

HUMAN HEALTH

ENVIRONMENTAL HEALTH

ChemOffice v22.0

Release Notes

Last Updated: September 14, 2022



Table of Contents

1 GENERAL DESCRIPTION..... 3

2 RELEASE QUALIFICATION..... 4

2.1 SCOPE OF TESTING 4

2.2 TESTING ENVIRONMENT..... 5

3 INSTALLATION INSTRUCTIONS..... 6

3.1 PREREQUISITES AND SYSTEM REQUIREMENTS 6

3.2 RELEASE INSTALLATION..... 6

4 KNOWN ISSUES, LIMITATIONS AND WORKAROUNDS 6

5 TECHNICAL SUPPORT 7

1 General Description

ChemOffice 22.0 is the latest release of the ChemOffice suite of productivity tools for chemists and biologists. ChemOffice helps scientists efficiently capture and share their work, visualize and gain a deeper understanding of their results, and correlate biological activity and other properties with chemical structures.

The release is qualified against the following:

- Windows 10 (64-bit) and Windows 11 (64-bit)
- Microsoft Office 2019, Microsoft Office 2021, and Microsoft Office 365
- macOS 11.6 (Big Sur) and 12.5 (Monterey) – (for ChemDraw only)
- Adobe Acrobat DC

Highlights of this release:

- ChemDraw now has support for hydrogen bonds. Formerly, dotted lines were used to represent hydrogen bonds, but now there is a specific bond tool for placement of such bonds. By explicitly recognizing a hydrogen bond, ChemDraw can handle them robustly and correctly. For example, hydrogen bonds are now correctly written to MOL files.
- ChemDraw now supports a new cartoon graphical style for monomers. To enable the display of the new style, use the “Sequence Graphics Monomers” stylesheet located in Files>Open Style Sheets. The style sheet is based on the ACS 96 format, with an extra flag to turn on the sequence cartoon support.
- ChemDraw can now fully support the FASTA format for sequences, including those monomers that are combinations of other monomers. We refer to those combination monomers as ‘OR monomers’ because they are defined as one of selection of monomers. For example, the monomer label ‘B’ is defined as D (Aspartic Acid) or N (Asparagine). A FASTA string pasted with any of these OR monomers will be interpreted correctly. In the cartoon representation, OR monomers display an integer that indicates how many monomers are included in the OR definition. For a full list of the supported FASTA monomers see the section ‘Sequence Representation’ in https://en.wikipedia.org/wiki/FASTA_format.
- FASTA strings can now be pasted into ChemDraw as HELM monomer sequences.
- The numbering of DNA/RNA sequences have been corrected. Formerly, each monomer got its own unique number. For DNA and RNA, where each “monomer” is really a triad of ribose, phosphate and base, each member of the triad was numbered. Now, the triads of DNA/RNA are numbered. So previously, a DNA sequence with bases ACG would be numbered 1-9 (with the ribose and phosphates getting their own numbers). Now this sequence would be counted as 1-3 correctly numbering the triads in the sequence.
- An additional default monomer library has been created: the Natural Monomers library. This contains only the naturally occurring amino acids and ribose, phosphates, and bases plus the OR monomers required to define FASTA sequences. This is provided as a convenience to users who only need to draw naturally occurring sequences.
- The default search order of HELM monomer libraries have been modified to be Natural Monomers, User, PerkinElmer and Pistoia libraries.
- The HELM Monomers dialog will now remember its settings between invocations of ChemDraw. This is very convenient because there are many options to select in these dialogs.
- New hotkeys are now available:
 - Bond hotkey ‘g’: places the drawing hotspot on the selected bond.
 - Atom hotkey ‘g’: places the drawing hotspot on the selected atom.
- Ring fill colors and Highlight colors are now supported when structures are exported to 3MF files. If these files are brought up in a 3MF viewer, the color filled rings and the color highlights will be seen.

- Improvements have been made to 3MF export to make the structures 3D-printable. Structures are reasonably scaled, have safeguards against parts of the model being too thin, and have fewer disconnects:
- ChemDraw now supports the “chem_comp_atom” schema in CIF files. This schema typically encodes the ligand in the CIF file. ChemDraw will attempt to deduce bond order and hydrogen counts from geometry in this case.
- A splitter has been added between the table and structure preview windows in the Monomer Manager. This allows the user to expose more columns in the table or give more space to the structure preview.
- Allene geometry modeling is improved in 3D clean.
- A toggle has been provided to show or hide explicit hydrogens under Structure>Toggle Hydrogen Display.
- A new set of shortcut key combinations (Shift + Alt/Option + Arrow keys) have been provided for the 3D rotation of molecules by + or - 12 degrees in the X or Y axis.

Chem3D

- A 64-bit version of Chem3D is now available. Also, the 64-bit version of ChemDraw now has the View/Show Chem3D Hotlink Window available and that feature is now complete in 64-bit.
- Chem3D now supports GAMESS 2021 R2 Patch 2 and will automatically detect this version if present. Instructions for setting up Chem3D with this version of GAMESS can be found at: <https://informatics-support.perkinelmer.com/hc/en-us/articles/8913001213588-How-do-I-install-GAMESS-to-work-with-Chem3D-> As always, Chem3D also supports older versions of GAMESS back to 2020.
- Chem3D also supports MOPAC2016 22.047W
- Chem3D also supports Gaussian 16W version C.01.

ChemScript

- ChemScript now supports Python versions 3.9 and 3.10.

