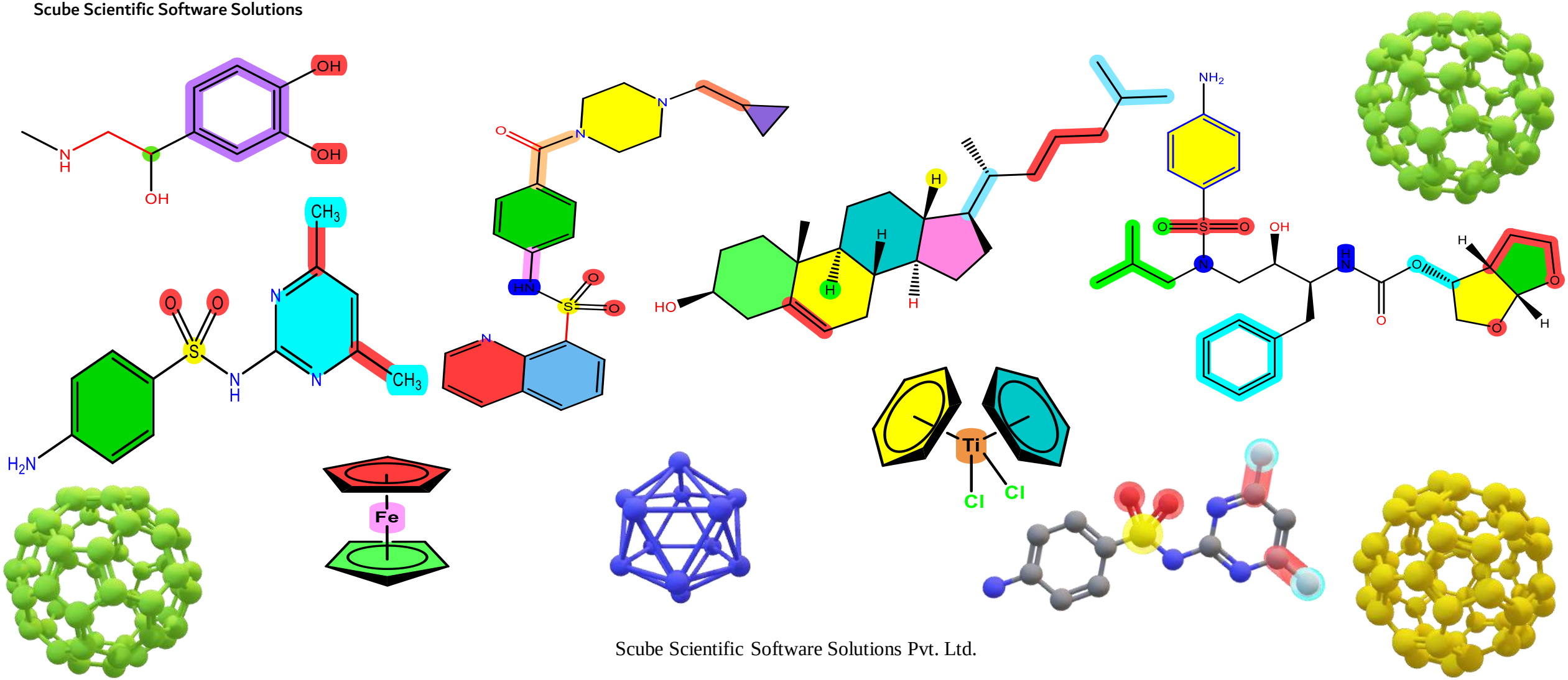
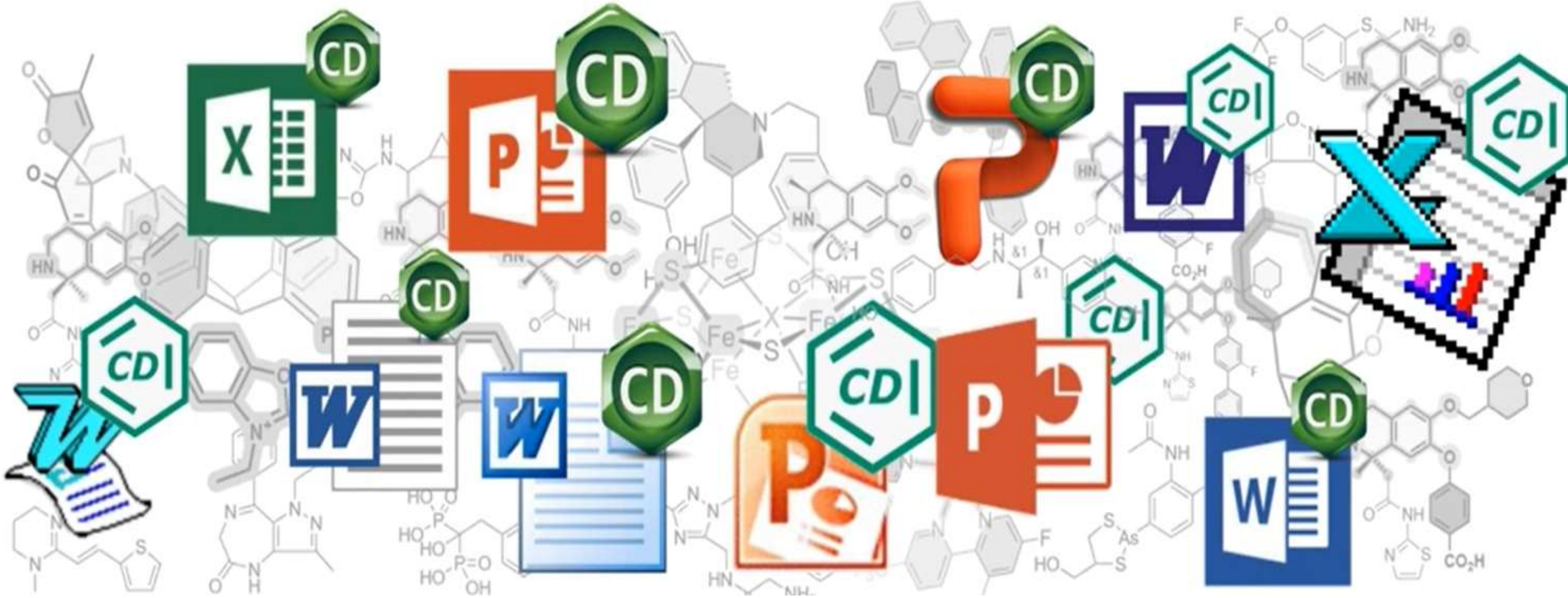
ChemDraw v23.0

Bobby Solanki

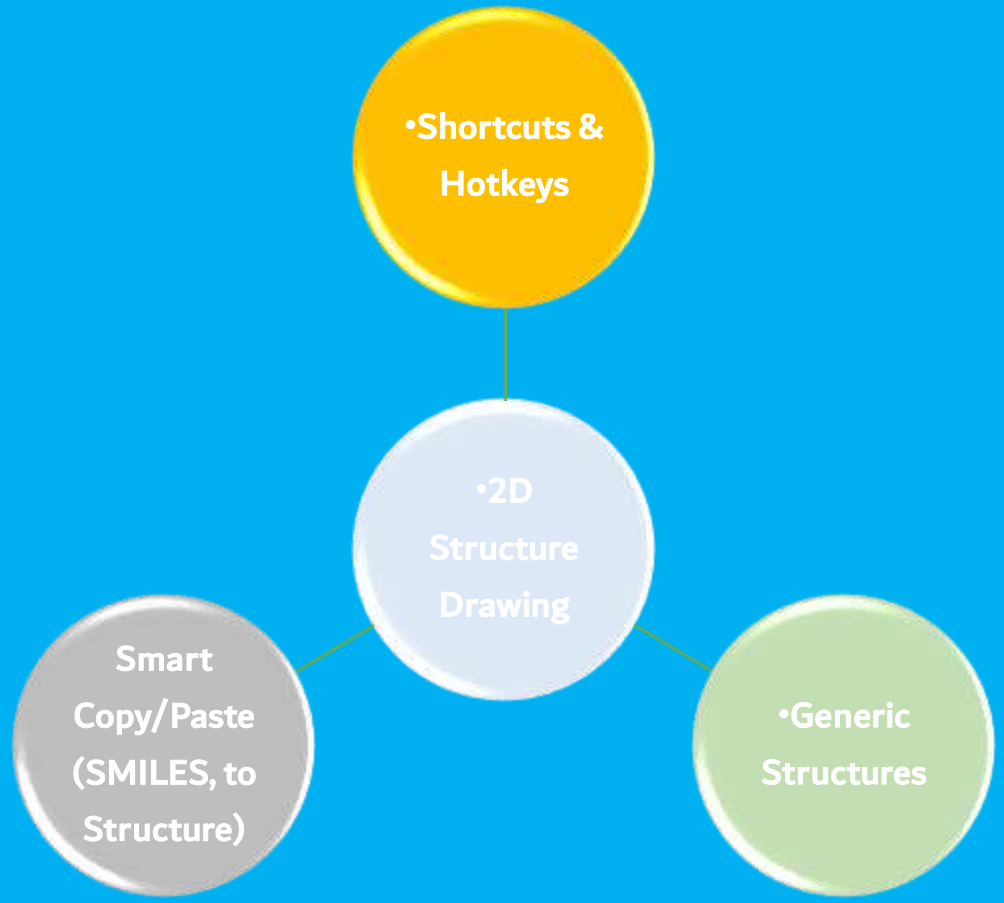
Technical Consultant
Scube Scientific Software Solutions



ChemDraw



ChemDraw Prime



ChemDraw Professional

ChemDraw
Integrated with the
Signals Platform

Signals ChemDraw 23.0

Features

- Most feature Rich ChemDraw Desktop
- Access to ChemDraw Products via Signals Platform
- Activation via Authentication (no activation codes)
- Signals Integration in Desktop
- Automatic Updates

Cloud Applications

ChemDraw+

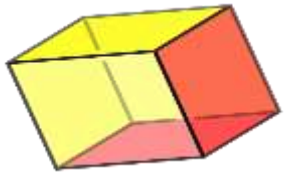
Create and organize publication quality drawings in the cloud

ChemDraw Collections

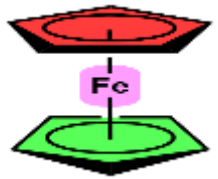
Unlock your chemistry data: capture, retrieve, store and share

HELM Monomer Curation

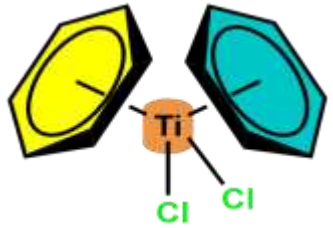
Manage & Curate Custom Monomer Libraries for use in ChemDraw+



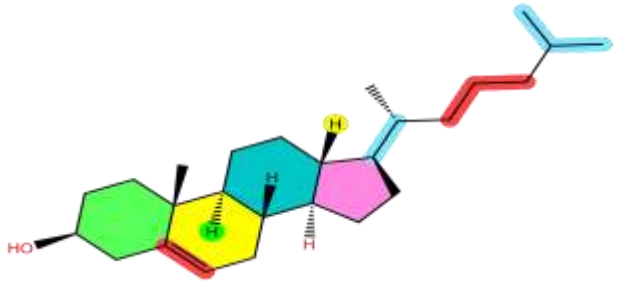
Molecular Weight: 104.15
Formula: C8H8
Exact Mass: 104.06
Chemical Name: cubane
CLogP: 2.30



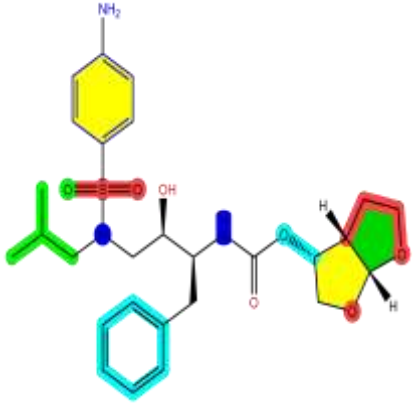
Molecular Weight: 186.04
Formula: C10H10Fe
Exact Mass: 186.01
Chemical Name:
CLogP: 1.78



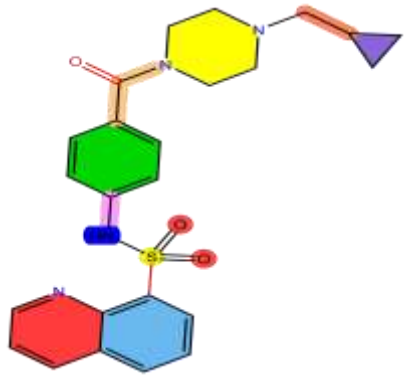
Molecular Weight: 275.00
Formula: C12H12Cl2Ti
Exact Mass: 273.98
Chemical Name:
CLogP: 2.14



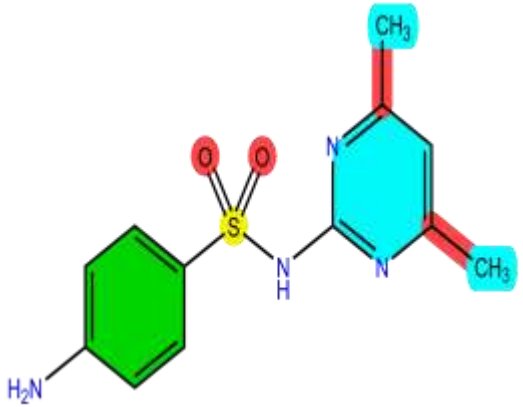
Molecular Weight: 372.64
Formula: C26H44O
Exact Mass: 372.34
Chemical Name: cholesterol
CLogP: 9.00



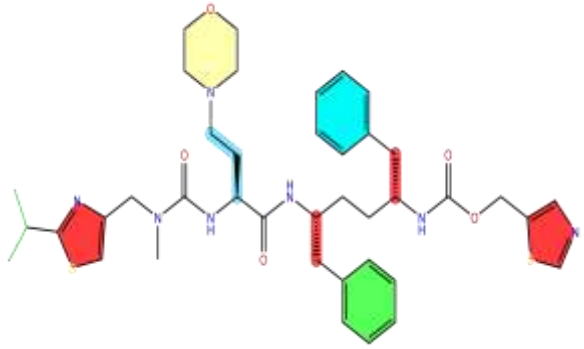
Molecular Weight: 547.67
Formula: C27H37N3O7S
Exact Mass: 547.24
Chemical Name: (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ((2S,3R)-4-((4-amino-N-isobutylphenyl)sulfonamido)-3-hydroxy-1-phenylbutan-2-yl)carbamate
CLogP: 2.89



Molecular Weight: 450.56
Formula: C24H26N4O3S
Exact Mass: 450.17
Chemical Name: N-(4-(4-(cyclopropylmethyl)piperazine-1-carbonyl)phenyl)quinoline-8-sulfonamide
CLogP: 3.44



Molecular Weight: 278.33
Formula: C12H14N4O2S
Exact Mass: 278.08
Chemical Name: 4-amino-N-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide
CLogP: 1.10



Molecular Weight: 776.03
Formula: C40H53N7O5S2
Exact Mass: 775.35
Chemical Name: thiazol-5-ylmethyl ((2R,5R)-5-((S)-2-(3-((2-isopropylthiazol-4-yl)methyl)-3-methylureido)-4-morpholinobutanamido)-1,6-diphenylhexan-2-yl)carbamate
CLogP: 3.98

ChemDraw Collections File Edit View Signals Collections Window Help Wed Mar 13 10:53 AM

ChemDraw Collections

Add to New Collection... Lindsey Rickershauser

Filter Duplicates All Drawings Reactions Structures Details

ChemDraw
- ChemDraw Connect
- ChemDraw Connect_Jan 2024...
- Demo
- Dissertation Docs
- Overflow

ACS Polym Au Abstract...

