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# ChemDraw and Chemoffice+ Cloud tips and tricks v21

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# CHEMDRAW®

AND CHEMOFFICE+ CLOUD  
TIPS AND TRICKS



2022 Edition



# No, you probably DON'T know how to use ChemDraw.

ChemDraw



INTRODUCTION

“ I have been using ChemDraw® for n years!  
I know how to use it” ( $5 < n < 35$ )... ”

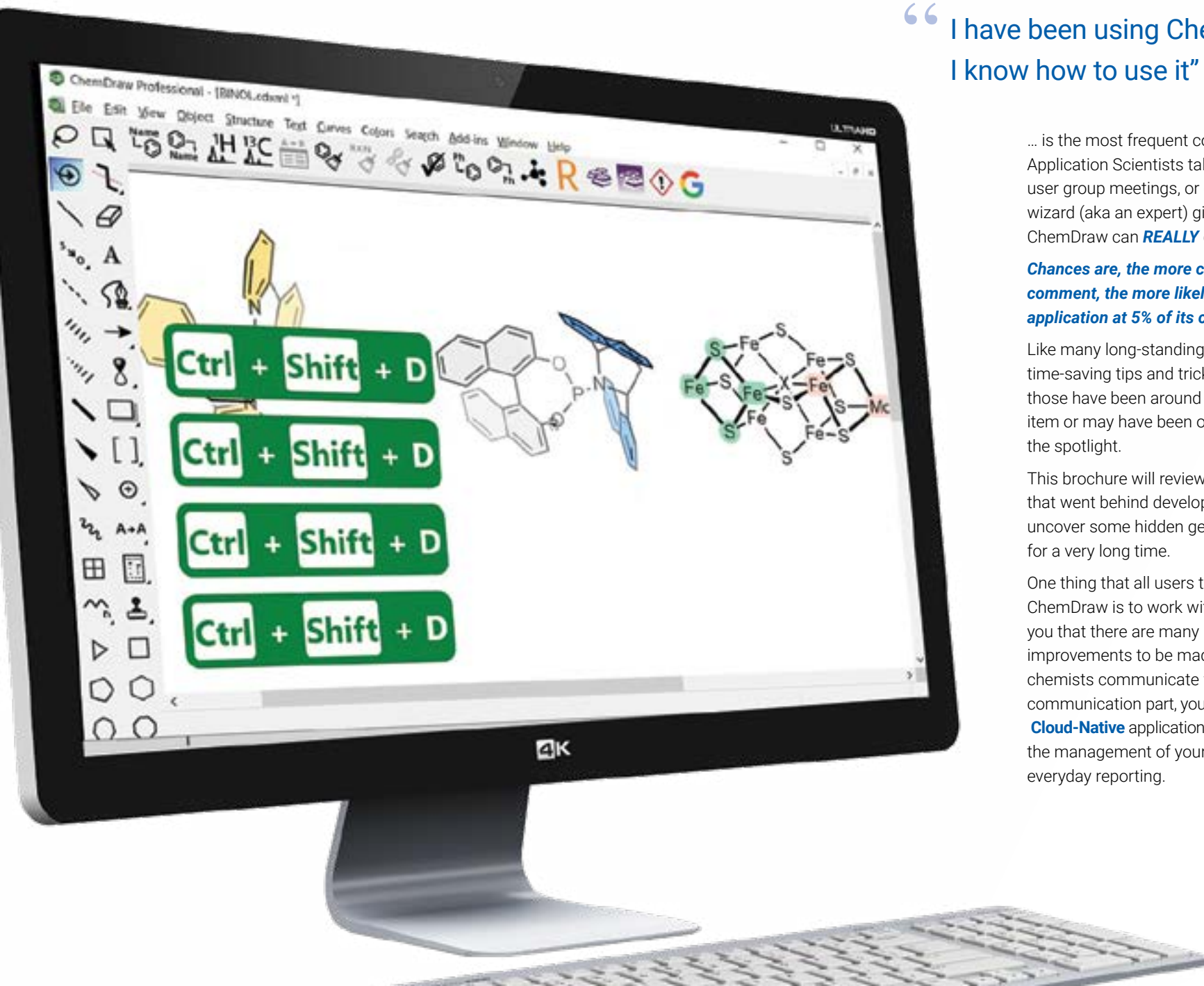
... is the most frequent comment heard when PerkinElmer Application Scientists talk to ChemDraw users at trade shows, user group meetings, or customer site visits. That is **BEFORE** a wizard (aka an expert) gives an actual demonstration of what ChemDraw can **REALLY** do.

***Chances are, the more confident you are at stating that comment, the more likely it is that you are using the application at 5% of its capacities.***

Like many long-standing applications, ChemDraw has a myriad of time-saving tips and tricks you'll benefit from as a chemist. Some of those have been around for a while but have been buried in a menu item or may have been overlooked due to some other feature getting the spotlight.

This brochure will review the latest improvements and the logic that went behind developing them in ChemDraw. It will also uncover some hidden gems that have been part of ChemDraw for a very long time.

One thing that all users tend to appreciate is how easy and intuitive ChemDraw is to work with. Hopefully, this brochure will convince you that there are many new things to learn, that there are still improvements to be made to chemical drawing, and the way chemists communicate with one another. To facilitate the communication part, you'll see how **ChemOffice+**, our new **Cloud-Native** application, can expedite mundane tasks such as the management of your molecules and reactions, as well as everyday reporting.





# DRAWING EFFICIENCY

## Hotkeys. Drawing is (literally) as easy as “1,2,3”

A long-time staple of ChemDraw, **HOTKEYS** – single keyboard key presses over an atom or a bond to elicit an action – have evolved dramatically in the last four years. Before version 17 of ChemDraw (2017), hotkeys were limited to intuitively changing atom and bond types: “**O**” over atoms to turn them into Oxygen, “**2**” over bonds to turn them into double bonds. The decision was then made to push this concept further to change text labels and allow sprouting of functional groups with simple keyboard presses. In other words, “**type**” molecules. After all, so many functional groups in organic chemistry are more than frequently found in small and large molecules (ketones, phenyl groups, amide linkages), so why not create hotkeys to produce those functional groups in one or two keypresses rather than time-consuming back-and-forth mouse movements?

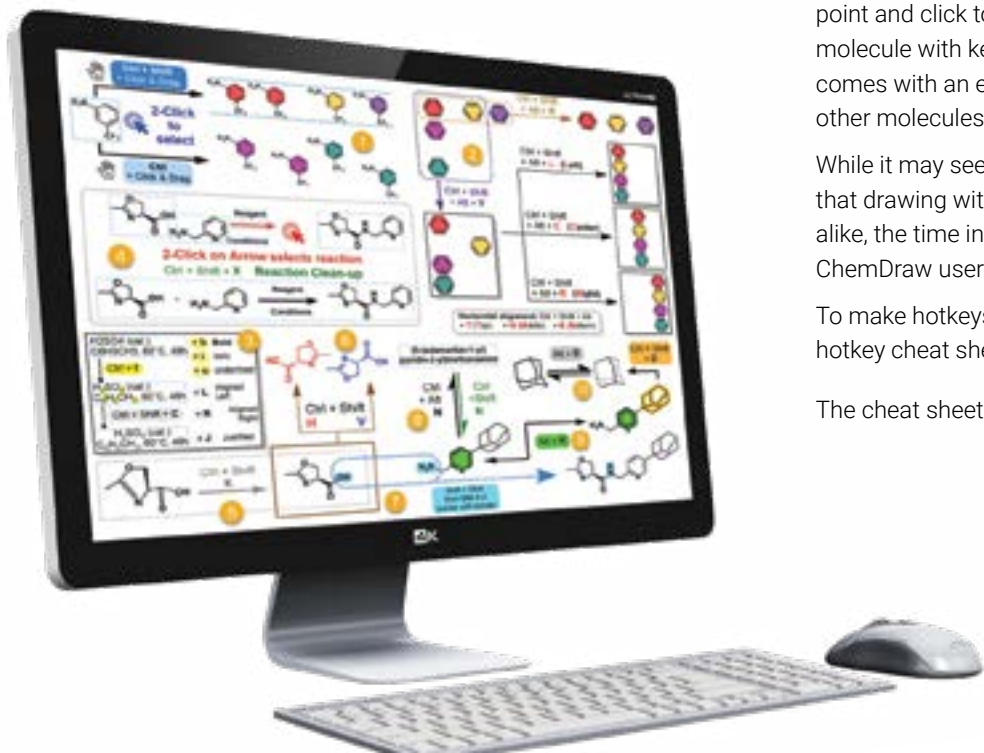
Every new release of ChemDraw sees a new set of hotkeys coming to life, and the latest 21.0 version is no exception. With organometallic complexes in mind, we made it possible to generate a p-bonded Cyclopentadienyl (Cp) ligand with the “**J**” hotkey on atom, while “**Shift + J**” gives a p-bonded phenyl ligand. It’s very convenient to draw, among others, ferrocene derivatives or Ruthenium cymene complexes.

Parallel to those improvements, we introduced another key concept in the drawing capabilities: the **hotspot**, equivalent to the text cursor of any word processing application. Imagine typing an e-mail and having to left-click after each letter you typed to re-introduce the cursor and type the following letter. This is, in essence, how inefficient the chemical drawing process with point and click tools has been. Introducing the hotspot gave our users the ability to move easily and precisely around the molecule with keyboard arrows and dramatically improved the drawing speed. Naturally, the latest 21.0 version of ChemDraw comes with an enhanced behavior for hotspot movement to efficiently move across a molecule (Shift+Arrows) but also onto other molecules (Shift+Alt+Arrows).

While it may seem like a daunting task to try and memorize **hotkeys**, we can safely say (with several years of user feedback) that drawing with hotkeys requires a day or two to get acclimated. According to newcomers and veteran users of ChemDraw alike, the time investment is more than worth it, as all saw their productivity with the application soar. Our most seasoned ChemDraw users often ask, “Where was THAT when I was a student?”.

To make hotkeys easier to discover, launching ChemDraw 20 for the first time will automatically display a comprehensive hotkey cheat sheet. Conveniently sized, the document can be printed and hung next to the computer for easier learning.

