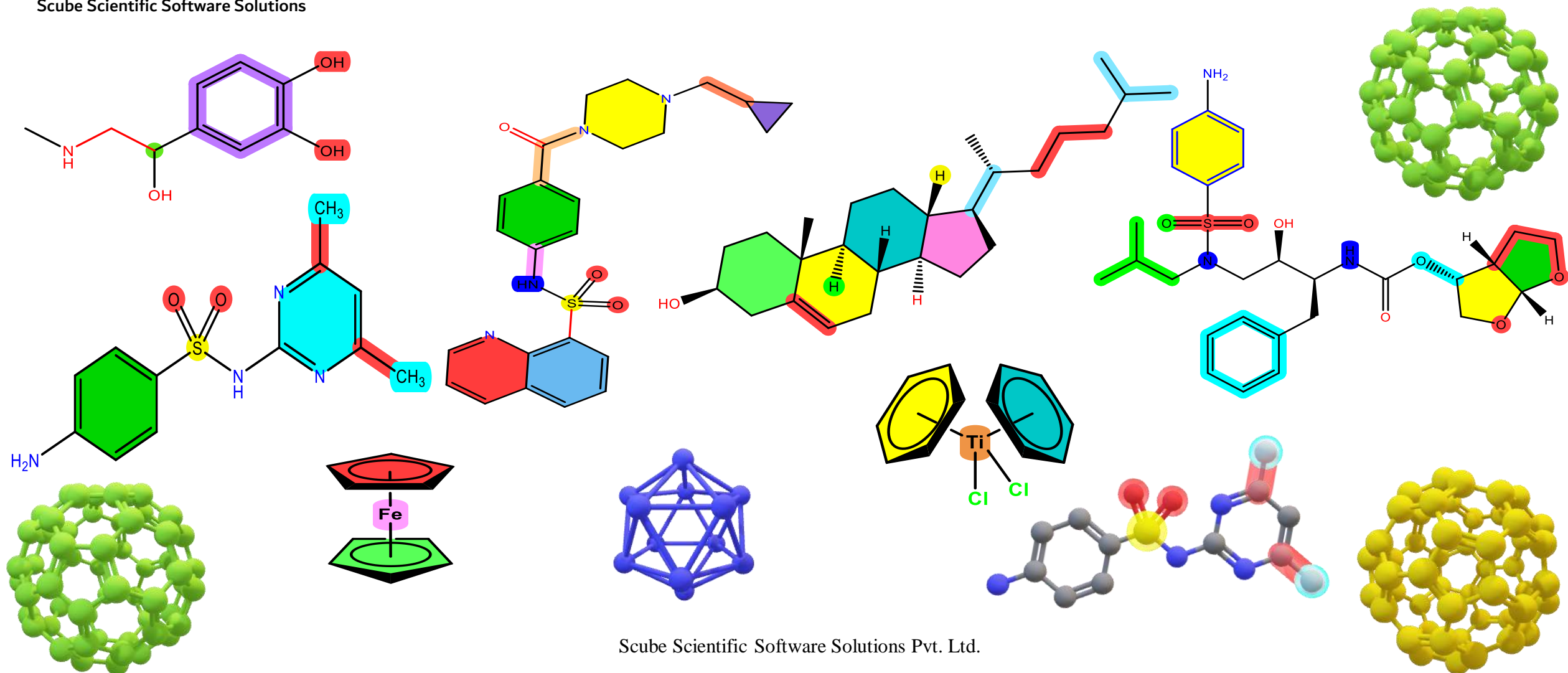




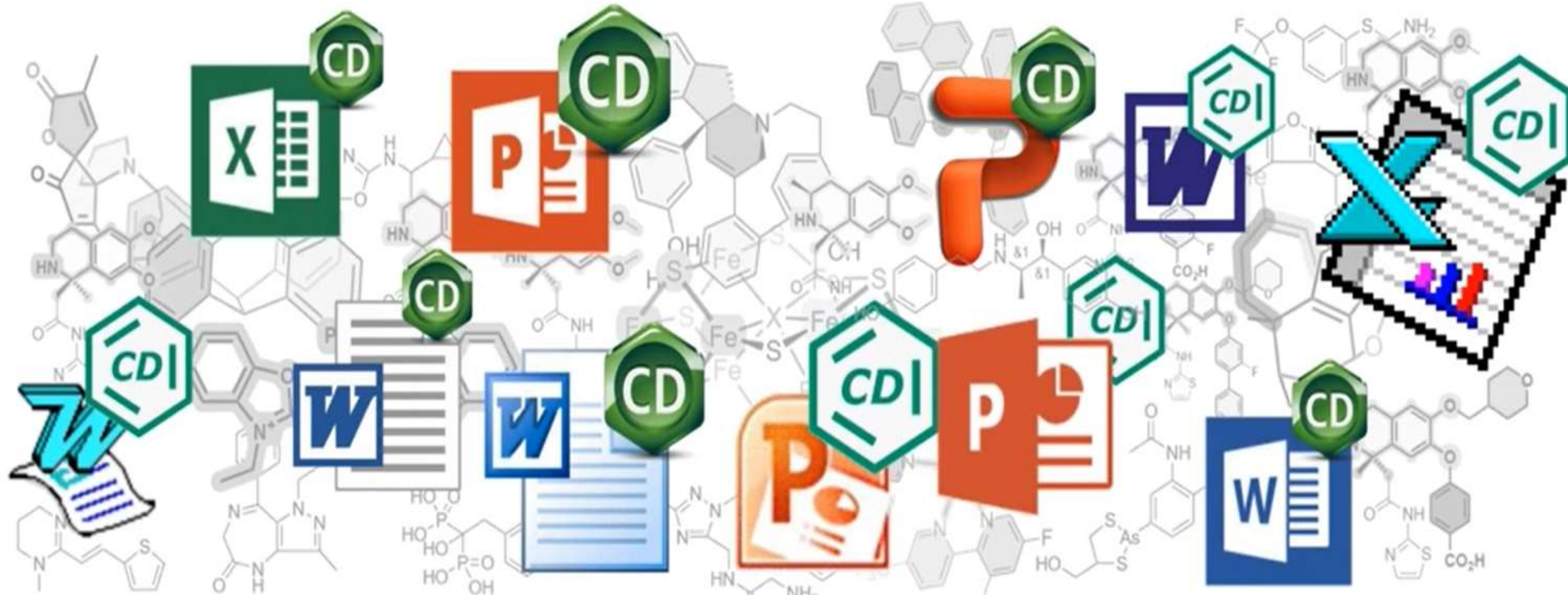
# ChemDraw v23.0

**Bobby Solanki**

Technical Consultant  
Scube Scientific Software Solutions

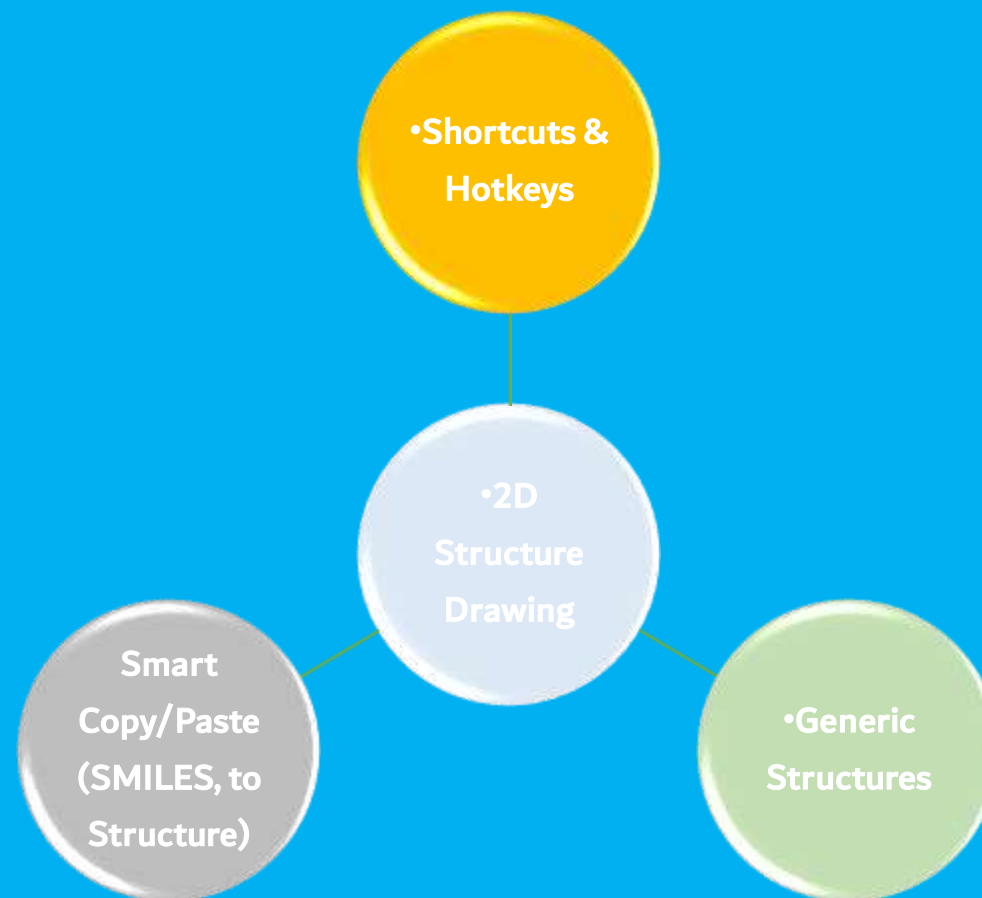


# ChemDraw





# 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

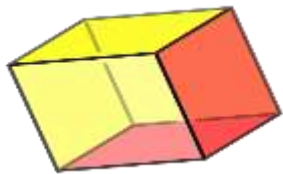


Unlock your chemistry data: capture, retrieve, store and share

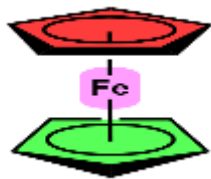
HELM Monomer  
Curation



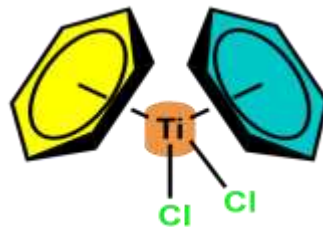
Manage & Curate Custom Monomer Libraries for use in ChemDraw+



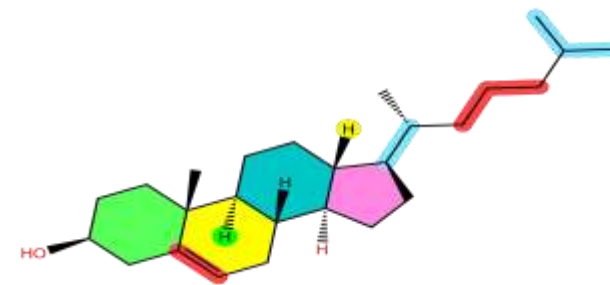
Molecular Weight: 104.15  
Formula: C<sub>8</sub>H<sub>8</sub>  
Exact Mass: 104.06  
Chemical Name: cubane  
CLogP: 2.30



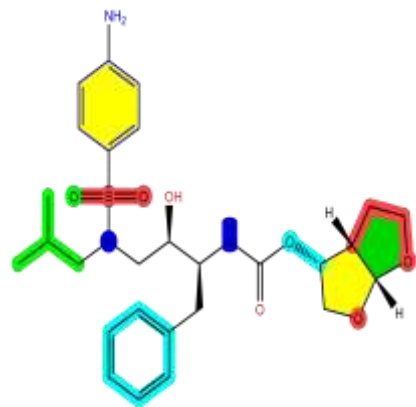
Molecular Weight: 186.04  
Formula: C<sub>10</sub>H<sub>10</sub>Fe  
Exact Mass: 186.01  
Chemical Name:  
CLogP: 1.78



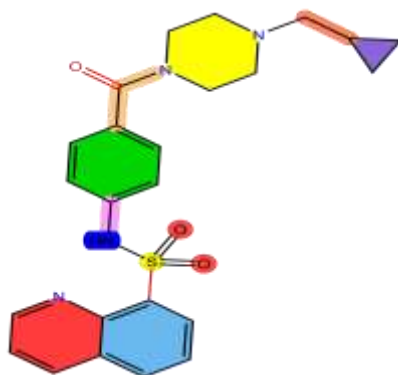
Molecular Weight: 275.00  
Formula: C<sub>12</sub>H<sub>12</sub>Cl<sub>2</sub>Ti  
Exact Mass: 273.98  
Chemical Name:  
CLogP: 2.14



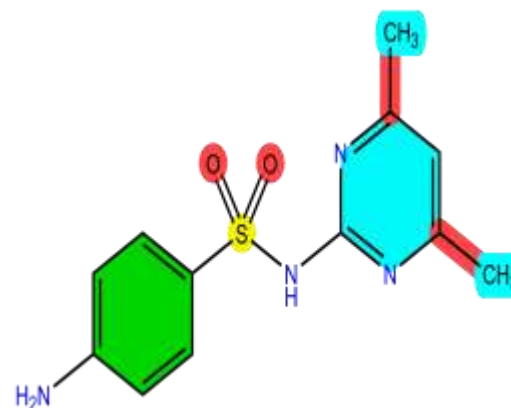
Molecular Weight: 372.64  
Formula: C<sub>26</sub>H<sub>44</sub>O  
Exact Mass: 372.34  
Chemical Name: cholesterol  
CLogP: 9.00



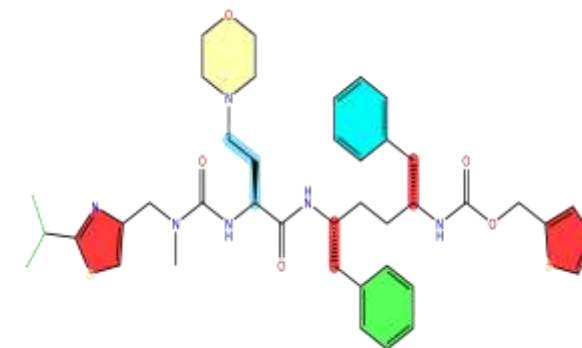
Molecular Weight: 547.67  
Formula: C<sub>27</sub>H<sub>37</sub>N<sub>3</sub>O<sub>7</sub>S  
Exact Mass: 547.24  
Chemical Name: (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ((2S,3R)-4-((4-amino-N-isobutylphenyl)sulfonamido)-3-hydroxy-1-phenylbutan-2-yl)carbamate  
CLogP: 2.89