Agelastatin_A.cdxml

ATR Kinase Inhibitor Sy...

AZD4747.cdxml

beta-cyclodextrin.cdxml

BRD 7_9 inhibitor VII sy...

Catenanes and Rotaxane...

Colored Drugs.cdxml

Cryptophane.cdxml

Reaction 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
Show 4 items

Reaction 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
NaI
66%
Show 3 items

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
NaI

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Reaction 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
81%
Show 3 items

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Reaction 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
NaOH
PhMe
65%
Show 2 items

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

Reaction 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...
Show 2 items

Structure 4 properties
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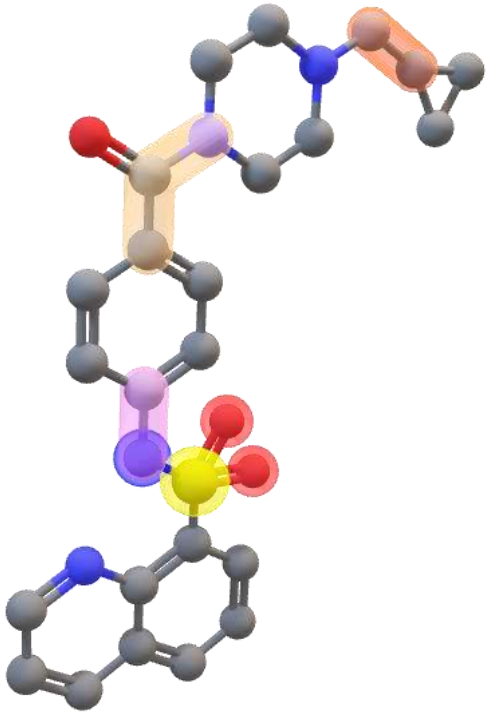
Structure 4 properties
ATR Kinase Inhibitor Synthesis - Reactio...