The cheat sheet can be found at any time in the **Help Menu** under **shortcuts and hotkeys**.

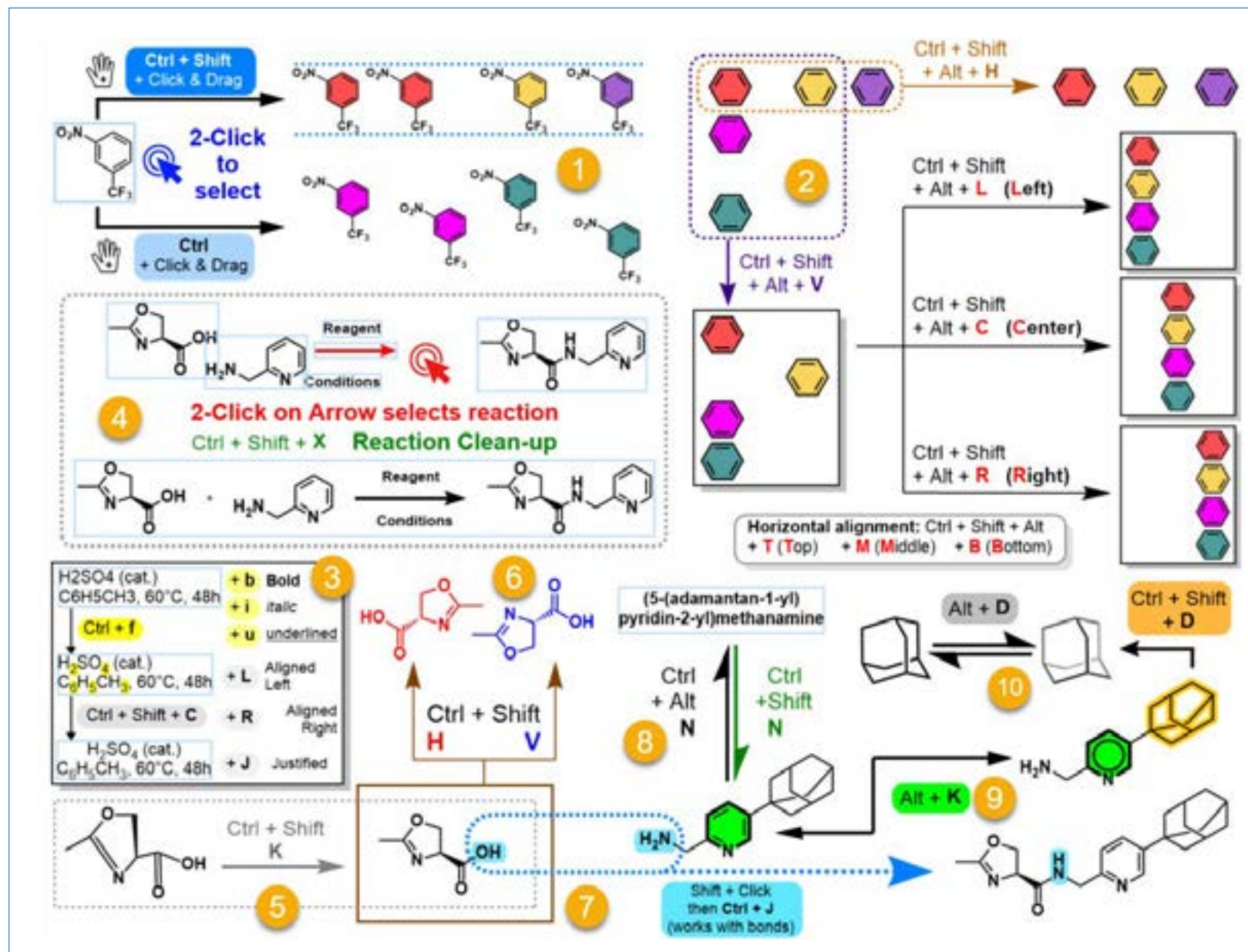


# DRAWING EFFICIENCY

The cheat sheet can be found at any time in the Help Menu under shortcuts and hotkeys.

The "Magic Hotkeys Cheat sheet" that appears upon first launch of ChemDraw 21.

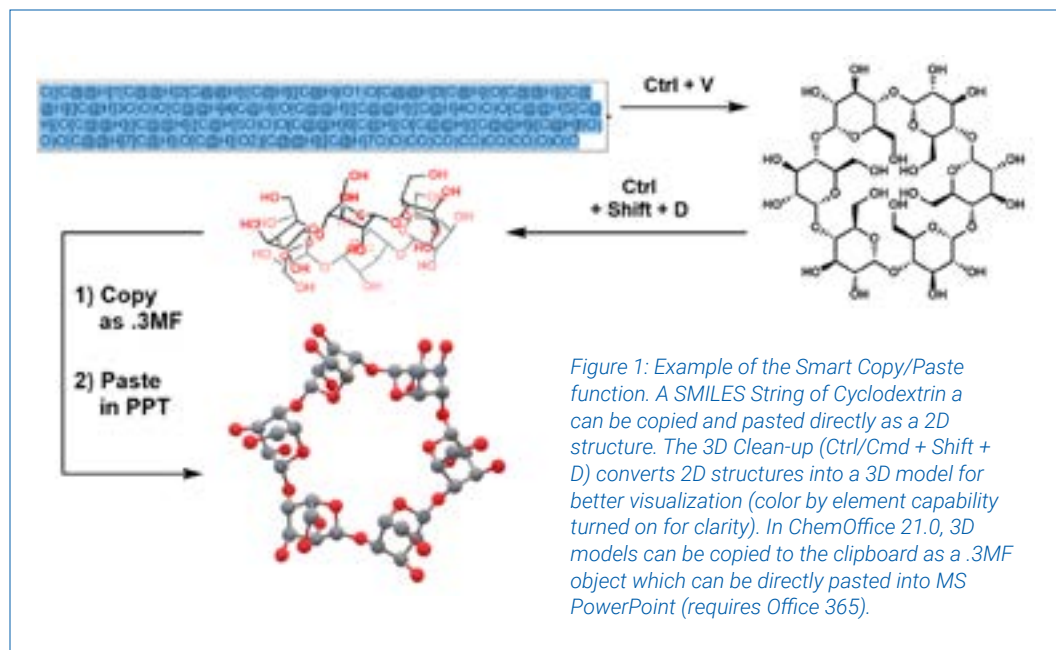
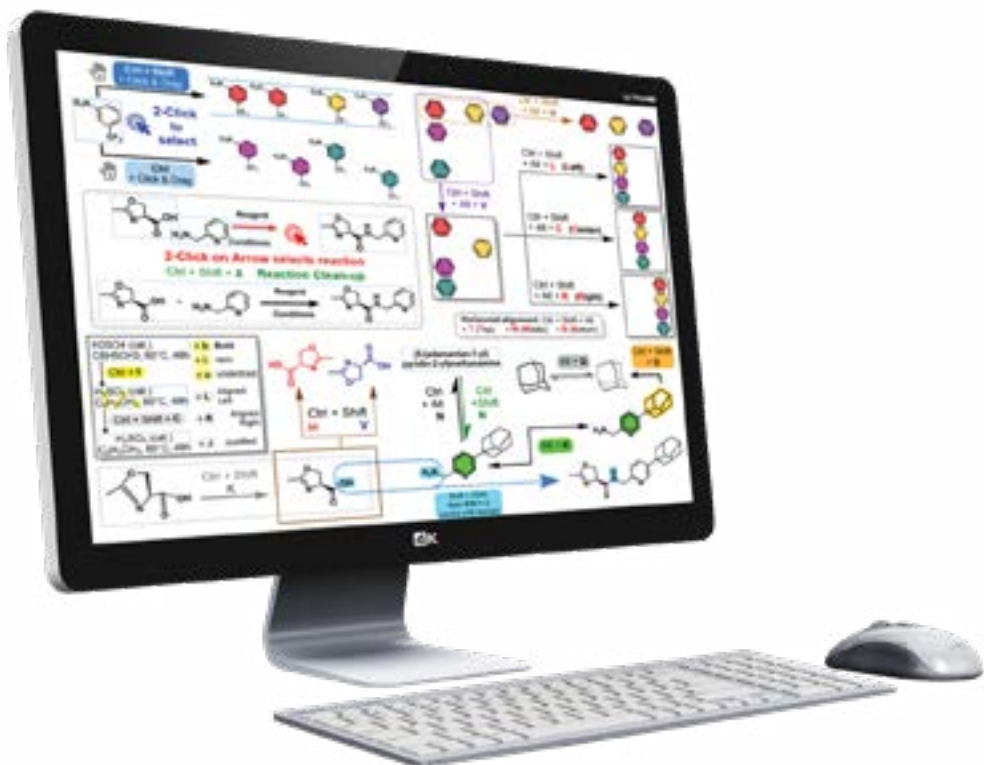
- 1 Atom hotkeys sprouting groups on primary carbons
- 2 Atom hotkeys sprouting groups on secondary carbons
- 3 Atom Label hotkeys
- 4 Reaction and rotation shortcuts
- 5 The Enter and Spacebar hotkeys to respectively insert the hotspot and select the current molecule
- 6 Bond hotkeys that change the nature of the bond.
- 7 Bond hotkeys that change bond order or fuse rings
- 8 Examples of hotkey sequences to build a molecule given a starting hotspot location
- 9 ?



# DRAWING EFFICIENCY

## Shortcuts

Shortcuts, another staple of ChemDraw, have also seen their fair share of enhancements since 2017. Shortcuts are technically different from hotkeys in that they involve combining one or more modifier keys (**Ctrl/Cmd, Shift, or Alt**) and a keyboard key. Long-standing shortcuts like the Structure Clean-up (**Ctrl/Cmd + Shift + K**) or Name-to-Structure function (**Ctrl/Cmd + Shift + N**) are almost universally known to regular ChemDraw users. Introduced with ChemDraw 17, the Reaction shortcut (**Ctrl/Cmd + keyboard arrows**) lets you quickly create reactions by selecting one or more molecules and quickly clone them on the other side of an arrow, where they can be joined together (**Ctrl + J**), now with its own icon in version 21.0). The rotation shortcut (**Alt + keyboard arrows**) is another recent introduction that allows you to rotate molecule(s), or part of a molecule by 1° or 15° increments. Back by popular demand, the "Move by 10 px" action is back with "Shift+Arrows" when a molecule is selected.



