HUMAN HEALTH

ENVIRONMENTAL HEALTH

ChemOffice v18.1

Release Notes

Last Updated: March 25, 2019

PerkinElmer
For the Better

Table of Contents

1 General Description

ChemOffice18.1 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 7 (32-bit and 64-bit), Windows 8.1 (64-bit) and Windows 10 (64-bit) including Creators Update
  - On Windows 10, IE 11 is supported, no support for Microsoft Edge browser.
- Microsoft Office 2019, Microsoft Office 2016 and Microsoft Office 365
- Mac OS X 10.13.6 (High Sierra) and 10.14.3 (Mojave) – (**for ChemDraw only**)
- Adobe Acrobat 11

Highlights to this release:

- The default format of HELM monomer JSON files has been switched from an internal proprietary format to the standard Pistoia Alliance 2.0 format. Monomer JSON files of the older (proprietary) format and the newer (Pistoia) format will be read successfully by ChemDraw. However, only the newer JSON format will be written on export of a monomer JSON file.

- The HELM toolbar has been improved to display the first 6 characters of a monomer name (as opposed to four as in ChemDraw 18.0 and earlier).

- ChemDraw 18.1 now supplies two HELM monomer databases out of the box:

  - A snapshot of the official Pistoia Alliance DB
  - An augmented monomer database from PerkinElmer that adds many extra monomer in all classes

- ChemDraw can now load add-ins from remote sources (i.e. accessed via a URL), as well as local and network sources. Add-ins loaded from remote sources are considered strictly read-only.

- An option has been added to control default representation of aromatic systems upon import. A user can choose to force the representation to alternating single/double bonds, aromatic circles or leave as-is. The representation is enforced regardless of the input method (files, drop-and-drop or smiles).

- Chem3D has been updated to support later version of 3rd party calculation engines. Specifically, Chem3D now supports:

  - Gaussian 16W (2016)
  - Mopac 2016
  - Games 2018 (gamess-64-2018-R1-pgi-mkl.msi)

- It is now possible to specify a proxy URL in the Reaxys interface. A user can override the default "https://www.reaxys.com" URL with a proxy URL when sending queries from ChemDraw to Reaxys.

- A new navigation paradigm has been introduced in ChemDraw to navigate between multiple molecule or reactions in a document. After selecting a structure, pressing "Tab" navigates to the next structure. Pressing "shift-Tab" navigates to the previous structure.

- The screening signatures generated in ChemFinder searches have been improved, necessitating an update in existing ChemFinder databases. If a database generated prior to ChemFinder 18.1 is imported in ChemFinder 18.1, the user will be prompted to upgrade the database. It is strongly recommended this action be permitted.

- The hotkey “F” has been mapped to the label “CF3”, when drawing structures.

2 Distribution Limitations

N/A

3 Release Qualification

3.1 Scope of Testing

For the ChemOffice18.1 release, the following testing conditions have been set and executed:

- **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) including Creators Update, Windows 8.1 (64-bit), Windows 7 (32-bit and 64-bit), Mac OS X 10.13.6 (High Sierra), Mac OS X 10.14.3 (Mojave)

    Note: *Only ChemDraw is compatible with Mac systems,* ***not*** *ChemOffice 18.1.*
  - *MS Office*: Office 365, 2016 (Mac & Windows), 2019 (Mac & Windows), where the latest MS Office updates used for testing are 1901 (11231.20130) on Windows and 16.22 (190211) on Mac.

    Note: *We test with the latest versions of MS Office available at the time, but that is no guarantee of full compatibly with future updates.*
  - *Browsers for ActiveX Controls*: Internet Explorer 11 and 10
  - *Calculation Engines for Chem3D*: Gaussian 09 Revision-D.01, Gaussian 16 Revision-B.01, MOPAC2016, Conflex7.2B, Autodock 4.2.6, MGL Tools 1.5.4 (for Autodock), msroll.exe (Archaic), and GAMESS 2018.

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

- **Regression Testing**:
  - Automated regression testing of many important functionalities in ChemDraw 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), High Sierra and Mojave systems.

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

- Qualification of the download executables.

