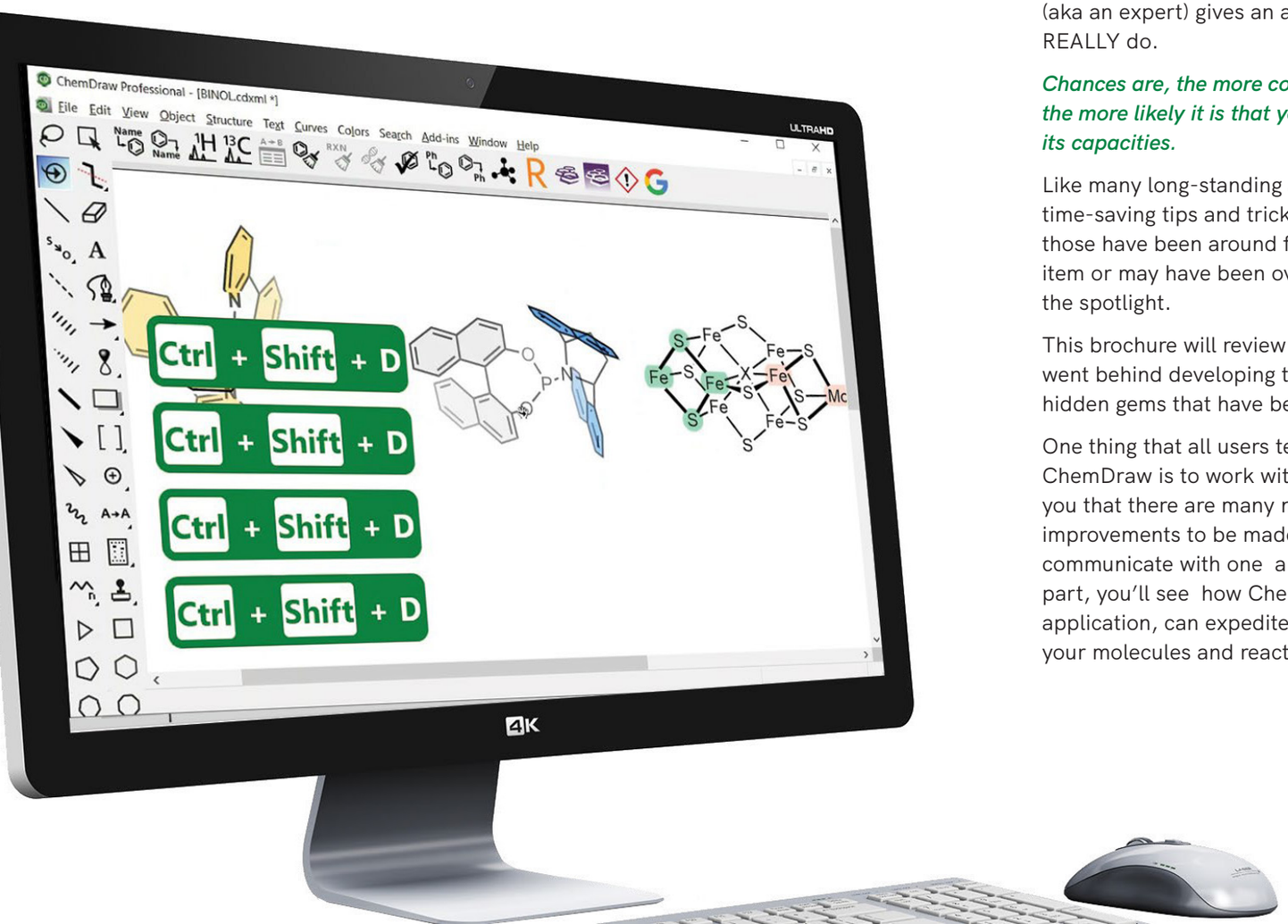
TIPS AND TRICKS

CHEMDRAW® AND SIGNALS CHEMDRAW® COLLECTIONS TIPS AND TRICKS



revvity signals | ChemDraw®

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



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

... is the most frequent comment heard when Revvity Signals 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 ChemDraw Collections, our new Cloud-Native application, can expedite mundane tasks such as the management of your molecules and reactions, as well as everyday reporting.

ChemDraw®

INTRODUCTION

- Drawing efficiency
- Visual communication
- Intergrations with key Research applications
- ChemDraw Collections

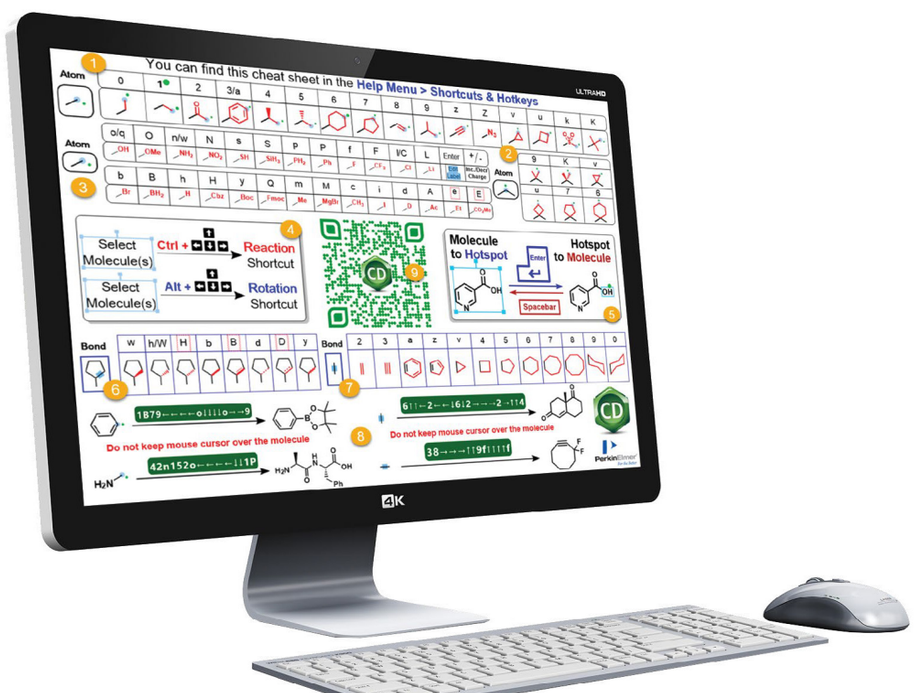
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DRAWING EFFICIENCY

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?

Since version 19.1 of ChemDraw, a cyclopropyl or a cyclobutyl group can be produced by respectively typing "v" or "u" over an atom. And with ChemDraw 20.0, a sulfonamide group can be created by pressing "k" over a primary carbon or a gem-dimethyl with stereochemistry by pressing "Shift+K" over a secondary carbon.



Parallel to those improvements, the hotspot, equivalent to the text cursor of any word processing application was introduced. 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 improve the drawing speed.

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.

