HUMAN HEALTH

ENVIRONMENTAL HEALTH

ChemOffice v21.0

Release Notes

PerkinElmer
For the Better

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1   General Description

ChemOffice 21.0 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)
    - On Windows systems, IE 11 is supported, with no support for the Microsoft Edge browser.
- Microsoft Office 2019, Microsoft Office 2021, and Microsoft Office 365
- macOS 11.6 (Big Sur) and 12.1 (Monterey) – (**for ChemDraw only**)
- Adobe Acrobat Pro DC

Highlights of this release:

- ChemOffice+ is now installed by default with ChemOffice. This new application allows users to upload structures to Signals, mine structures out office documents and build curated collections of structures for export to reports in PowerPoint or as SDF files.
- HELM monomer management has been completely redesigned
    - There is now a monomer viewer that lists all the monomers in the current library in a convenient tabular form. This is further described in section *Accessing the Monomer Manager* of the *ChemDraw User Guide*.
    - Monomer creation and editing are now in their own dialog, invoked from the monomer viewer. This is further described in sections *Creating Monomers* and *Editing Monomers* of the *ChemDraw User Guide*.
    - Two new concepts have been introduced into monomer management
        - Versioning: Monomers can now have multiple versions. This is useful when a monomer's topology has been corrected. The corrected version may be in the database as a later version, while a CDXML document may contain the older incorrect version. It may also be useful to have multiple versions of monomers, for example to represent the presence of absence of R groups side chains, or depict different tautomers. If a monomer has multiple versions, the HELM Monomer Toolbar will display only the latest active version of it for drawing. This is further described in section *Editing Monomers* of the *ChemDraw User Guide*.
        - Deprecation: Monomers can now be deprecated in the Monomer Viewer. This is useful when a monomer's topology has been corrected in the database, we still have to be able to parse documents with the older incorrect version. This is further described in section *Deprecating and Activating Monomers* of the *ChemDraw User Guide*.
        - As part of this work, some monomers in the shipped PerkinElmer monomer databases were corrected.
- ChemDraw can now export 3D structures to 3MF files. These files can be imported into any application that renders 3MF files (e.g. PowerPoint). Additionally, a new copy operation has been added: Copy As 3MF. In the copy or export operation, the user can select a ball-and-stick, or a stick representation in the 3MF file. This copied 3MF file can be pasted directly into PowerPoint. This is further described in *Creating a 3MF 3D model of Structures* of the *ChemDraw User Guide*.
- Highlights drawn on atom or bonds can also be exported to 3MF. These will appear as continuous translucent meshes over the selected atoms and bonds. This is further described in section *Color Highlighting* of the *ChemDraw User Guide*.

- The PNG format has been added as a new option to the Copy As: Copy As PNG.

- 3D clean has been enhanced to support ferrocene-like structures. A new handler has been implemented to handle the bond from the metal of the ferrocene to the aromatic ring. This bond will be preserved in the 3D clean.

- Drawing ferrocene-like structures has been enhanced with two new hotkeys. With a metal atom selected that has 0 or 1 incident bonds:
  - Hotkey "j" sprouts a cyclopentadienyl orthogonal to the metal.
  - Hotkey "shift-j" sprouts a phenyl ligand orthogonal to the metal

- Hotspot hopping has been improved. The hotspot is an editing convenience and represents the next place a bond or group will be placed. Shortcuts have been provided to make it easier to move this hotspot around on the molecule.

- To move a hotspot within a fragment:
  - Shift->Up Arrow- moves 3 bonds up
  - Shift->Down Arrow- moves 3 bonds down
  - Shift->Left Arrow- moves 3 bonds left
  - Shift->Right Arrow- moves 3 bonds right

- To move hotspot between 2 fragments:
  - Shift->Alt->Up Arrow- moves hotspot to nearest fragment above
  - Shift->Alt->Down Arrow- moves hotspot to nearest fragment below
  - Shift->Alt->Left Arrow- moves hotspot to nearest fragment left
  - Shift->Alt->Right Arrow- moves hotspot to nearest fragment right
  - Wraps around if there is no fragment

- The join function (Ctrl-j on windows, Cmd-j on Mac) has been enhanced. Now multiple atoms can be joined in a single operation. When multiple atoms are selected, they can be joined with the new atom being placed at the geometric center of the selected atoms and the identity of the atom being set to the selected atom with the highest atomic number.

- The hotkey '0' has been improved when invoked on a secondary carbon. In this circumstance, the spouted bond is made 75% longest to improve the visual affect by making the drawing appear less crowded. This is further described in section *Atom Hotkeys* of the *ChemDraw User Guide*.