3.2 Testing Environment

The following table details the testing environments for ChemOffice v18.1:

Machine Type	Operating System	Database Version	MSOffice Version	Browser	Adobe Version	IIS
Client	Windows 10 Professional 64-bit (including Creators Update)	N/A	2016 (32-bit and 64-bit), 2019 (32-bit and 64-bit)), Office 365	IE11	Acrobat 11	N/A
Client	Windows 8.1 Professional 64-bit	N/A	2016 (32-bit and 64-bit), 2019 (32-bit and 64-bit)), Office 365	IE11	Acrobat 11	N/A
Client	Windows 7 Professional 32-bit	N/A	2016, 2019), Office 365	IE10, IE11	Acrobat 11	N/A
Client	Windows 7 Professional 64-bit	N/A	2016 (32-bit and 64-bit), 2019 (32-bit and 64-bit)), Office 365	IE10, IE11	Acrobat 11	N/A
Client	Mac OS X 10.13 (High Sierra) (**ChemDraw only**)	N/A	2016 (16. 21), 2019), Office 365	Safari 12.0.1	Acrobat 11	N/A
Client	Mac OS X 10.14.3 (Mojave) (**ChemDraw only**)	N/A	2016 (16. 21), 2019), Office 365	Safari 12.0.1	Acrobat 11	N/A

4 Installation Instructions

4.1 Prerequisites and System Requirements

For information about system requirements please refer to the *DT-18.1 Hardware Software Guide* (part of this release package).

4.2 Release Installation

Please note the following when installing ChemOffice v18.1:

- **Windows:** For a clean installation, we recommend running the downloaded *cos18.1.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:
  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 18.1.
- The Desktop 18.1 packages can be installed side-by-side with older Desktop packages.

4.3 Manifest

The Desktop v18.1 release includes the following SKUs and components:

- **ChemOffice Suite**
  - *** Installation**
    - Windows\Install.exe
    - Windows\Install.ini
    - Windows\MSCOMCTL.OCX
    - Windows\QProGIF.ocx
    - Windows\RICHTX32.OCX
    - Windows\PerkinElmer\Activation\Activate.exe
    - Windows\PerkinElmer\Activation\activationhelp.html
    - Windows\PerkinElmer\Activation\FlxComm.dll
    - Windows\PerkinElmer\Activation\FlxCore.dll
    - Windows\PerkinElmer\Activation\concrt140.dll
    - Windows\PerkinElmer\Activation\msvcp140.dll
    - Windows\PerkinElmer\Activation\vccorlib140.dll
    - Windows\PerkinElmer\Activation\vcruntime140.dll
    - Windows\PerkinElmer\Activation\FNEactivationhelp.html
    - Windows\PerkinElmer\Activation\registerproduct.html
    - Windows\PerkinElmer\Activation\registerproductemail.html
    - Windows\PerkinElmer\Activation\registerproductfax.html
    - Windows\PerkinElmer\Activation\registerredirect.html
    - Windows\PerkinElmer\ChemOffice\PerkinElmer_ChemOffice_64-bit_Support_18.1.msi
    - Windows\PerkinElmer\ChemOffice\PerkinElmer_ChemOffice_Suite_2018.msi
    - Windows\PerkinElmer\ChemScript\PerkinElmer_ChemScript_18.1.msi
    - Windows\ThirdParty\Microsoft\VCRedist\vcredist_x64.exe
    - Windows\ThirdParty\Microsoft\VCRedist\vcredist_x86.exe
    - Windows\ThirdParty\Microsoft\WinInstaller4.5\Windows6.0-KB942288-v2-x64.msu
    - Windows\ThirdParty\Microsoft\WinInstaller4.5\Windows6.0-KB942288-v2-x86.msu
    - Windows\ThirdParty\Microsoft\WinInstaller4.5\WindowsServer2003-KB942288-v4-x64.exe

- Windows\ThirdParty\Microsoft\WinInstaller4.5\WindowsServer2003-KB942288-v4-x86.exe
- Windows\ThirdParty\Microsoft\WinInstaller4.5\WindowsXP-KB942288-v3-x86.exe
- Windows\ThirdParty\NETInstaller\dotNetFx40_Full_x86_x64.exe
- Windows\ThirdParty\Python\python-3.2.2.msi
- Windows\ThirdParty\PythonExt\pywin32-217.win32-py3.2.exe
- Windows_images\progress.gif

- **ChemDraw Active-X Enterprise Const (admin)**
  - *** Installation**
    - PerkinElmer_ChemDraw_ActiveX_Enterprise_Constant_18.1.msi
    - Install.exe
    - Install.ini
    - MSCOMCTL.OCX
    - QProGIF.ocx
    - RICHTX32.OCX
    - ThirdParty\Microsoft\VCRedist\vcredist_x86.exe
    - ThirdParty\Microsoft\NETInstaller\dotNetFx40_Full_x86_x64.exe
    - _images\progress.gif

- **ChemDraw Active-X Enterprise Const Non Admin**
  - ***Installation**
    - PerkinElmer_ChemDraw_ActiveX_Enterprise_Constant_NA_18.1.msi

5 Known Issues, Limitations and Workarounds

The following list describes the known issues, limitations, and workarounds for ChemOffice18.1:

- ChemDraw allows users to enable and disable add-ins. The enable/disabled state of add-ins is persisted between launches of ChemDraw. However, when ChemDraw is upgraded from 18.0 to 18.1, the enable/disabled state is lost, and all add-ins will appear to be enabled. These add-ins can be disabled, and this state will be persisted by ChemDraw 18.1.