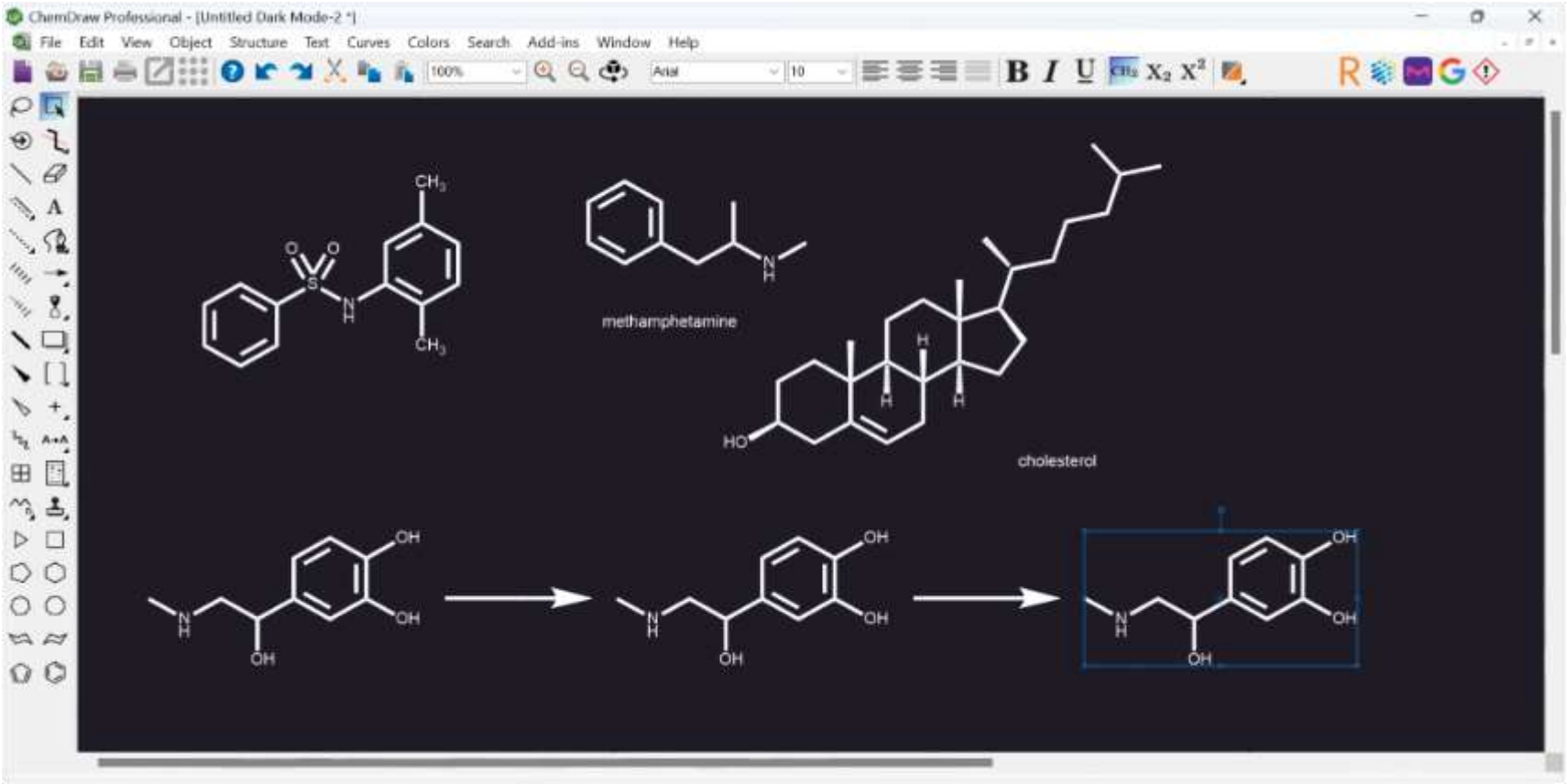
15 items

Signals ChemDraw

ChemDraw
Integrated with the
Signals Platform

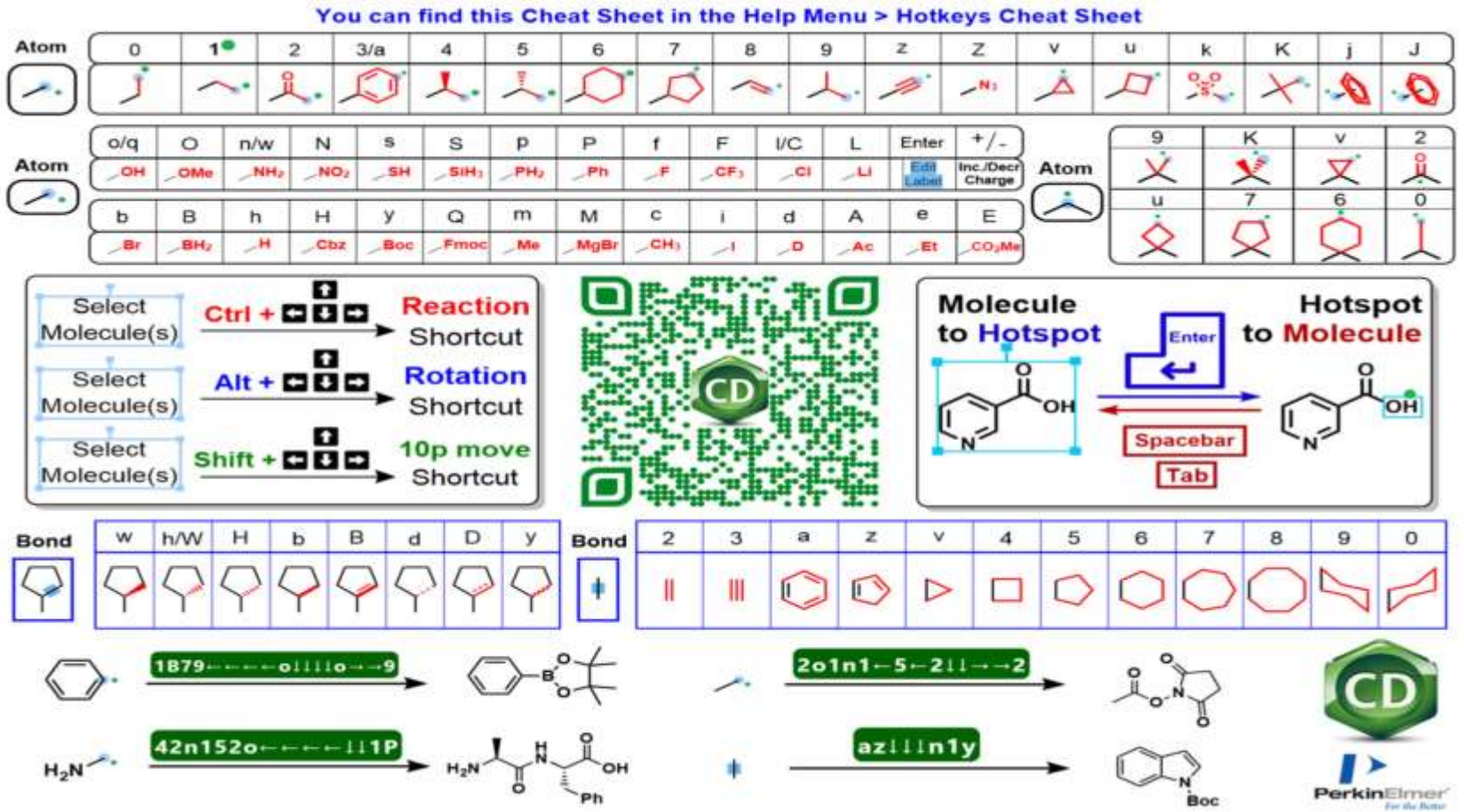


Signals ChemDraw



Shortcuts and Hotkeys

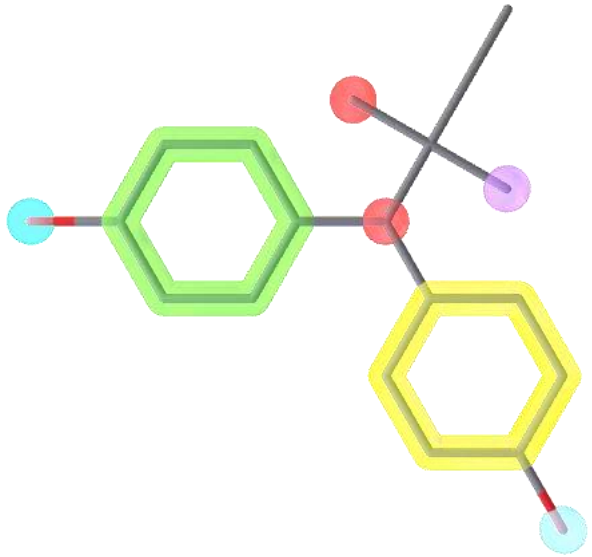
Help →Shortcuts and Hotkeys



Shortcuts and Hotkeys

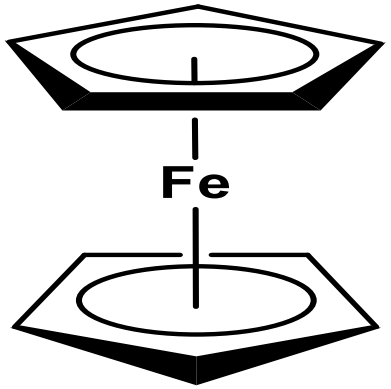
'0' on **secondary** or

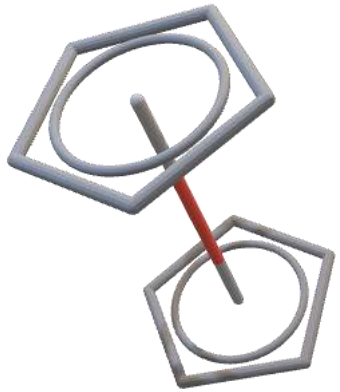
tertiary carbon atom



'j' shortcut key sprouts

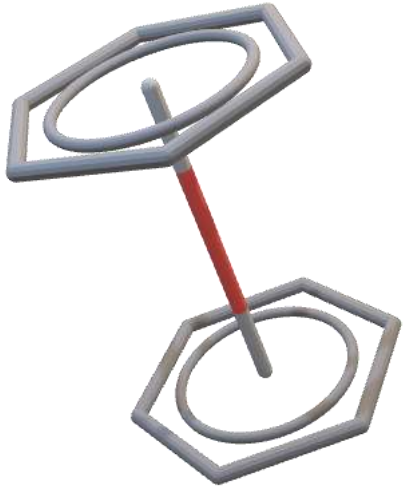
a **cyclopentadienyl ring**

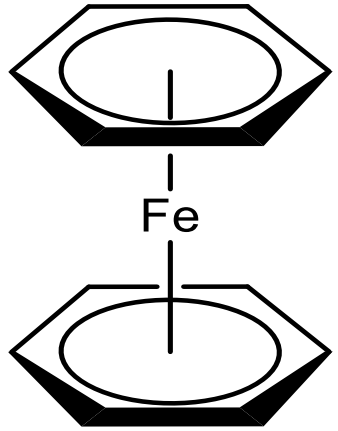




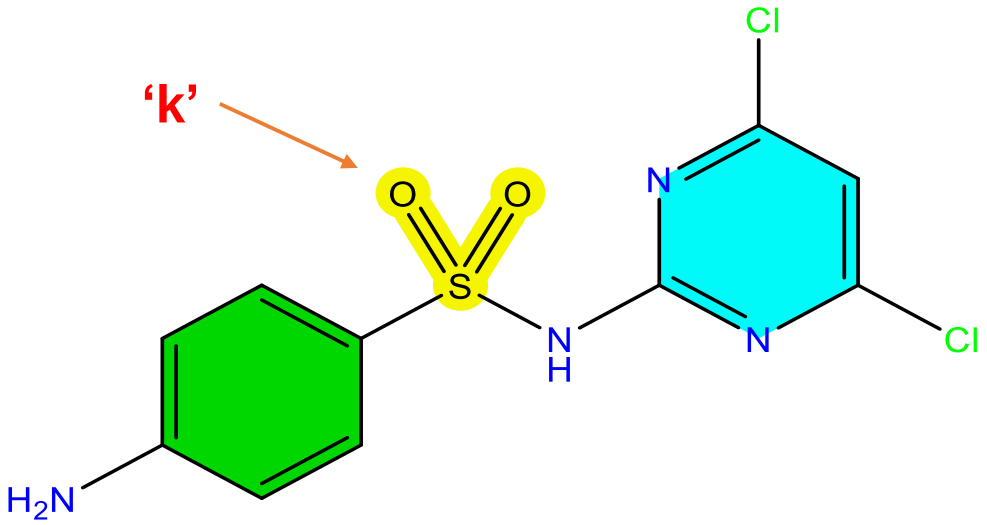
'J' shortcut key sprouts

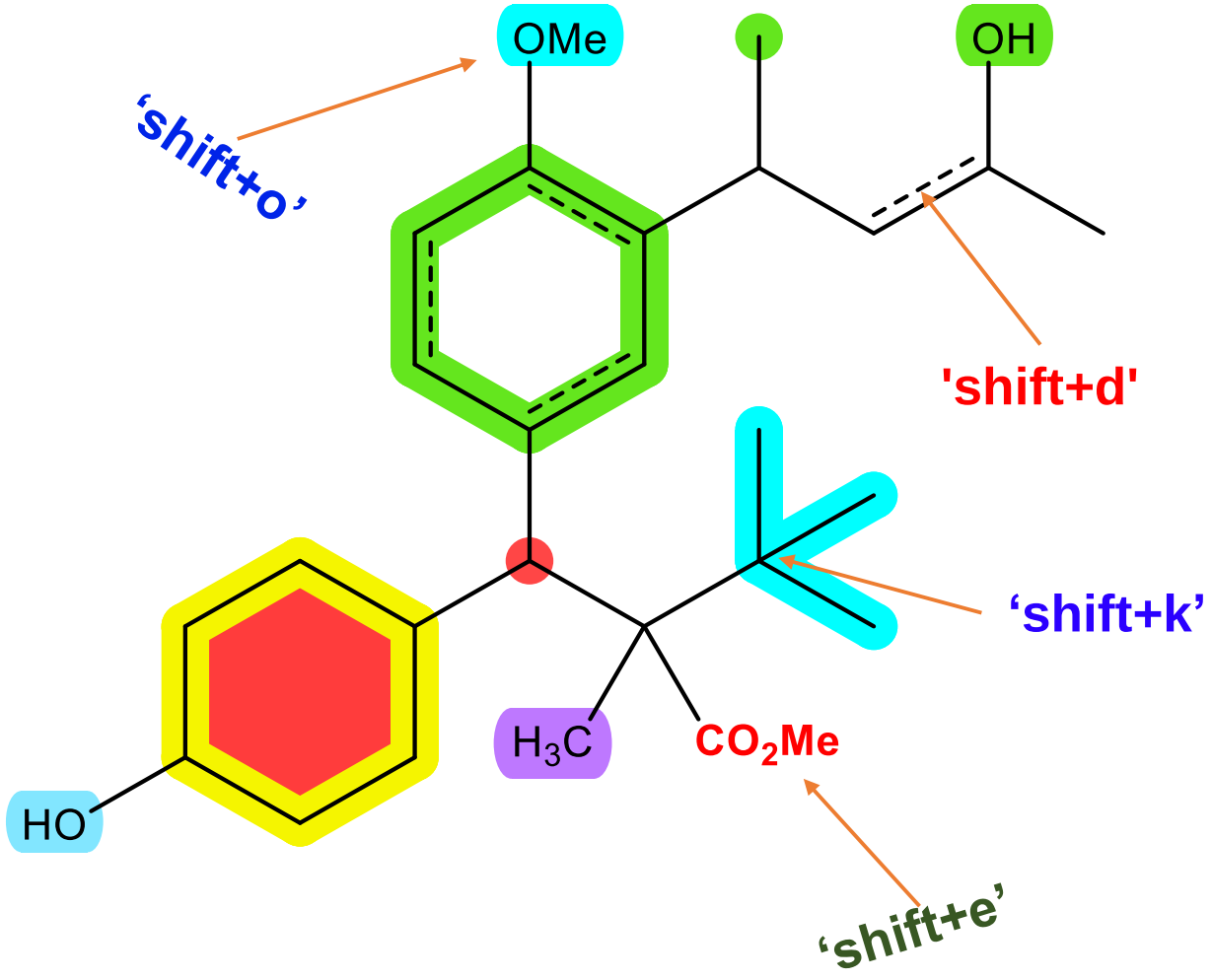
a **Phenyl Ligand**





- **'shift+d'** key places a **dashed double bond**.
- **'k'** key sprouts a **sulfonyl group**.
- **'shift+k'** key sprouts a **t-butyl group**.
- **'shift+o'** atom hotkey for **OMe group**.
- **'shift+e'** atom hotkey for **CO_2Me group.**



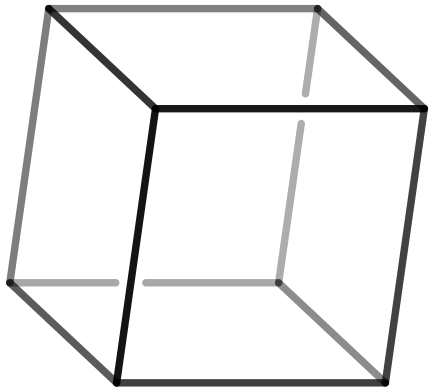


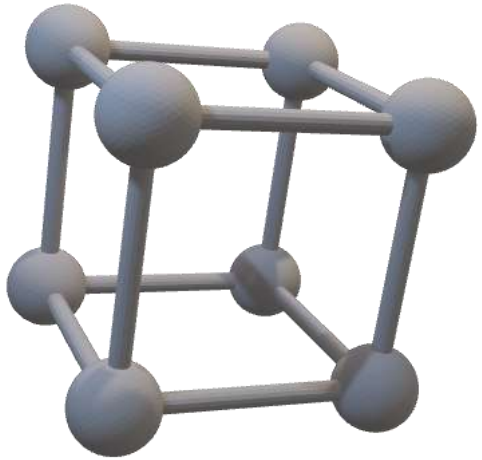
Copy as PNG

- ChemDraw now lets you copy a structure in **.png format** and paste it directly into **Outlook or Gmail**.

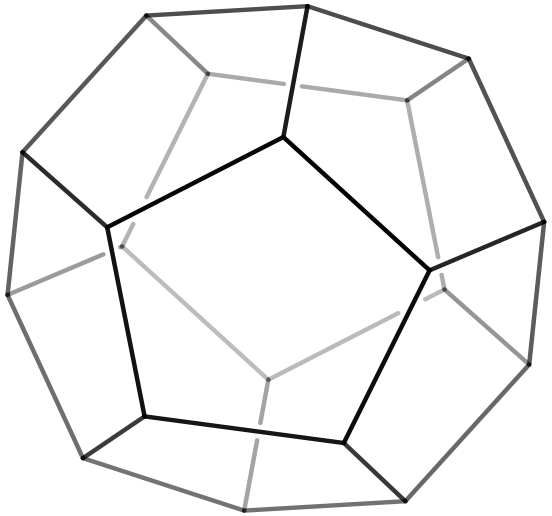
'ctrl+J'

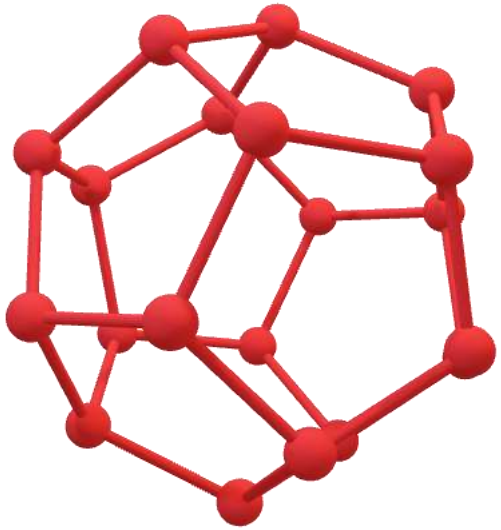
- Joining the two or more atoms or molecules together.





