Rowan Patents Drafting
Life and Material Sciences
Small Molecule Support

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Accessing Life and Materials Sciences Features

Rowan drafting features supporting patent applications in the fields of life and material sciences, such as chemistry, pharmaceuticals, and biotechnology, are not currently available as part of our general Rowan Patents drafting release, but can be provided to users interested in helping us exercise and improve functionality designed for these fields. If you or your colleagues want to learn more about our life and materials science features and perhaps become beta-testers, please contact Tracy Campbell at tcampbell@rowantels.com.

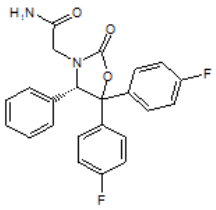
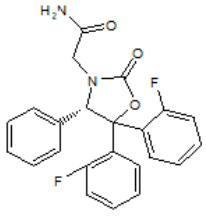
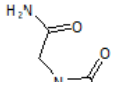
This document focuses on features we've designed to support these particular fields of invention. Information on Rowan Patents drafting's general functionality is available in the Rowan Patents Drafting Complete User Manual.

Molecular Compound Management

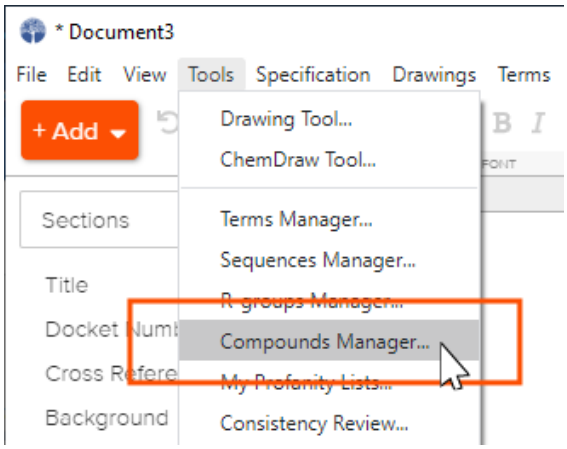
Importing Compounds from a Spreadsheet

1. If needed, adjust your molecular compound data spreadsheet as follows:

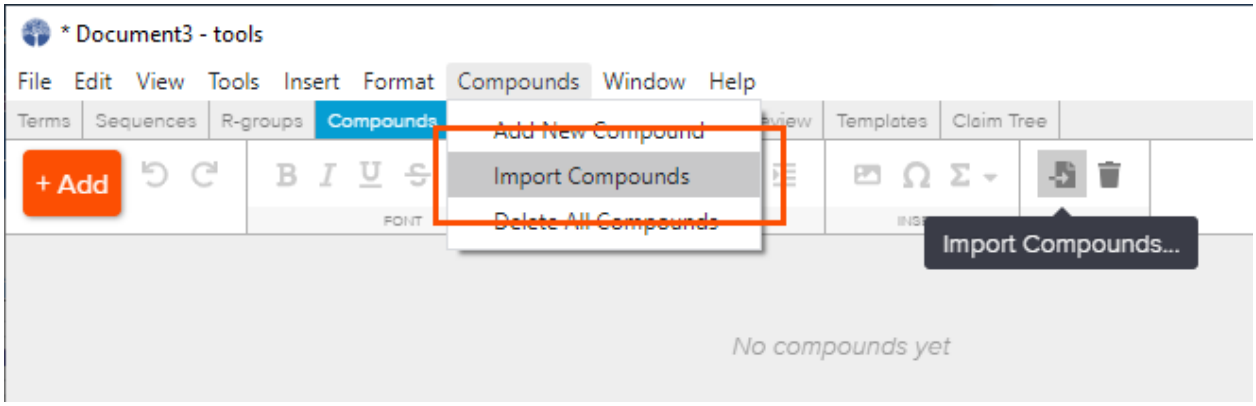
    a. First column: Compound reference number (required)
    b. Second column:Compound structure image (required)
    c. Third column: Compound molecular weight (optional)
    d. Fourth column: Compound name (optional).