When it comes to copy/pasting, shortcuts in ChemDraw have become "smarter" over the years to facilitate the drawing process. SMILES strings are one such example: you can now copy a SMILES string to the clipboard (from Wikipedia, ChemSpider, vendors' websites) and paste (**Ctrl / Cmd + V**) onto the canvas to paste directly as a chemical structure (figure 1). Beyond small molecules, it is also possible to paste an **N -> C** peptide sequence in one-letter code through the **Edit > Paste Special > FASTA Peptide** (capital letters for natural configuration, lower case for unnatural configuration). Peptides and nucleic acids can then be easily expanded by pressing the **"Expand Label"** button in the Structure toolbar.

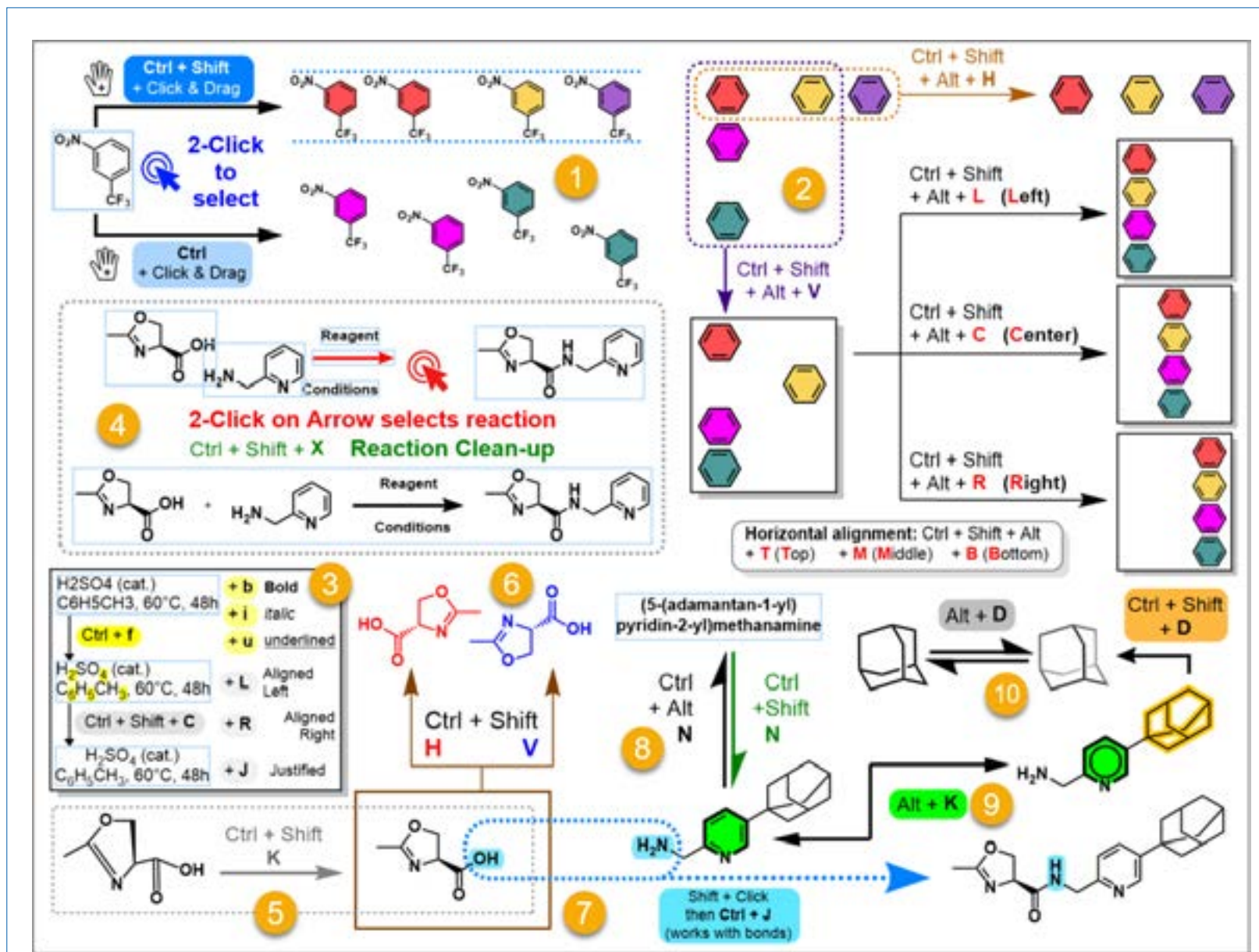


# DRAWING EFFICIENCY

## Shortcuts

A comprehensive list of 30 commonly used shortcuts in ChemDraw.

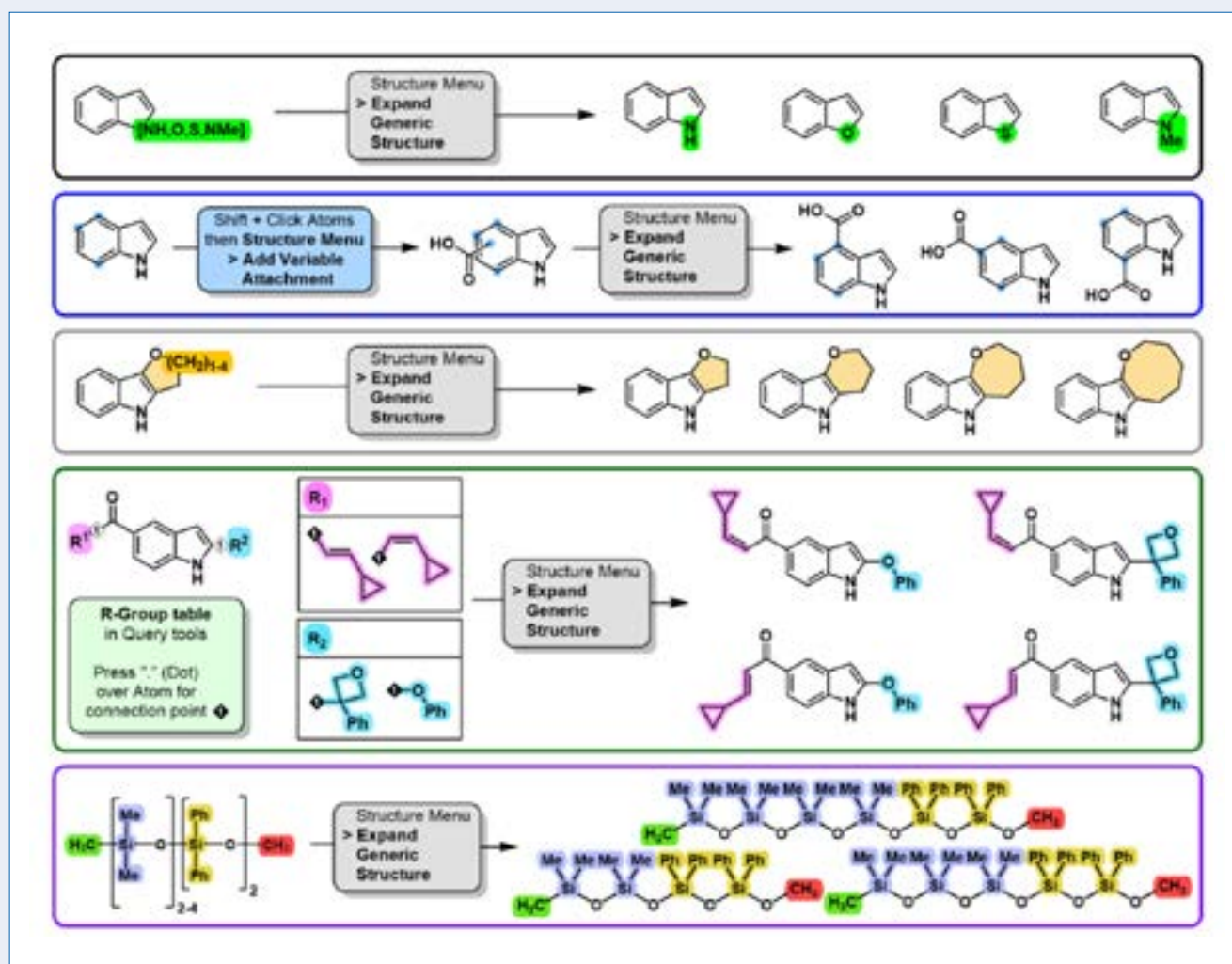
- 1 Selection and cloning shortcuts
- 2 Object alignment and distribution shortcuts
- 3 Atom Label hotkeys
- 4 Reaction selection and clean-up shortcuts
- 5 Structure clean-up shortcut
- 6 180° rotation shortcut
- 7 Joining shortcut
- 8 Name-to-Structure / Structure-to-Name shortcuts
- 9 Kekulize / De-kekulize aromatics shortcuts
- 10 3D Clean-up shortcut (works on sub-selection) and Structure Perspective shortcut (toggles depth shading)



# DRAWING EFFICIENCY

## Hidden Gems: Generic Structures for Library Enumeration

Lastly, when it comes to smarter ways of drawing it's important to mention generic structures (sometimes broadly referred to as "Markush structures"). Generic structures are condensed representations of multiple molecules, typically used as a chemical search query, that can also be enumerated to generate all possible combinations.



### Five types of generic structures exist in ChemDraw.

1. Atom lists (highlighted in green)
2. Variable attachments (blue dots)
3. Label range (highlighted in orange)
4. R-group tables (highlighted in pink and light blue)
5. Parameterizable Brackets (highlighted in grey blue and gold)

When drawn, the structure can be selected and expanded by going to the **Structure Menu > Expand Generic Structure**. Generic structures can be combined to generate up to 200 molecules in ChemDraw. Above 200 structures the molecules can be enumerated directly to a SDF File, which can then be used in other applications more suited to work with large batches of molecules, like the new Cloud-Native application ChemOffice+.