Cube

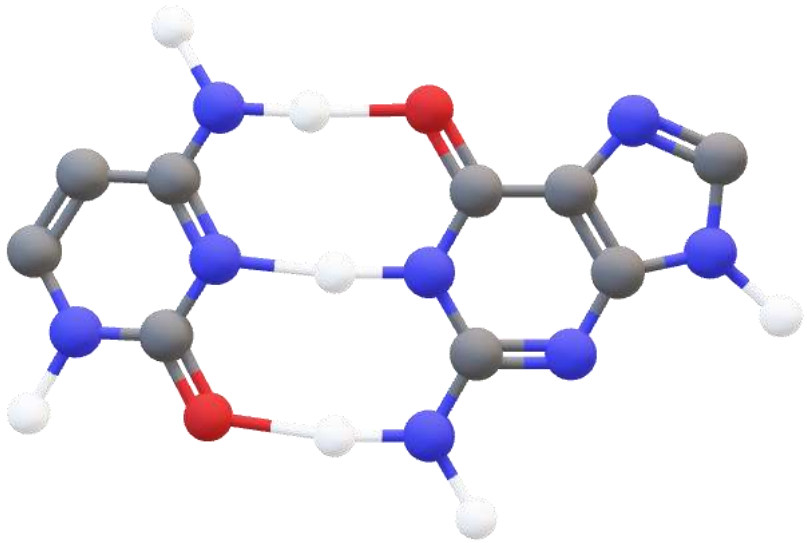


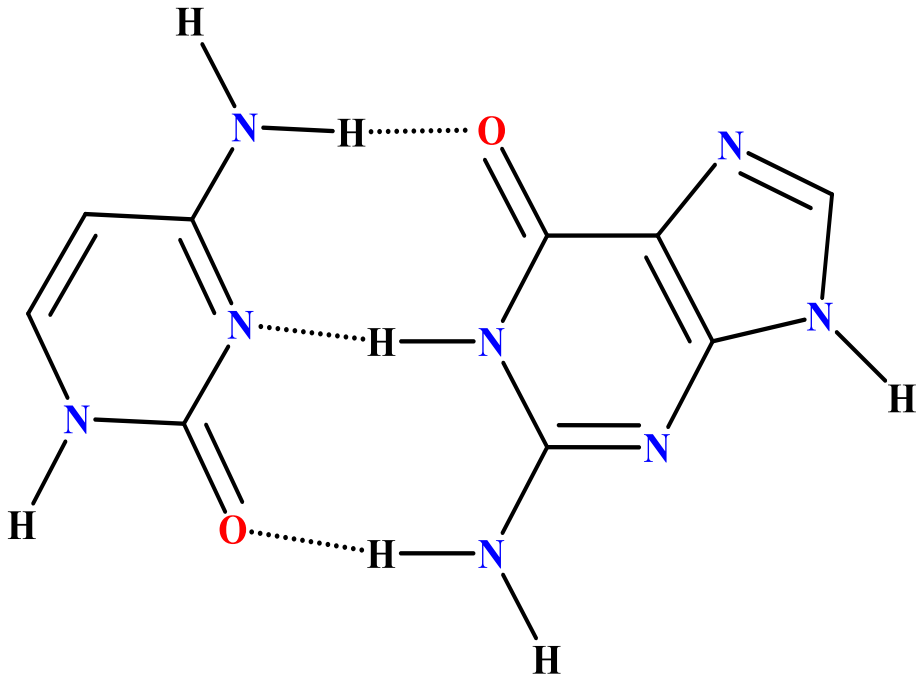


Dodecahedron

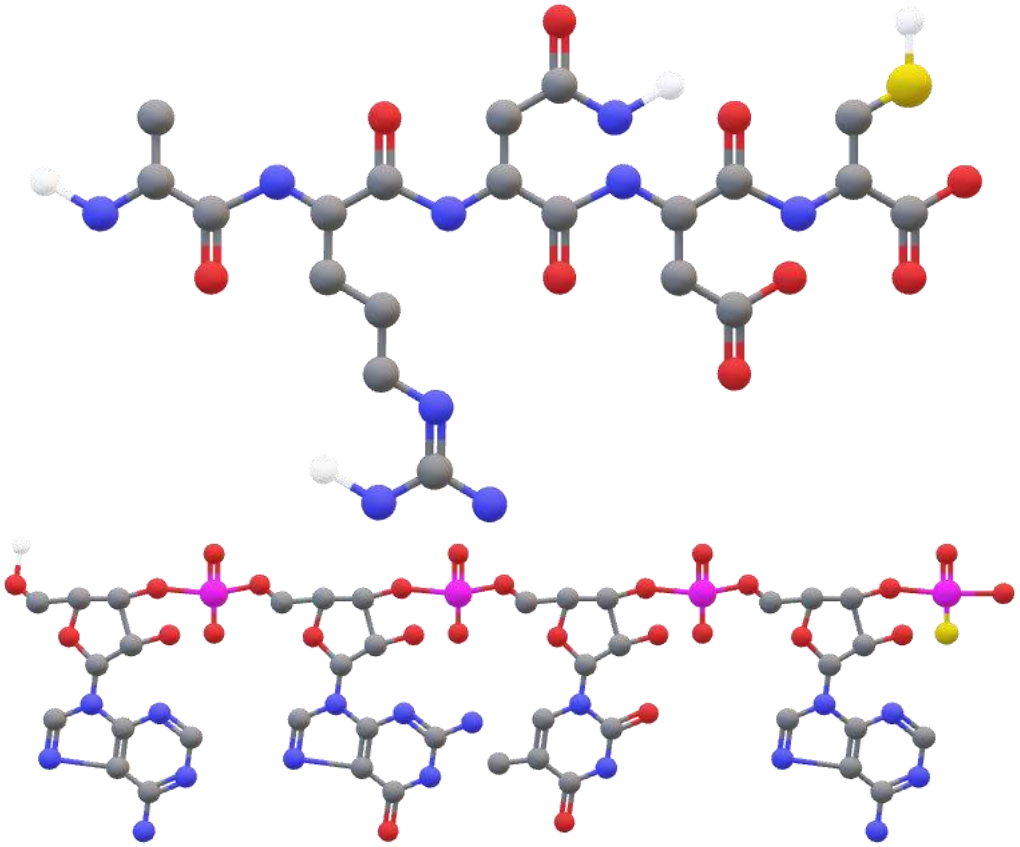
Hydrogen bonds

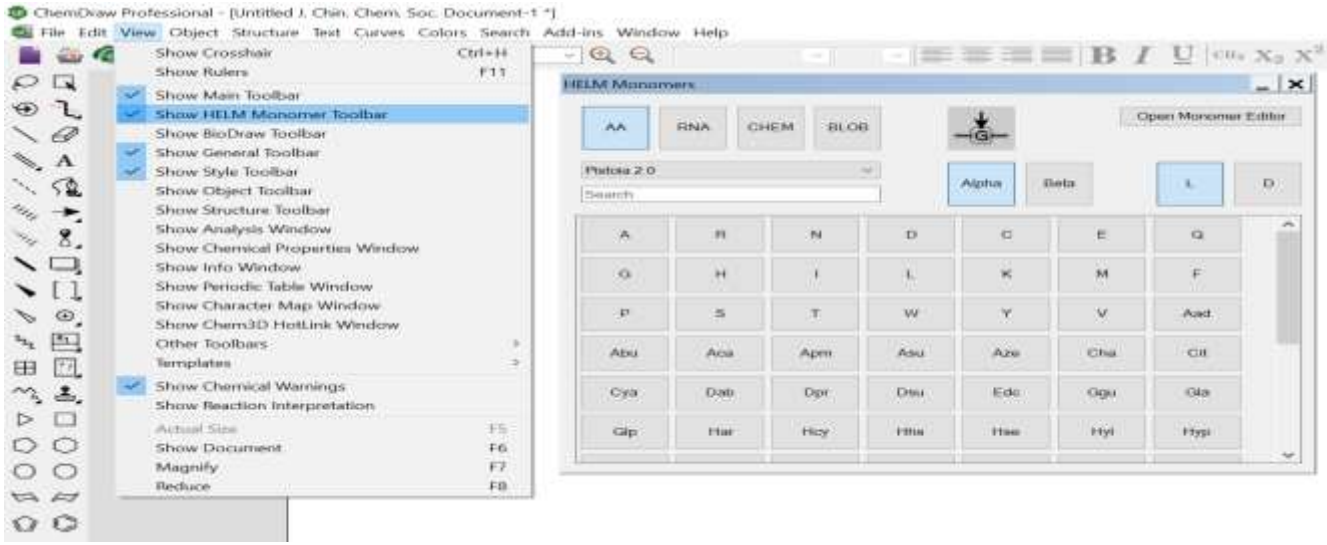
Formerly, dotted lines were used to represent hydrogen bonds, but now there is a specific bond tool for placement of such bonds. By explicitly recognizing a hydrogen bond, ChemDraw can handle them robustly and correctly. For example, hydrogen bonds are now correctly written to MOL files.

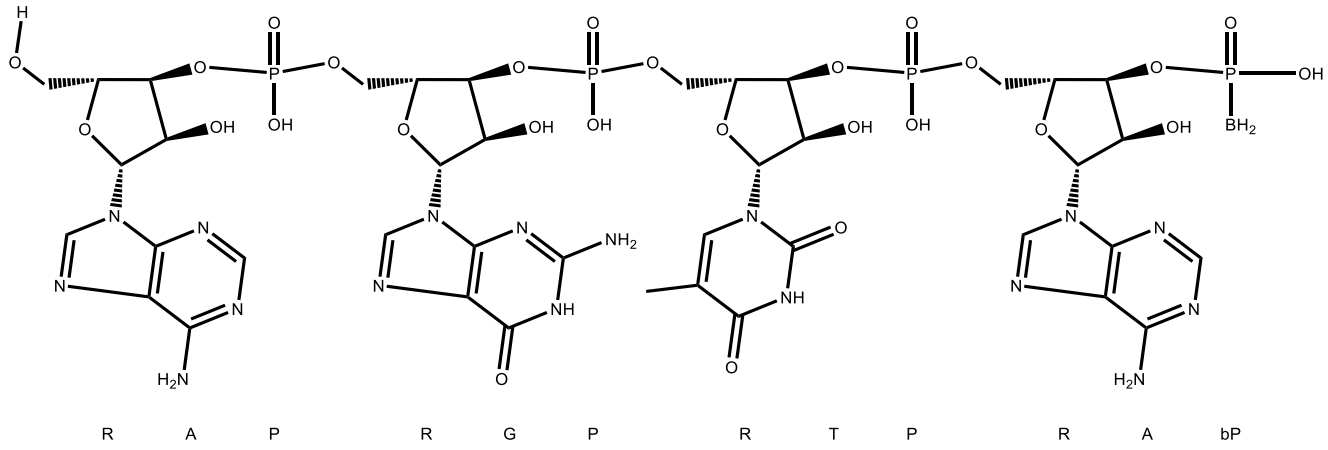




HELM Monomer Toolbar

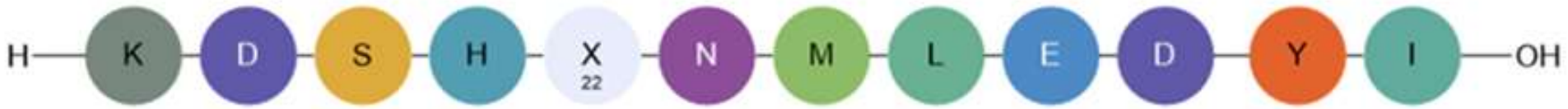




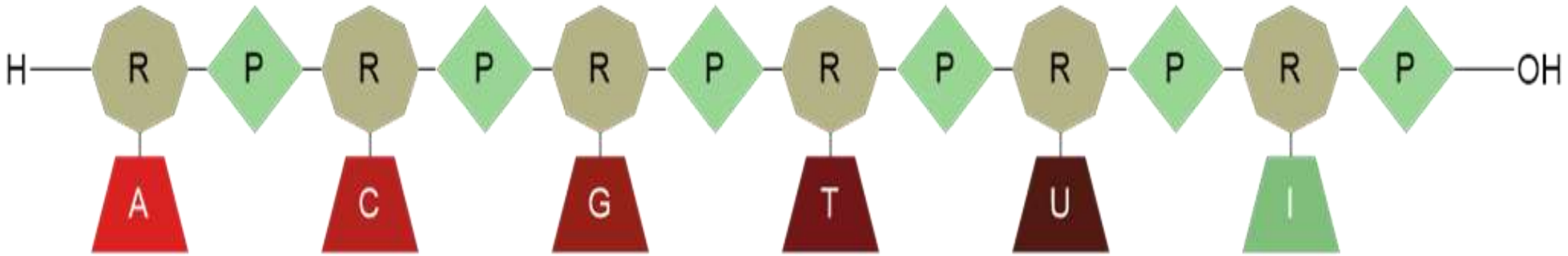


Sequence Graphic Monomers" stylesheet

- In case of the presence of **OR monomers**, a count indicating the number of members in the OR relationship is displayed as shown in the following image.

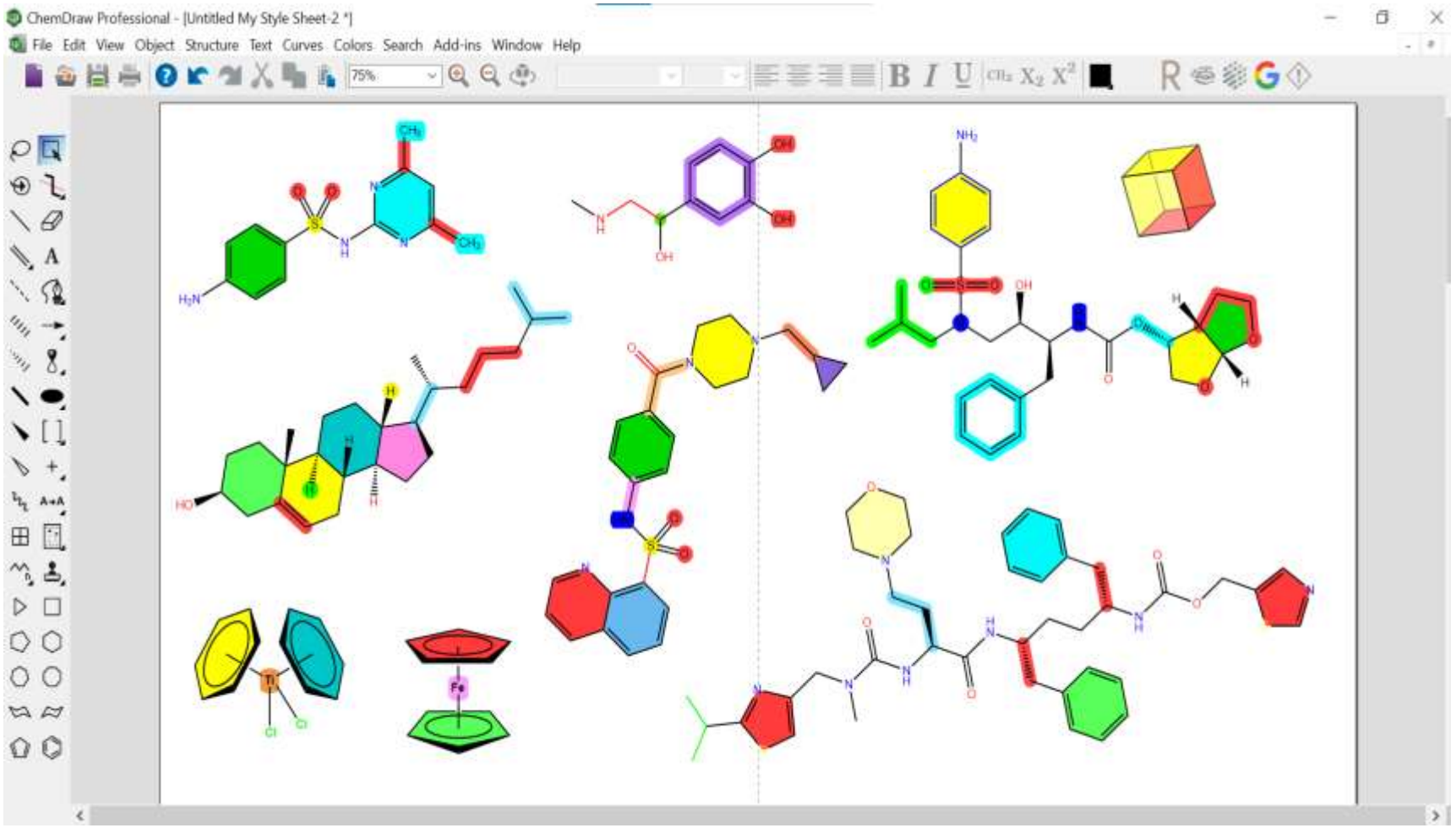


- In the case of DNA/RNA sequences

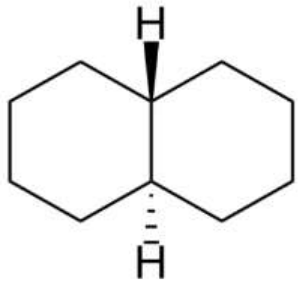


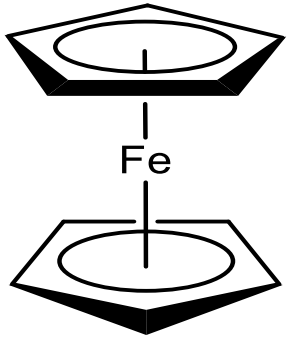
Highlight Colours

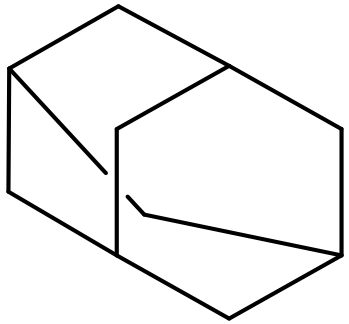
- Produce publication-worthy drawings with selected **atoms**, **bonds**, and **ring** colouring.