2 Release Qualification

2.1 Scope of Testing

The following testing conditions have been set and executed for this release:

- **Installations:**
 - Default mode
 - Custom mode
 - Side-by-Side compatibility modes
- **Enhanced Functionality:**
 - The Flexera activation system is now used.
- **Third-Party Compatibility:**
 - *Operating Systems:* Windows 10 (64-bit), Windows 11 (64-bit), macOS Big Sur 11.6 and macOS Monterey 12.5
Note: Only ChemDraw is compatible with Mac systems, **not** ChemOffice 22.0.
 - *MS Office:* Office 365, 2019 (Mac & Windows), 2021 (Mac & Windows), where the latest MS Office updates used for testing are 2208 Build (16.0.15601.20078) on Windows and 16.64 (22081401) on Mac.
Note: We test with the latest versions of MS Office available at the time, but that is no guarantee of full compatibility with future updates.

- *Browsers for ActiveX Controls:* MS Edge 105 (IE Mode)
- *Calculation Engines for Chem3D:* Gaussian 16 Revision-C.01, MOPAC2016, Conflex7.2B, Autodock 4.2.6, MGL Tools 1.5.4 (for Autodock), msroll.exe (Archaic), and GAMESS 2021 R2 Patch2.
Note: Chem3D supports the 64-bit version of GAMESS only.
- *Python for ChemScript:* 3.9, 3.10
- *Visual C# for ChemScript:* 2022
- *Visual Studio 2022*
- **Regression Testing:**
 - Automated regression testing of many important functionalities in ChemDraw, ChemFinder, and ChemScript.
 - Verification of issue fixes and regression testing of related features.
- **Backward & Forward Compatibility:**
 - Limited testing with files created using current and past versions of ChemOffice applications.
- **Japanese Localization:**
 - Limited testing on Windows 10 (64-bit), and Monterey.
- **Release Candidate Qualification Testing:**
 - Digital signature verifications.
 - Sanity/Smoke test executions with all packages in mixed environments.
 - Qualification of the download executables.
 - Qualification of test orders in the Flexera Live system.

2.2 Testing Environment

The following table details the testing environments for this release:

Machine Type	Operating System	Database Version	MSOffice Version	Adobe Version
Client	Windows 10 Professional 64-bit	N/A	2019 (32-bit and 64-bit), 2021 (32-bit and 64-bit), Office 365	Acrobat DC
Client	Windows 11 Professional 64-bit	N/A	2019 (32-bit and 64-bit), 2021 (32-bit and 64-bit), Office 365	Acrobat DC
Client	macOS Big Sur (11.6) (ChemDraw only)	N/A	2021, Office 365	Acrobat DC
Client	macOS Monterey (12.5) (ChemDraw only)	N/A	2021, Office 365	Acrobat DC

3 Installation Instructions

3.1 Prerequisites and System Requirements

For information about system requirements, please refer to the *DT-22.0 Hardware Software Guide* (part of this release package).

3.2 Release Installation

Please note the following when installing ChemOffice:

- **Windows:**
 - For a clean installation, we recommend running the downloaded *cos22.0.exe* (or the extracted *Install.exe*) executable as *Administrator*.
 - When the installer is run, prior versions of *ChemDraw/ChemOffice* and ChemOffice 64-bit Support (as far back as v15.0) are detected.
 - A **"Yes/No"** dialog listing all the packages found and offering the option to remove them all, with: "Warning: This operation cannot be undone" appears.
 - If prior versions of *ChemScript* (as far back as v12.0) are detected, a similar dialog is presented. In both dialogs:
 - i. If **"Yes"** is selected, the packages are uninstalled.
 - ii. If **"No"** is selected, the packages are left as they are.
 - The installation automatically creates desktop shortcuts for ChemDraw 22.0 executable(s) (32-bit and/or 64-bit).
- The ChemOffice/ChemDraw 22.0 (Windows/Mac) can be installed side-by-side with older ChemOffice/ChemDraw versions.

4 Known Issues, Limitations and Workarounds

The following list describes the known issues, limitations, and workarounds for this release of ChemOffice:

- Chem3D does not currently support hydrogen bonds drawn in ChemDraw. They will be rendered and treated as a single bond. The workaround is to delete the single bond and replace it with the dotted bond in Chem3D.
- Hydrogen bonds are currently not supported in 3MF export or import from CDXML/CDX written from V22.0 into older versions of ChemDraw (V21.0 or earlier). In each of these cases, the hydrogen bond will be converted to a single bond. There is no workaround, because older versions of ChemDraw do not support hydrogen bonds.
- The validation of hydrogen bonds is currently limited to those that involve an explicit acceptor atom and an explicit hydrogen. Hydrogen bonds to labels that include these atoms will generate an incorrect warning. The workaround is to suppress the hydrogen bond warnings in Preferences>Warnings>Hydrogen Bonds.
- This release includes a lot of work around making structures exported to 3MF printable. Some of the measures taken to improve the success of printing are:
 - Scaling the print model in a reasonable range (50-150mm).
 - Making sure bonds are not too thin so the model does not break apart.
 - Ensuring all parts of the model are connected.
 - If the model fails to print correctly, try scaling up slightly to make for a robust model.
- The "chem_comp_atom" schema parsed from CIF files is limited to reading the ligand only without any unit cell information: in other words, a single instance of the ligand is imported. Hydrogen atoms are added after inferring bond order from distances. Sometimes this can fail. The workaround is to correct the hydrogen count manually.

5 Technical Support

PerkinElmer Informatics Support supports this software. Please contact your Sales or Services representative for more information about ChemOffice v22.0.

<https://informatics.perkinelmer.com/Support/Contact/>

PerkinElmer Inc. | For the Better

HUMAN HEALTH | ENVIRONMENTAL HEALTH

940 Winter Street | Waltham, MA 02451