	A	B	C	D
1	Internal Reference		Weight	Systematic Name
2	ABC1			2-[(S)-5,5-Bis-(4-fluoro-phenyl)-2-oxo-4-phenyl-oxazolidin-3-yl]-acetamide
3	ABC2			2-[(S)-5,5-Bis-(2-fluoro-phenyl)-2-oxo-4-phenyl-oxazolidin-3-yl]-acetamide
				

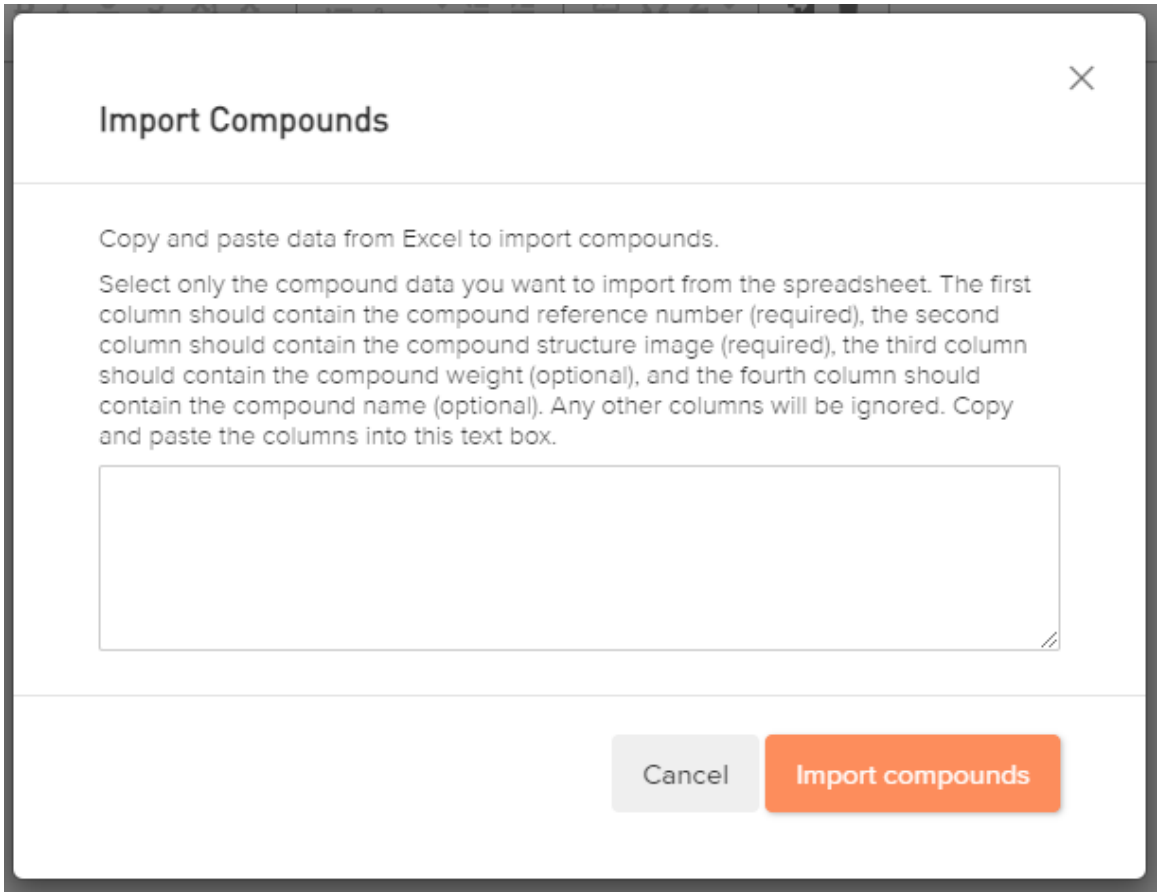
2. Open the Rowan Compounds Manager from the Tools menu.



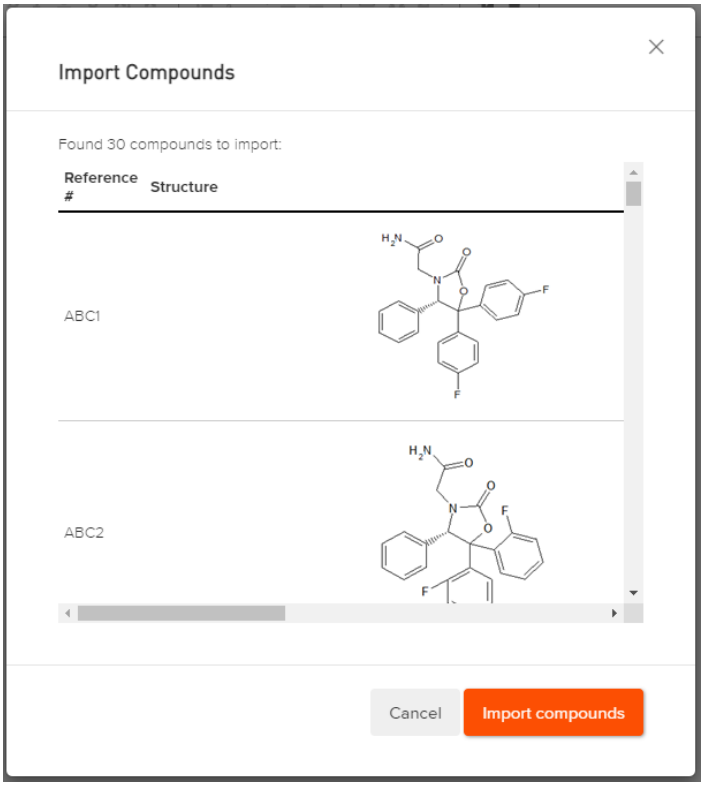
3. Select the Import Compounds option from the toolbar or the Compounds menu.