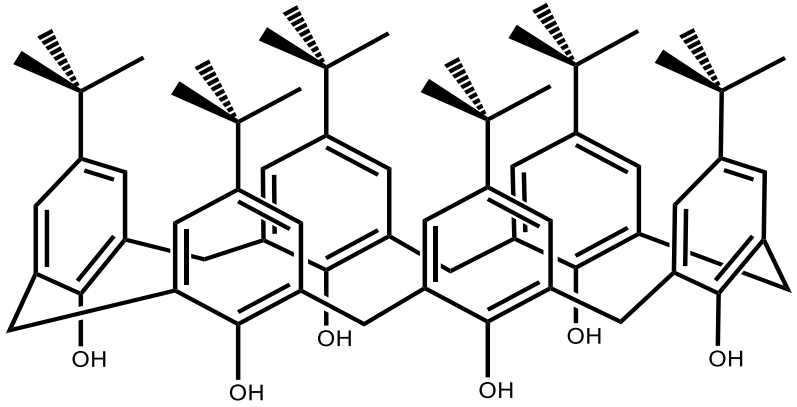


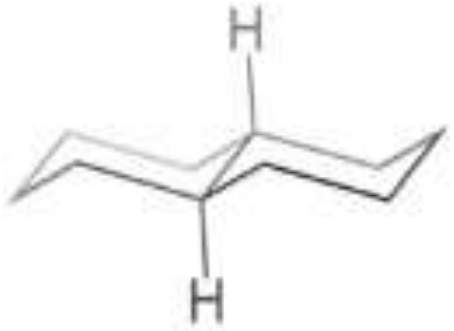
3D Clean-up

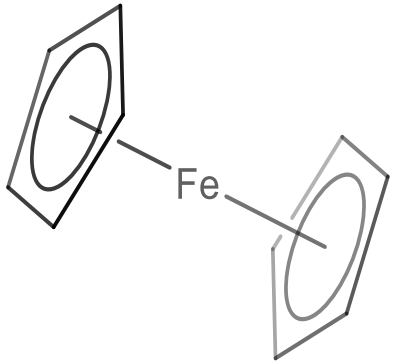


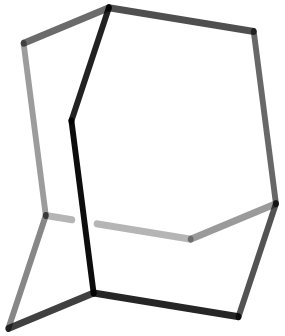


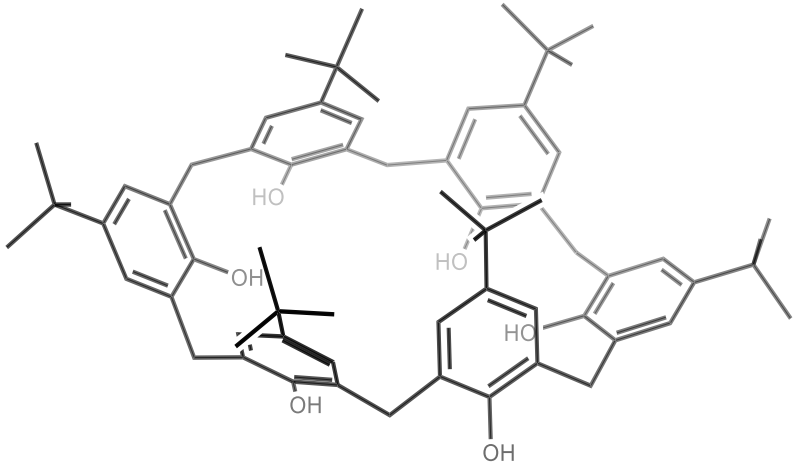




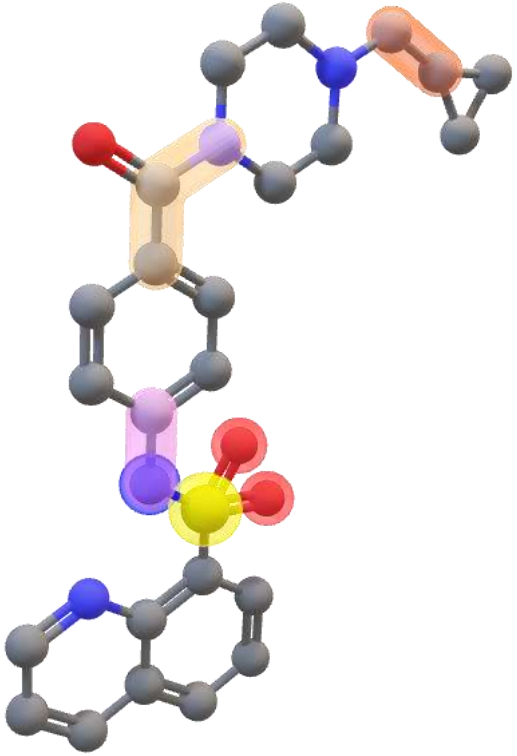


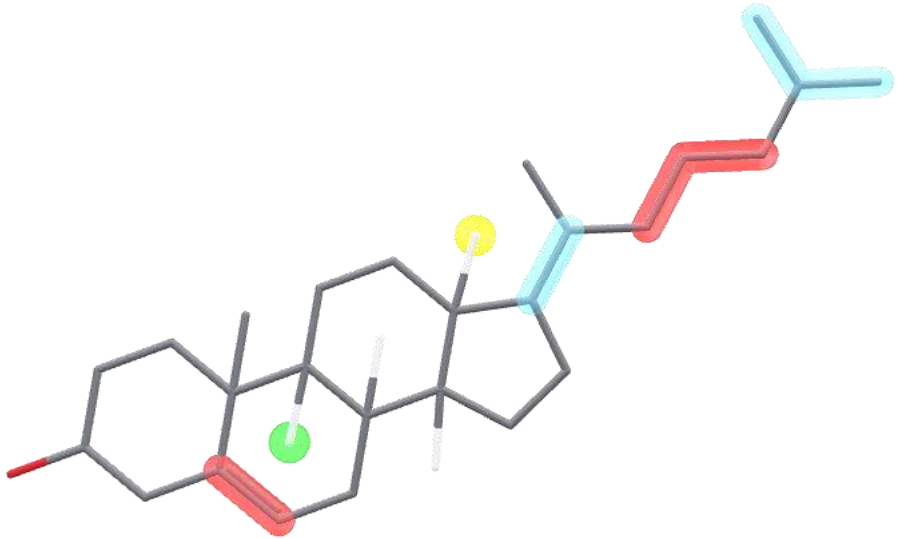


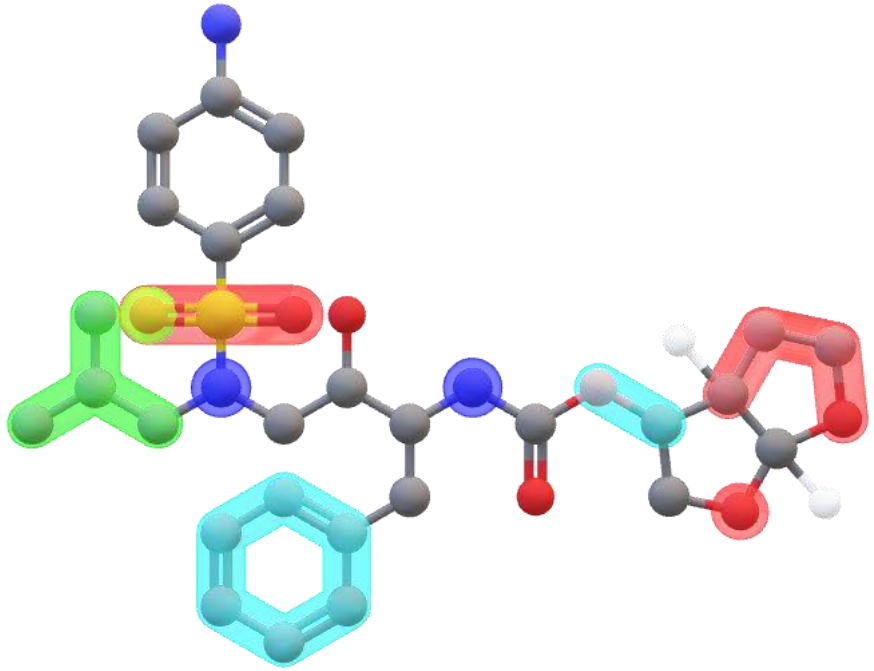


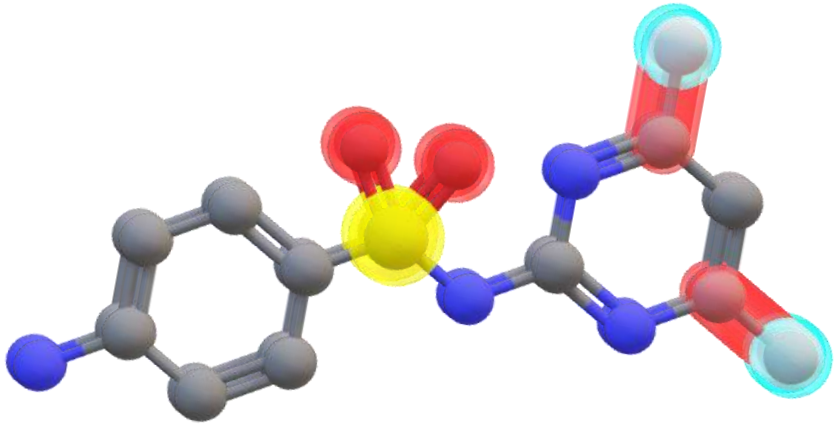


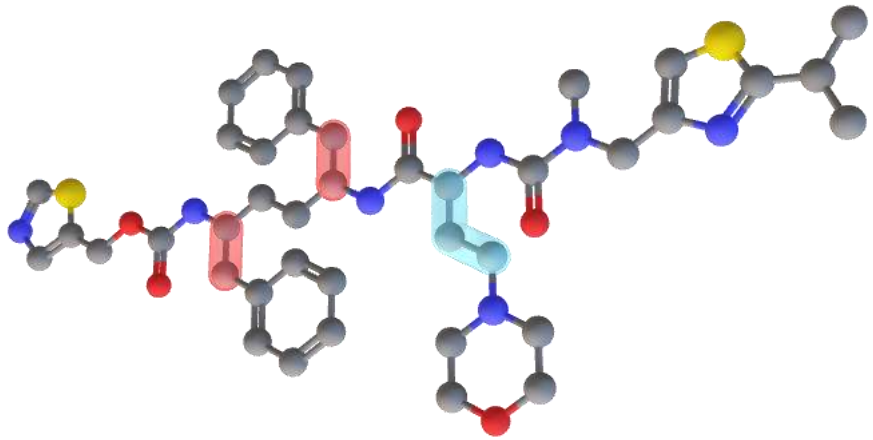
3D Printable Format (.3MF)











Signals Notebook

- Cloud-based collaborative platform,
- Available anytime, anywhere and on multiple devices.

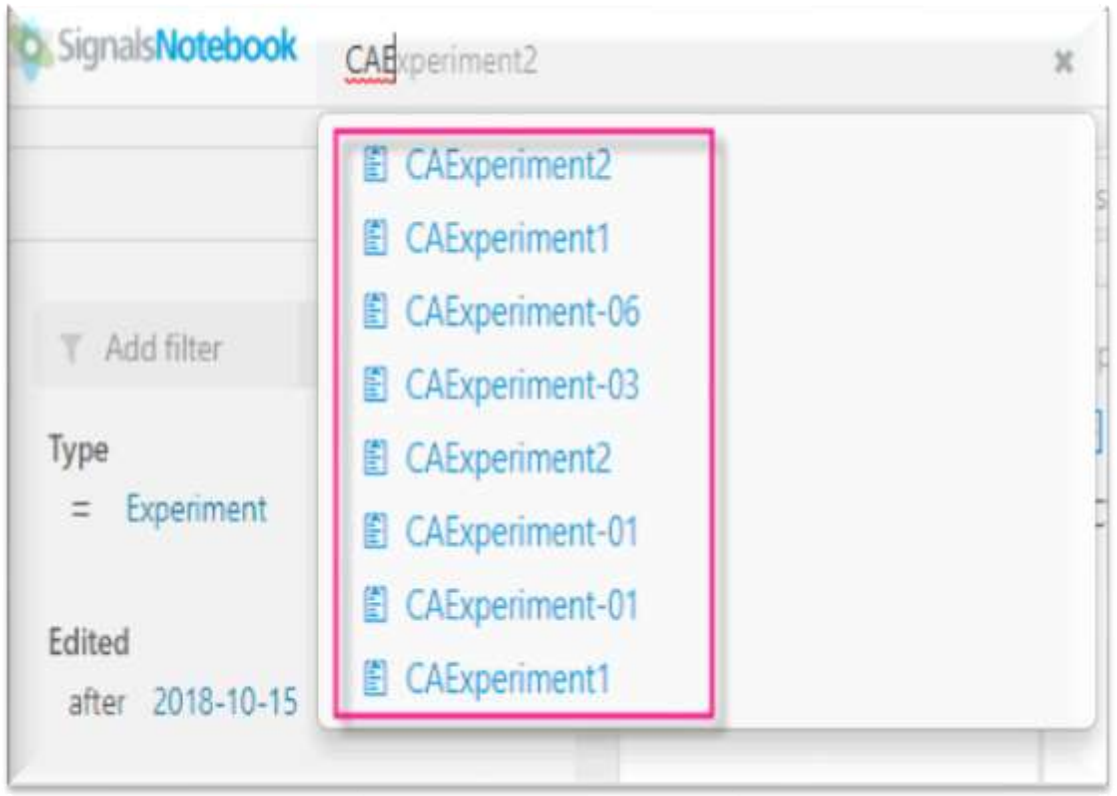
- Manage, Record, and Share your Experiments with Cloud Based Revvity Signals Notebook

- Connect and share data with colleagues and collaborators.

Searching Option

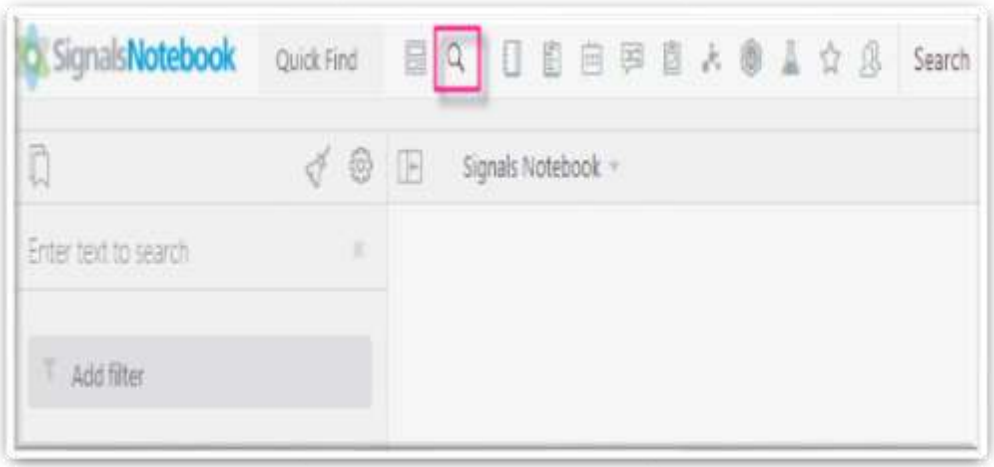
Two types of searches are available:-

- **Quick Find:-** Contains a text field where you enter the text that you are looking for.
- **Advanced Search:-** Provides you multiple query fields that you can combine to create and run a query. Advanced search allows you to perform a text search as well.