VIEW THE CHEAT SHEET HERE

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Shortcut
Generic Structure

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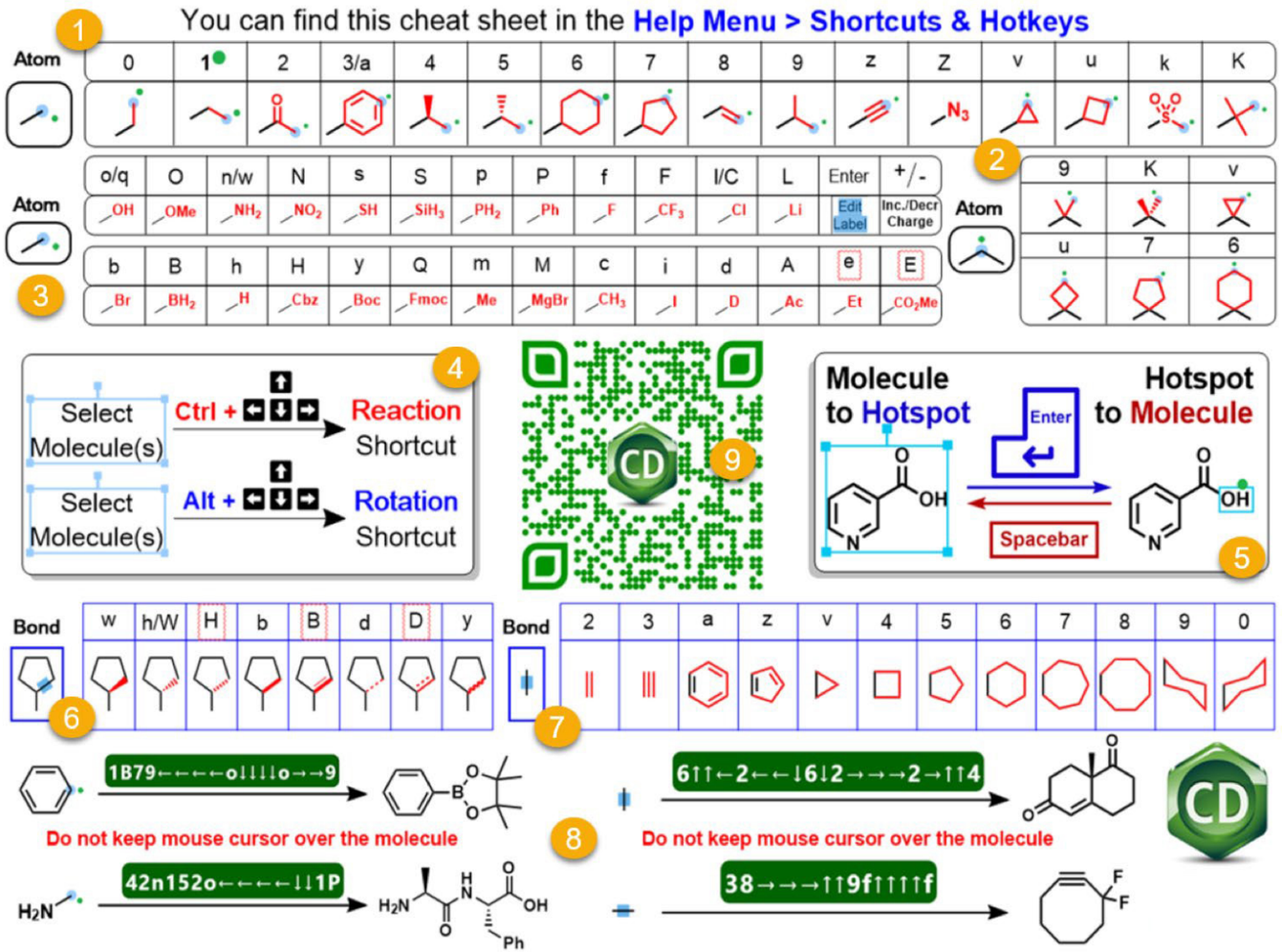
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DRAWING EFFICIENCY

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 20.

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. ?



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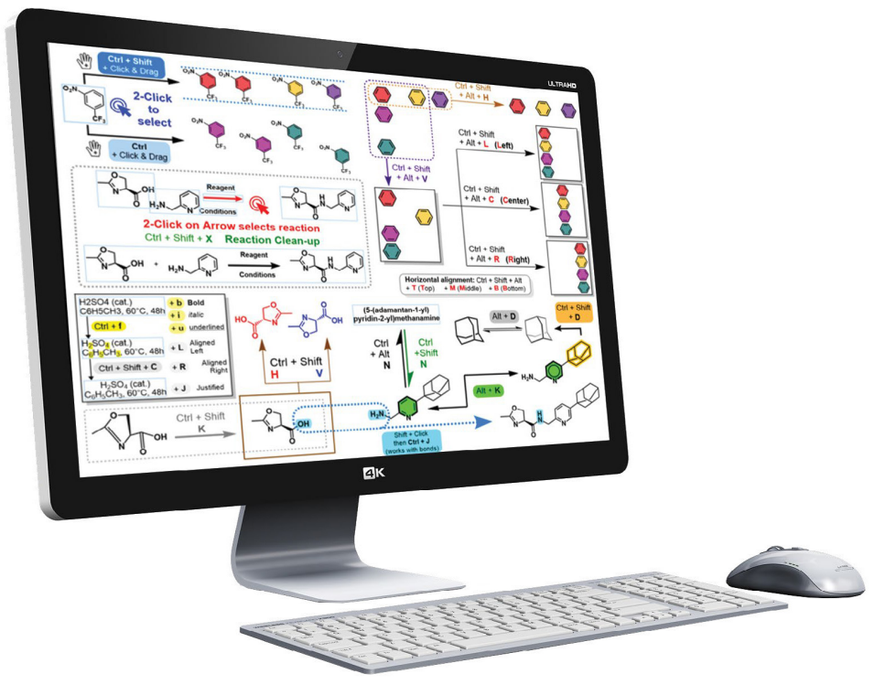
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ChemDraw Collections

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). 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.



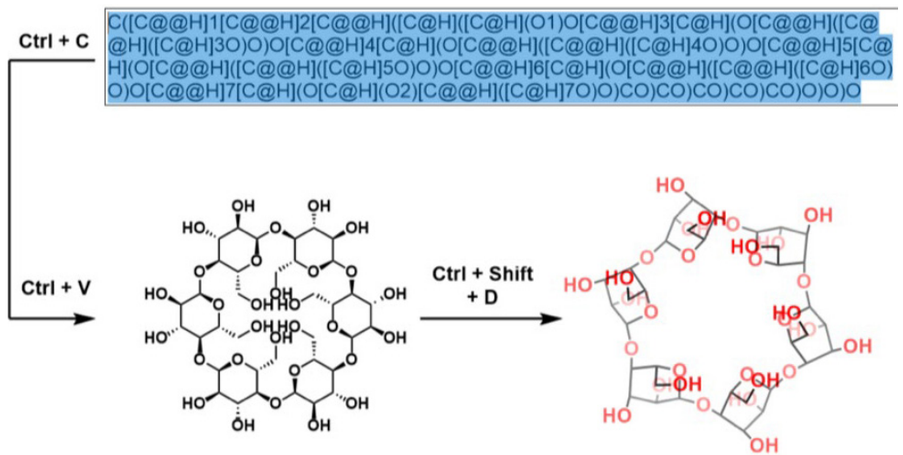


Figure 1: Example of the Smart Copy/Paste function. A SMILES String of Cyclodextrin a can be copied and pasted directly as a structure. It can now be converted to a 3D structure for better visualization (color by element capability turned on for clarity).

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.

