Search.asmx
KEGG™: Kyoto Encyclopedia of Genes and Genomes	http://www.kegg.jp/
	http://rest.kegg.jp
	https://proxy.online-licensing.net
BioCyc	https://biocyc.org/
	https://biocyc.org/web-services.shtml

Specifying the IP Address of the Proxy Server

If the communication tests fail but you can access the online databases through your browser, follow this procedure to specify the IP address of the proxy server.

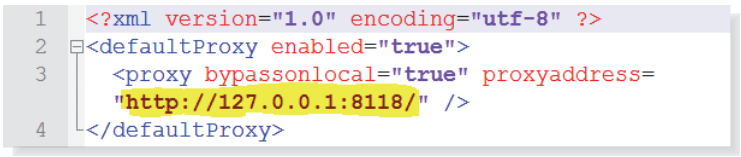
❖ **To configure the IP address of the proxy server**

1. Go to *drive*:\Program Files\Thermo\Compound Discoverer 3.1\bin\Config.
2. Open the **Proxy.config** file in Notepad.
3. Remove the text that is highlighted in yellow in Figure 2—that is, remove the XML comment delimiters: <!-- and -->.

Figure 2. Proxy configuration setting with XML comment delimiters

4. Replace the text that is highlighted in yellow in Figure 3 with your company proxy address.

Figure 3. Default proxy address highlighted in yellow

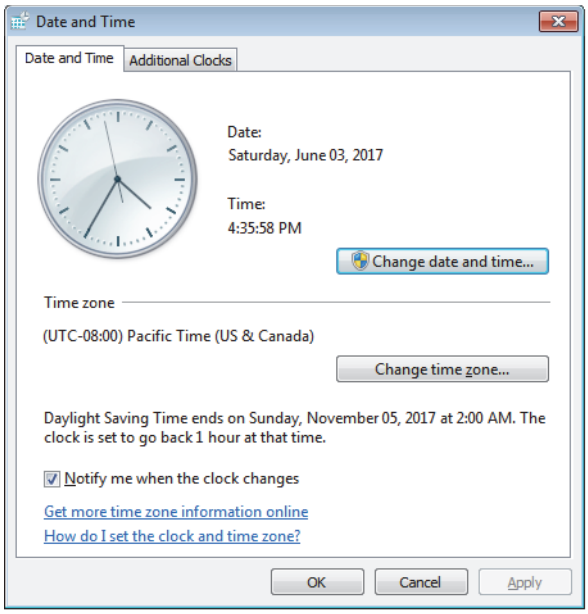


Setting the Correct Time and Time Zone on the Processing Computer

The mzCloud communication test includes a validation of the date and time settings on the processing computer. If the mzCloud communication test fails, but the other communication tests succeed, check the date and time settings for the processing computer.

❖ To check the time and time zone settings

1. Open the Date and Time dialog box. For the Windows 7 operating system, open the Control Panel. In the View By list, select **Category**. Then choose **Clock, Language, and Region > Date and Time**.



2. Make sure that the date, time, and time zone settings are correct.
3. If the Internet Time tab is available, synchronize the Internet time.

> **Note** If your computer is not part of a network domain that synchronizes the computer's clock to the network server, you can use an Internet server to synchronize the computer's clock.

Setting Up a BioCyc Account or Subscription

Follow the instructions in the BioCyc User Login view to set up your BioCyc subscription or user account. You must have an organization subscription or an individual subscription to access all BioCyc databases. A user account allows you to access only the EcoCyc database.

To set up a BioCyc account or individual subscription and enter your credentials in the BioCyc User Login view, follow these procedures as needed:

- To open the BioCyc User Login page
- To set up a BioCyc account or individual subscription
- To enter, test, and save your account information

> **Note** To set up a user account or an individual user subscription, you must have Internet access.