Molecular Weight: 450.56  
Formula: C<sub>24</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>S  
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: C<sub>12</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>S  
Exact Mass: 278.08  
Chemical Name: 4-amino-N-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide  
CLogP: 1.10



Molecular Weight: 776.03  
Formula: C<sub>40</sub>H<sub>53</sub>N<sub>7</sub>O<sub>5</sub>S<sub>2</sub>  
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

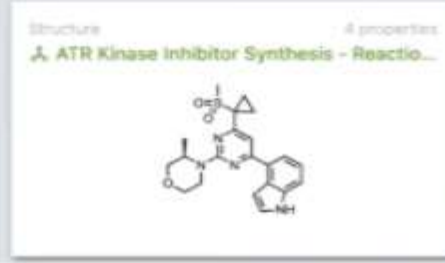
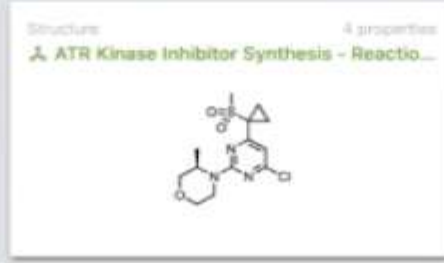
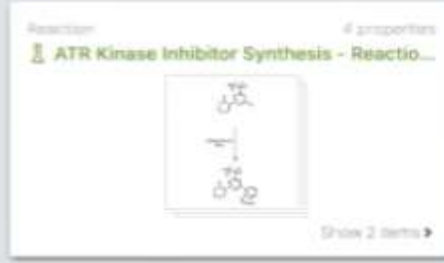
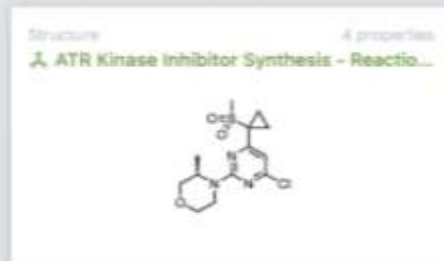
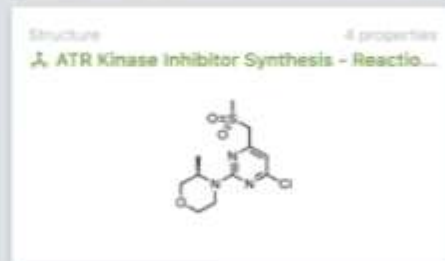
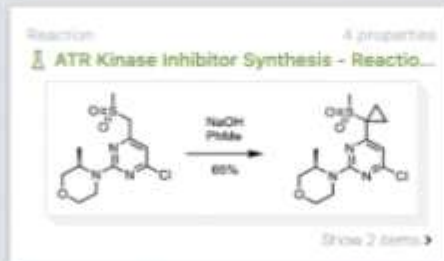
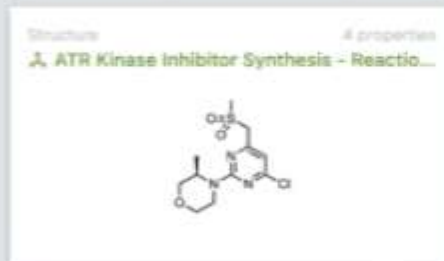
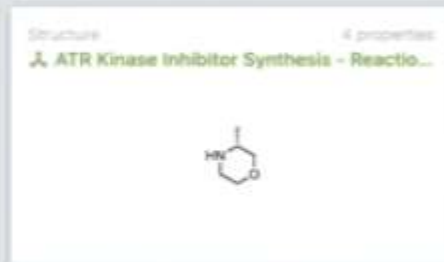
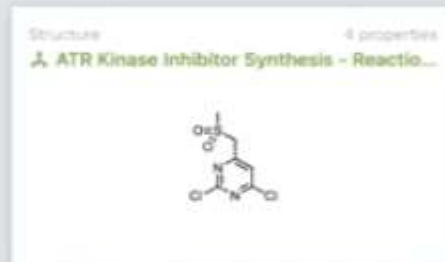
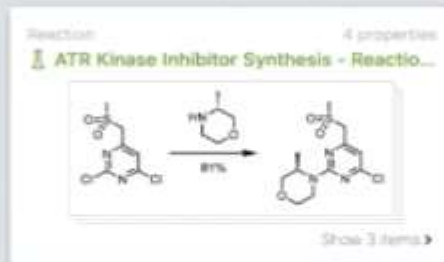
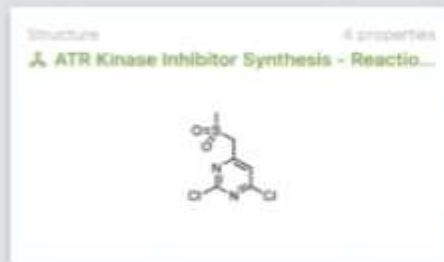
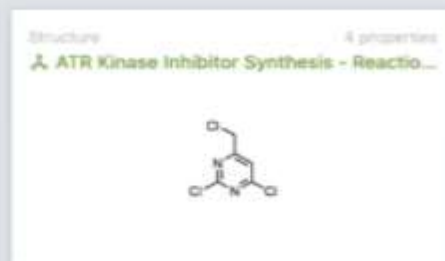
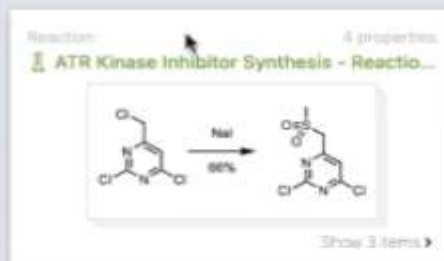
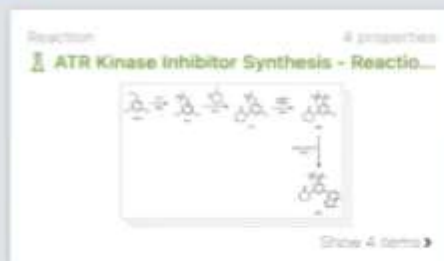


Filter X

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
- Cvrotorhane.cdxml





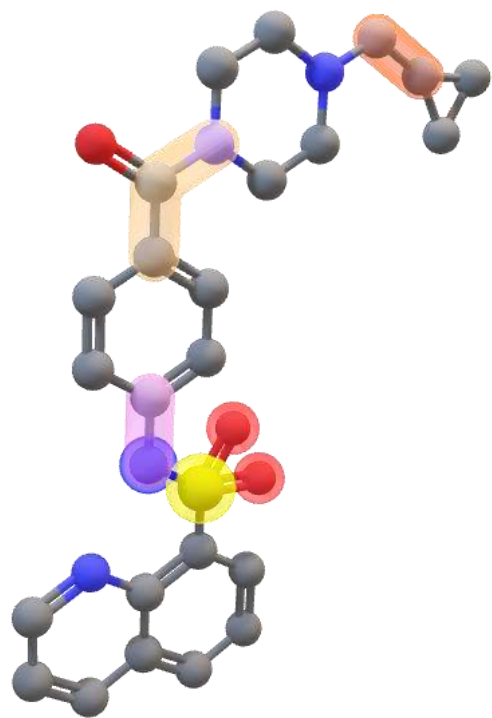
# Signals ChemDraw



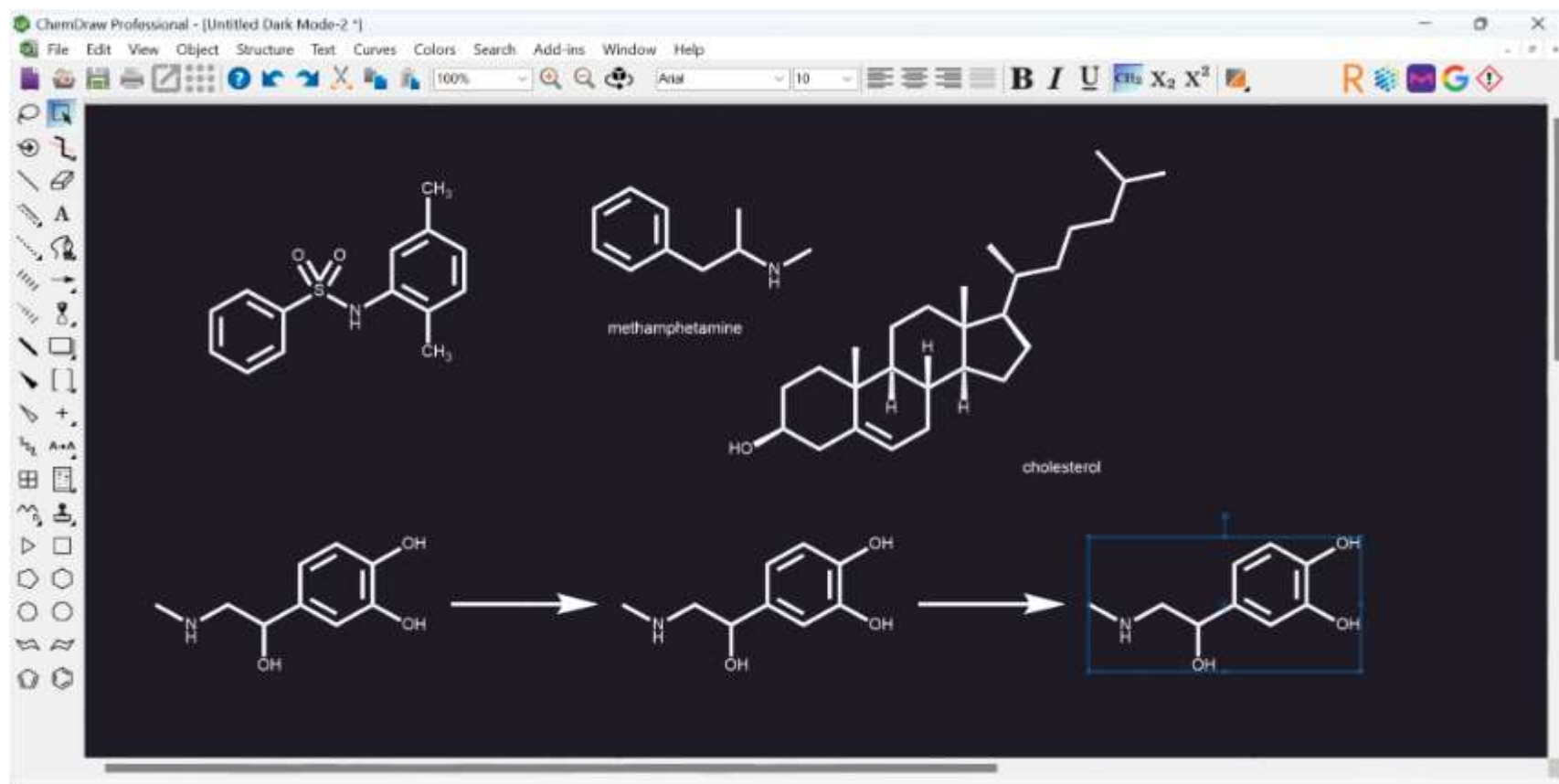




# ChemDraw *Integrated with the* **Signals Platform**



# Signals ChemDraw



# Shortcuts and Hotkeys

Help → Shortcuts and Hotkeys

You can find this Cheat Sheet in the Help Menu > Hotkeys Cheat Sheet

Atom	0	1	2	3/a	4	5	6	7	8	9	z	Z	v	u	k	K	j	J
Atom	o/q	O	n/w	N	s	S	p	P	f	F	/C	L	Enter	+/-	9	K	v	2
	b	B	h	H	y	Q	m	M	c	i	d	A	e	E	u	7	6	0
	-Br	-BH <sub>2</sub>	-H	-Cbz	-Boc	-Fmoc	-Me	-MgBr	-CH <sub>3</sub>	-I	-D	-Ac	-Et	-CO <sub>2</sub> Me				

Select Molecule(s) → **Ctrl +** → **Reaction Shortcut**

Select Molecule(s) → **Alt +** → **Rotation Shortcut**

Select Molecule(s) → **Shift +** → **10p move Shortcut**

**Molecule to Hotspot** → **Hotspot to Molecule**

Enter →

Spacebar / Tab →

Bond	w	h/W	H	b	B	d	D	y	Bond	2	3	a	z	v	4	5	6	7	8	9	0

c1ccccc1 → **1B79** → c1ccccc1B(C)(C)OC(C)(C)C

N → **42n152o** → N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)C(=O)O

C1=CC=CC=C1 → **2o1n1-5-2** → C1=CC=CC=C1C(=O)N1C(=O)CC1

N → **az** → C1=CC=C2C(=C1)N(C2)C(=O)OC(C)(C)C

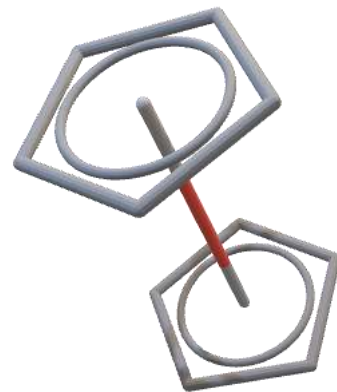
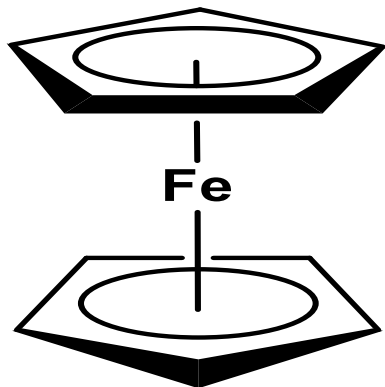