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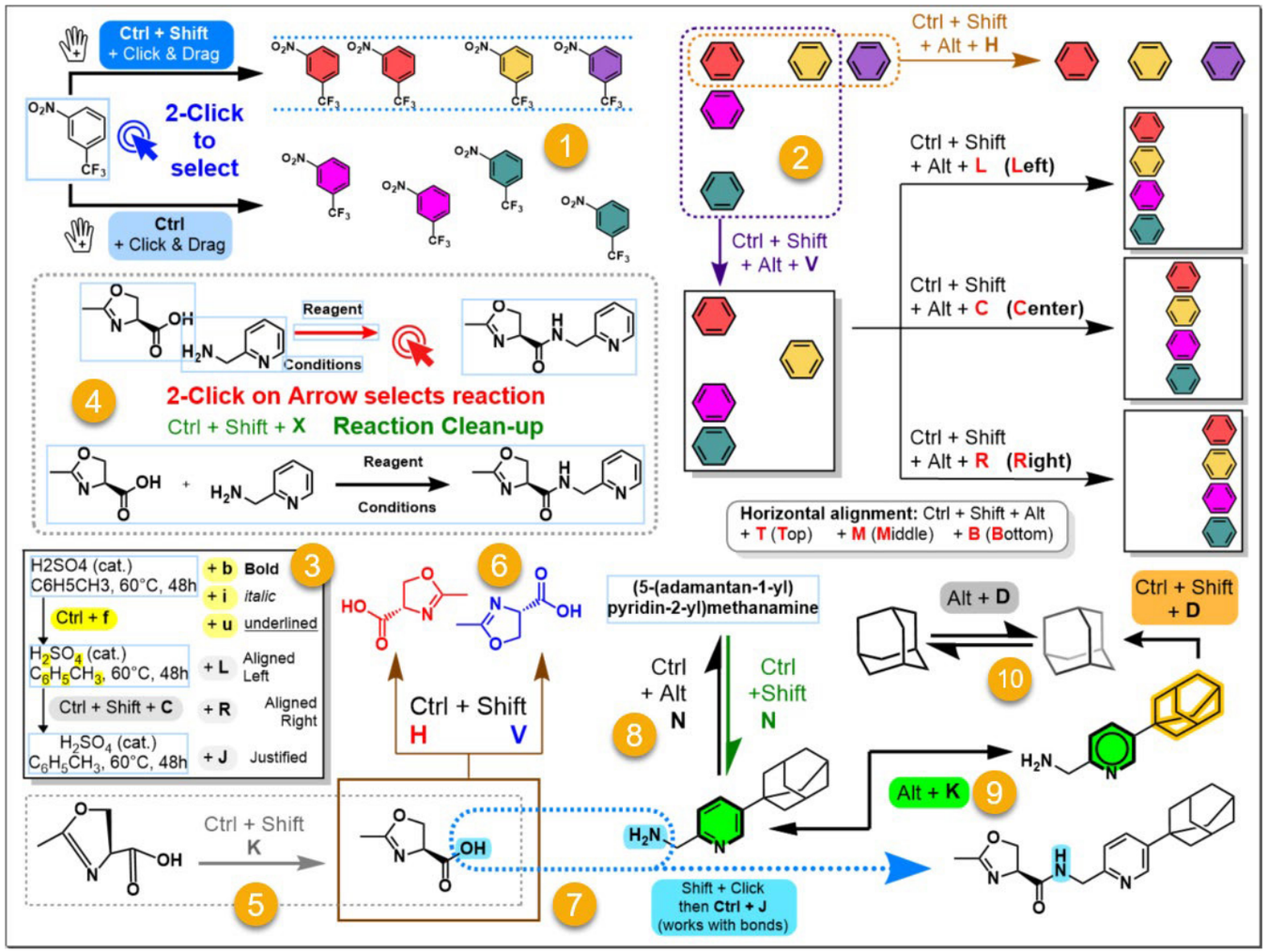
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DRAWING EFFICIENCY

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
5. clean-up shortcuts
6. Structure clean-up shortcut 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)



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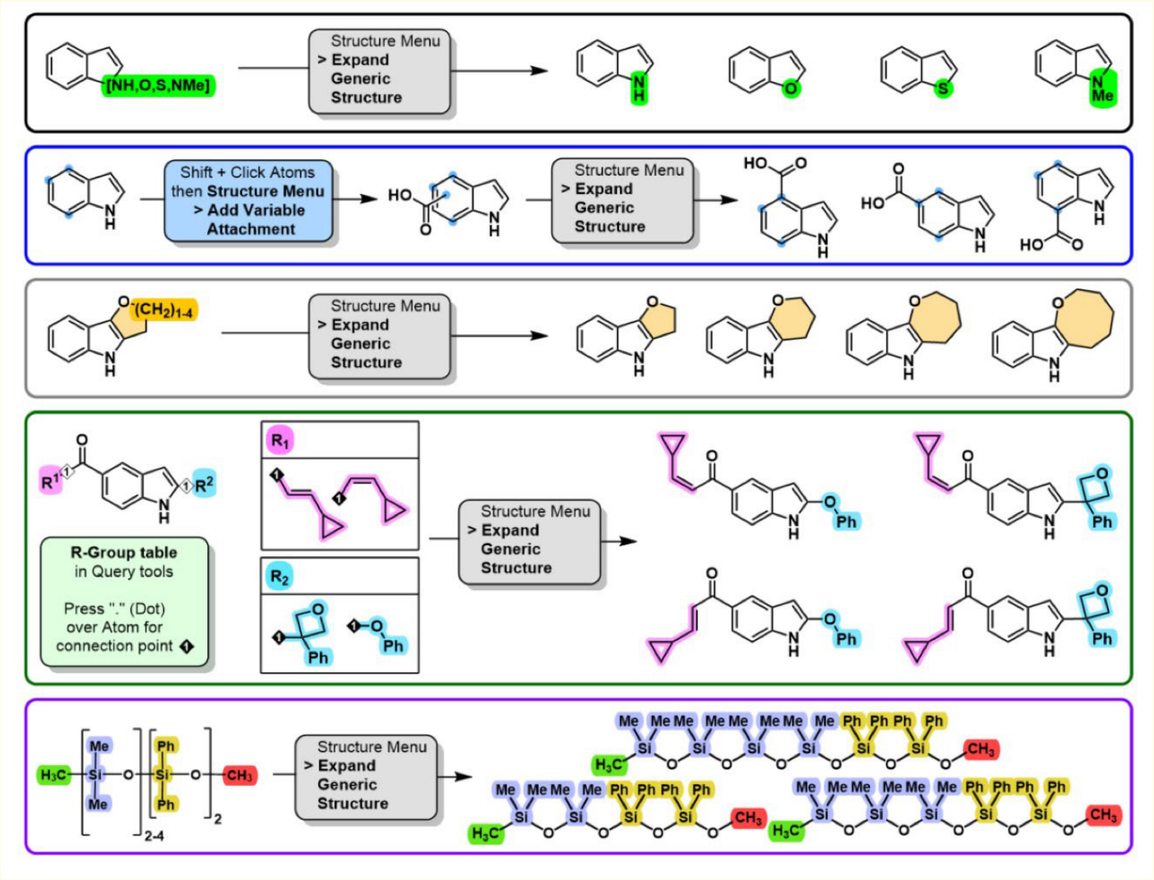
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DRAWING EFFICIENCY

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 ChemDraw Collections.