- The legacy biopolymer toolbar has been removed from ChemDraw 18.1. However, all sequences (peptide, DNA/NA and ad-hoc) can be drawn using the newer HELM monomer toolbar. The keyboard shortcut for drawing the 20 standard amino acids and 4 standard DNA/RNA bases have not been preserved. This functionality is far less valuable when the monomer toolbar supports hundreds or thousands of monomers.

- When ChemOffice Suite is installed in a 64-bit system, it installs a 64-bit version of the ChemDraw executable also in addition to the usual x86 version. This 64-bit executable was qualified only to the extent of its full functioning for ChemDraw for Excel features. Hence, it is recommended to use only the default x86 (32-bit) version of ChemDraw for all other functionalities until a full support is declared for the 64-bit version.

- There is no 64-bit version of the Python Extension available to install along with the 64-bit ChemScript / Python. Hence, to continue using the Python Extension feature in ChemFinder even after installing ChemScript 64-bit, re-run the installer package and select to install the 32-bit version of ChemScript, Python and Python Extension. Both the 32-bit & 64-bit versions of ChemScript can co-exist in the same 64-bit system.

- ChemDraw Cloud feature will work only if your Windows system contains Internet Explorer 11 installed. Any system containing a prior version of Internet Explorer needs to be upgraded to version 11 for the use of ChemDraw Cloud feature.

- IUPAC atom numbering scheme after Structure to Name conversion will be displayed only in the expanded regions of the molecule.

- The Paste as HELM feature does not support parsing of the following information in HELM strings:
  - Monomer ambiguity
  - Hydrogen parings for DNA
  - List of polymer groups
  - Extended annotations

- 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 persist HELM sequences.

- Open and Save to ChemDraw Cloud fails on Japanese systems. If a file containing Unicode characters is in a cloud location, ChemDraw will fail to open the file, saying that the file cannot be found.
  - **Workaround:** Use ASCII characters only in file names that are located in the Cloud.

- When files with filenames consisting of 12 or more characters are saved on a system with Japanese locale, an error message ("Invalid UTF-8 text") will be displayed, but the file will be generated and the contents saved successfully. However, ChemDraw will fail to read the file back.
  - **Workaround:** Rename the file to have 11 or fewer characters.

- The Enhanced Retrosynthesis feature may not provide all desired reaction results if:
  - Query product contains stereochemistry undefined stereo-center atoms.
    1. **Workaround**: For optimum results, present such queries with all stereo-center atoms defined using relevant stereo-bond connectivity.
  - Query product contains erroneous atom definition (e.g., valence errors, wrong atom types etc.).
    1. **Workaround**: Make sure to rectify atom errors in the query product before doing enhanced retrosynthesis.

- Enhanced Retrosynthesis results will show only the queried product as the end product of each reaction even if more side products are expected for any reaction.

- Cannot import pre-18 version of ChemScript module in default Python after installing ChemScript 18.1 64-bit.

  The ChemOffice Suite 2018 ships with 32 and 64-bit versions of ChemScript and Python, which in turn requires that a version of ChemScript is used with bitness matching the "default" Python version. The ChemScript Python library will not load if it's bitness does not match that of the default Python from which it was launched.

  This issue can be seen if 32-bit ChemScript is used when the last installed version of Python is 64-bit and vice versa.
  - **Workaround**: Run the bit-correct version of Python IDLE and invoke the ChemScript Python script through it. This can be done by creating a 32-bit Python IDLE shortcut for running 32-bit Python. Windows 10 steps are given below:
    a. Go to the Python installation path "C:\Python32\Lib\idlelib" and locate the file "idle.py".
    b. Right-click on "idle.py" and choose "Send to > Desktop (create shortcut)".
    c. Specify a name for the shortcut (For example, "IDLE (Python GUI) 32-bit").
    d. Right-click on new shortcut in desktop and choose “Properties”.
    e. Set "Target" in Shortcut tab as: *C:\Python32\python.exe C:\Python32\Lib\idlelib\idle.py.*
    f. Set "Start in:" in as: *C:\Python32\.*
    g. Click "Apply" and "OK".