# Shortcuts and Hotkeys

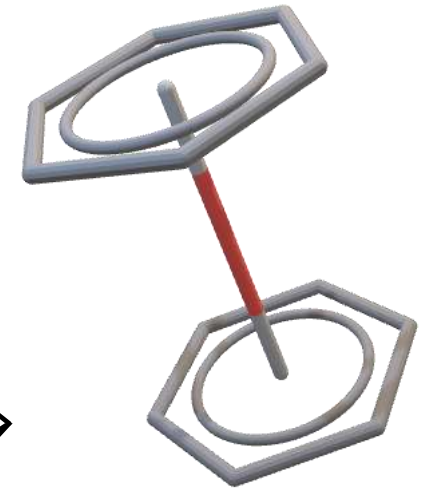
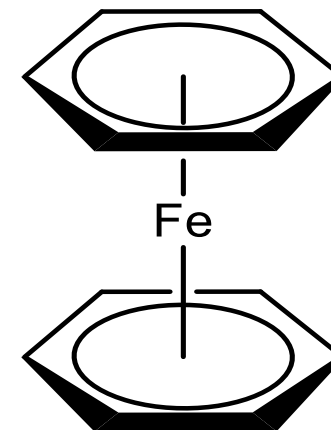
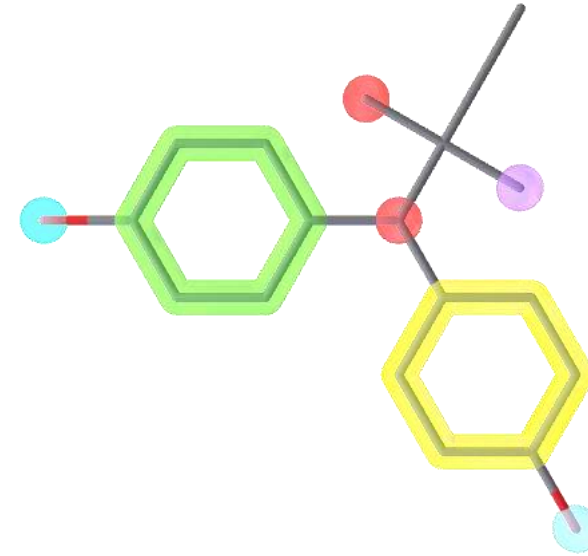
'0' on secondary or tertiary carbon atom



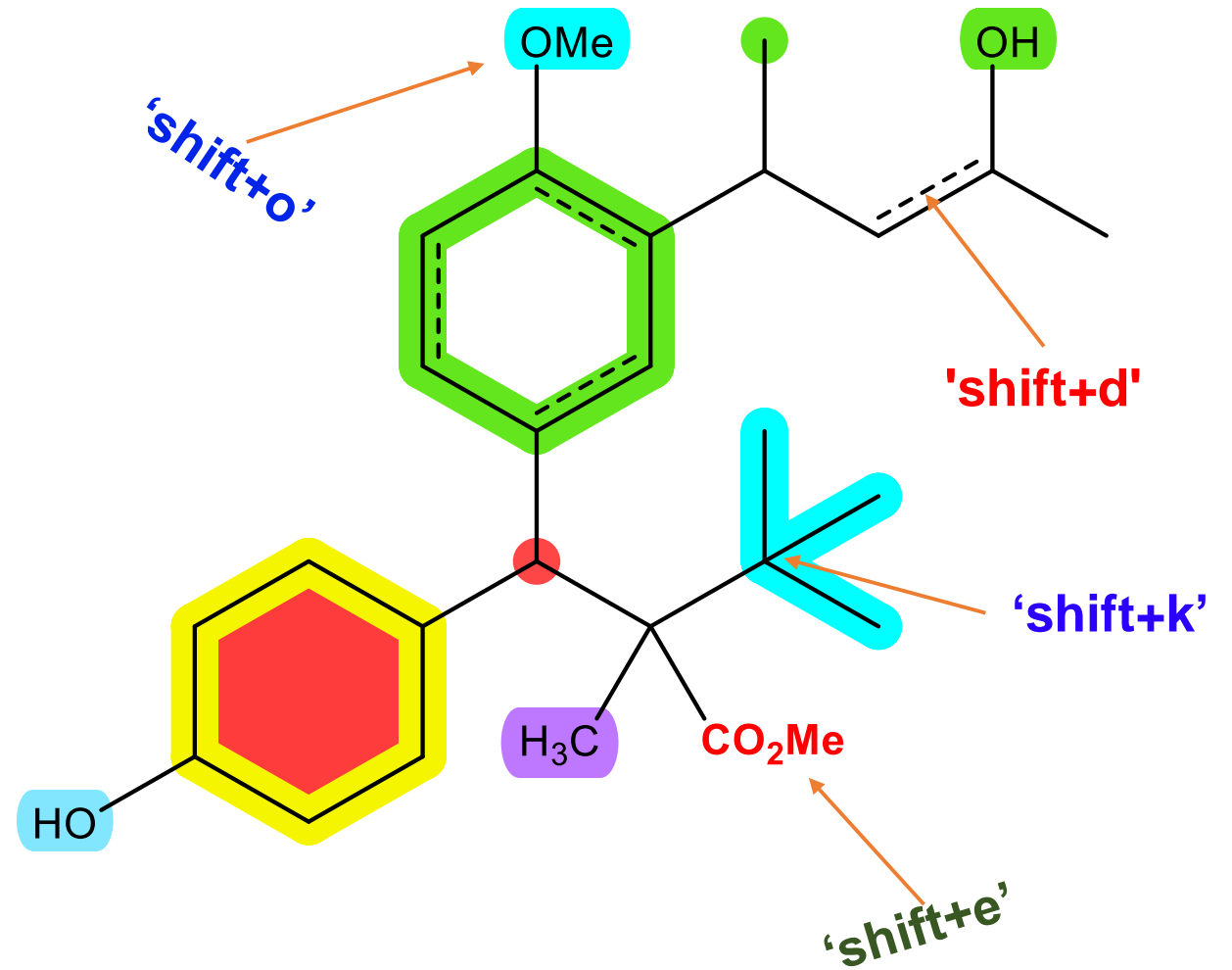
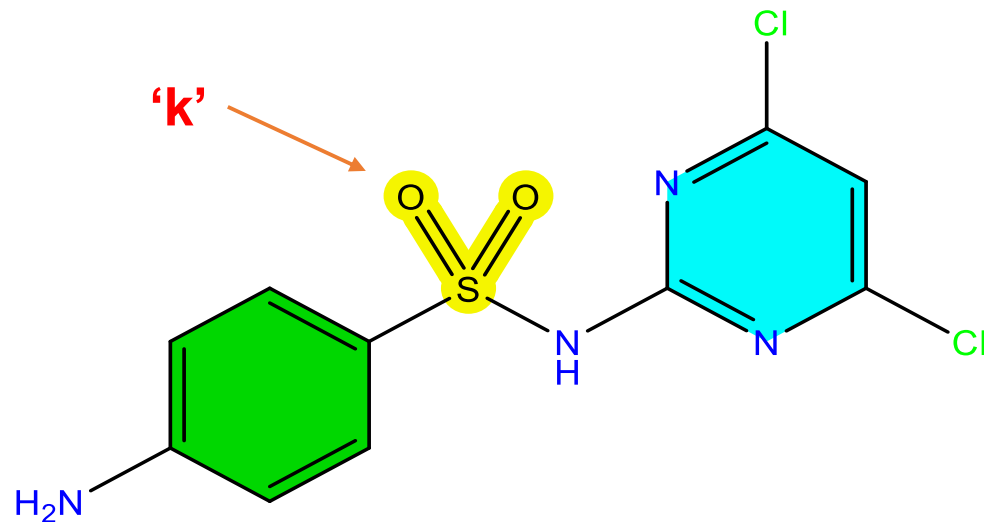
'j' shortcut key sprouts a cyclopentadienyl ring



'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<sub>2</sub>Me group**.

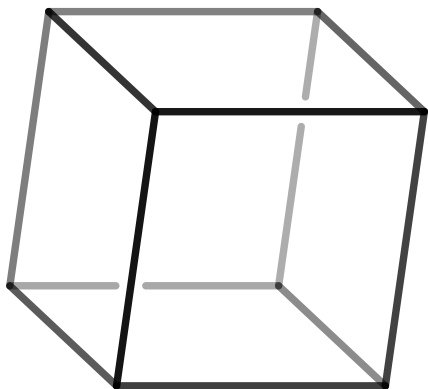


## Copy as PNG

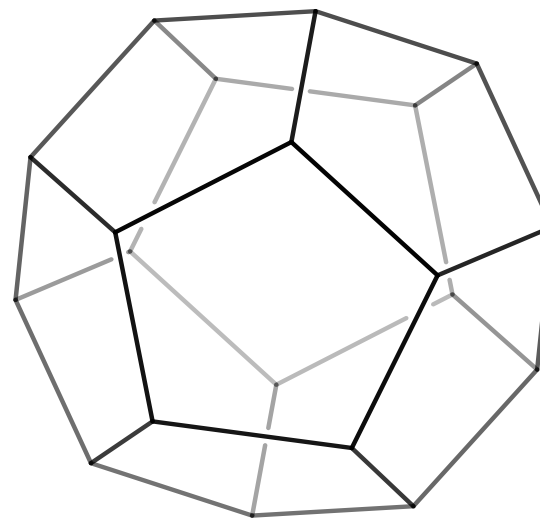
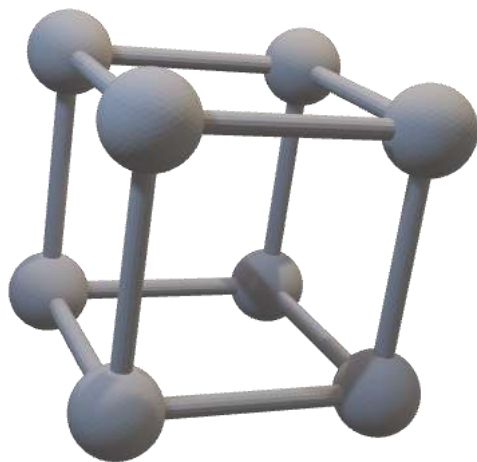
- ChemDraw now lets you copy a structure in **.png format** and paste it directly into **Outlook or Gmail**.

## 'ctrl+J'

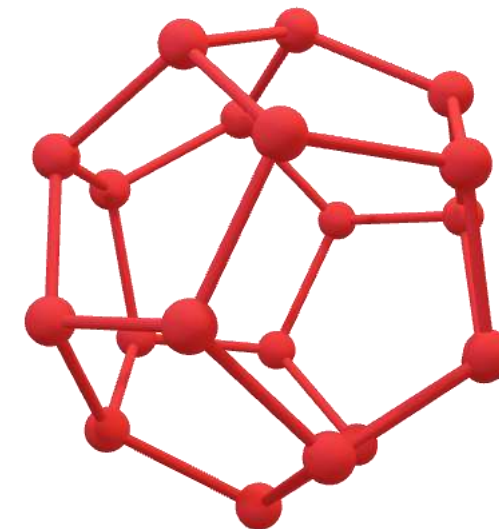
- Joining the two or more atoms or molecules together.



**Cube**

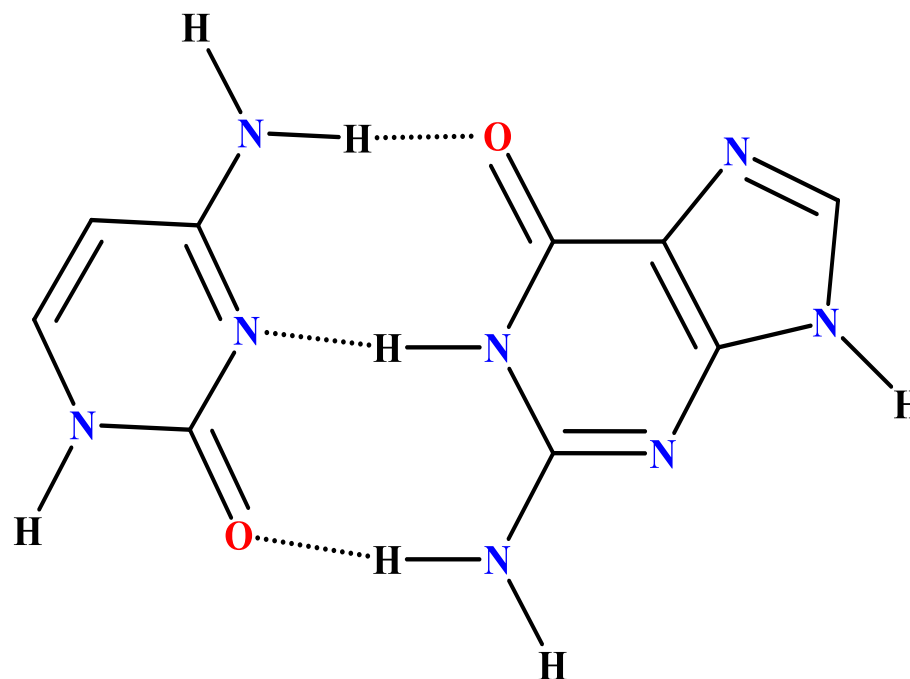
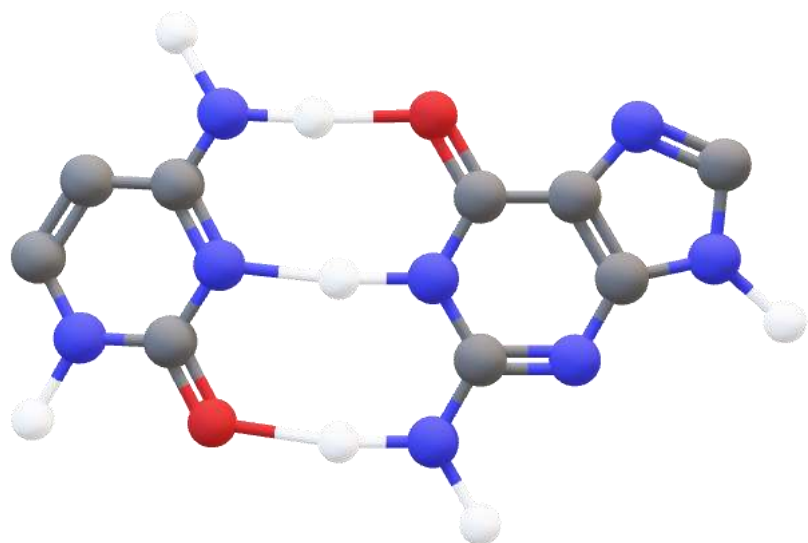