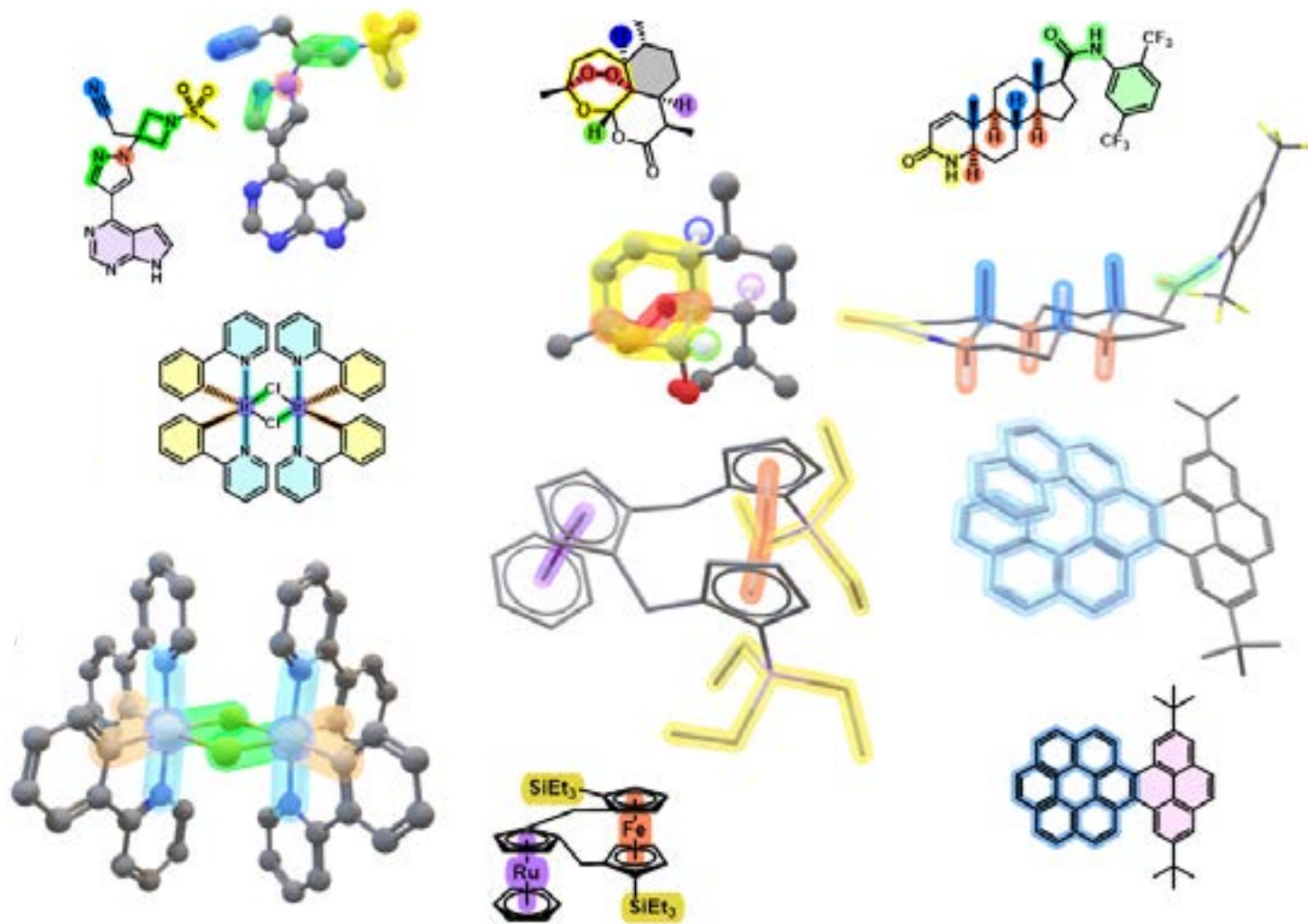
# VISUAL COMMUNICATION

*Chemistry to be proud of.*

Making small (and large) molecules look their best .



VISUAL COMMUNICATION



# VISUAL COMMUNICATION - 3D

## Color 3D and Color Provoke reactions (and facilitate perception)

For a long time, organic chemistry has been represented in black and white. However, as visual animals, we Humans tend to understand things more clearly when color is involved. Until recently, users could only color atom types by element or change the color of atoms and bonds in ChemDraw. In practice, this worked reasonably well with red and dark blue bonds but started becoming less and less useful when a third color was needed, especially when projecting on a low-quality beamer in a room with no blinds. To tackle that problem, we introduced the ring fill coloring for carbocycles in ChemDraw 19 to facilitate visualization and communication.

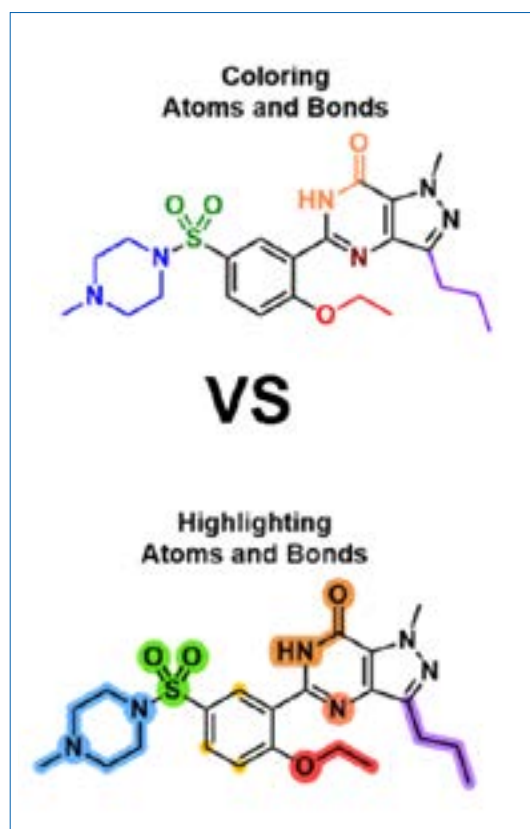


Figure 2: Differences of visibility between functional groups or atoms and bonds simply colored or highlighted with identical colors.

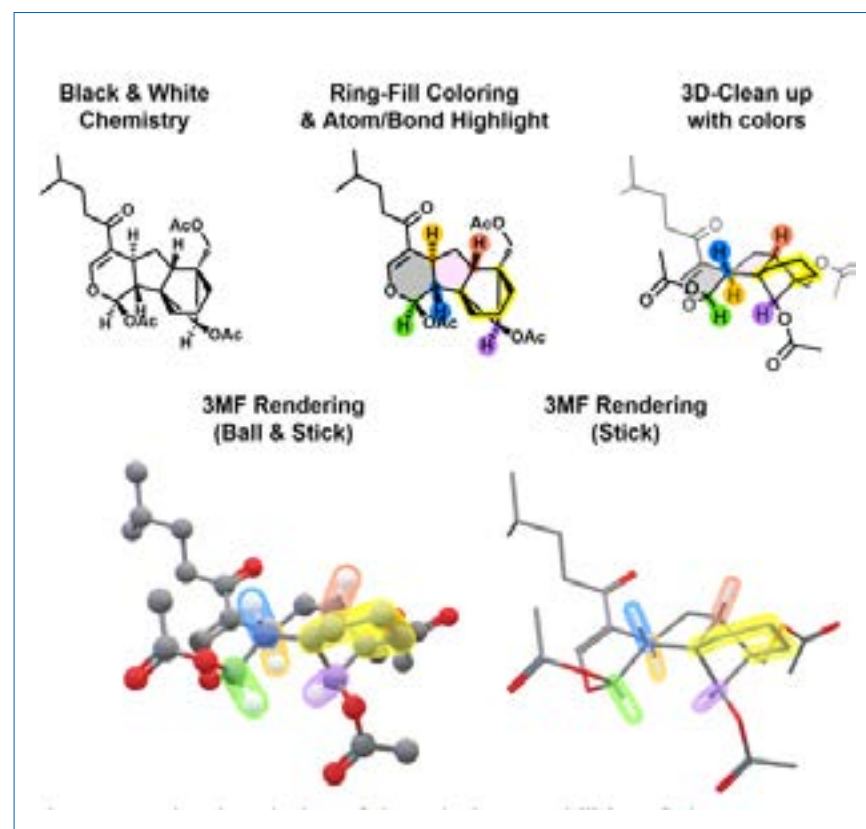


Figure 3: Generating platonic solids in ChemDraw is now easier than ever. Follow the instructions and use the "Join" shortcut (Ctrl+J) on atoms or bonds with the same color highlight and press the new "3D Clean-up" shortcut (Ctrl+Shift+D).

### The 3D Clean-up (Ctrl/Cmd + Shift + D)

With ChemDraw 20, we added the complementary capability to highlight bonds and atoms with color. In addition, a critically acclaimed new feature and its corresponding shortcut were introduced: the **3D Clean-up (Ctrl/Cmd + Shift + D)**, which produces an energy-minimized conformation of a molecule with Z axis-based color shading (Figure 3).

This way, when presenting to your peers at a conference or to your colleagues during your weekly lab meeting, you can say "the double bond in green" or "the amide bond in yellow" with the confidence that your audience will know what you are talking about (Figure 2). Importantly the color-filled rings also fade when used with the 3D clean-up feature, further facilitating the perception of 3D in drawings of complex molecules.

# VISUAL COMMUNICATION

## Wait, you've been saying 3D a lot. Can you do 3D within ChemDraw?

The 3D Clean-up algorithm introduced with version 20.0 of ChemDraw Professional has been improved with version 21.0. It was enhanced to handle metal complexes better while supporting aromatic circles in 3D (Figure 9), and render in-perspective double bonds in a better way, i.e., double bonds viewed “from the side” in 3D do not stick out of the plane anymore (Figure 10). While improving this important capability, we recognized its limitation in the context of the communication of Chemistry: a rotatable 3D model may be useful to the chemist viewing it in ChemDraw but displaying and sharing it outside of ChemDraw in an audience-facing presentation required (until now) a lot of extra steps. Serendipitously, we observed that native, interactive, and animatable 3D objects – including molecules – were available in Microsoft PowerPoint and learned about the .3MF format ourselves, an open-source 3D-printing format co-developed by major companies involved in 3D printing, including Microsoft. With that use case in mind, we first implemented a “Save as 3MF” option to save 3D molecules for 3D.