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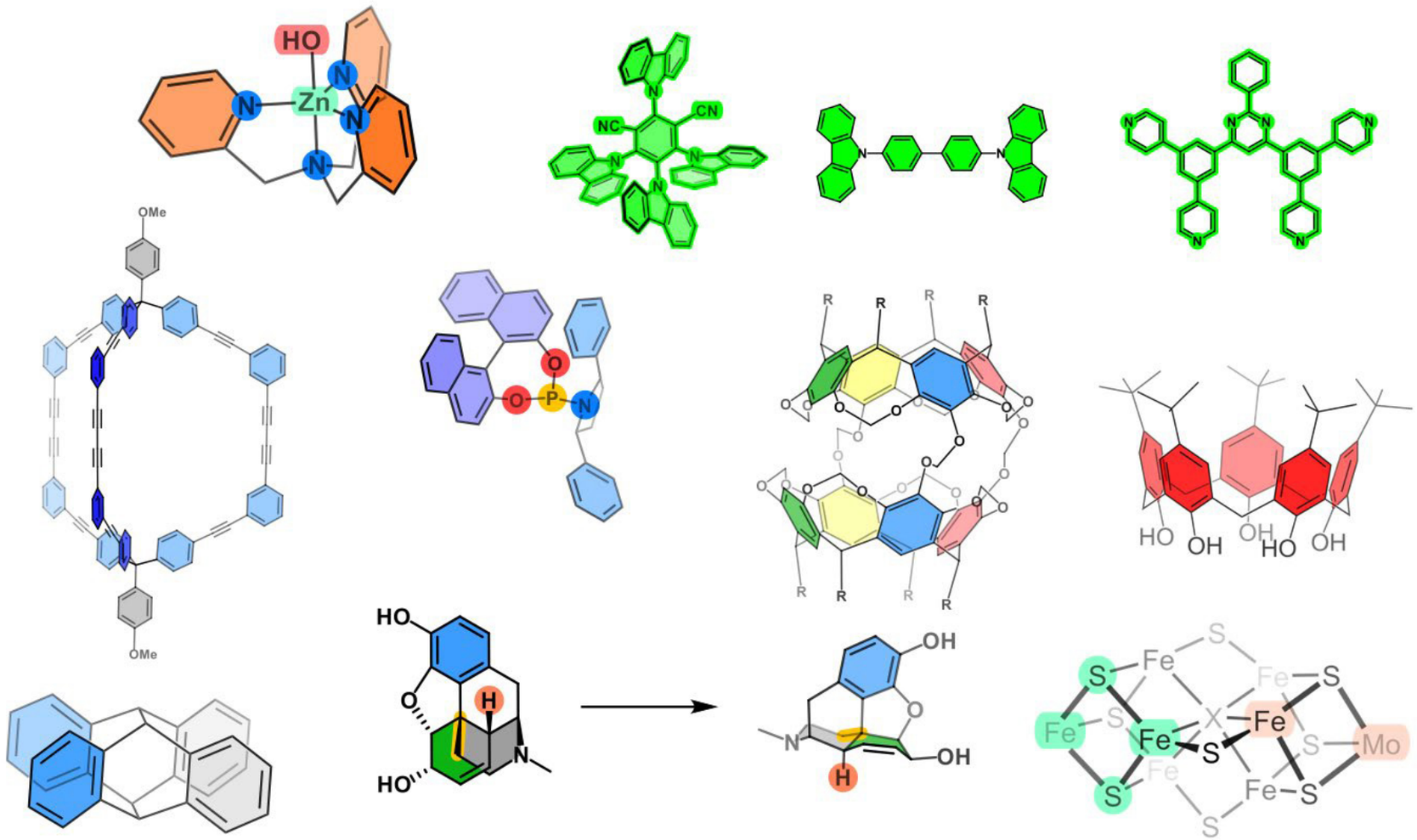
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VISUAL COMMUNICATION

Chemistry to be proud of.

Making small (and large) molecules look their best.



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VISUAL COMMUNICATION

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.

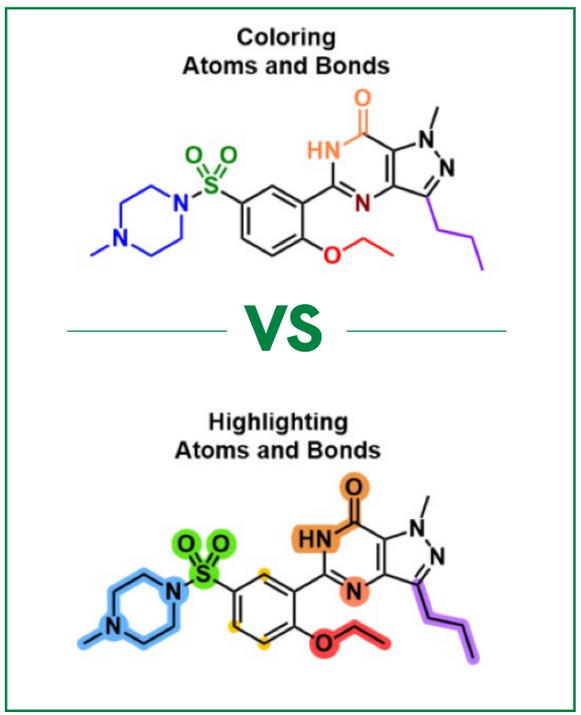


Figure 2: Differences of visibility between functional groups or atoms and bonds simply colored or highlighted with identical colors.

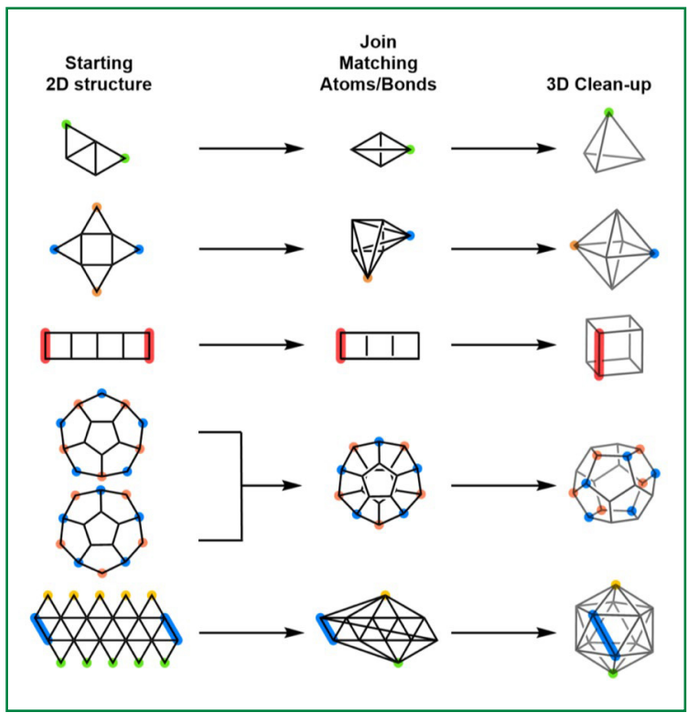


Figure 3: Generating platonic solids in ChemDraw is now easier than ever. Follow the instructions and use the "Join" shortcut (Ctrl+J) on atoms or bonds with the same color highlight and press the new "3D Clean-up" shortcut (Ctrl+Shift+D).

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?

Yes you can! Talking to and listening to our users, we realized that chemists have a need to represent increasingly complex chemical structures, inherently 3-dimensional, through a 2D representation. For chemists, needing to represent a molecule in 3D does not necessarily equate to "I need a space-filling 3D model of my molecule". It often means getting help representing their molecule. With the 3D Clean-up function of ChemDraw 20, you can generate energy-minimized conformations of molecules in just a few clicks. Combining the coloring capabilities with the 3D Clean-up lets you better perceive and appreciate the depth and the real shape of molecules (Figure 4 and 5).