**Dodecahedron**

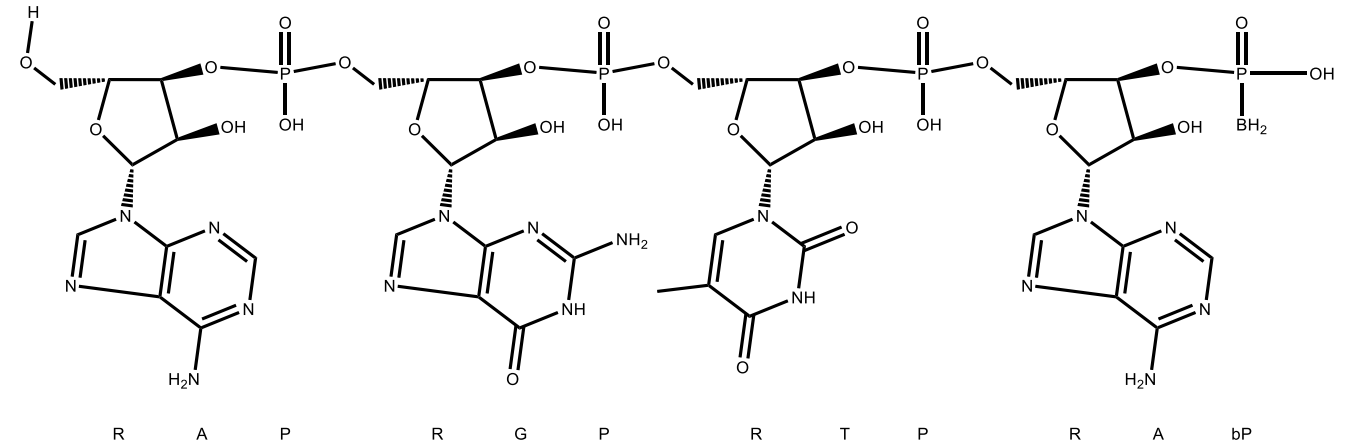
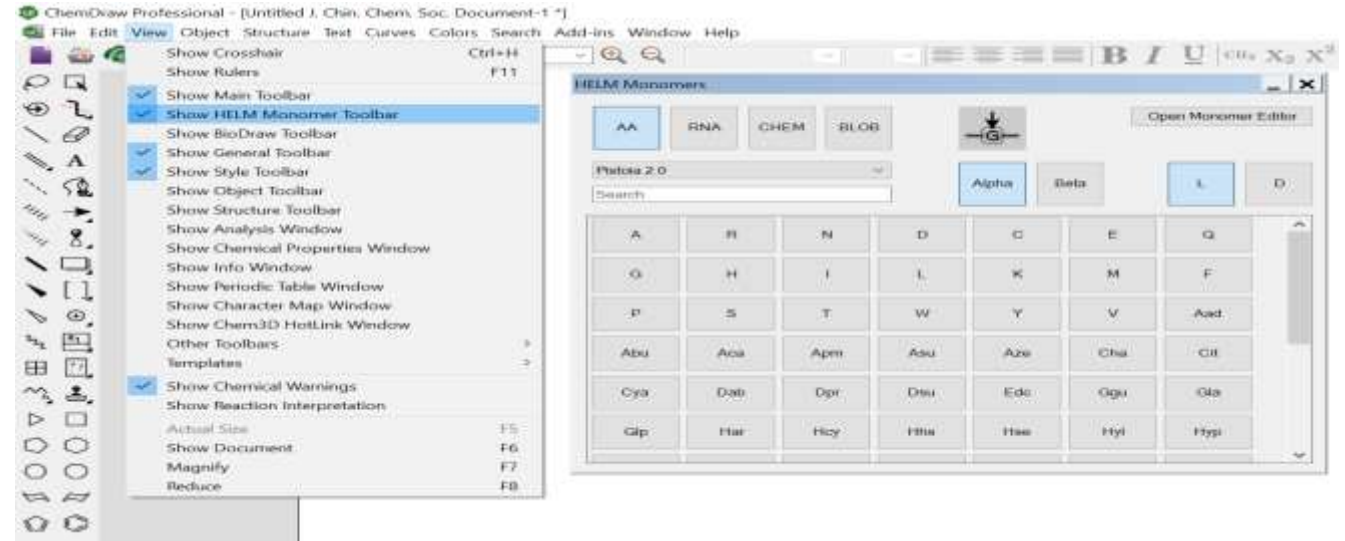
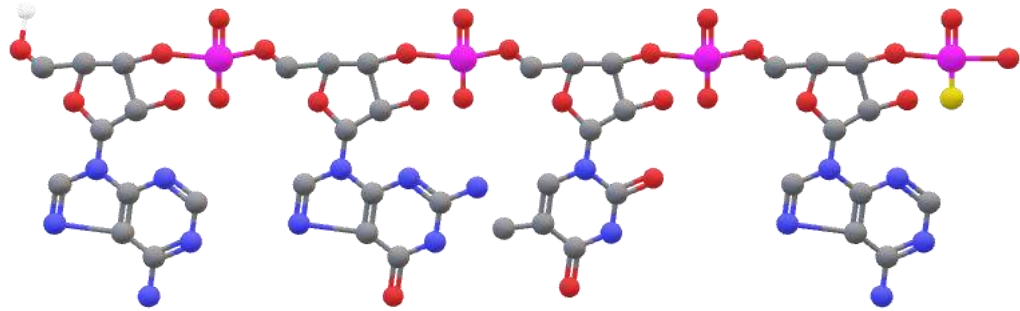
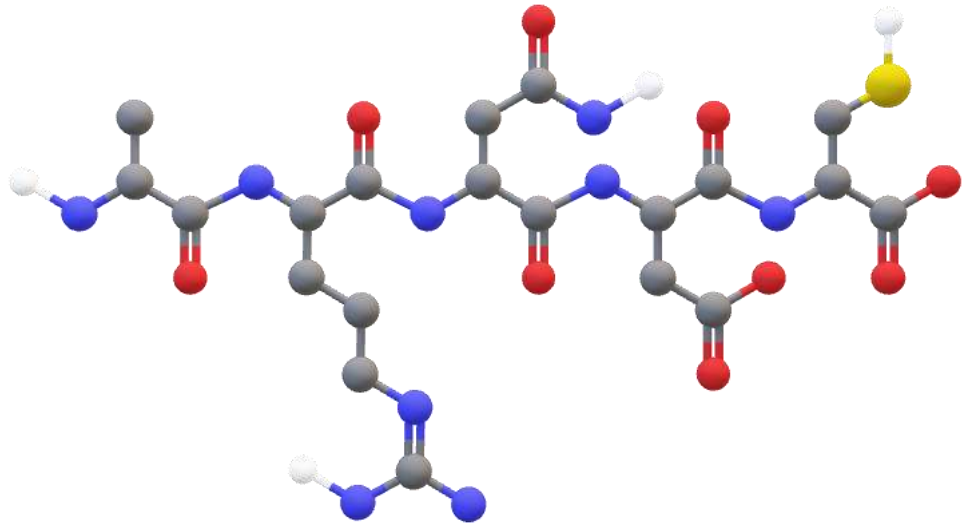


## Hydrogen bonds

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

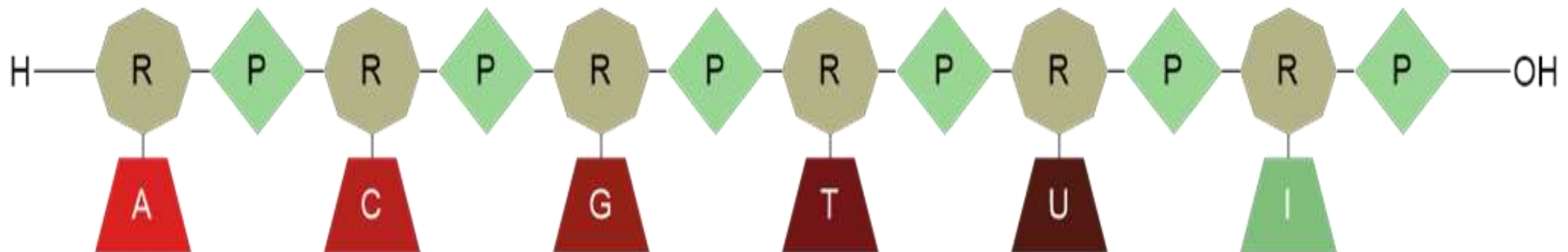


## Sequence Graphic Monomers" stylesheet

- 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.