Advanced Search

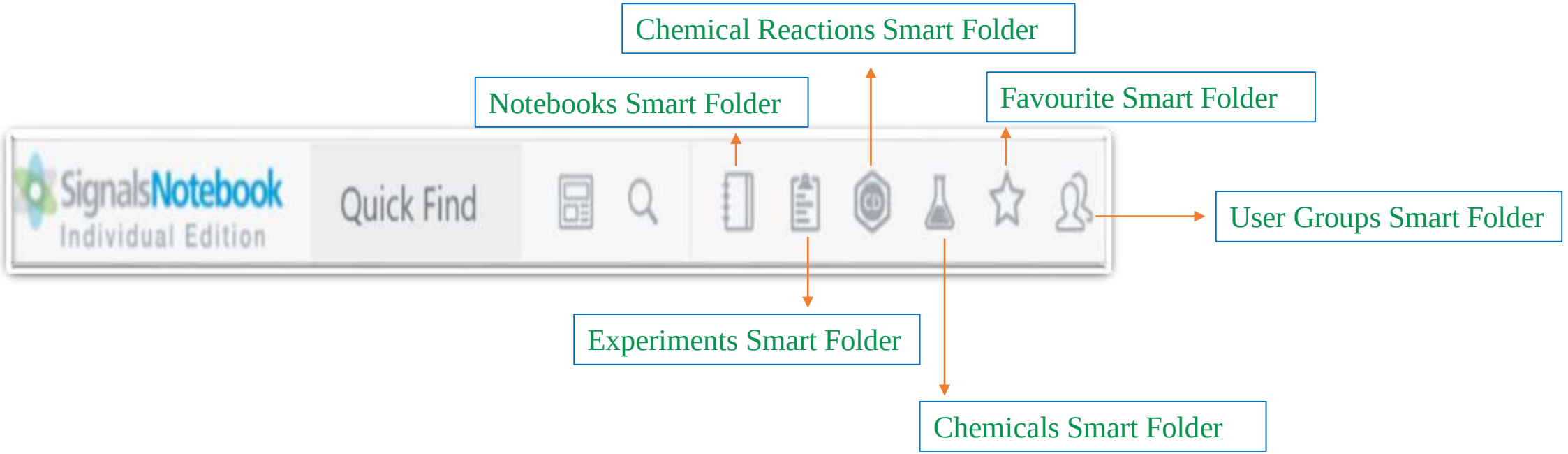
- Using the Advanced Search page you can run chemical, text or combined chemical and text searches.
- You can access the advanced search page by clicking on the Search icon in Signals Notebook toolbar.



Field Filter	Description
Chemical	Allows you to draw and search for chemical structure.
Text	Allows you to add text field type such as product name, reactant name, MF, resource name, project name, supplier name, etc....
Key	Allows you to add resource type and state fields.
Numeric	Allows you to add numeric fields such as actual mass, purity, sample mass, pressure, etc....
Date	Allows you to add date fields such as created date, modified date, etc....
Boolean	Allows you to add a boolean field type such as Sequence Confirmed, etc....
User	Allows you to add user types fields such as creator, reviewer, etc

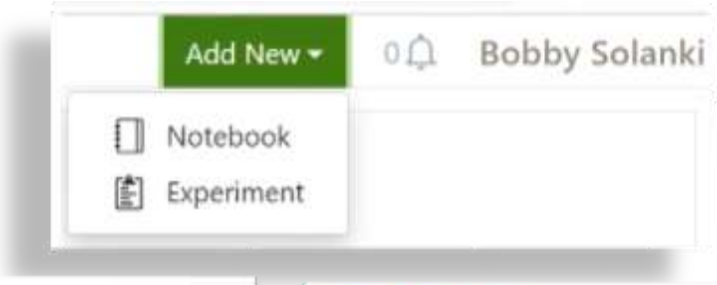
Smart Folders

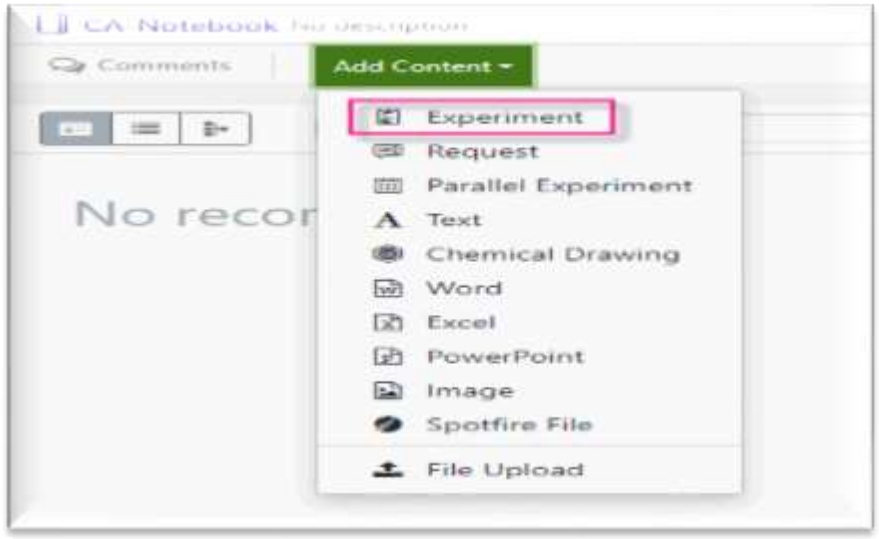
- Smart folders are available in the Signals Notebook header and allow you to navigate to your notebooks, experiments, requests, tasks, materials, chemical reactions, chemicals, favourites items and user groups with a single click.

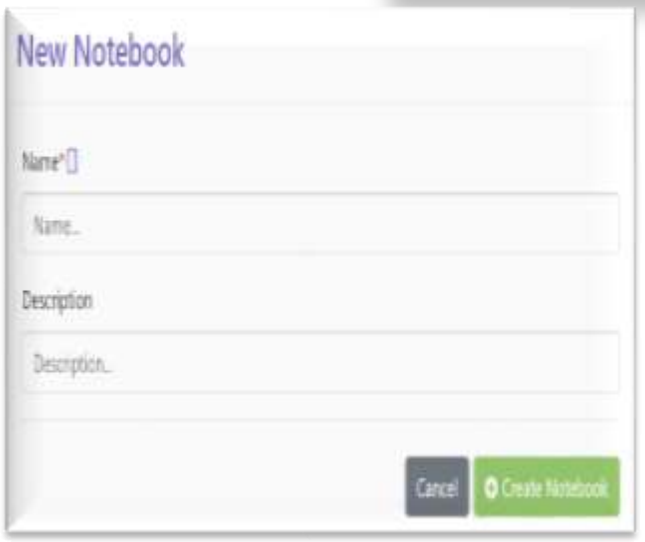


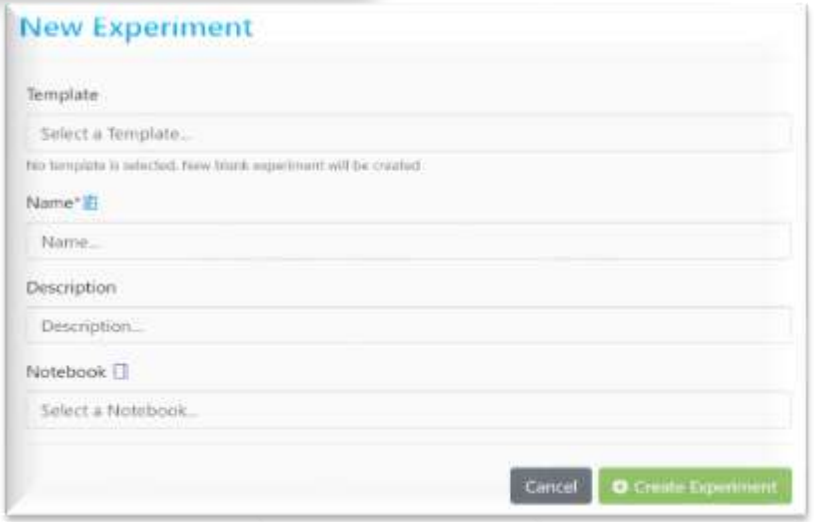
Creating Notebook/Experiment

- You can create an experiment under a notebook or an independent experiment not as a part of any notebook.



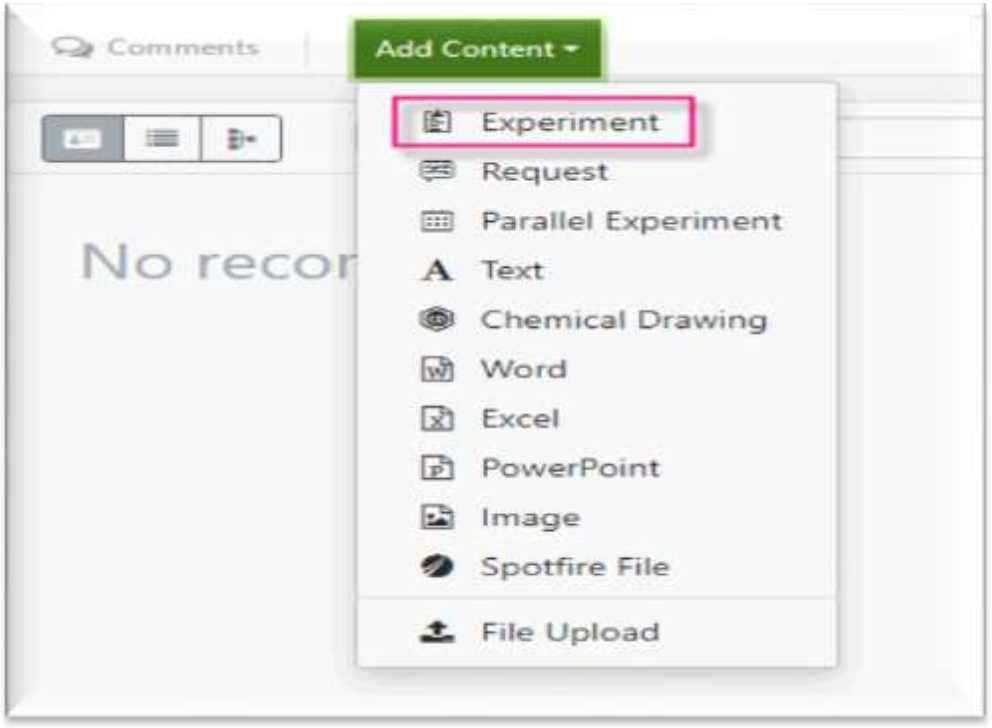






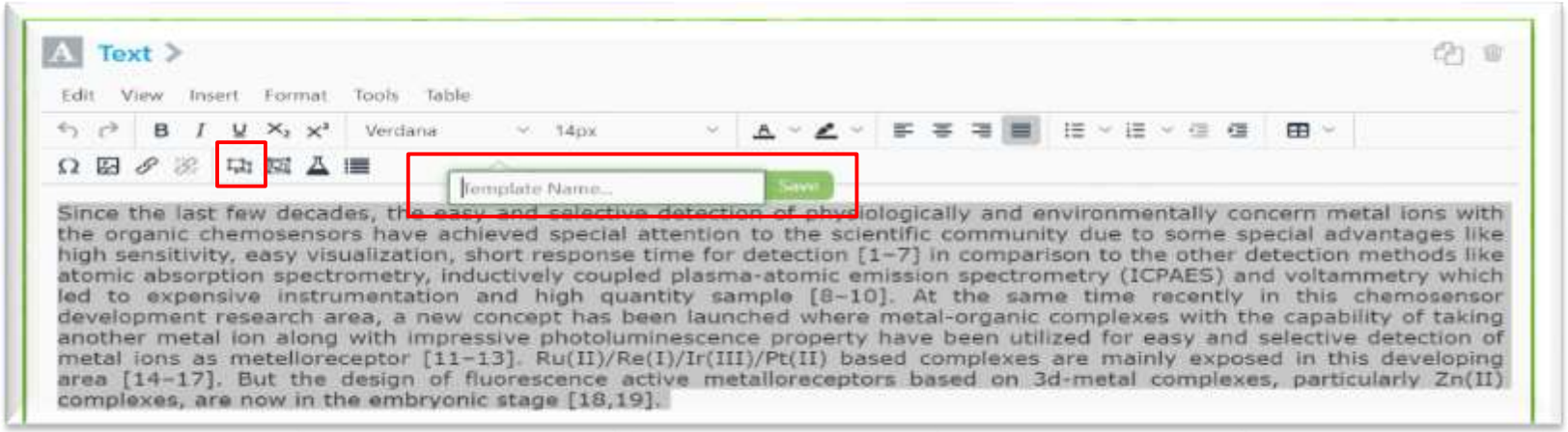
Adding Information Items to an Experiment

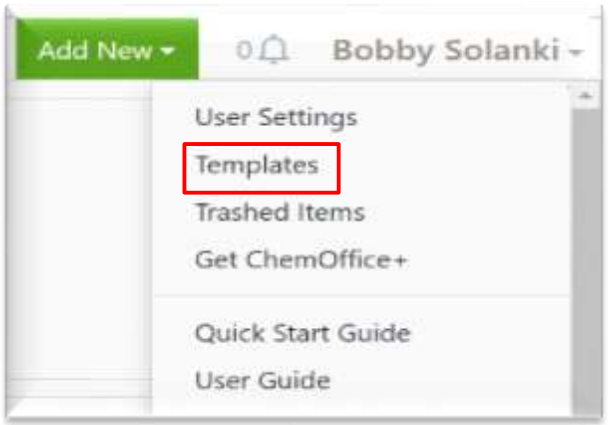
- Once you create an independent experiment or within a notebook, you are ready to start adding content by adding files to your experiment.
- You can also add files to your experiment using the drag and drop method.