- Hotkey behavior has been enhanced to make rotation of objects easier; With one or more objects selected:
  - Alt->Up Arrow- rotates the objects 15 degrees counter-clockwise
  - Alt->Down Arrow- rotates the objects 15 degrees clockwise
  - Alt->Left Arrow- rotates the objects 1 degree counter-clockwise
  - Alt->Right Arrow- rotates the objects 1 degree clockwise

- ChemDraw has been enhanced to make the hotpsot smarter and persist over a number of state changes for the active molecule. The hotspot location is retained when the molecule is selected/deselected, when parts of it are deleted, or when it is copied. For more information, see *Shortcuts and Hotkeys* section of the *ChemDraw User Guide.*

- Improved continuity of hot object state with Enter key / Esc key

- ChemDraw, ChemFinder and Chem3D now use an updated version of molecular weights, taken from https://iupac.qmul.ac.uk/AtWt/

- A new acknowledgement section has been added to ChemDraw for open source or other libraries used in the product.

- The activation window in the ChemOffice installers now shows all the activation options by default instead of the user have to click an expand control to see them. This makes for a better installation experience

- Chem3D now supports GAMESS 2020 R2

2   Release Qualification

2.1   Scope of Testing

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

- **Installations**:
  - o   Default mode
  - o   Custom mode
  - o   Side-by-Side compatibility modes

- **Enhanced Functionality**:
  - o   The Flexera activation system is now used

- **Third-Party Compatibility**:
  - o   *Operating Systems*: Windows 10 (64-bit), Windows 11 (64-bit), macOS Big Sur 11.6 and macOS Monterey 12.1

    Note: *Only ChemDraw is compatible with Mac systems, **not** ChemOffice 21.0.*
  - o   *MS Office*: Office 365, 2019 (Mac & Windows), 2021 (Mac & Windows), where the latest MS Office updates used for testing are 2112 (16.0.14729.20254) on Windows and 16.57 (22011101) 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.*
  - o   *Browsers for ActiveX Controls*: Internet Explorer 11
  - o   *Calculation Engines for Chem3D*: Gaussian 16 Revision-B.01, MOPAC2016, Conflex7.2B, Autodock 4.2.6, MGL Tools 1.5.4 (for Autodock), msroll.exe (Archaic), and GAMESS 2020 R2.

    Note: *Chem3D supports the 64-bit version of GAMESS only.*
  - o   *Python for ChemScript*: 3.2 and 2.5
  - o   *Visual C# for ChemScript*: 2017
  - o   *Visual Studio 2017*

- **Regression Testing**:
  - o   Automated regression testing of many important functionalities in ChemDraw and ChemScript.
  - o   Verification of issue fixes and regression testing of related features.

- **Backward & Forward Compatibility**:
  - o   Limited testing with files created using current and past versions of ChemOffice applications.

- **Japanese Localization**:
  - o   Limited testing on Windows 10 (64-bit), and Monterey.

- **Release Candidate Qualification Testing**:
  - o   Digital signature verifications.
  - o   Sanity/Smoke test executions with all packages in mixed environments.
  - o   Qualification of the download executables.

o   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	Browser	Adobe Version
Client	Windows 10 Professional 64-bit	N/A	2019 (32-bit and 64-bit), Office 365, 2021 (32-bit and 64-bit)	IE11	Acrobat 11
Client	Windows 11 Professional 64-bit	N/A	2019 (32-bit and 64-bit), Office 365, 2021 (32-bit and 64-bit)	IE11	Acrobat 11
Client	macOS Big Sur (11.6) (**ChemDraw only**)	N/A	Office 365	Safari 15.2	Acrobat DC
Client	macOS Monterey (12.1) (**ChemDraw only**)	N/A	Office 365	Safari 15.2	Acrobat DC

3   Installation Instructions

3.1   Prerequisites and System Requirements

For information about system requirements, please refer to the *DT-21.0 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 *cos21.0.exe* (or the extracted *Install.exe*) executable *as Administrato*r.
  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:
  If "**Yes**" is selected, the packages are uninstalled.
  If "**No**" is selected, the packages are left as they are.
- **Windows:** The installation automatically creates a desktop shortcut for ChemDraw 21.0.
- The ChemOffice 21.0 packages can be installed side-by-side with older ChemOffice packages.

4   Known Issues, Limitations and Workarounds

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

- When a molecule has ring colors set, and a part of that molecule is selected where the selection contains ring highlighting, moving the selection will cause the colors to bleed. This does not happen when the whole molecule is selected and moved, and is cleared upon a screen refresh.

- 2D/3D does not generate the correct structure on 1-n allenes, where N is odd and greater than or equal to 3. The attachments at each end of the motif should have a dihedral angle of 90 degrees (instead of the 180 degrees produced).

- 2D/3D may invert stereo for molecules rendered with Fischer projections.

- The Structure Perspective tool can occasionally result in clipping of the rendered structure.

- When bonds that cross are highlighted, the drawing order is undefined and the highlights will appear to be crossed incorrectly.

- Structures containing either (i.e. crossed) bonds when converted to smiles lose their "either" designation when pasted into ChemFinder. They are converted to cis or trans depending on the representation the smiles were generated from.

- RGroup data gets lost when exporting to and re-importing from an RDF file. If a set of substituents are presented in a RGroup table, these molecules will be reimported as a simple list of molecules (i.e. no longer in the RGroup table).