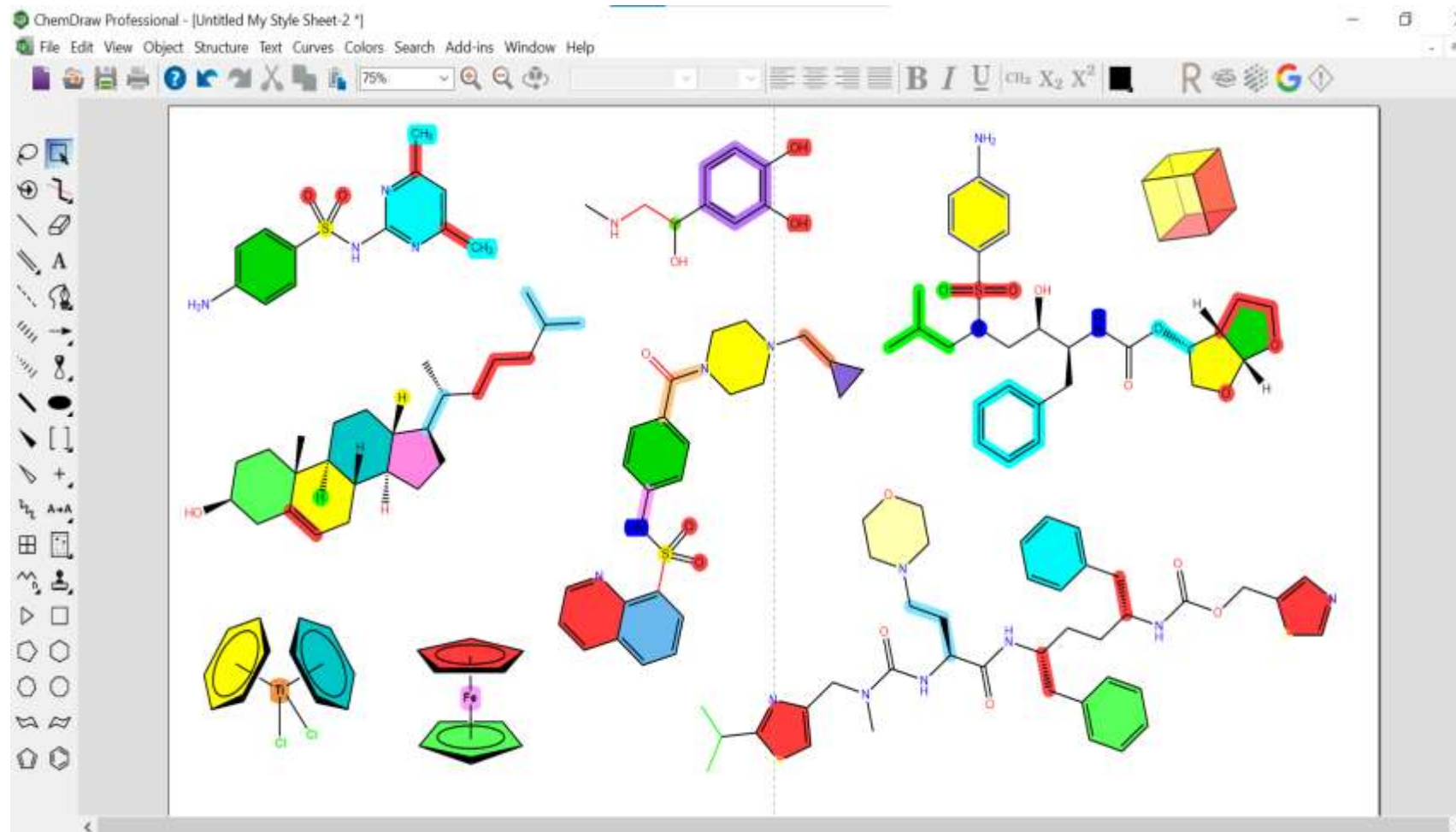
- In the case of DNA/RNA sequences



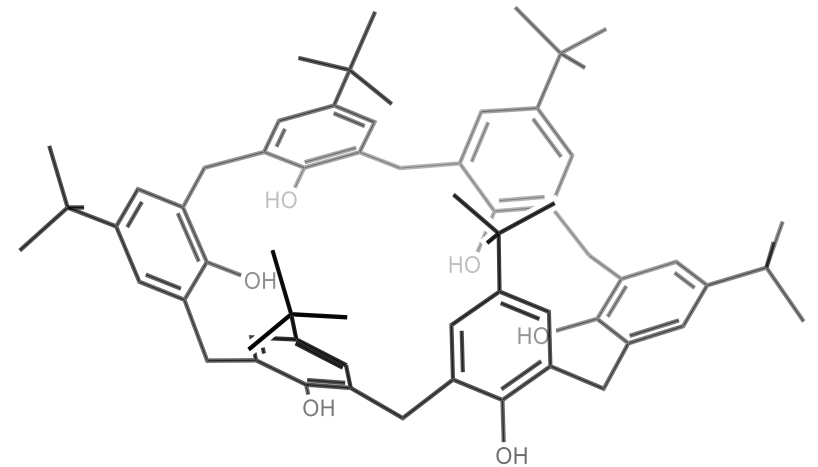
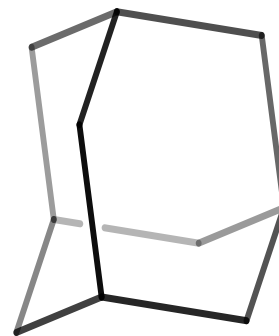
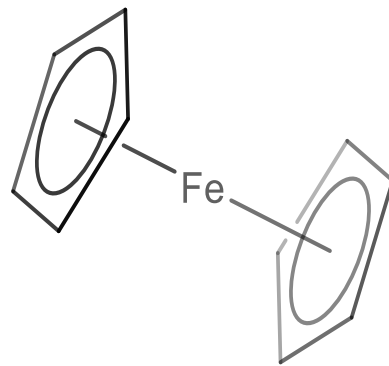
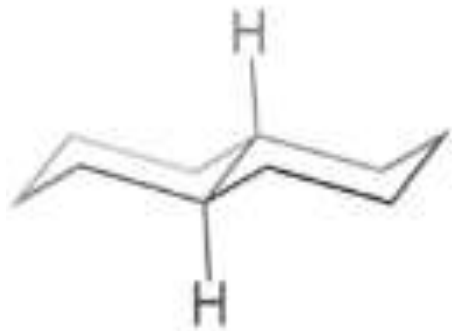
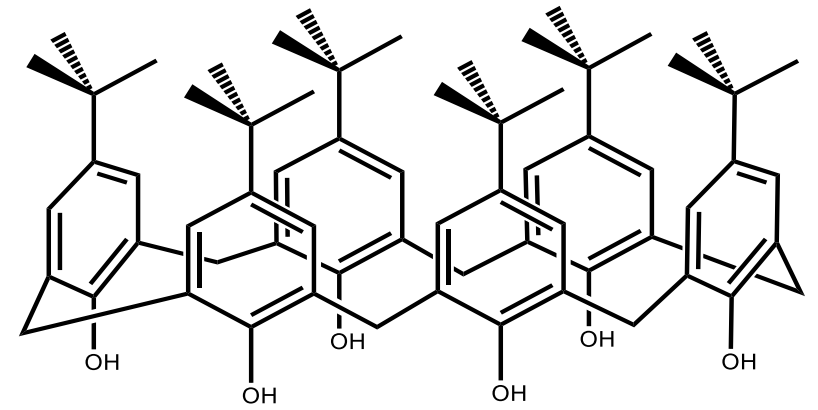
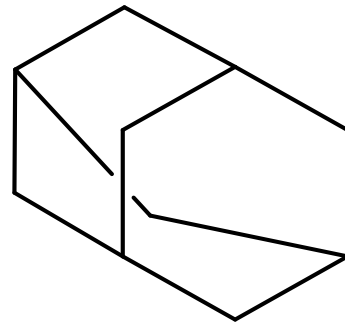
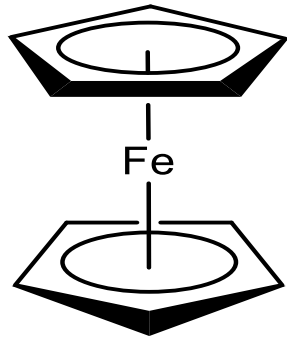
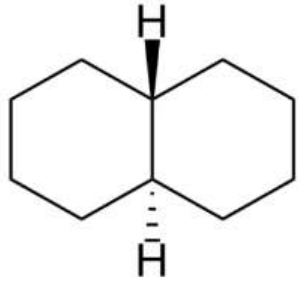


# Highlight Colours

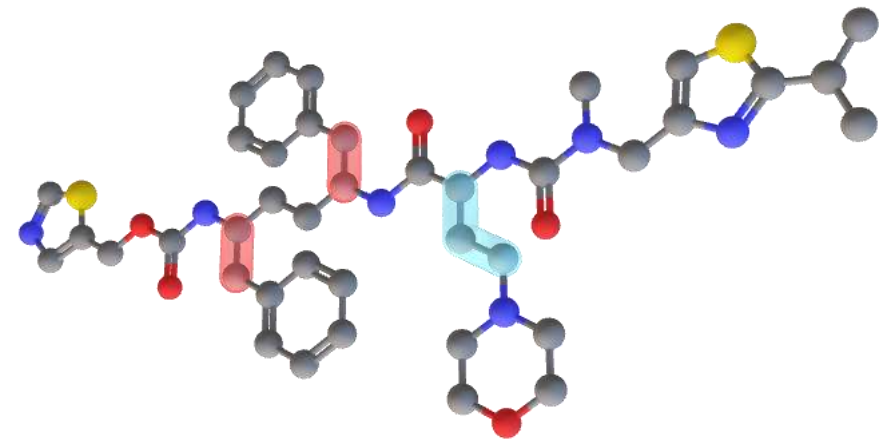
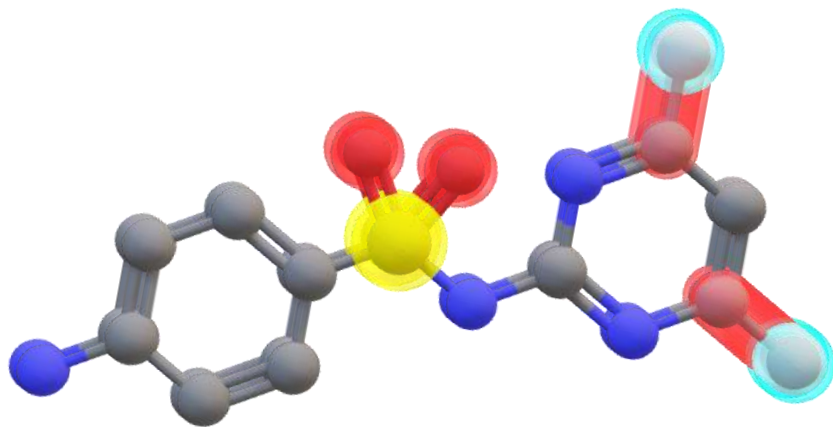
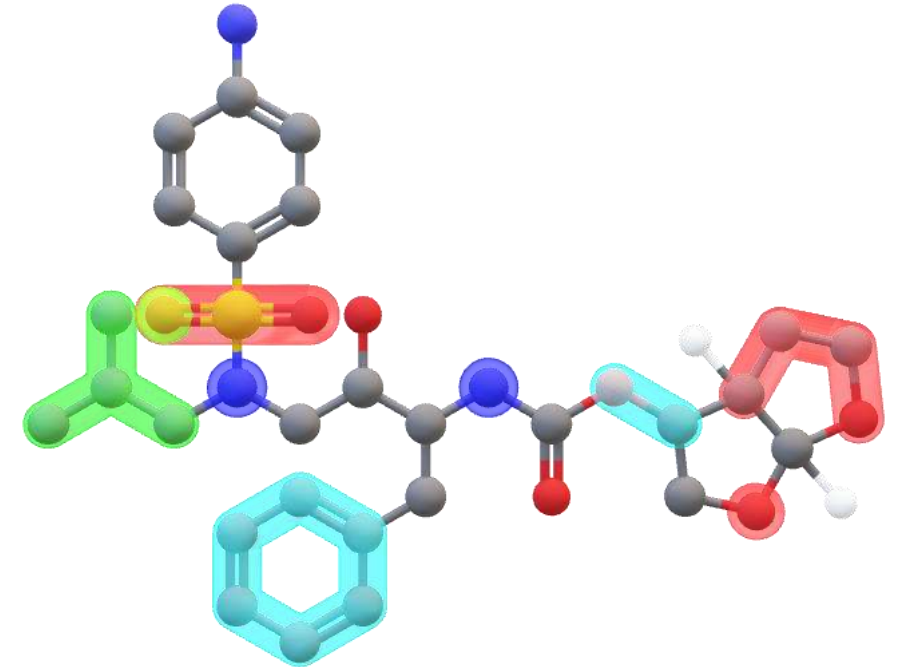
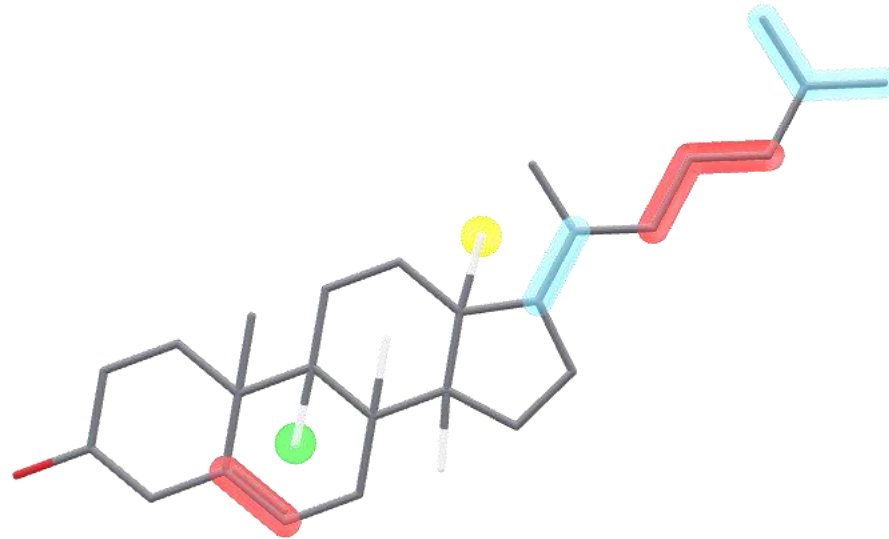
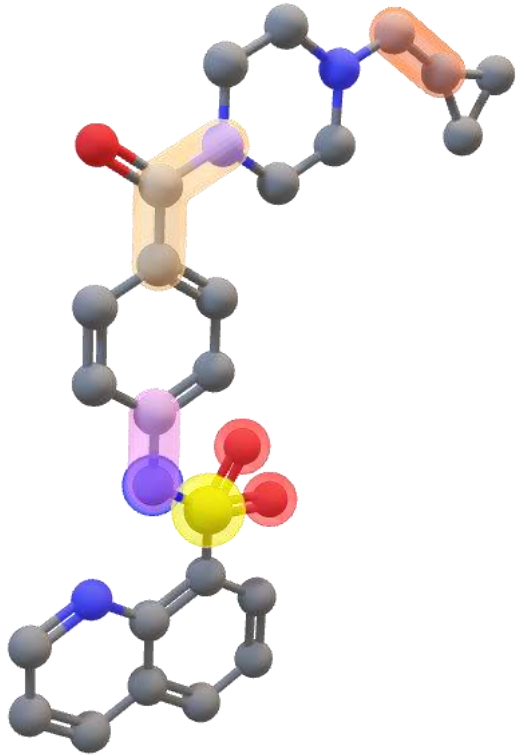
- Produce publication-worthy drawings with selected **atoms**, **bonds**, and **ring** colouring.



# 3D Clean-up



# 3D Printable Format (.3MF)



# Signals Notebook

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

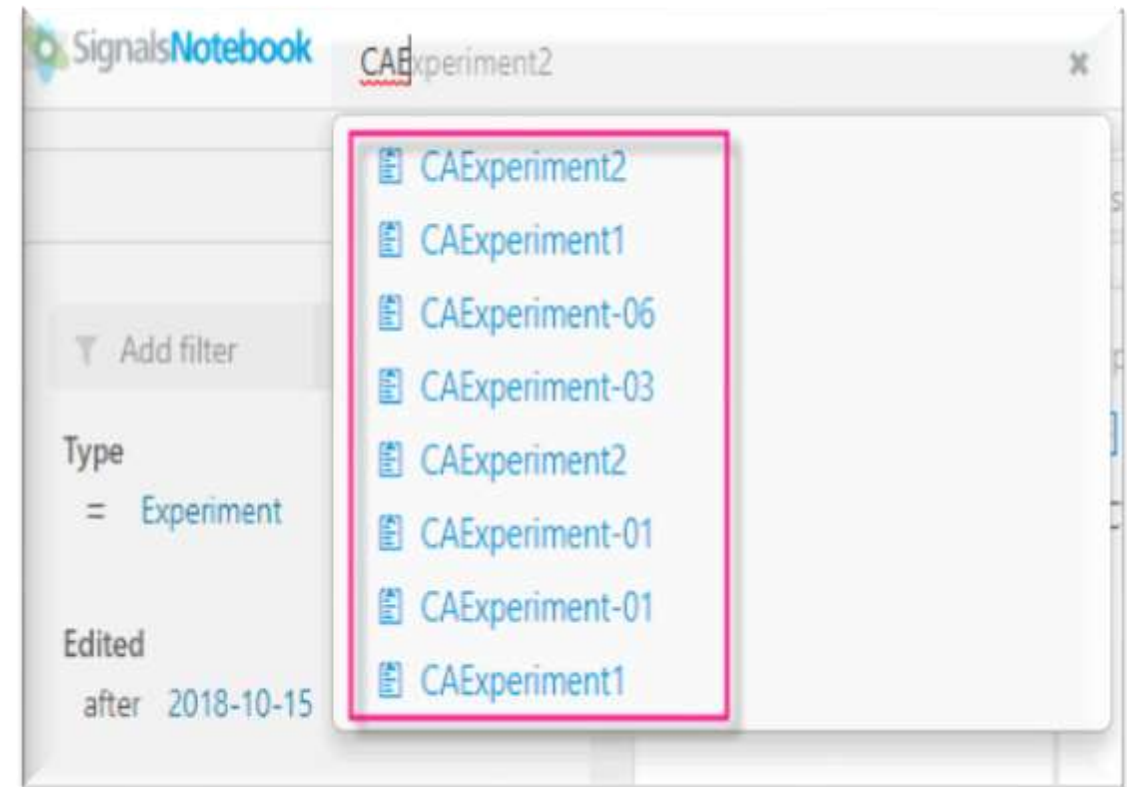
- Manage, Record, and Share your Experiments with Cloud Based Revvity Signals Notebook

- Connect and share data with colleagues and collaborators.