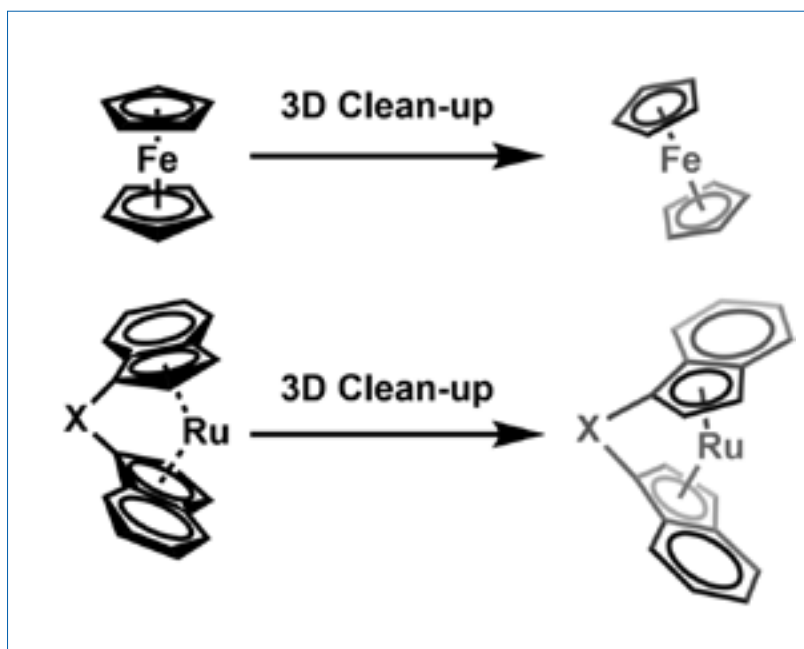


Figure 4: Two examples of 3D-rendered metallocenes in version 21.0 of ChemDraw Professional, using their 2D representation from the ChemDraw metallocene templates and the 3D Clean-up algorithm. Aromatic circles and multi-center attachments points are properly rendered in 3D.

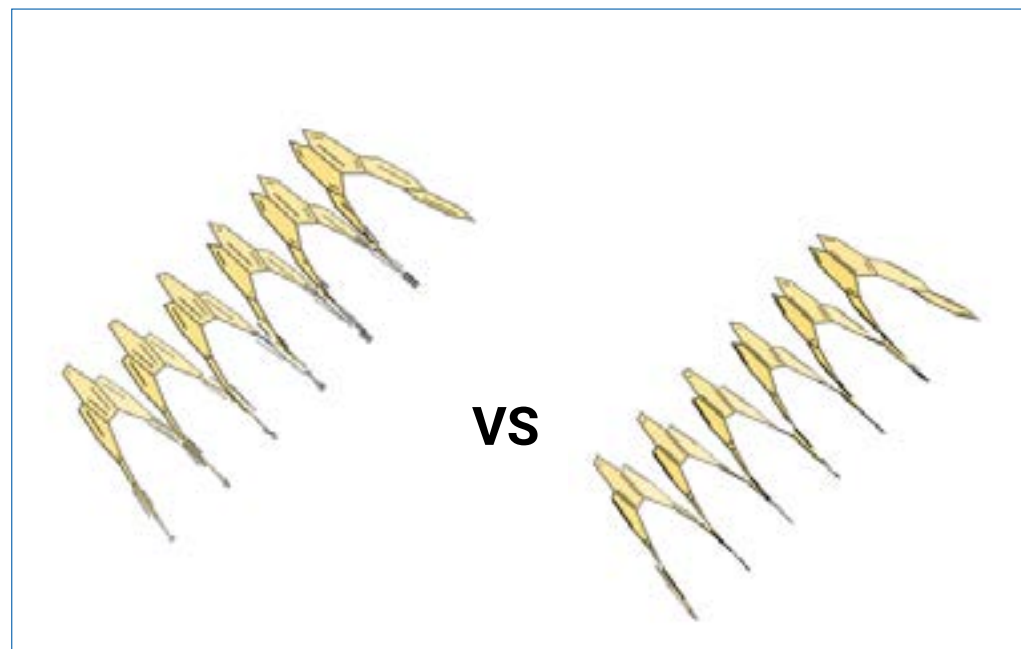


Figure 5: An example of improved rendering of double bonds in 3D in ChemDraw, shown with a 3D Cleaned-up helicene molecule in version 20.0 (left) and in version 21.0 (right). Double bonds do not stick out of the plane anymore when looking “from the side”.



# VISUAL COMMUNICATION

## Color Highlights In 3D Representation

As we were developing the feature and testing it with complex molecules like natural products, we felt that we needed to address a fundamental problem when presenting 2D and 3D chemistry: the difficulty to establish a visual correspondence between the skeletal representation and the 3D representation of molecules, in other words, correlate wedges, hashed wedges and overly elongated crossing bonds with a 3D shape can be intellectually challenging. While testing and developing the new 3MF export feature, we thought this would be the perfect use case to show the power of the color highlighting capability introduced in version 20. Therefore, we investigated how to easily transfer color highlights from the 2D representation of the molecule to the 3D model so that when presenting to an audience, a chemist could easily convey the right message or easily focus attention on the relevant parts of the molecule.

Thanks to open-source code (Available in [GitHub: QuickHull by Akuukka](#)), we were able to generate 3D color “transparent tubes” from the 2D highlights and add them around the bonds on the 3MF models (Figure 11). We were quite excited to be releasing such a neat feature to our users, and it’s no wonder the full 3MF / Color highlights capability has been getting [rave reviews on Social Media](#).

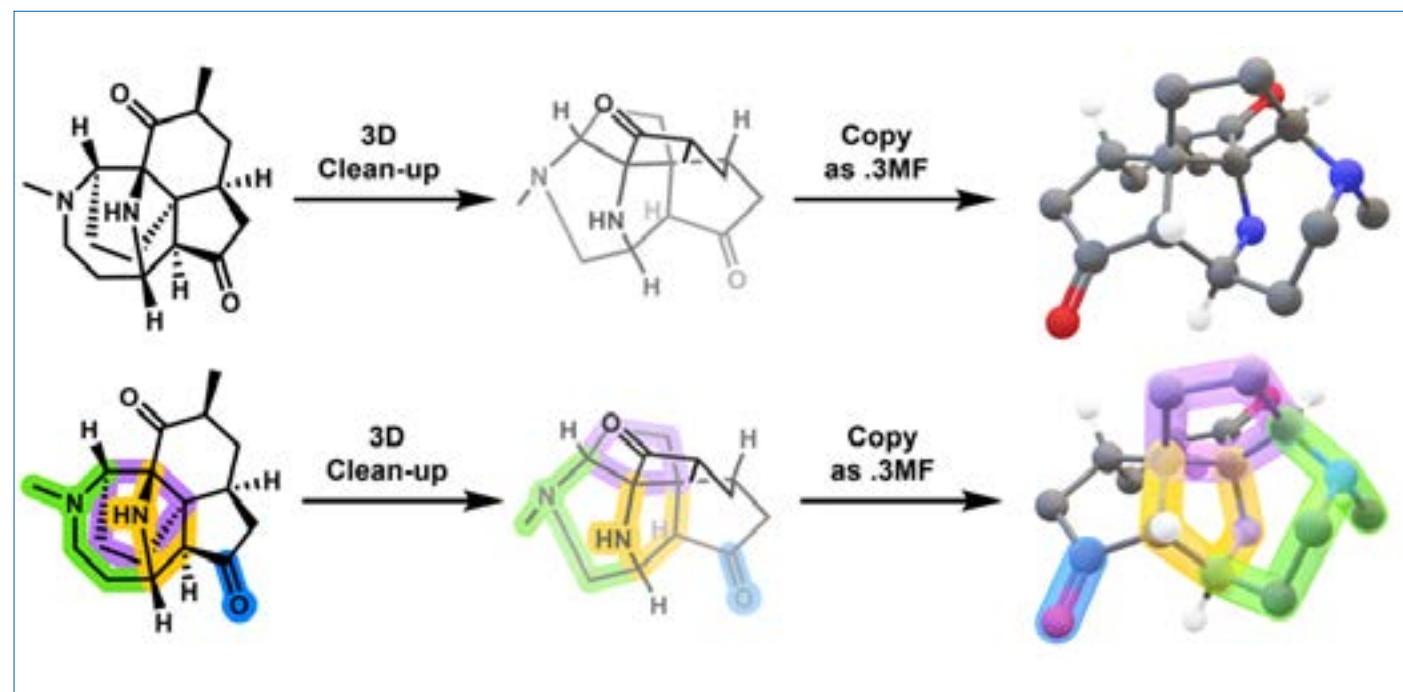


Figure 6: Which ring is which? Top row: the successive transformation of a colorless 2D molecule of Phlegmadine C into a 3D model exported to 3MF. Bottom row: the same molecule of Phlegmadine C with color highlights transferred all the way to the 3MF model to greatly facilitate the perception of 3D.



VISUAL COMMUNICATION

# INTEGRATIONS WITH KEY RESEARCH APPLICATIONS

## SciFinder<sup>n</sup> and Reaxys

As a chemist, you don't just start making something out of the blue. You search the literature and prior art to understand if the compound/material you are trying to prepare hasn't been created already, and if so, how that was accomplished (also, what was the yield?). Back in 2014, and upon request from many chemists, the first integration between ChemDraw 14 and CAS' **SciFinder**<sup>®</sup> was introduced and perceived as a significant improvement, greatly benefitting users from both applications. The slogan was "The Choice for Chemistry Research meets the Choice for Chemistry Drawing." The Choices were clear. Since 2014 more and more integrations have been introduced to help remove existing barriers between ChemDraw and key research applications to increase researchers' productivity and the speed of their research. In 2018, the integration between ChemDraw and **Reaxys**<sup>®</sup> was introduced, followed by ChemDraw and SciFinder<sup>n</sup> in 2019 (Figure 7).

Those add-ins conveniently allow users of ChemDraw to select a molecule or a reaction from a chemical drawing and perform a search of the existing literature.