- On Mac, SDF files can only be generated with an extension ".sdf". On windows, SDF files can be saved with the extension ".sdf" or ".sd".

- On multiple monitors:
  - When ChemDraw is dragged to the second monitor, the main toolbar remains on the primary monitor. If that toolbar is then moved, it can disappear. On quit and relaunch, the toolbar reappears on the primary monitor.
  - Add-in always appear on the primary monitor, even if ChemDraw is on the secondary monitor.

- For the ChemDraw 19.1 and future versions on Mac, the default location in which the user stores and accesses the Add-ins, User Monomers, Templates, Samples has been changed from **~/Documents/ChemDraw/** folder to a more secure location **~/Library/Application Support/com.perkinelmer.ChemDraw/.** For the users who have custom files created for any prior version of ChemDraw, those need to be transferred to the new location in order to access using ChemDraw 20.1 and future versions by following the steps from the workarounds listed below.
  - **Workaround 1 - *Upgrading from 18.2 or older versions of ChemDraw:***
    1. Launch and quit ChemDraw 21.0 after successful setup and activation.
    2. Copy all folders and contents from ~/Documents/ChemDraw/ to ~/Library/Application Support/com.perkinelmer.ChemDraw/
    3. Re-launch ChemDraw and make sure that those items are accessible.
  - **Workaround 2A - *Upgrading from ChemDraw 19.0 after deactivating the license:***
    1. Deactivate ChemDraw 19.0 and quit.
    2. Launch and quit ChemDraw 21.0 after successful setup and activation using the same Activation key.
    3. Copy all folders and contents from ~/Documents/ChemDraw/ to ~/Library/Application Support/com.perkinelmer.ChemDraw/
    4. Re-launch ChemDraw and make sure that those items are accessible
  - **Workaround 2B - *Upgrading from ChemDraw 19.0 without deactivating the license:***
    1. If already setup ChemDraw 21.0 without deactivating ChemDraw 19.0, then launch ChemDraw 21.0 and go to **ChemDraw > Preferences.. > Directories tab**.

2. Click the **Reinstall…** button and then the Install button to create the ~/Library/Application Support/com.perkinelmer.ChemDraw/ location and its default contents.

3. Click the **Restore** button to add the new location to the ChemDraw items location search priority list.

4. Go to **Monomer Libraries** tab, click twice on the Location cell for the User library to make it editable and replace the existing path with that of the newly added user-monomers.json file (full path needed)

5. Copy all folders and contents from ~/Documents/ChemDraw/ to ~/Library/Application Support/com.perkinelmer.ChemDraw/

6. Quit and re-launch ChemDraw and make sure that those items are accessible.

- Applying Contract Label option to a fully/partially selected color-filled ring removes the fill color from it.

- There is an issue with copying and pasting ChemDraw structures from Microsoft Excel and PowerPoint applications on Mac to ChemDraw. An image is copied instead of the editable ChemDraw structures. This is due to a change in Microsoft security policy and we are working with them to find an alternate solution.

- You may experience some issues with in-place OLE editing in MS Office applications from version 2016 onwards, such as the image moving out of sight in Word after an inline OLE editing operation.
    o **Workaround:** Switch off in-place OLE editing by unchecking "File->Preferences->General->Use In-Place Editing for OLE Objects Embedded in Other Applications" to force editing of the OLE object in a separate ChemDraw window.

- Cannot embed Chem3D models in MS PowerPoint 2010, 2013, 2016 and 2019.

- Annotations are not displayed correctly when applied to multiple structures. If annotations are added to multiple selected objects, and the document persisted to a file, when the file is re-read the annotation may move from being located on the group to being located a member of that group. It is not lost; just relocated.

- Some property annotations for the components of different reactions were observed as misplaced or lost after exporting as RDFile from ChemDraw.

- Reaction Components with disproportional dimensions, overlaps and failed reaction interpretations were observed after importing RDFiles from some external sources in ChemDraw. This is mainly due to the non-standard coordinate definitions in those files.

- If an NMR spectrum is calculated for a structure and the structure is subsequently edited, the spectrum will not be updated.
    o **Workaround:** Select the modified structure and recalculate the spectrum using Structure->Predict 1H-NMR Shifts.

- If a part of a ring with color is selected and turned into a label, using Structure->Contract Label, the ring color will be lost.
    o **Workaround:** Re-select the ring and fill with color using Color->RingFillColors.

- ChemDraw's look and feel and high DPI displays have been improved in this release, but the windows buttons (minimize, maximize and close) do not scale well on these displays.

- HELM sequences do not display correctly when opening SDF files in ChemDraw for Excel. The full representation of HELM sequences is only supported using CDX or CDXML files, and HELM strings. Other file formats, such as mol or sdf, lack the ability to fully represent the sequences and are not supported as a way to correctly persist HELM sequences.

5 Technical Support

PerkinElmer Informatics Support supports this software. Please contact your Sales or Services representative for more information about ChemOffice v21.0.

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

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