# Searching Option

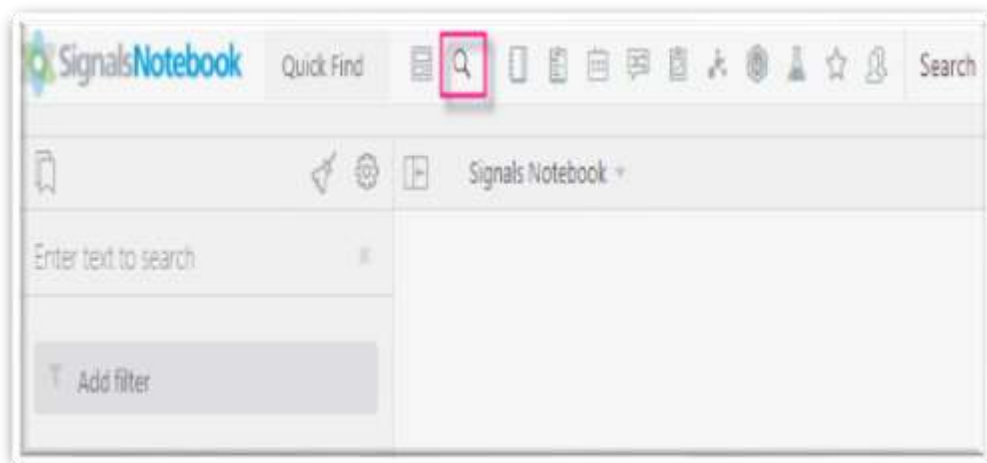
## Two types of searches are available:-

- **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

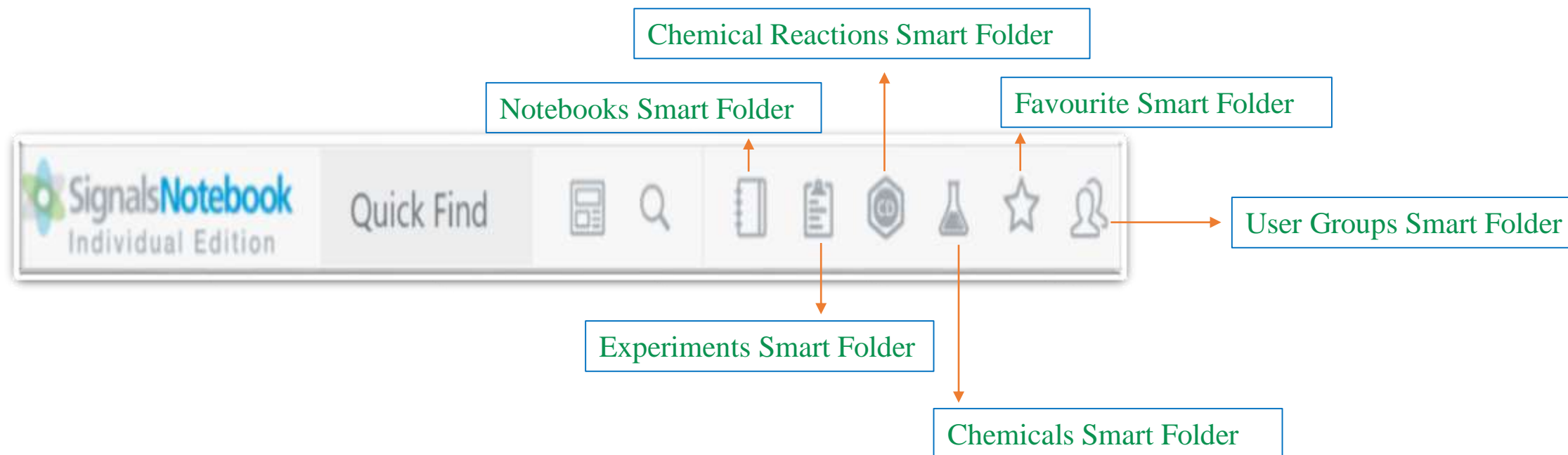
- Using the Advanced Search page you can run chemical, text or combined chemical and text searches.
- You can access the advanced search page by clicking on the Search icon in Signals Notebook toolbar.



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

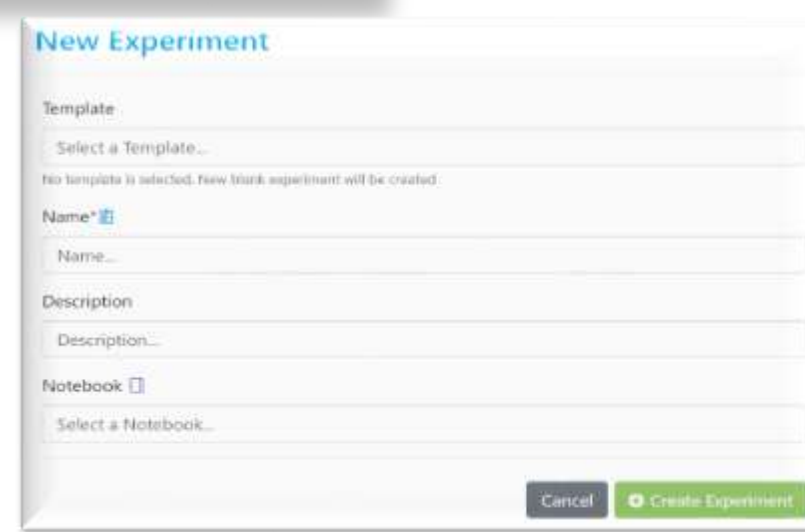
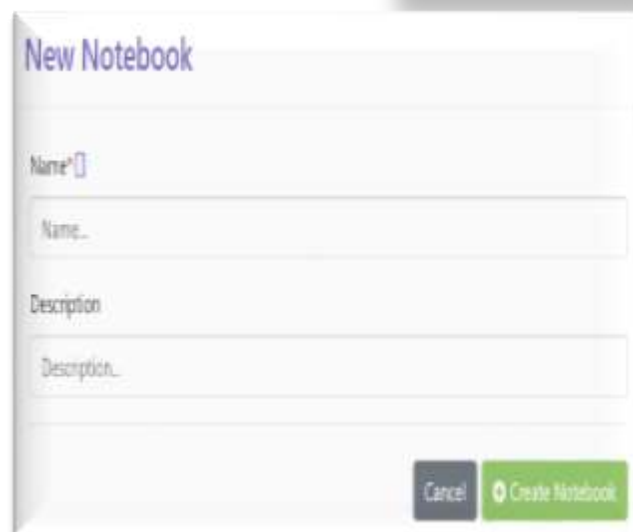
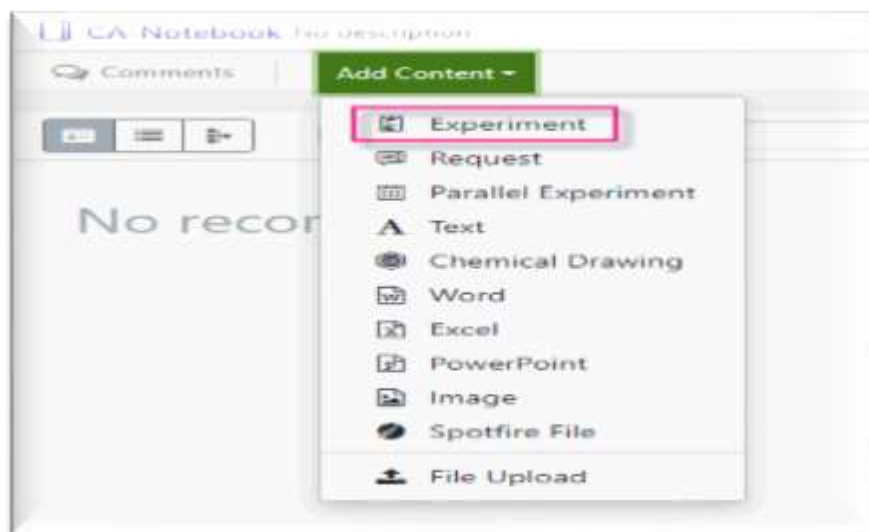
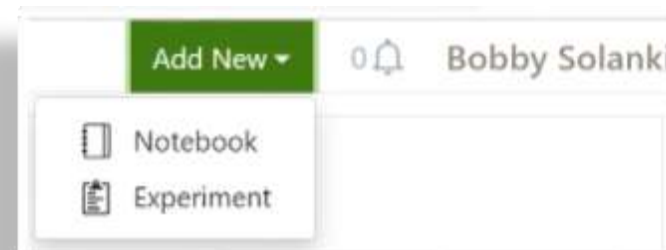
# Smart Folders

- 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

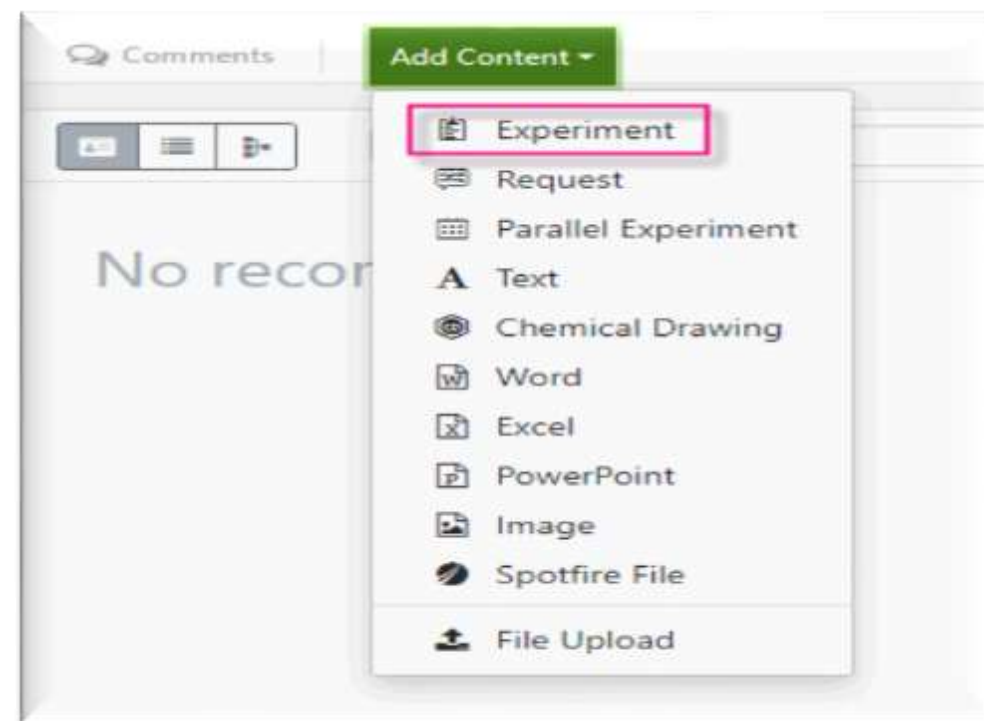
- You can create an experiment under a notebook or an independent experiment not as a part of any notebook.





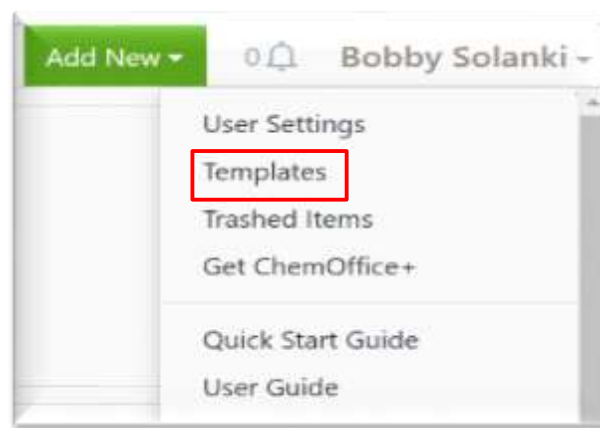
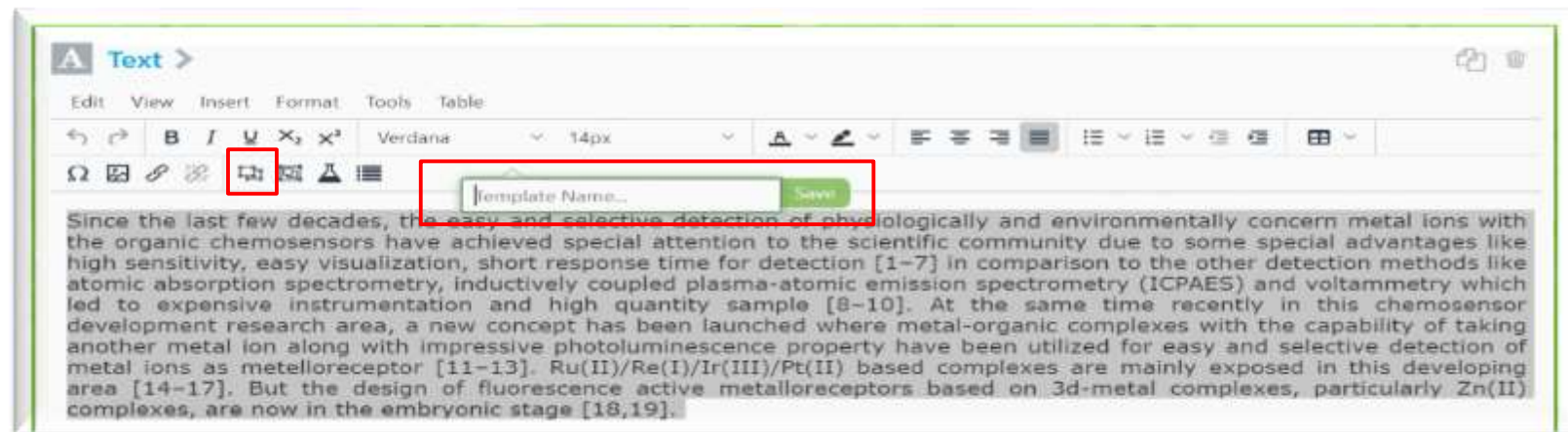
# Adding Information Items to an Experiment

- 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.