    Double clicking on this shortcut will launch the 32-bit version of Python IDLE and now if you open any other script through the ‘File>Open’ menu, it will be run as a 32-bit version. You can even move this file to "C:\ProgramData\Microsoft\Windows\Start Menu\Programs\Python 3.2" so that it will appear in "All Programs->Python 3.2".

- Unable to Repair/Change the PerkinElmer ChemOffice software on Windows.

  During the installation of ChemOffice Suite 2018, the installation goods are extracted to a temporary directory during installation. During a repair operation the files necessary to apply the repair may become unavailable because they were written to a temporary location.

  - **Workaround:** On running this version of ChemOffice Suite, a dialog titled "Extracting ChemOffice Suite <version>" shows up with the default extraction path displayed in it. Choose one of these options:
    1. Change the Extraction path to a desired location and proceed with the extraction and installation:
       - Repair/Change operations should work fine as long as the installer goods are retained in that location, OR
    2. Copy the default Extraction path displayed there, browse that location and copy the extracted goods to a desired location after once the installation is complete.
       - During a Repair/Change operation the corresponding installer can be located from that location, if prompted to locate and complete it successfully

- It was observed that ChemDraw OLE editing in MS Office 2010/2013/2016 applications failed to work after installing Windows 10 Anniversary update (1607).
  - This was later **fixed** by Microsoft update:
    Cumulative Update for Windows 10 Version 1607 for x64-based Systems (KB4013429) (OS Build 14393.953)

- 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 Office applications from version 2016 onwards, such as the image moving out of sight in Word after an inline OLE editing operation.

  - **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.

- The ChemDraw & Chem3D Plugins are no longer part of any ChemOffice/ChemDraw 18.1 Windows packages (ChemOffice, ChemDraw Professional & Prime). However, users can continue to use any older version of the ChemDraw & Chem3D Plugin along with ChemDraw 18.1 applications. The ChemDraw & Chem3D ActiveX controls are still included and can be used with IE.

- When try to add/edit a structure in a ChemOffice sheet that was created in a system with opposite bit architecture (32 or 64) compared to the current system bit architecture (64 or 32) via 'Edit in Excel' option from Office 365 Online portal, a (1) 'Cannot run Macro …' error or (2) 'Link update' failure may appear by blocking that operation.
  - **Workaround**: (1) Keep your local MS Excel running before selecting the 'Edit in Excel' option from Office 365 online portal.
    or
    (2**)** Choose Edit Links option and remove the existing *.xla link by clicking the Break Link button. Now you will be able to edit the contents in that file and save the changes. This step may need to be repeated in the other system if you want to edit the same document there.

- When a ChemDraw structure is copied from Keynote/Pages/Numbers document and pasted to ChemDraw Document, it loses the structure information.

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

- The contents in a document uploaded to ChemDraw Cloud with a Japanese file name may lose when modify contents in it and save. This issue will not appear if the file name is in English.

- The Search SciFinder feature may not provide accurate results for the following query types:
  - Query bond types 'Any', 'S/A', 'D/A', and 'S/D'
  - Stereo bond types: Dashed, Hashed, Bold, Hollow Wedged, and Wavy
  - Multiple bond types: Quadruple, Dative, Tautomeric (Dashed Double), Aromatic (Double Dashed Double), and Double Either
  - Resonance delocalized ring forms
  - Chemical Symbols Radical, Lone Pair, Radical Cation, and Radical Anion
  - Isotopic labels
  - Multiple Group Bracket Repeat Patters 'Either/Unknown' and 'Head-To-Head'
  - Multiple Group Brackets crossing multiple bonds or no bonds of the query structure
  - Nested bracketed groups
  - Anonymous alternative group labels with more than (1) non-H atoms
  - Generic atom labels for Exact Search

- ChemScript18 may not work properly after installing ChemOffice on a Windows 8.1, 64-bit machine.
  - **Workaround**: Reboot your machine after installing ChemOffice on a Windows 8.1, 64-bit system. ChemScript should operate normally.

- With systems running Windows 8.1 (64-bit) and Visual Studio C# 2010 Express, the demo (Demo.csproj) might crash due to a possible error in VS 2010 Express conversion process.
  - **Workaround**: Manually remove the "Demo.exe.config" file from the "C:\ProgramData\PerkinElmerInformatics\ChemOffice2018\ChemScript\Examples\Demo". This will prevent this issue from recurring on systems with Visual C# 2010 Express.

6 Technical Support

PerkinElmer Informatics Support supports this software. Please contact your Sales or Services representative for further information about ChemOffice v18.1.

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

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