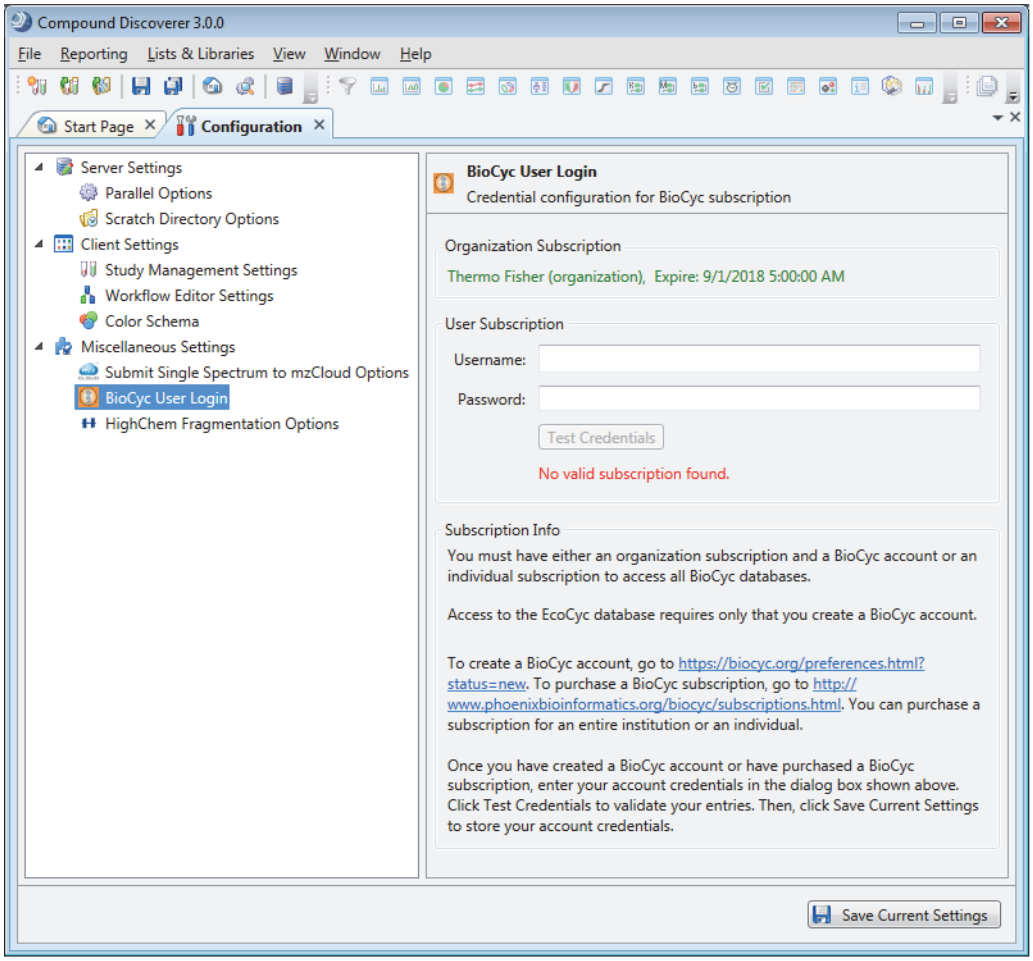
❖ To open the BioCyc User Login page

1. From the application window, choose **Help > Configuration**.

   The Configuration page opens.
2. In the left pane, under Miscellaneous settings, select **BioCyc User Login**.
   - In the Organization Subscription area, if you have a subscription, the organization name appears in green. Otherwise, this area displays, "No Valid Subscription Found" in red.
   - In the User Subscription area, if you already created a BioCyc user account, entered and tested your credentials, and saved the settings, the User Name box displays your email address. Otherwise, the following text appears in red below the Test Credentials button: No Valid Subscription Found.

   Figure 4 shows a BioCyc User Login page for a user without a subscription.

Figure 4. BioCyc User Login page for a user without a subscription



❖ To set up a BioCyc account or individual subscription

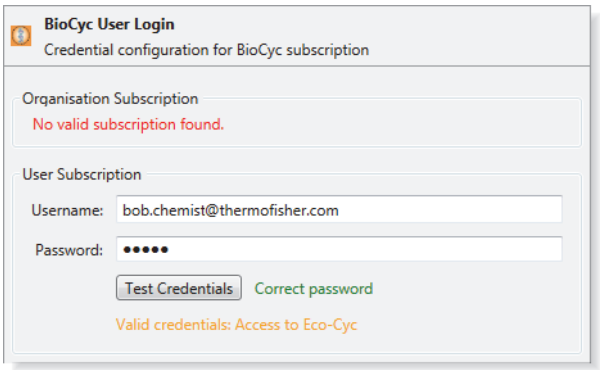
Follow the instructions in the BioCyc User Login view.

❖ To enter, test, and save your account information

1. In the User Subscription area, enter your email address in the User Name box and your BioCyc password in the Password box.
2. Click **Test Credentials**.
3. Click **Save Current Settings**.