Quick Add

Hide Column

Reactants													
Rxn ID	Reactant	MF	FM	MW	EM	Limit?	Eq	Sample Mass	Moles	Molarity	Vol	d	% Wt
I	2-hydroxybenzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138.12	138.12	138.03169	<input checked="" type="checkbox"/>	1	6 g	29 mmol	1 molar	29 mL	0.2 g/mL	
II	acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.05	60.05	60.02113	<input type="checkbox"/>	2,1	4 g	60 mmol	1.5 molar	40 mL	0.1 g/mL	

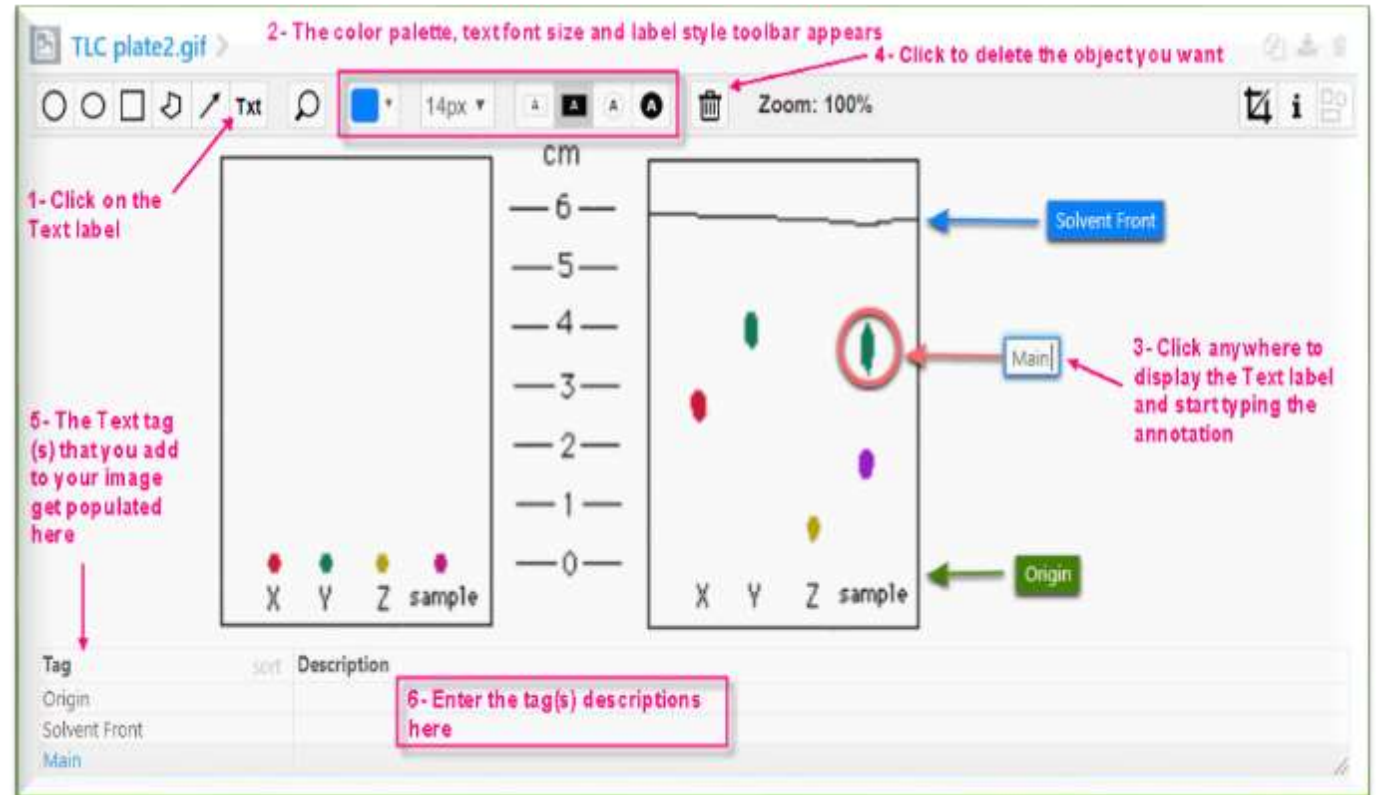
Total Volume: 94 mL    Reaction Molarity: 0.31 molar

Products												
Rxn ID	Product ID	Product	MF	FM	MW	EM	Theo Mass	Actual Mass	Purity	Yield	Theo Mol	Actual Mol
III	P1	2-acetoxybenzoic acid	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	180.16	180.16	180.04226	5.2 g	4.8 g	85 %	78 %	29 mmol	23 mmol

Reaction Conditions			
	Pressure	Temperature	Reaction Time
⚙			
▼			

# 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.



1- Click on the Text label

2- The color palette, text font size and label style toolbar appears

3- Click anywhere to display the Text label and start typing the annotation

4- Click to delete the object you want

5- The Text tag(s) that you add to your image get populated here

6- Enter the tag(s) descriptions here

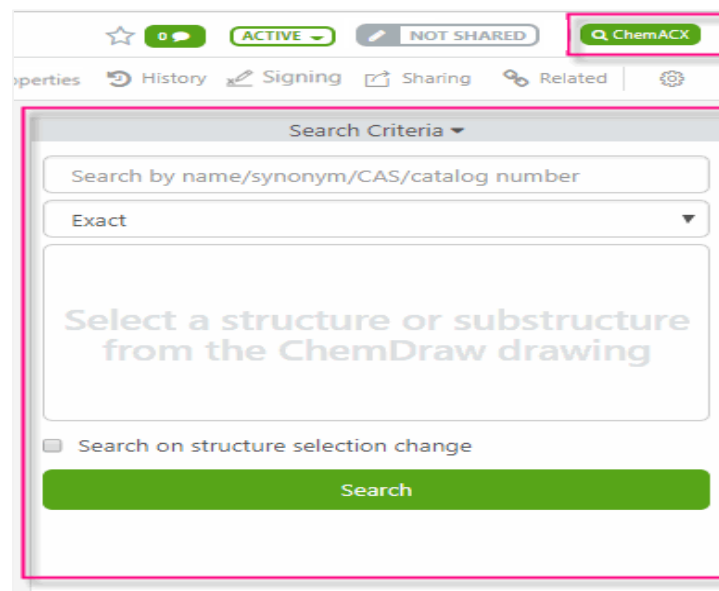
Tag	Description
Origin	
Solvent Front	
Main	

# 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



Search Criteria

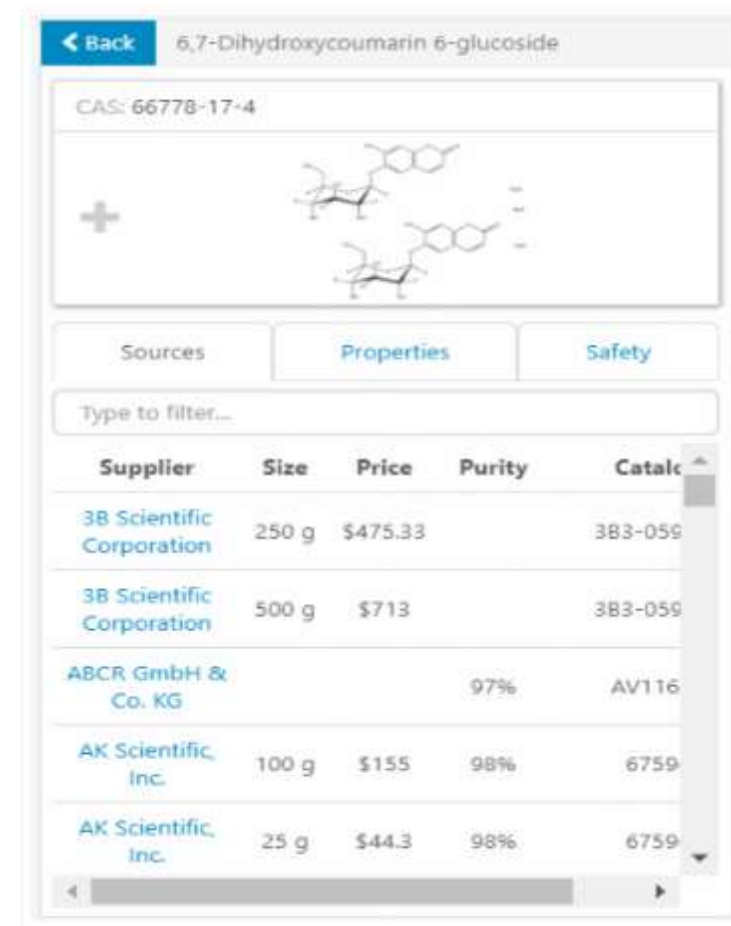
Search by name/synonym/CAS/catalog number

Exact

Select a structure or substructure from the ChemDraw drawing

Search on structure selection change

Search



6,7-Dihydroxycoumarin 6-glucoside

CAS: 66778-17-4

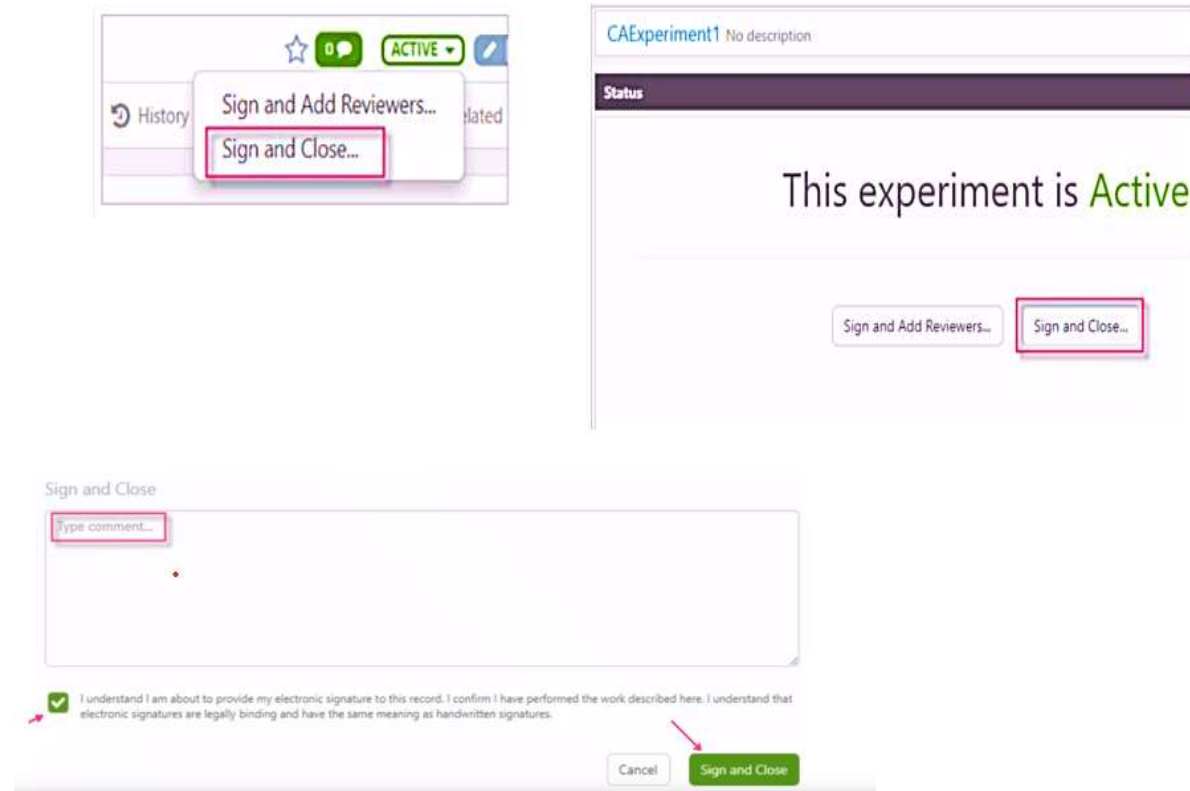
Sources Properties Safety

Type to filter...

Supplier	Size	Price	Purity	Catalog
3B Scientific Corporation	250 g	\$475.33		383-059
3B Scientific Corporation	500 g	\$713		383-059
ABCR GmbH & Co. KG			97%	AV116
AK Scientific, Inc.	100 g	\$155	98%	6759
AK Scientific, Inc.	25 g	\$44.3	98%	6759