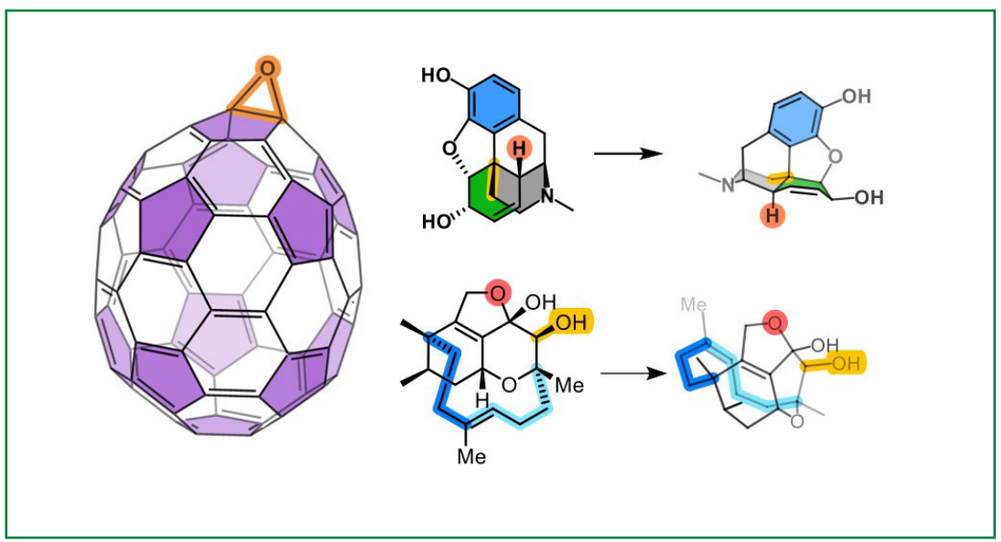


Figure 4: Left: an epoxidized C70 fullerene generated from a SMILES string and a 3D Clean-up operation. 5-membered rings are colored in purple. Right: examples of improved spacial perception of molecule when combining the 3D clean-up capability with coloring options (Top: Morphine; Bottom: Phomactin A).

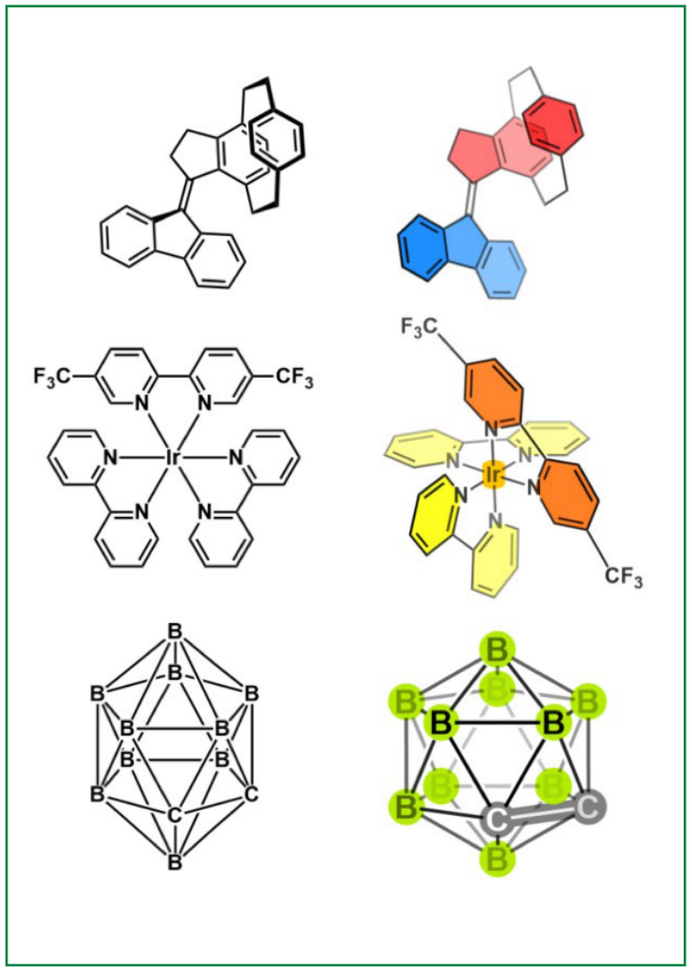


Figure 5: Examples of black and white 2D representations of molecules (Left column) and their corresponding 3D, colorized version (Right Column) to facilitate perception and turn them into a pleasing-to-the-eye format.

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INTEGRATIONS WITH KEY RESEARCH APPLICATIONS

SciFindern 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® 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® was introduced, followed by ChemDraw and SciFindern® in 2019 (Figure 6)

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.

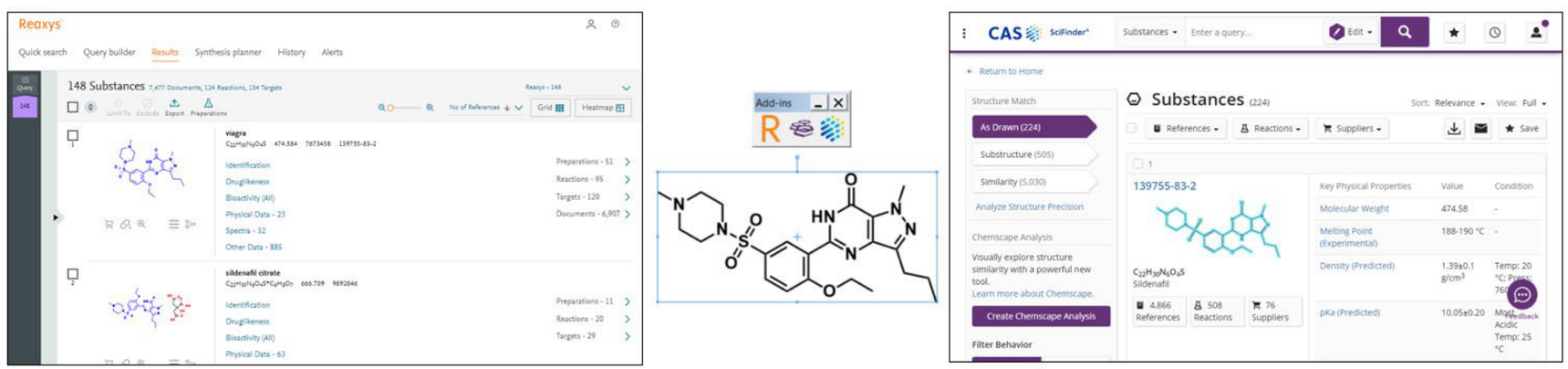


Figure 6: Illustration of the search results for a molecule of sildenafil into the Reaxys (Left) and SciFinder-n (Right) databases.

ChemDraw

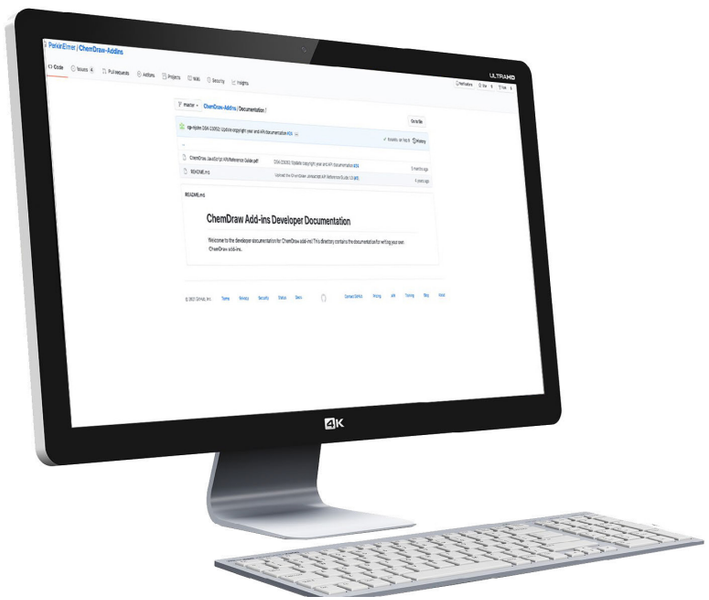
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INTEGRATIONS WITH KEY RESEARCH APPLICATIONS

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/Revvity/ChemDraw-AddIns/tree/master/Documentation). We then started adding new integrations with every new version of ChemDraw Desktop in Signals ChemDraw (Figure 7).