INTEGRATIONS WITH KEY  
RESEARCH APPLICATIONS

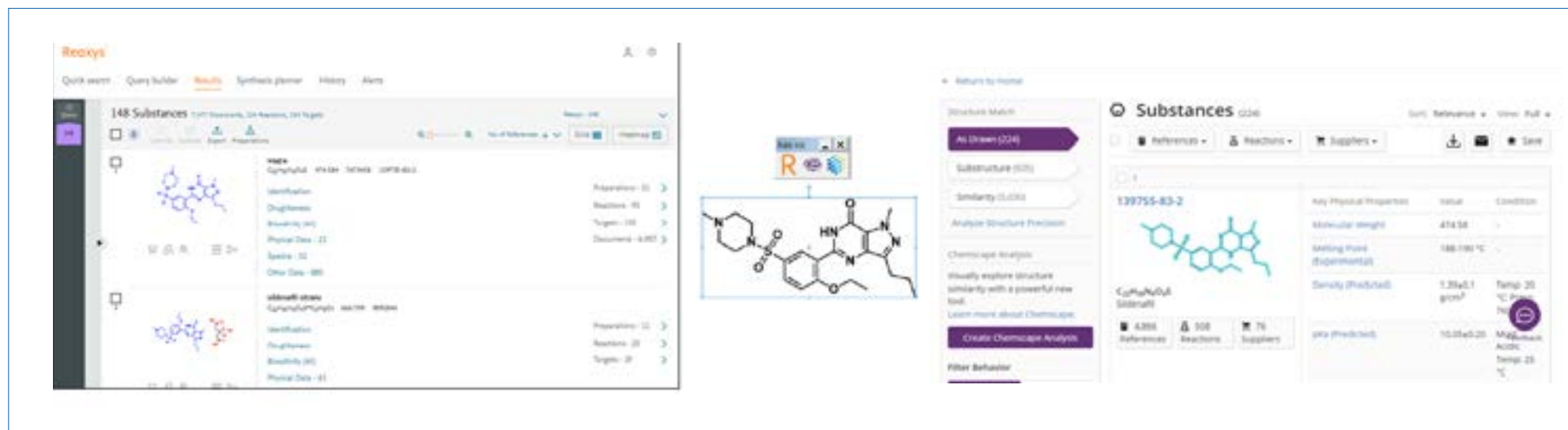


Figure 7: Illustration of the search results for a molecule of sildenafil into the Reaxys (Left) and SciFinder-n (Right) databases.

# INTEGRATIONS WITH KEY RESEARCH APPLICATIONS

## PubChem Safety, Google Scholar/Patents and Customization

Realizing the importance of those integrations, we also refactored the underlying architecture of ChemDraw to enable developers to create custom add-ins with third party applications using JavaScript and (<https://github.com/PerkinElmer/ChemDraw-AddIns/tree/master/Documentation>). We then started adding new integrations with every new version of ChemOffice, formerly known as ChemOffice Professional (Figure 8).

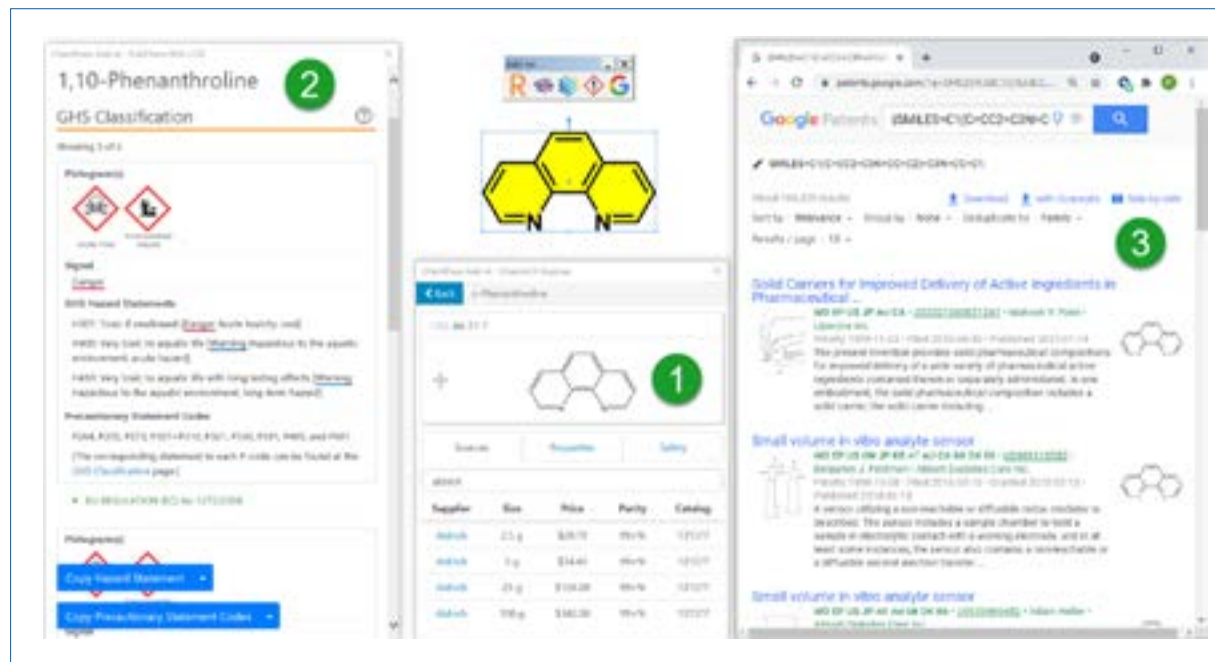
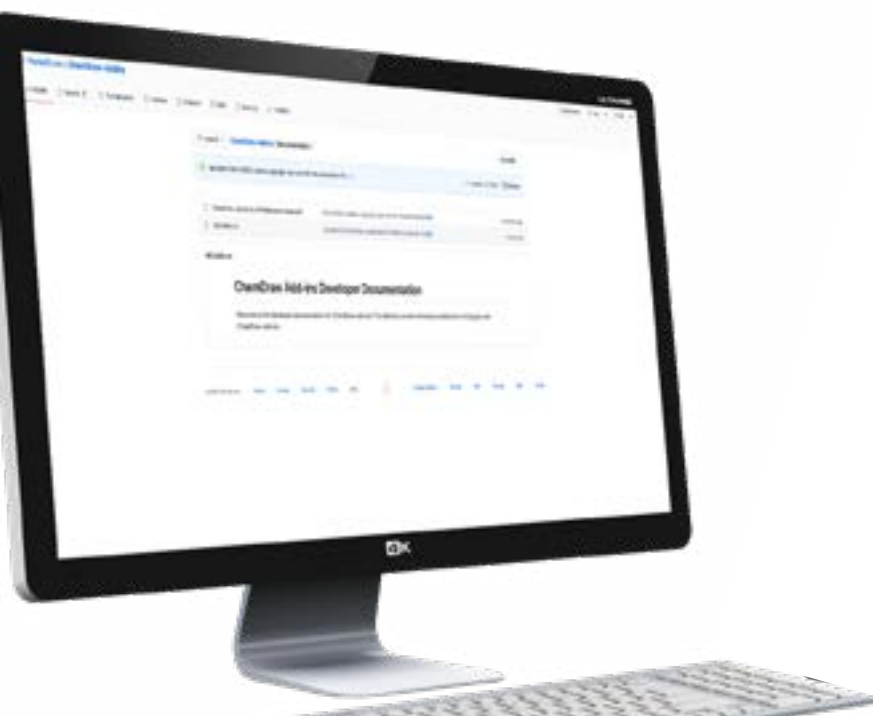


Figure 8: The various Out-Of-The-Box add-ins available within ChemDraw when licensed with ChemOffice+ Cloud, using ortho-phenanthroline as an example:

- 1 The ChemACX Explorer allows users to look up molecules by structure, name, or CAS Number in PerkinElmer's database of >20M commercially available substances and find pricing and commercial availability.
- 2 The PubChem Laboratory Chemical Safety Summary (Fig8: 2) enables chemists to view GHS pictograms and Hazard Statements and Precautionary Statement Codes associated with a given molecule.
- 3 The Google Scholar/Patents add-in, allowing users to draw molecules from the comfort of ChemDraw and look up research articles or patents where the structure can be found.



INTEGRATIONS WITH KEY RESEARCH APPLICATIONS



# ChemOffice

*Turning Chemical Drawings  
Into Chemical Knowledge*



CHEMOFFICE+ CLOUD

# CHEMOFFICE+ CLOUD - SEARCH

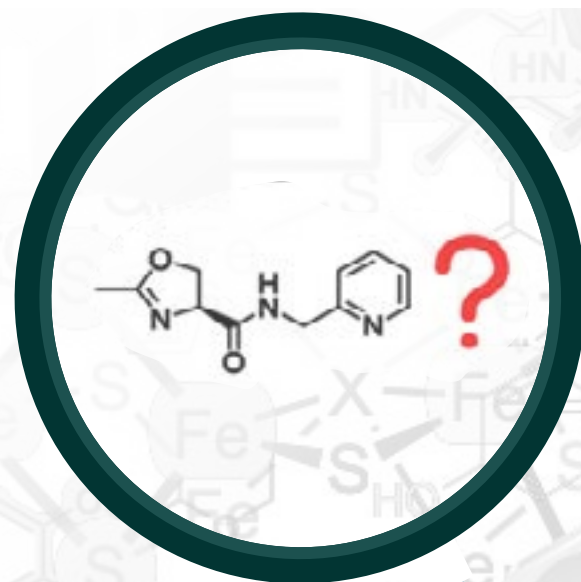
## *A chemist's Life: the literal search for molecules.*

A chemical drawing is just the beginning of an idea.

This idea needs to grow, evolve, and communicate and share to a broader audience or readership. In this context, ChemDraw is a place of birth for drawings but, more often than not, not the place where those drawings retire. As part of what may be called the standard digital communication workflow, drawings get pasted in MS PowerPoint for presentations, in MS Word for reports and publications, or in MS Excel to manage and share lists of molecules or reactions. Sadly, MS Office documents often represent the end of the line for the drawing, as an overwhelming majority of ChemDraw users store their ChemDraw drawings as embedded objects inside MS Office documents that slowly get forgotten over time.