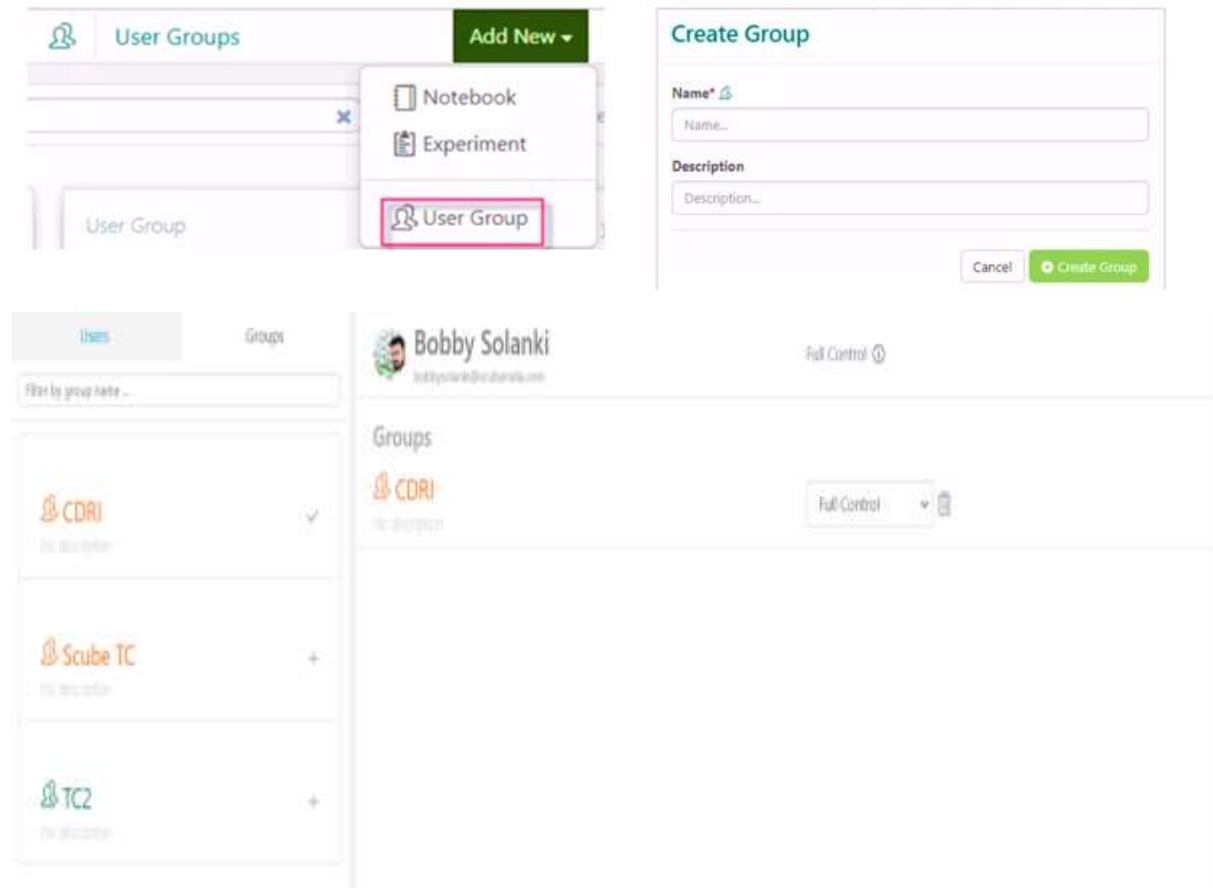
# Signing and Closing an Experiment

- 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

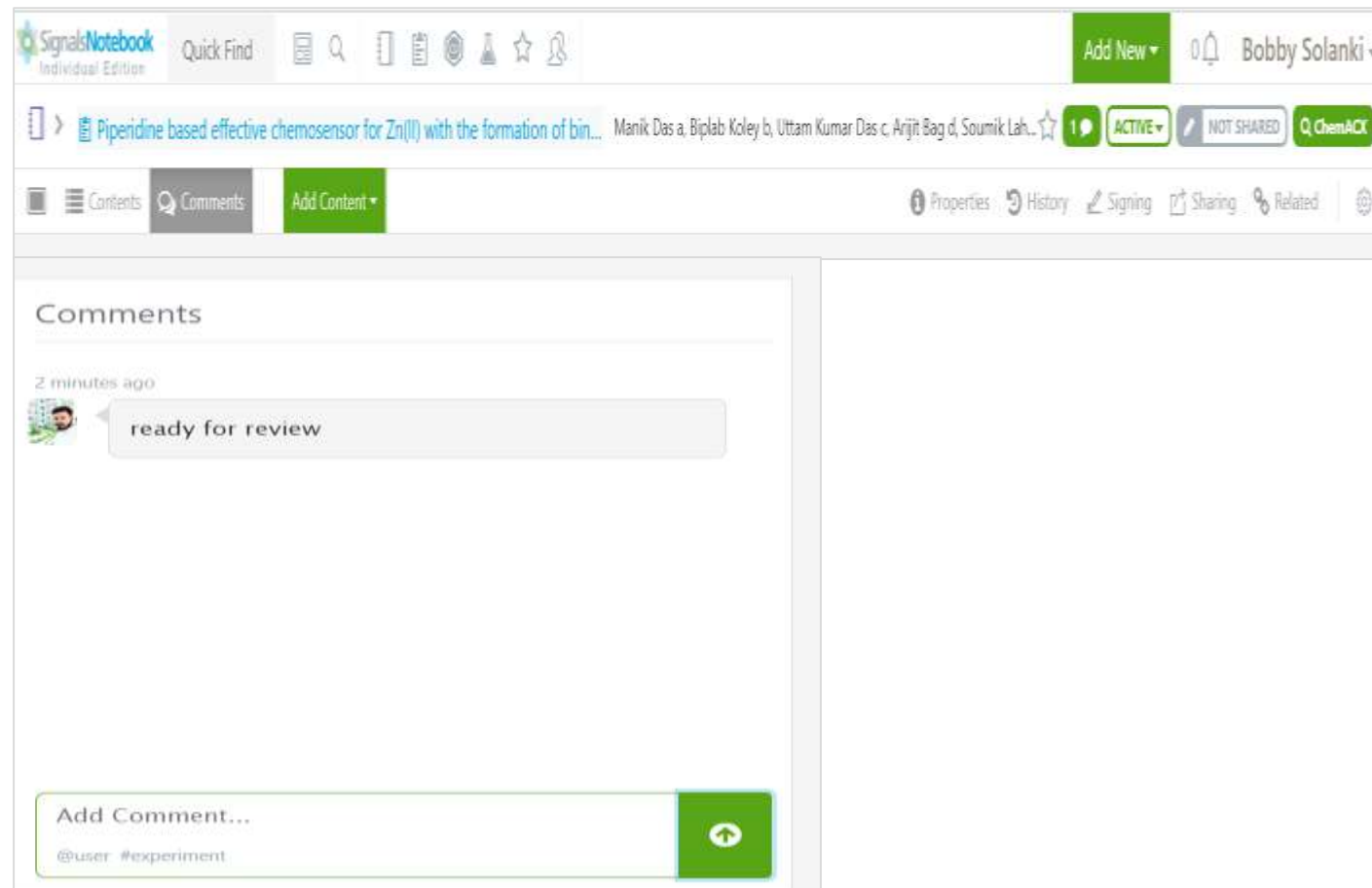
- You can create a group for sharing or collaboration.
- A system group is a set of users who have the same interests and privileges.
- For example, as a laboratory supervisor, you might want to create a laboratory technicians group so you can share assignments with them or as a professor or teacher's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



The screenshot displays the SCUBE software interface for managing user groups. At the top, the 'User Groups' section includes an 'Add New' button. A dropdown menu is open, showing options for 'Notebook', 'Experiment', and 'User Group', with 'User Group' highlighted. To the right, the 'Create Group' form is visible, featuring input fields for 'Name\*' and 'Description', and 'Cancel' and 'Create Group' buttons. Below this, a user profile for Bobby Solanki is shown with 'Full Control' permissions. A list of groups is displayed, including 'CDRI', 'Scube TC', and 'TC2', each with a 'Full Control' dropdown menu.

# 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.

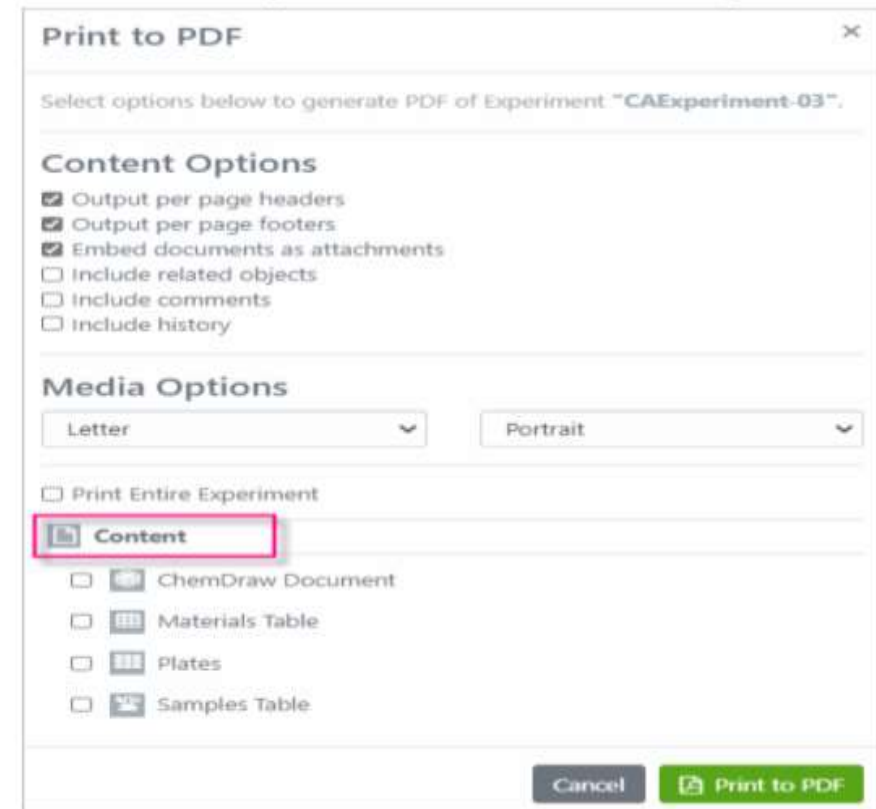
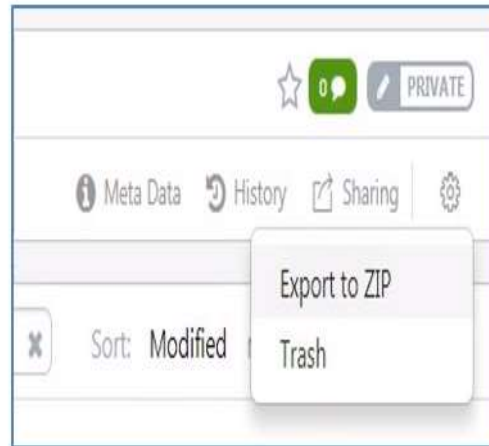
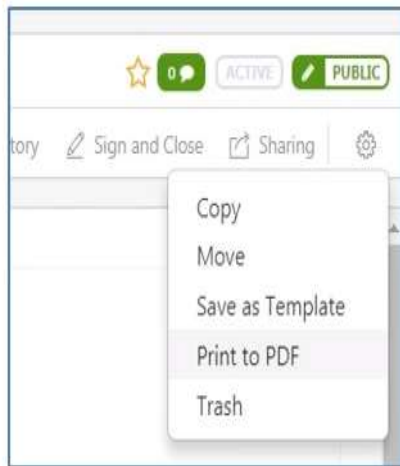


The screenshot displays the Signals Notebook interface. At the top, the title bar shows "Signals Notebook Individual Edition" and "Quick Find" with various icons. The user "Bobby Solanki" is logged in. The main content area shows a resource titled "Piperidine based effective chemosensor for Zn(II) with the formation of bin..." with authors "Manik Das a, Biplab Koley b, Uttam Kumar Das c, Arijit Bag d, Soumik Lah..." and status "ACTIVE" and "NOT SHARED". The "Comments" tab is selected, and a comment "ready for review" is visible, posted "2 minutes ago" by a user with a profile picture. At the bottom, there is a text input field "Add Comment..." with a placeholder "@user #experiment" and a green "Post" button.



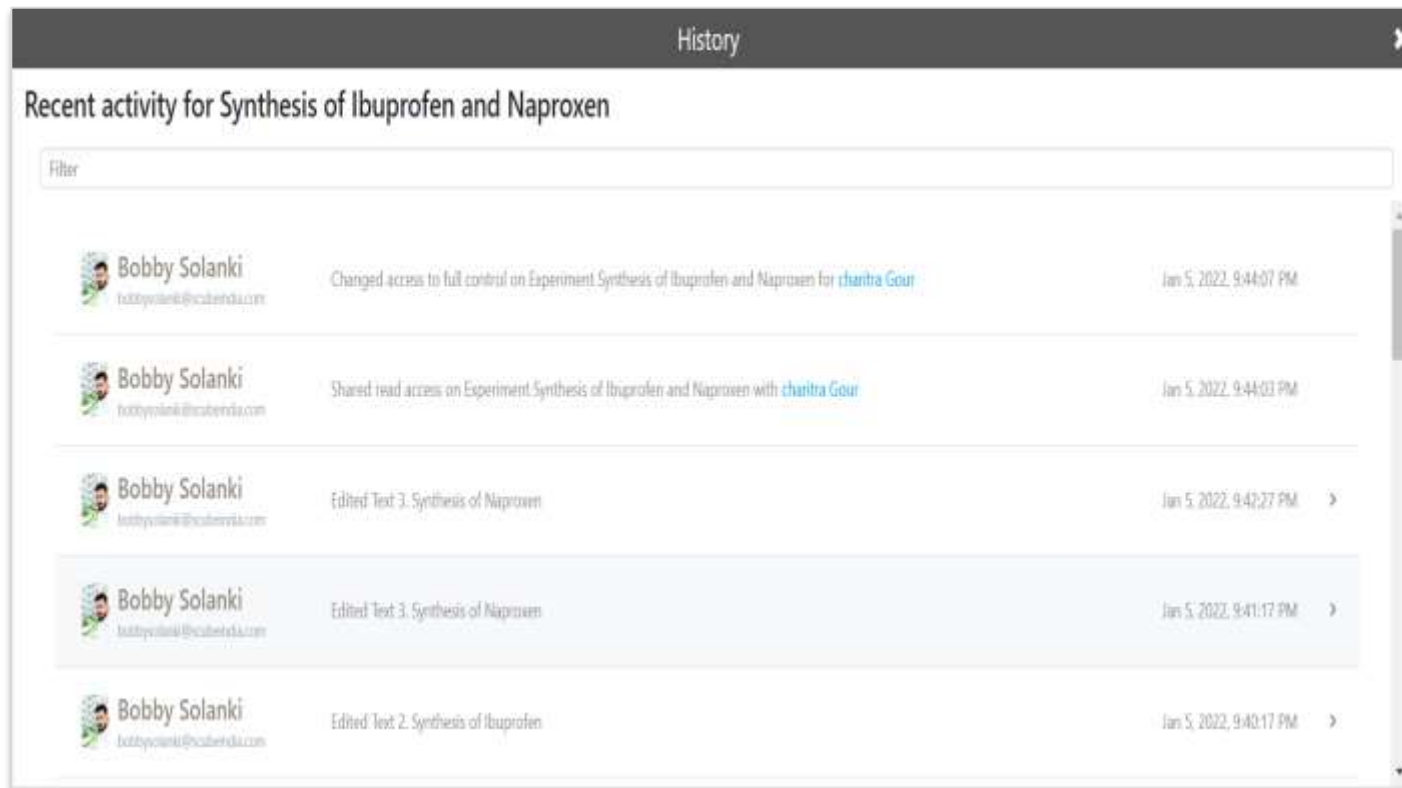
# Exporting Notebooks/Print to Pdf






- 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.



Recent activity for Synthesis of Ibuprofen and Naproxen		
Filter		
 Bobby Solanki bobbysolanki@scubenda.com	Changed access to full control on Experiment Synthesis of Ibuprofen and Naproxen for <a href="#">charitra Gour</a>	Jan 5, 2022, 9:44:07 PM
 Bobby Solanki bobbysolanki@scubenda.com	Shared read access on Experiment Synthesis of Ibuprofen and Naproxen with <a href="#">charitra Gour</a>	Jan 5, 2022, 9:44:03 PM
 Bobby Solanki bobbysolanki@scubenda.com	Edited Text 3. Synthesis of Naproxen	Jan 5, 2022, 9:42:27 PM >
 Bobby Solanki bobbysolanki@scubenda.com	Edited Text 3. Synthesis of Naproxen	Jan 5, 2022, 9:41:17 PM >
 Bobby Solanki bobbysolanki@scubenda.com	Edited Text 2. Synthesis of Ibuprofen	Jan 5, 2022, 9:40:17 PM >



***Thank You***

***bobbysolanki@scubeindia.com***