Figure 5 shows the subscription information if you have a user account but do not have an organization subscription or an individual subscription. When running analyses that map compounds to the BioCyc pathways, you can access only the EcoCyc database.

Figure 5. Settings for a user account only



Suggested Recovery Actions

- For some issues, restarting the application or data system computer is the appropriate recovery action.
- As a fix we generally do not recommend reinstalling the software or the operating system, which more commonly occurs after you install a new hard drive.

Feature Requests and Other Removed Items

- We do not include issues where there is insufficient information logged to successfully reproduce the reported problem.
- We do not list feature requests as software issues, regardless of the reported significance or severity of the request. Product managers evaluate logged feature requests for future releases.
- We report only discrepancies in the documented software as known issues.

Terminology Tables

Severity	Interpretation
Critical	A problem that renders the system unusable because either an entire function is unusable and no workaround exists, or use of the current system compromises data integrity or results in data loss. Catastrophic problems also include significant and non-obvious quantitative errors, and all human and instrument safety issues.
High	A serious issue that does not affect data integrity (meaning data loss, corruption of data, or the wrong answer), but affects the customer's ability to use the product as designed. It can be a failure, design issue, or documentation error or omission. A workaround might or might not exist.
Medium	A minor error or poor behavior of a product feature. There is probably a workaround.
Low	An issue that has a limited effect on customer usage of the product; for defects with visibility so low that a customer might never see it; or for ease of use issues or other items not causing any performance degradation.

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 4 contains known defects in the software, categorized by software section, with a brief abstract and information related to each defect's severity and risk. The Item ID is the internal number assigned to each issue. Product management assesses risk, which can differ significantly from the reported severity.

Table 4. Software defects (Sheet 1 of 2)

Software section	Severity	Abstract	Risk	Item ID
Alignment	Medium	Inadequate alignment can cause reported peak areas being too low.	Medium	87877
Alignment	Medium	Insufficient alignment for samples with low feature density.	Medium	87433
Compound Editor	Low	Atom Properties dialog box | Periodic Table | Terrestrial Isotopes: The mass numbers displayed as superscript are not aligned for some elements.	No Risk	29737

Table 4. Software defects (Sheet 2 of 2)

Software section	Severity	Abstract	Risk	Item ID
Compound Editor	Medium	Charged compound is not supported in Compound Editor.	Medium	29739
Find Expected Compounds	Medium	In chromatograms with many adjacent peaks, some smaller peaks are not detected.	Medium	96464
Job Queue	Medium	When expanding the details on a job a red X is displayed and an error message is shown (does not affect data processing).	Medium	77747
mzCloud search	Medium	Some compounds are not identified when DIA scans are used for the search.	Medium	94443
mzVault Library	Low	Spectral library—Bamba Lab 538 polar metabolite library has all ID=1 for mzCloud.	Low	78269
Reporting	Medium	MS2 spectrum is not supported in reporting.	Medium	29748
Reporting	Low	Report Template View: When you delete multiple items, part of the warning message is cut off.	No Risk	58156
Reporting	Low	The structure annotations on MS/MS spectra are not clear in the PDF report.	No Risk	58157
Reporting	Medium	HTML file is not generated for a report that contains 1000 or more entries.	Low	29752
Reporting	Medium	Color-coding can be inconsistent between XIC overlays in the Compound Discoverer result view.	Low	29758
Reporting	Medium	Unable to report the expected compounds associated with radio trace in RT order.	Low	53722
Scatter Chart	Low	The ToolTip for the data point is not displayed after docking the scatter chart in the data review window.	No Risk	58158
Unknown Detector	Medium	Ambiguities during component assembly can cause erroneous assignment of M+NH4 adduct.	Medium	88848
Unknown Detector	Medium	D-labeled compounds are not detected in certain cases.	Medium	33662
Unknown Detector	Medium	Two M+H adducts are grouped into one hit.	Low	29742
Unknown Detector	Medium	Unknown Detector occasionally assigns A1 isotope peaks as A0.	Medium	29747
Unknown Detector	Medium	Adduct grouping issue causes duplicated compounds in the Compounds result table.	Medium	29759
Unknown Detector	Medium	Unknown Detector does not correctly assemble the isotopic pattern for Boron-containing compounds.	Low	29756
Unknown Detector	Medium	[M+H]+ is assigned as [M+NH4]+ for amine compounds, for example, amino acids.	Medium	30367

Trademarks