Create Templates

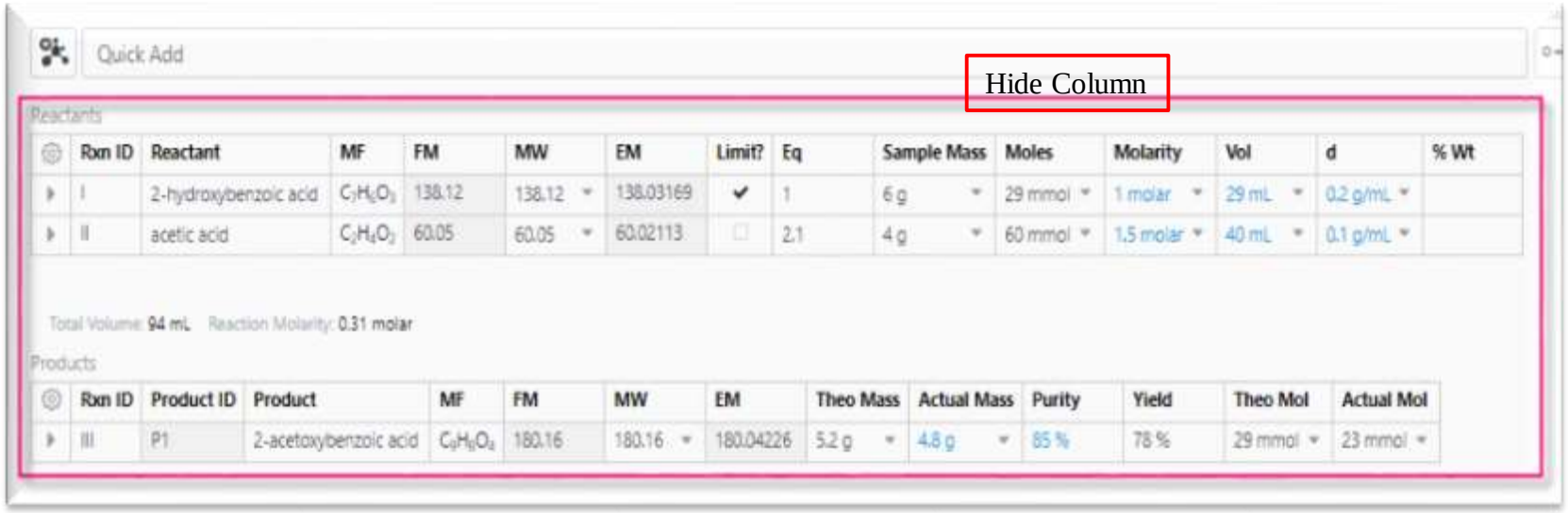
- A text template is a set of instructions which are common to different text information items. If you create a text template to contain the instruction set, you do not have to re-type them for each text information item to which they apply. You can create text templates for the Text information item.





Working with Stereometry Grid

- The Stoichiometry grid analyzes the reaction drawing automatically. It consists of reactant's details and product's details. It automatically calculates and stores sample mass, moles, density, volume, and many other variables of the reactions.
- The Stoichiometry grid shows "The reaction has no Reactants" and the "The reaction has no Products" messages when there are no structures in the drawing area.



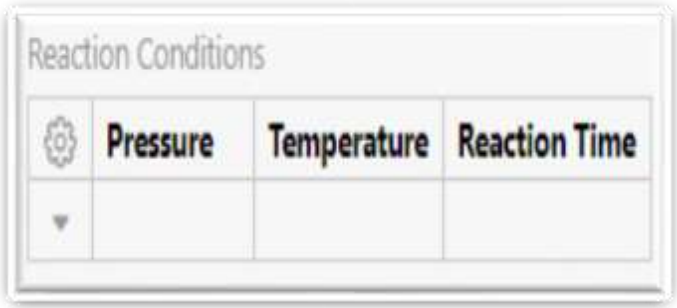
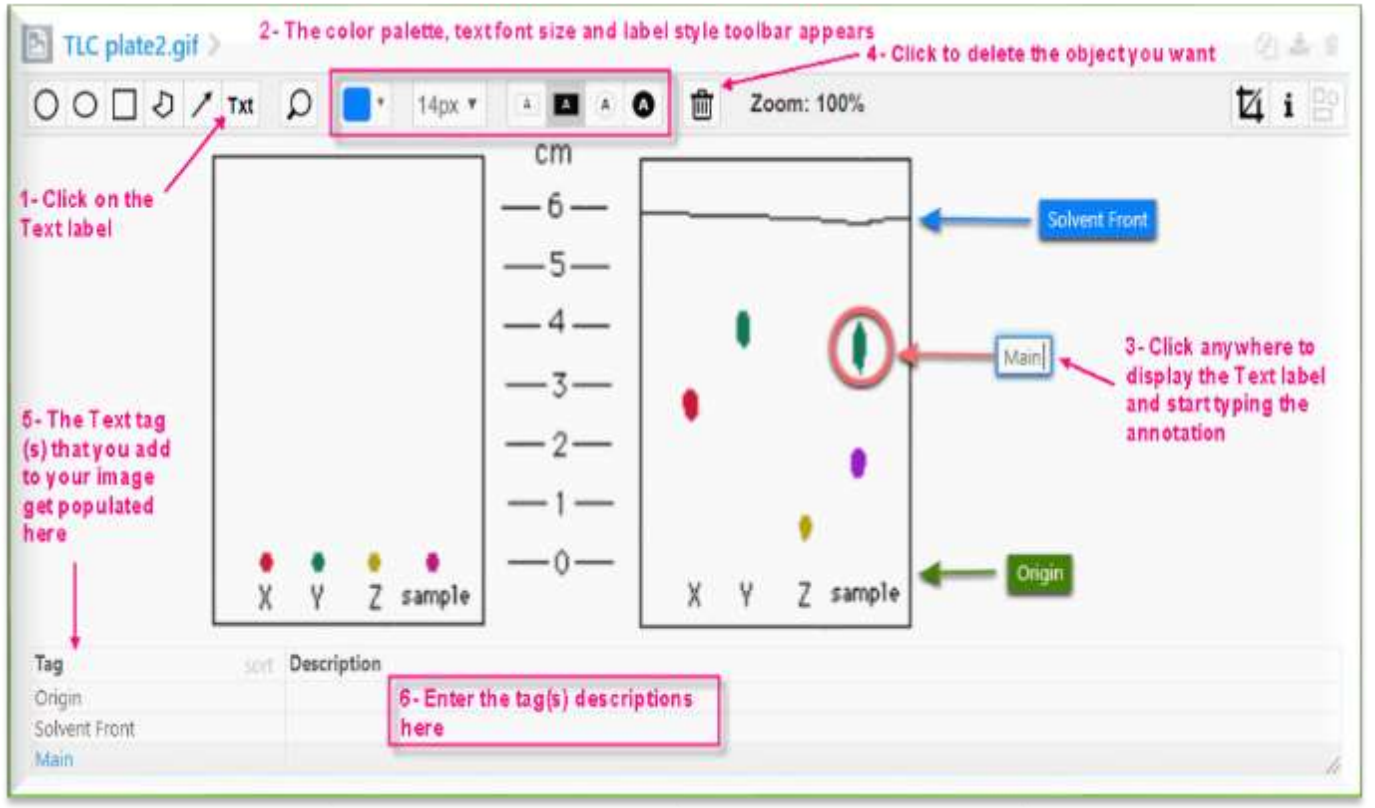


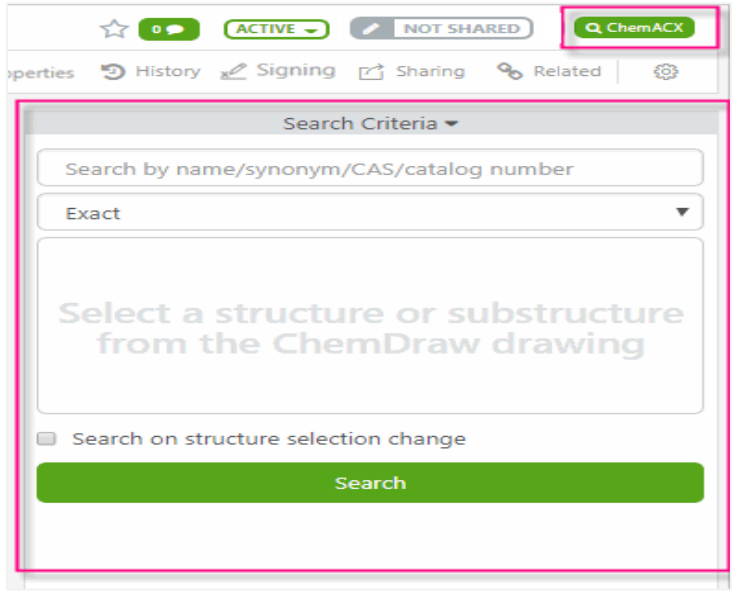
Image Annotation

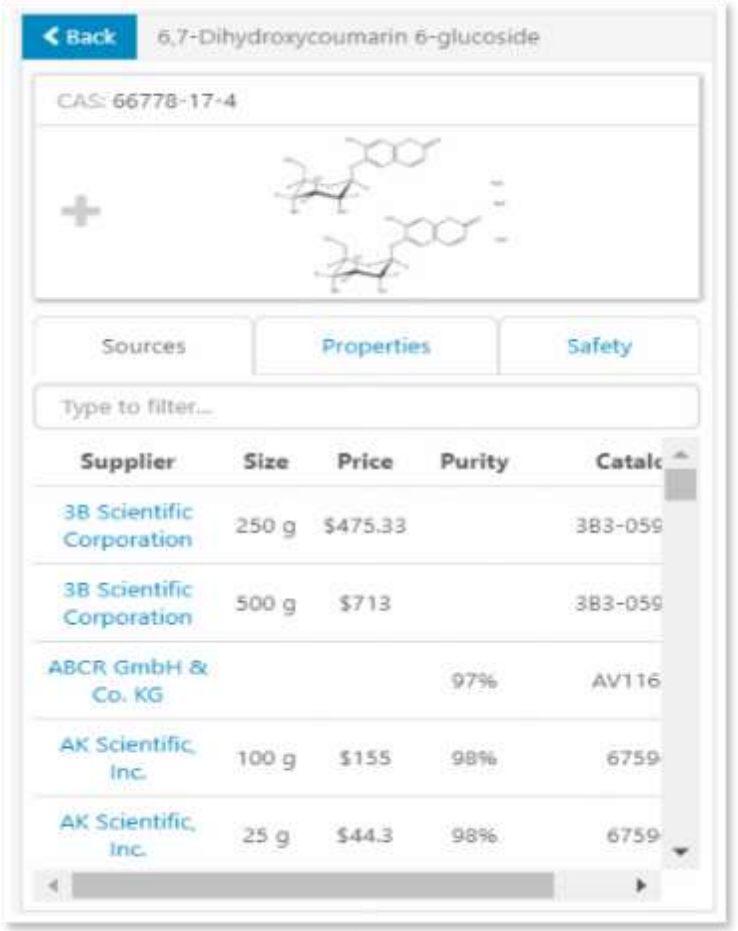
- You can add a tag to an image as an annotation. When you reference the tag again in the future, it can help you remember image details and also collaborate on those details with colleagues. You can also use tags to search for images.



Chem ACX Integration

- ChemACX (Available Chemicals Exchange) is your guide to commercially available chemicals worldwide. Whether you are planning a bench synthesis, scale-up, or a commercial process, you can search these databases to determine the availability and sources for the chemicals you need.
- You can access ChemACX and search for chemicals from the Signals Notebook interface.



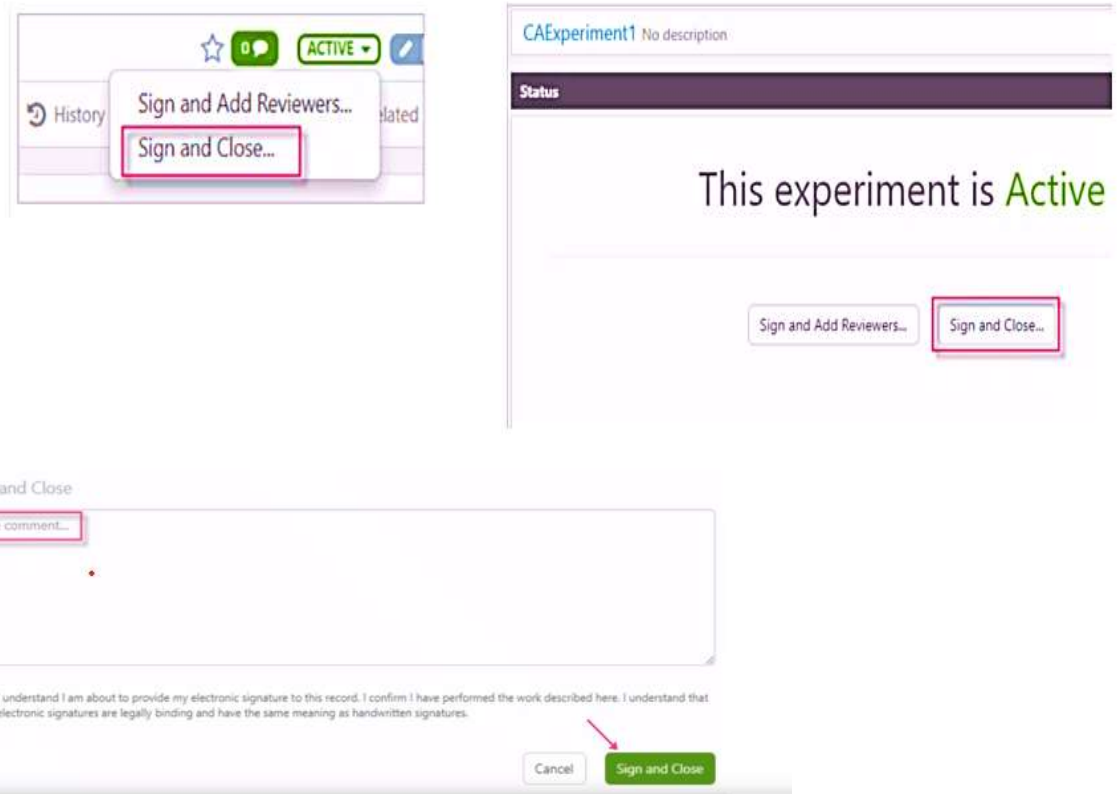


You can search ChemACX by:

- Chemical structure
- Chemical substructure
- Compound name
- Compound synonym
- CAS Register number
- Catalog number