There is a wealth of chemical information buried inside MS Office documents that is very difficult to excavate unless you have an excellent memory or the patience to open and scroll through entire documents to find out which page the structures/reactions were pasted in. Often, chemists end up re-creating schemes they have already drawn because they cannot find them anymore. That is until **ChemOffice+** came along.

ChemOffice+ is a **Cloud-Native** application purpose-built to circumvent this horribly inefficient process by allowing chemists to quickly view and re-purpose chemical drawings without opening the Office document itself. They can then be pasted in ChemDraw to be modified. And that is only ONE of the many things it can accomplish.



CHEMOFFICE+ CLOUD

# CHEMOFFICE+ CLOUD

## *It's Friday evening, do you know where your molecules are?*

Wouldn't it be nice if you could search for molecules in your documents? Now you can. By uploading documents to the Cloud, you can use the lightning-fast ChemSearch capability, which indexes chemical drawing content, including content embedded inside MS Office documents.

This means that you can now search for documents based on their created and edited dates (Figure 9: 1) and based on a specific exact or substructure (Figure 9: 2). With the document filter (Figure 9: 3), you can look for particular molecules embedded in a given type of document (MS Word, MS Powerpoint, MS Excel, and Signals Notebook Experiment).

Documents, where the substructure can be found, are displayed within the middle column (Fig 9: 4), and their content can then be viewed in the rightmost column (Fig 9: 6). A **"Hide Duplicate"** filter reduces the number of items displayed in this column if multiple occurrences of the same molecule happen within a document.

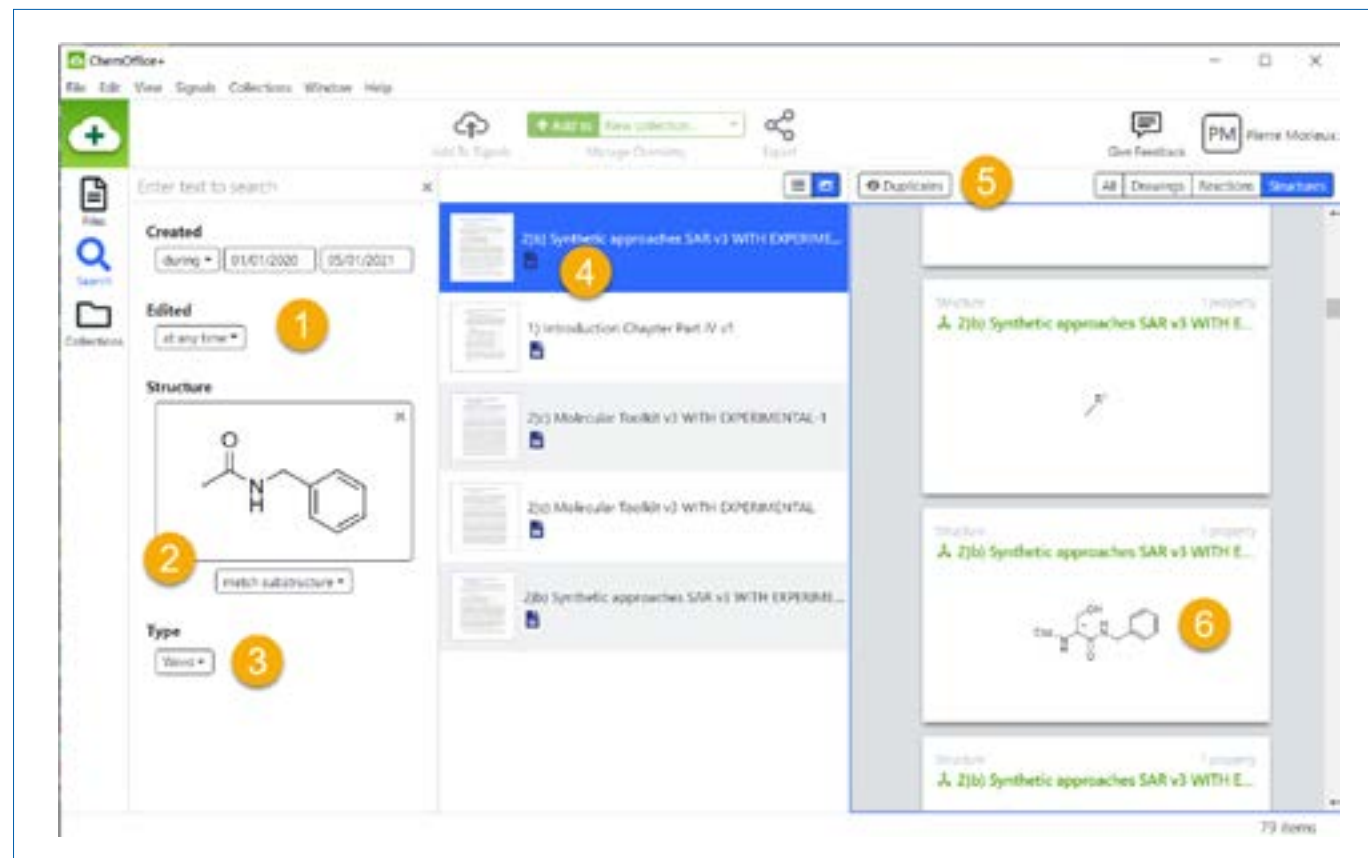


Figure 9: The Search View of ChemOffice+.





# CHEMOFFICE+ CLOUD

## Green Chemistry: easily recycle your drawings.

The first time-consuming workflow tackled by ChemOffice+ allows chemists to quickly re-use and re-purpose chemical drawings stored on a computer. A **File Explorer** is available on the left (Figure 10: 1), where one or multiple documents can be selected to have their chemical drawing content displayed on the right-hand side. Mousing over a drawing shows a blown-up view of the drawing (Figure 10: 2). Multiple items can be selected through the tickbox (Figure 10: 3).

Once items are selected, they can be copied to the clipboard (**Ctrl/Cmd+C**) to be pasted into ChemDraw to be re-used or modified. Drawings can be drilled into (Figure 10: 4) to view individual reaction components or individual structures and interact with them to re-use them.

Filters at the top (Figure 10: 5) enable the view of only the chemical drawings, the reactions, the individual structures comprising those reactions, or all those items at the same time. Lastly, they can be sent to a collection (Figure 10: 6).

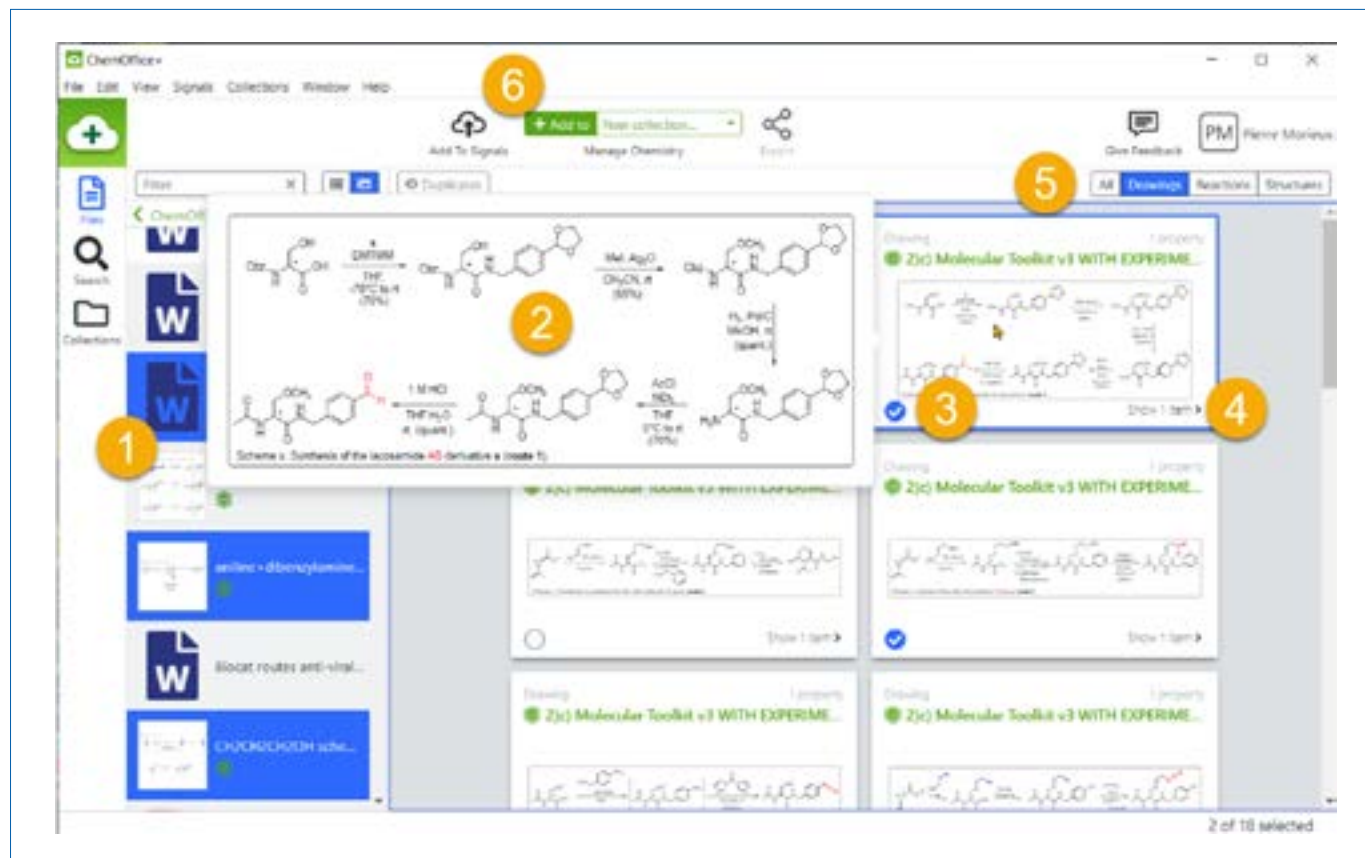


Figure 10: The File Explorer view of ChemOffice+.