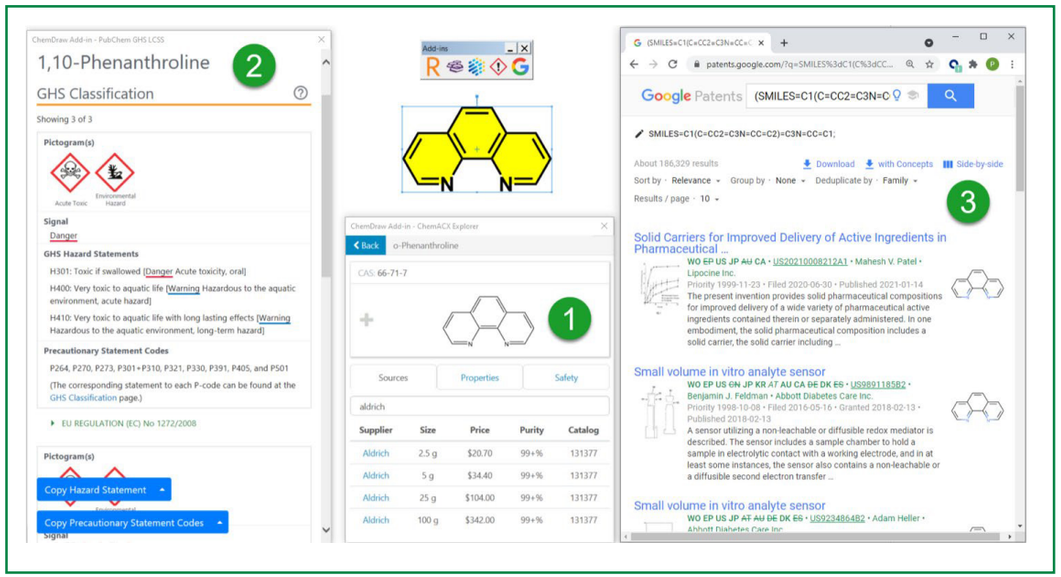


Figure 7: The various Out-Of-The-Box add-ins available within ChemDraw when licensed with Signals ChemDraw, using ortho-phenanthroline as an example:

1. The ChemACX Explorer allows users to look up molecules by structure, name, or CAS Number in Revvity's database of >20M commercially available substances and find pricing and commercial availability.
2. The PubChem Laboratory Chemical Safety Summary (Fig7: 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.

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ChemDraw Collections

Turning Chemical Drawings Into Chemical Knowledge

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CHEMDRAW COLLECTIONS - *SEARCH*

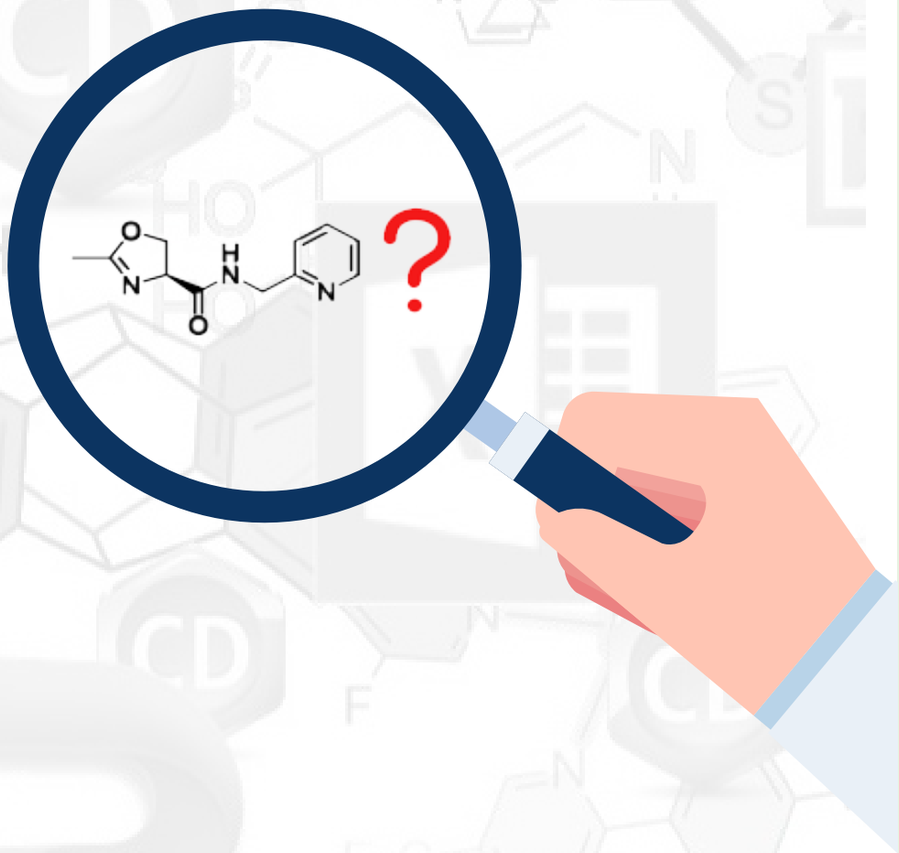
A chemist's Life: the literal search for molecules.

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 **ChemDraw Collections** came along.

ChemDraw Collections 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.

Read more on searching molecules on the next page.



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CHEMDRAW COLLECTIONS

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 8: 1) and based on a specific exact or substructure (Figure 8: 2). With the document filter (Figure 8: 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 8: 4), and their content can then be viewed in the rightmost column (Fig 8: 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.

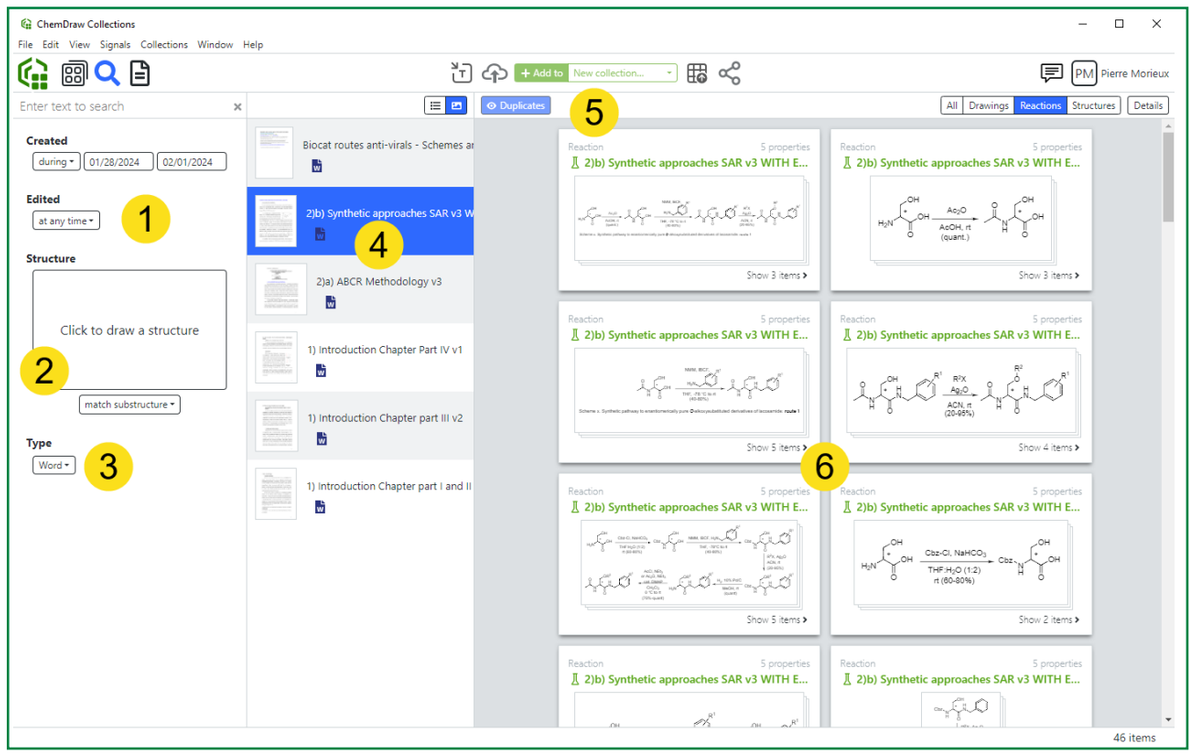


Figure 8: The Search View otf ChemDraw Collections.