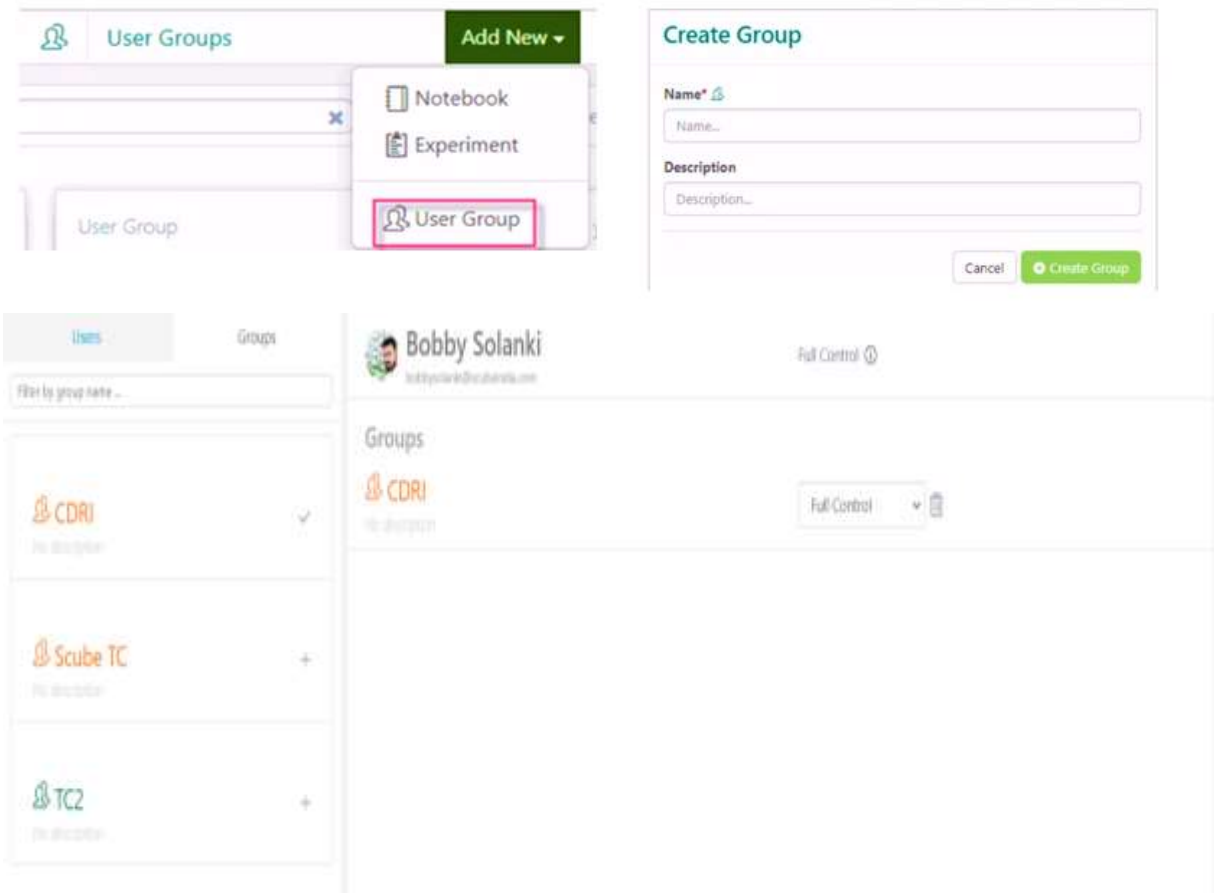
Signing and Closing an Experiment

- When you have completed your experiment, you can electronically sign it without a reviewer.
- Once you complete and electronically sign your experiment, you can select a Signals Notebook user to electronically accept or reject your experiment as a reviewer.



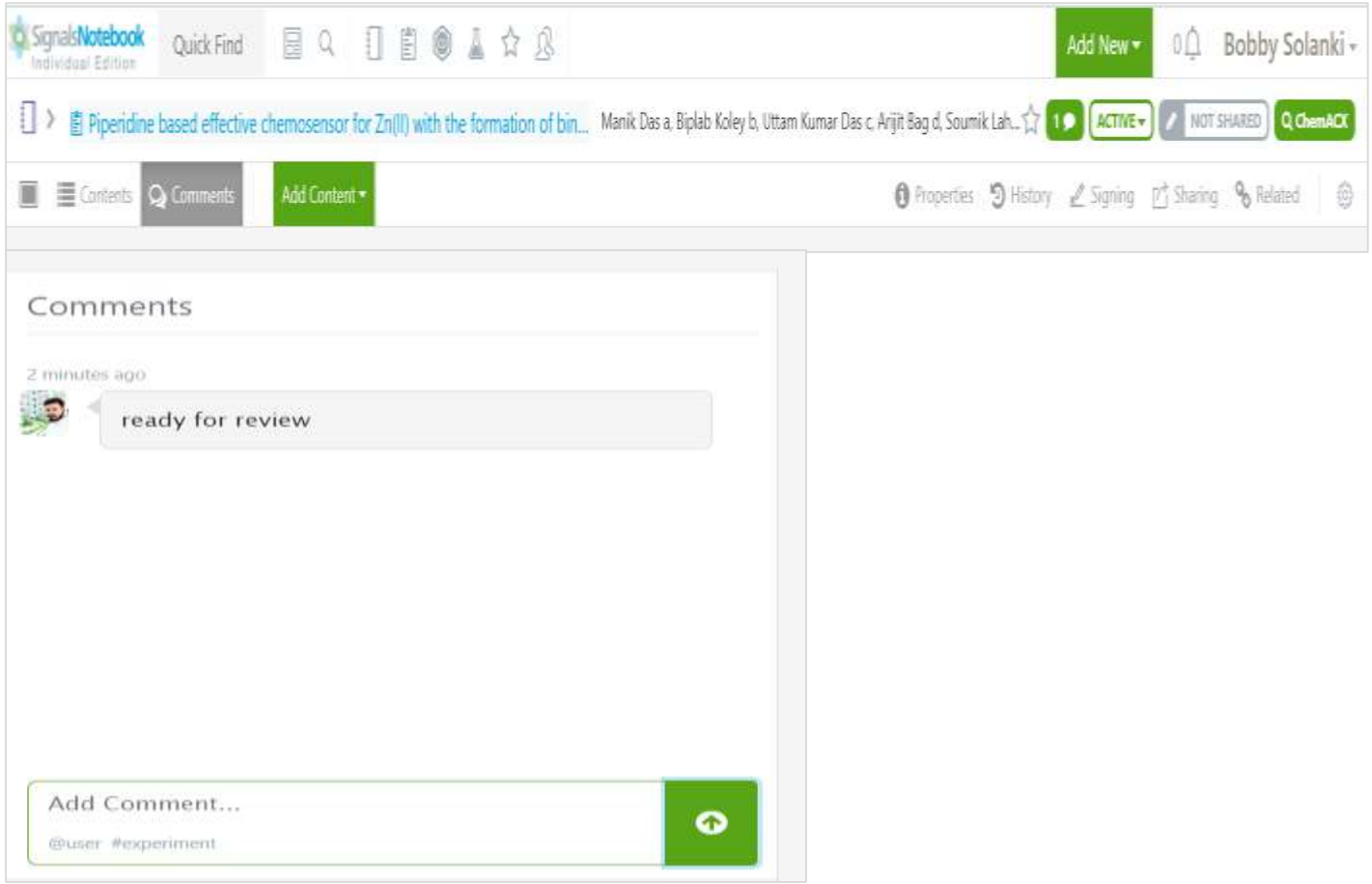
Creating a Group

- You can create a group for sharing or collaboration.
- A system group is a set of users who have the same interests and privileges.
- For example, as a laboratory supervisor, you might want to create a laboratory technicians group so you can share assignments with them or as a professor or teacher's assistant (TA), you might want to create a Students Group so you can share assignments with them.



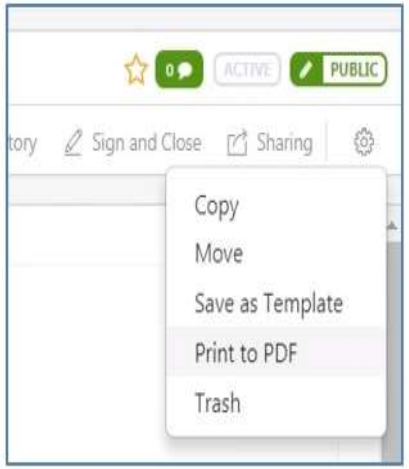
Adding Comments

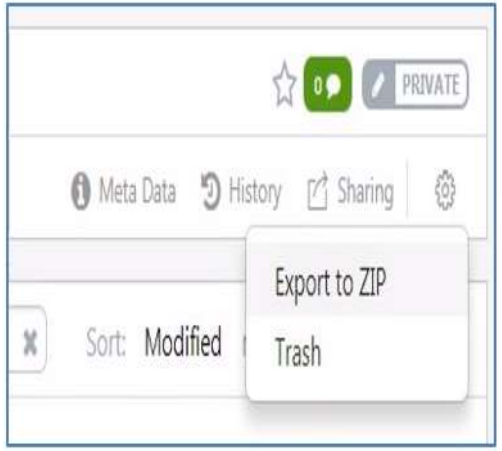
- You can add comments to the resources. The number of comments added by you or by the collaborators to the resources appears in the header.

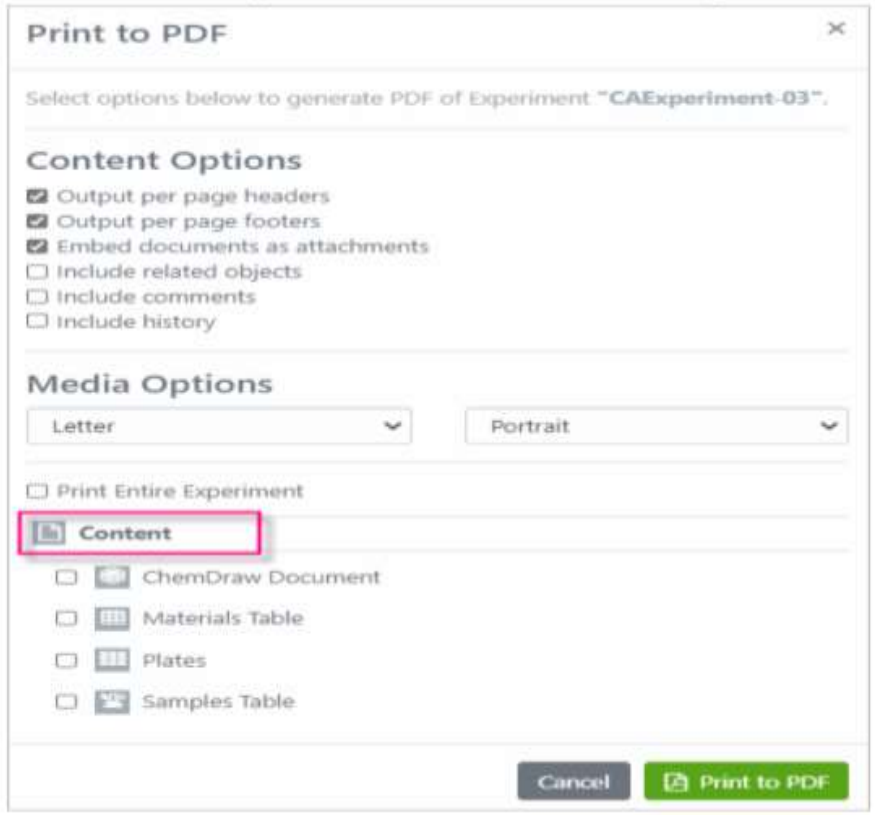


Exporting Notebooks/Print to Pdf

- You can print the content of your experiments into a PDF format and save it locally. That way, you can have access to your experiments outside of the Signals Notebook application.

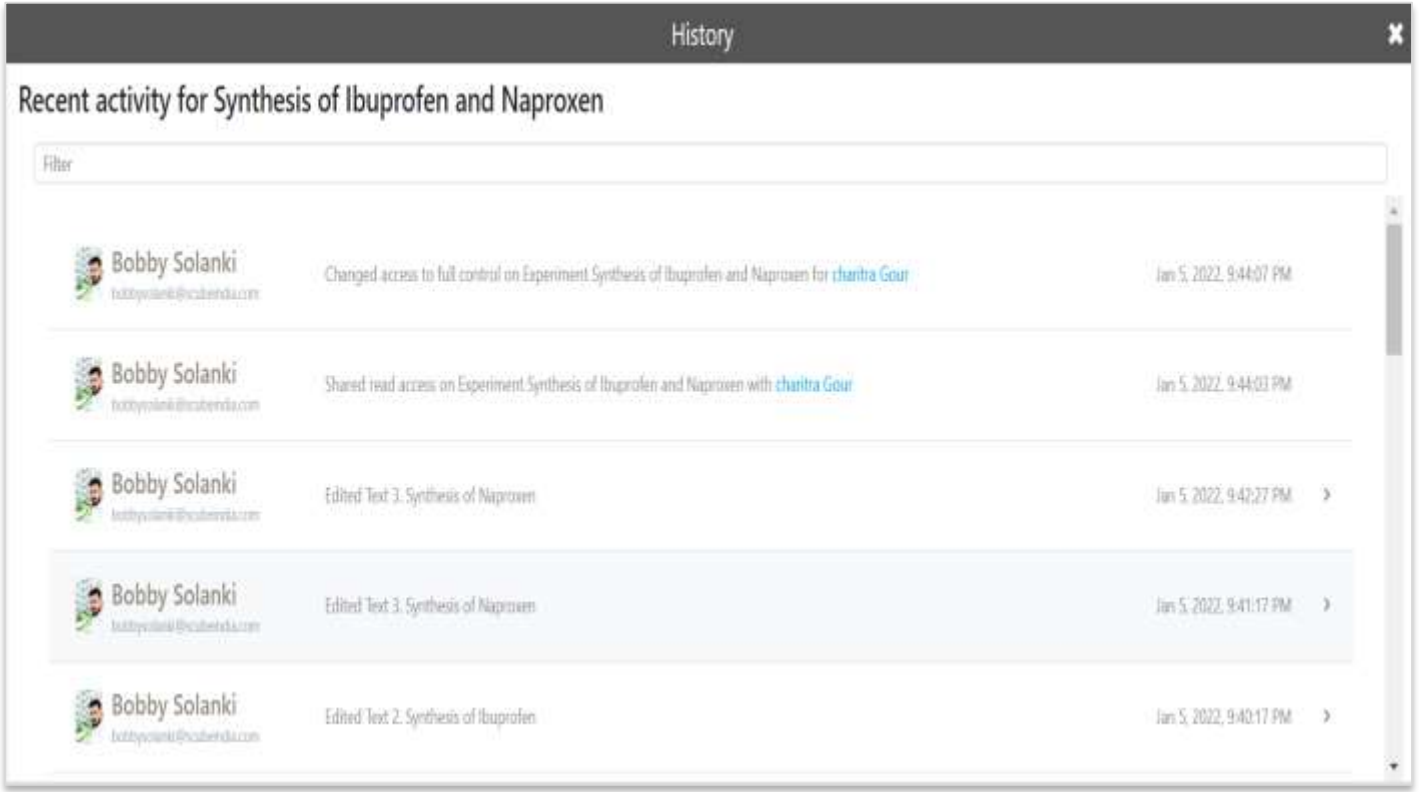






History

- For all actions such as creation, edit, rename, trash, restore, etc a log (revision) is created in the History tab for the resources.



Thank You

bobbysolanki@scubeindia.com