# CHEMOFFICE+ CLOUD

## Collections: Easily manage and share your chemistry.

Collections are a new way to manage lists of compounds and molecules with their associated properties in ChemOffice+. Collections are designed for chemists to **“apply actions to batches of molecules.”**

When selected (Fig 11: 1), the collection's content is displayed on the right. Hovering over a molecule preview (Fig 11: 2) will blow up the corresponding structure. Resizing the Preview column will enlarge the structures.

When creating a collection from an SD File, existing properties will be inserted as columns, which can be filtered. Custom properties can also be inserted. All or a sub-selection of entries can then be structurally modified (Fig 11), added to another collection (Fig 11: 4), exported to SD File, or Powerpoint (Fig 11: 5).

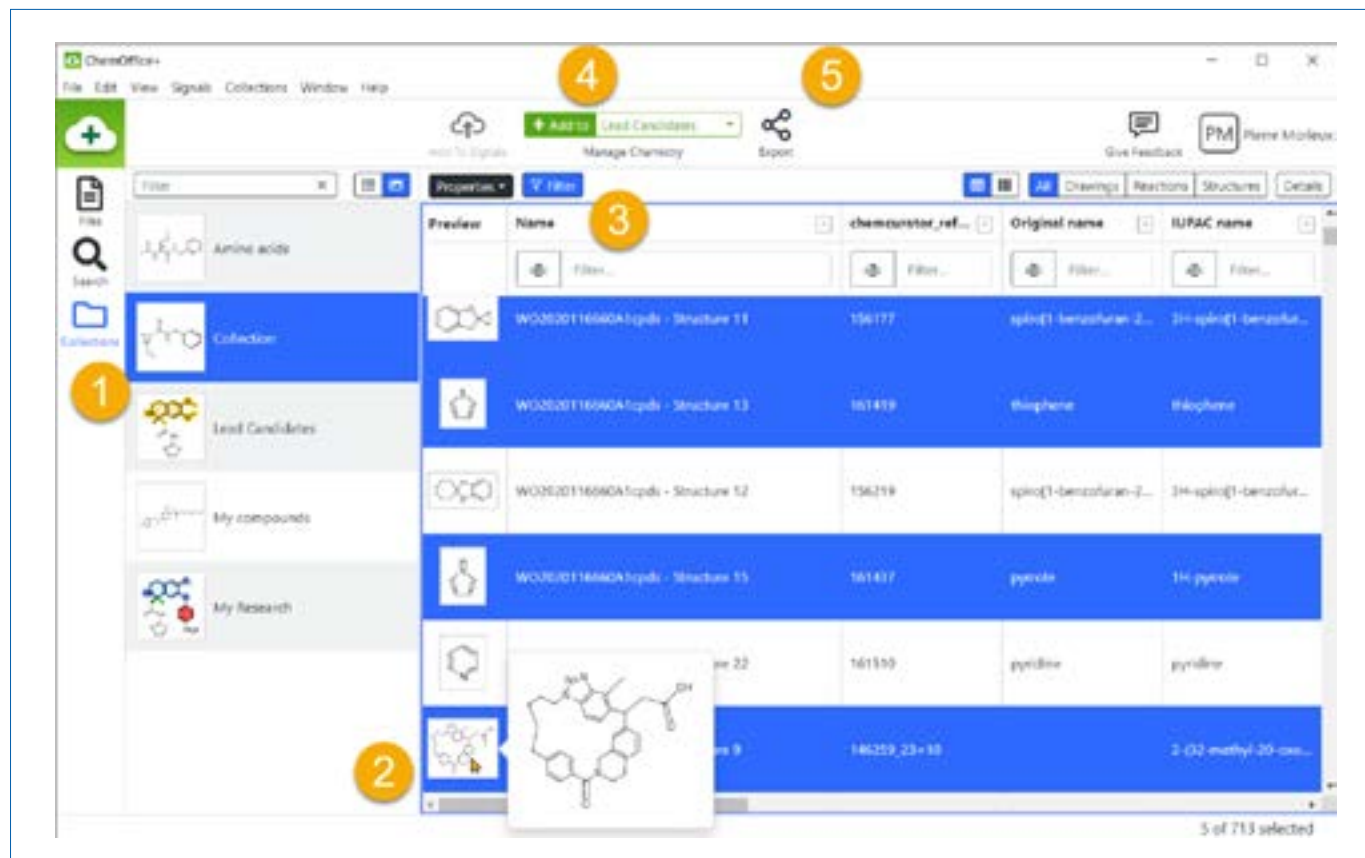


Figure 11: The Collection View of ChemOffice+.



# CHEMOFFICE+ CLOUD

## Manage Multiple Objects Simultaneously

The ability to handle and manage multiple objects at the same time is a central aspect of ChemOffice+. Multiple compounds can be selected and edited within a “collection”. The ChemDraw JS editor lets users modify multiple molecules via a convenient carousel. (Figure 12.). The full or partial content of collections can then be conveniently selected and readily exported to an SD File or to a PowerPoint document to create the normally time-consuming lab weekly report in just a few minutes. Molecules and their properties are conveniently output and displayed in a pleasing-to-the-eye format, with molecules and text boxes nicely positioned and formatted (figure 12).



Figure 12: ChemOffice+ lets you easily modify structures in batches.



CHEMOFFICE+ CLOUD



# CHEMOFFICE+ CLOUD

## Cloud Means Easy and Frequent New Capabilities

ChemOffice+ is the most recent Cloud-Native application added to the Signals Platform Ecosystem (innovative solutions that support research workflows). It is an evergreen application, i.e. users are always on the latest available version and as ChemOffice+ evolves, its reporting capabilities will cross over other applications like Signals Notebook.

Over the past year, we have added numerous improvements stemming from user requests. One of those is the ability to easily configure and report on SNB Experiments (figure 17).

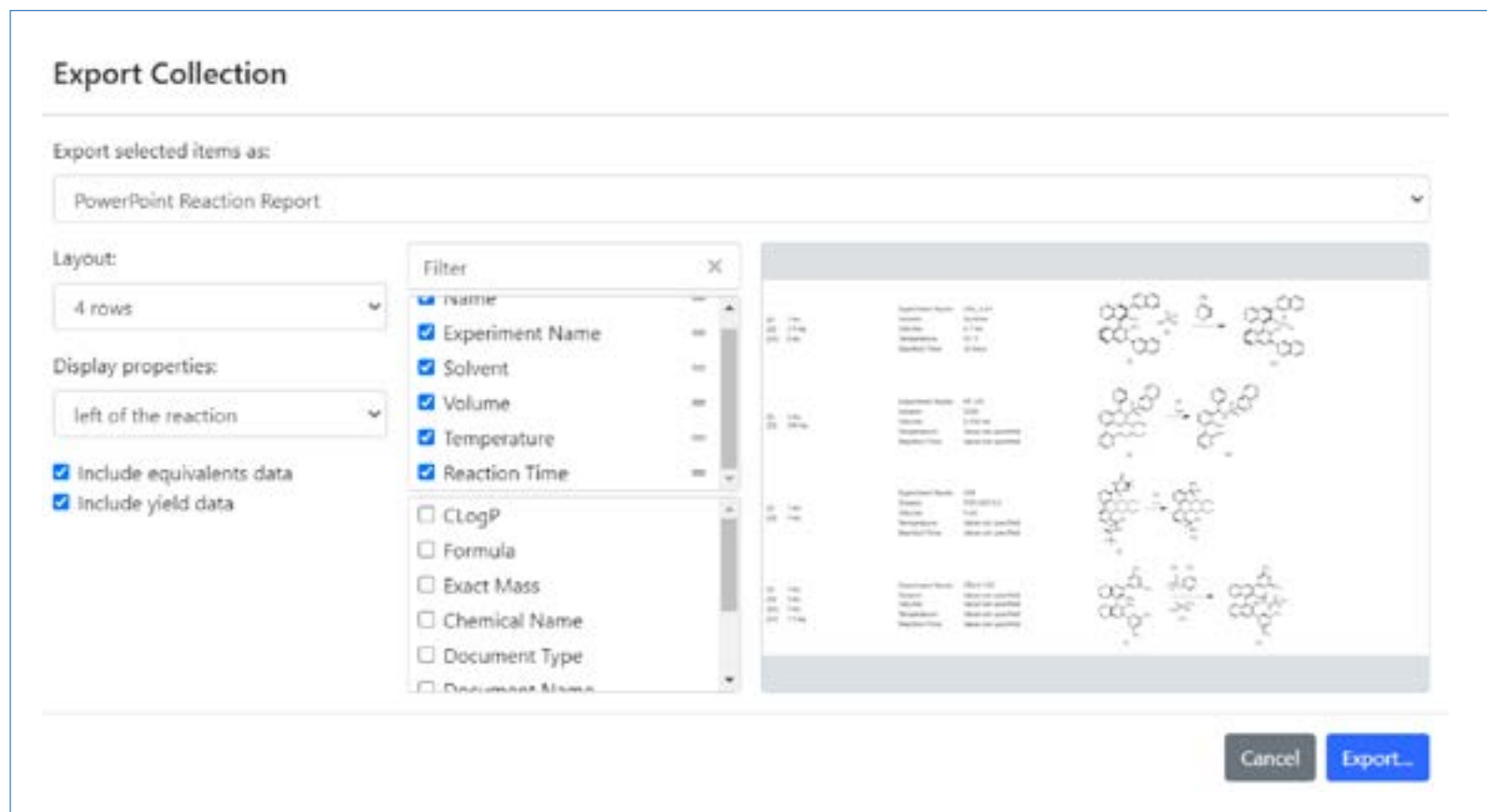


Figure 13: A recent improvement of ChemOffice+: the configuration of PowerPoint reports from a collection with a preview window. The layout and the exported properties can be selected through tickboxes before PowerPoint slides are generated.

# CHEMOFFICE+ CLOUD

*Now that you REALLY know more about ChemDraw...*

HERE'S HOW TO ACCESS IT.



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**New to ChemDraw?**

Give the latest version a test run.



**FIND OUT ABOUT ELIGIBILITY HERE**

**Already a ChemDraw user?**

Did you know you may be entitled to the latest version of ChemDraw?

If you are unable to install a free trial on your company computer,  
**CLICK HERE** to request a live demonstration.



CHEMOFFICE+ CLOUD