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CHEMDRAW COLLECTIONS

Green Chemistry: easily recycle your drawings.

The first time-consuming workflow tackled by ChemDraw Collections allows chemists to quickly re-use and re-purpose chemical drawings stored on a computer. A File Explorer is available on the left (Figure 9: 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 9: 2). Multiple items can be selected through the tickbox (Figure 9: 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 9: 4) to view individual reaction components or individual structures and interact with them to re-use them.

Filters at the top (Figure 9: 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 9: 6)

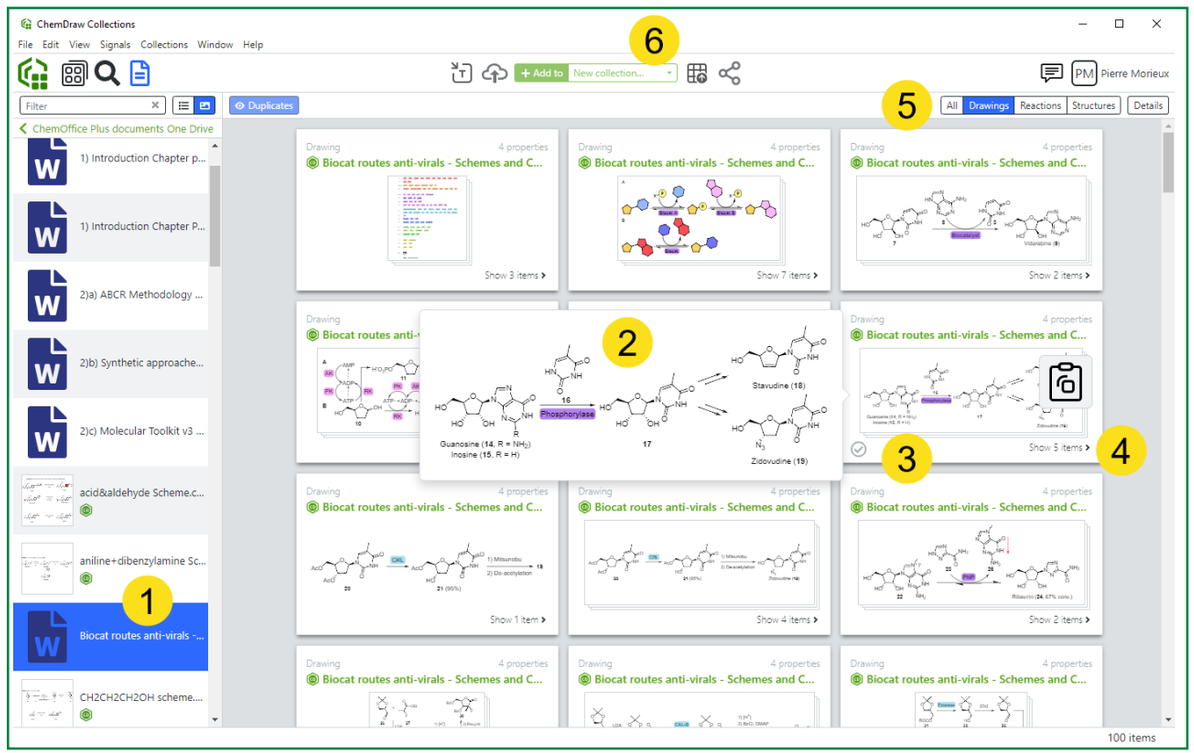


Figure 9: The File Explorer view of ChemDraw Collections.

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CHEMDRAW COLLECTIONS

Collections: Easily manage and share your chemistry.

Collections are a new way to manage lists

of compounds and molecules with their associated properties in ChemDraw Collections. Collections are designed for chemists to **“apply actions to batches of molecules.”**

When selected (Fig 10: 1), the collection’s content is displayed on the right. Hovering over a molecule preview (Fig 10: 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 10: 4), exported to SD File, or Powerpoint (Fig 10: 5).

Read more on managing compounds on the next page.

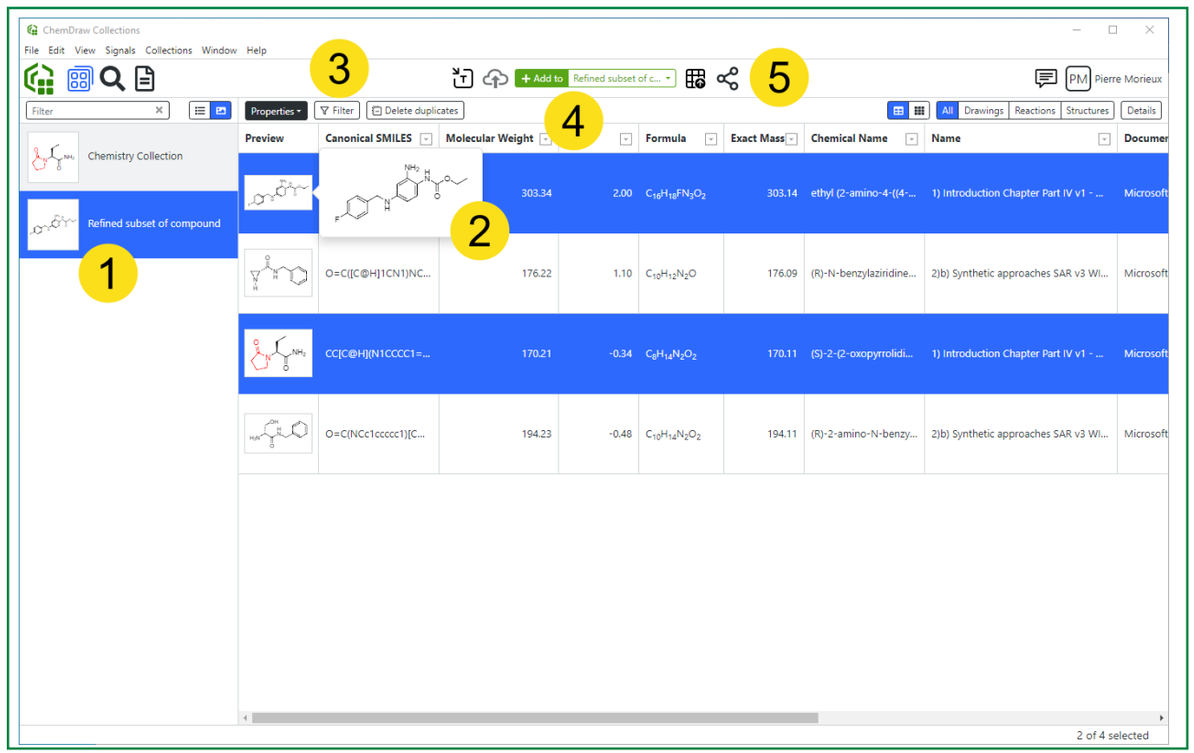


Figure 10: The File Explorer view of ChemDraw Collections.

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CHEMDRAW COLLECTIONS

Manage Multiple Objects Simultaneously

The ability to handle and manage multiple objects at the same time is a central aspect of ChemDraw Collections. Multiple compounds can be selected and edited within a "collection". The ChemDraw JS editor lets users modify multiple molecules via a convenient carrousel. (Figure 11.). 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).

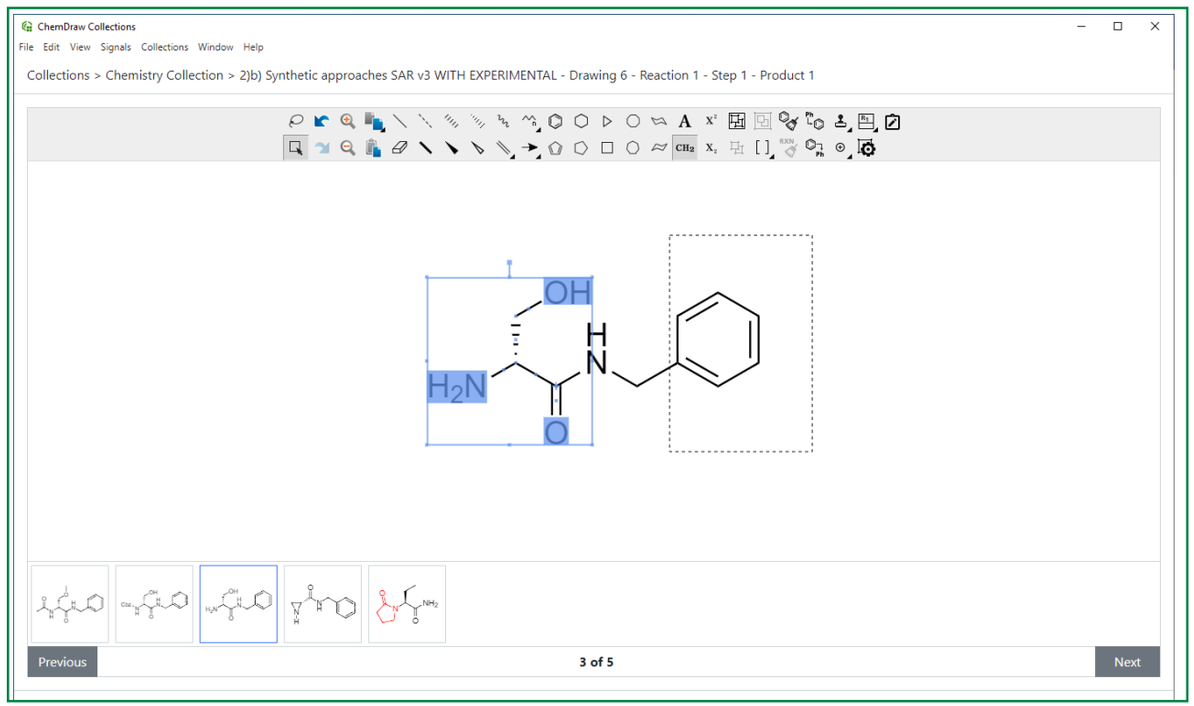


Figure 11: ChemDraw Collections lets you easily modify structures in batches.

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CHEMDRAW COLLECTIONS

Reporting capabilities

ChemDraw Collections 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 ChemDraw Collections evolves, its reporting capabilities will cross over other applications like Signals Notebook.
In the upcoming future, Signals Notebook Experiment data will become easily "reportable" through ChemDraw Collections. The ChemDraw Collections client can be downloaded from the user's Signals Notebook User Profile.

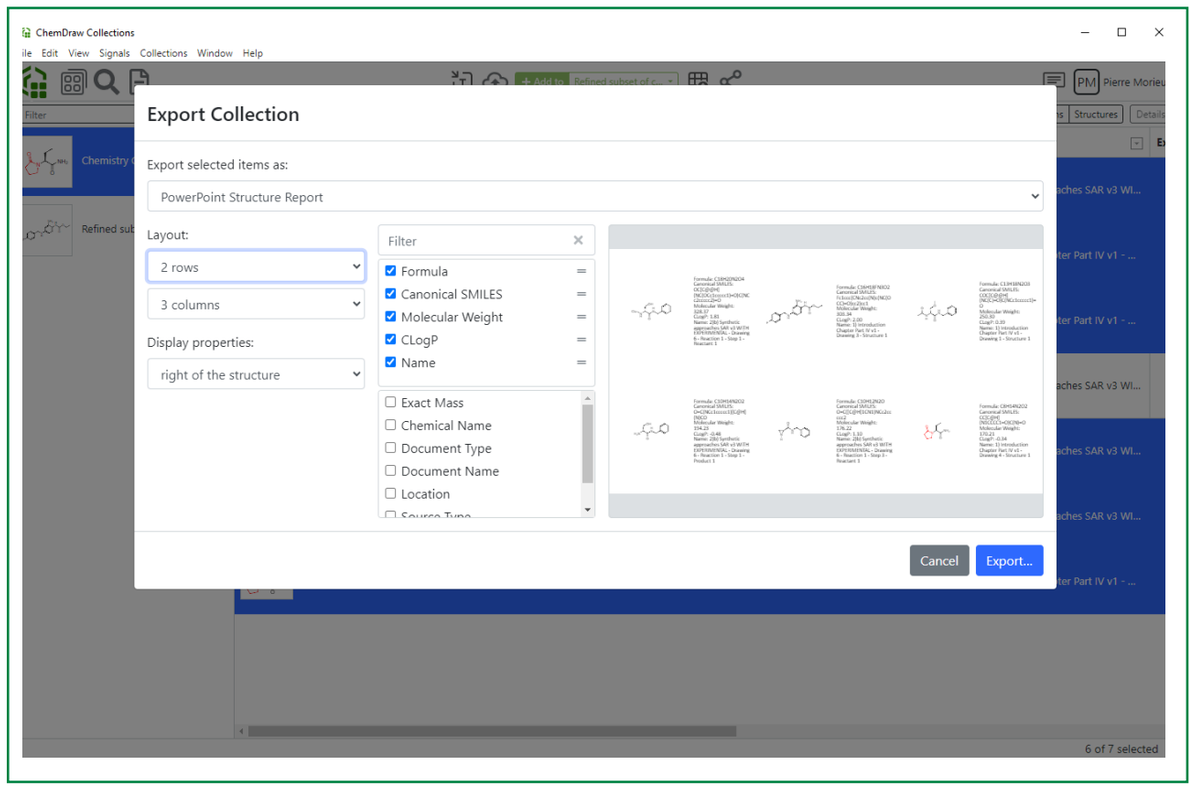


Figure 12: An example of a Powerpoint Report slide generated from a collection.

ChemDraw

- Introduction
- Drawing efficiency
- Visual communication
- Intergrations with key Research applications
- **CHEMDRAW COLLECTIONS**
  - Search
  - Recycle
  - Manage
  - **Report**
  - Get Started

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CHEMDRAW COLLECTIONS

Now that you REALLY know more about ChemDraw...

Here's how to access it.
New to ChemDraw? Give the latest version a test run.

GET A FREE TRIAL HERE

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

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