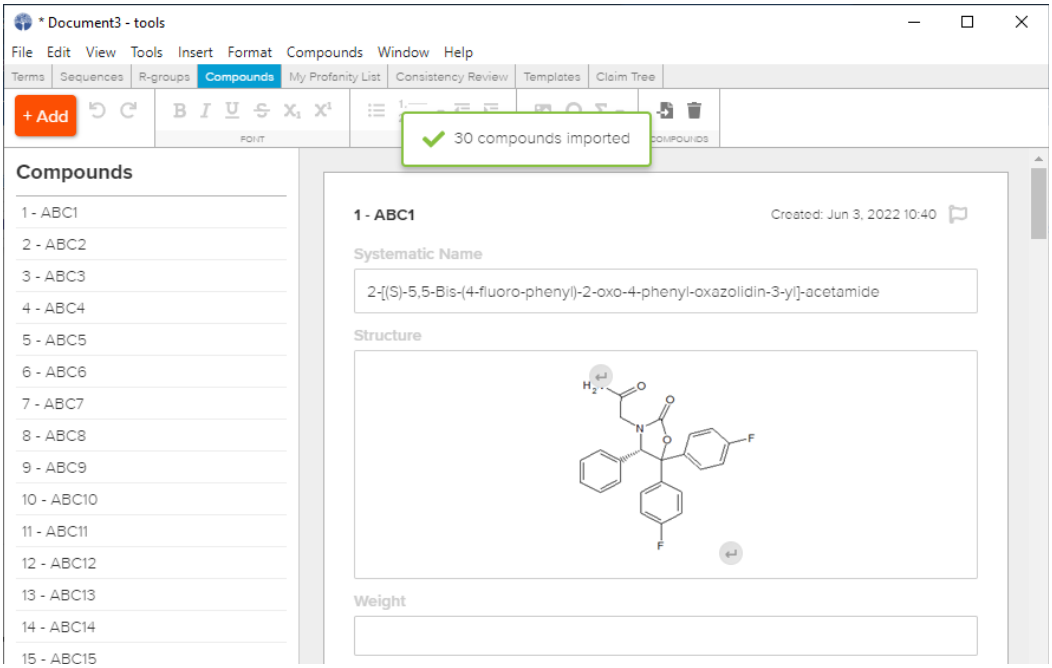
4. Copy and paste your spreadsheet data, following the instructions in the import dialog.



5. Once your imported data is ready, click the Import Compounds button.

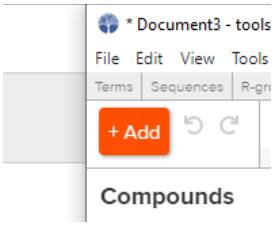


6. Your compounds and associated data will be imported and automatically numbered in the tool.

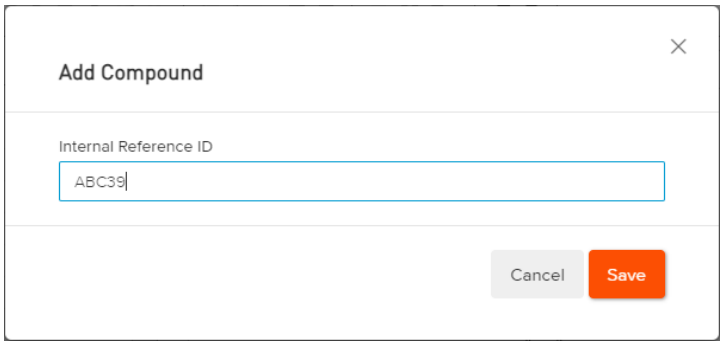


Adding an Individual Compound

1. Open the Rowan Compounds Manager from the tools menu, and click the +Add button to the upper left.

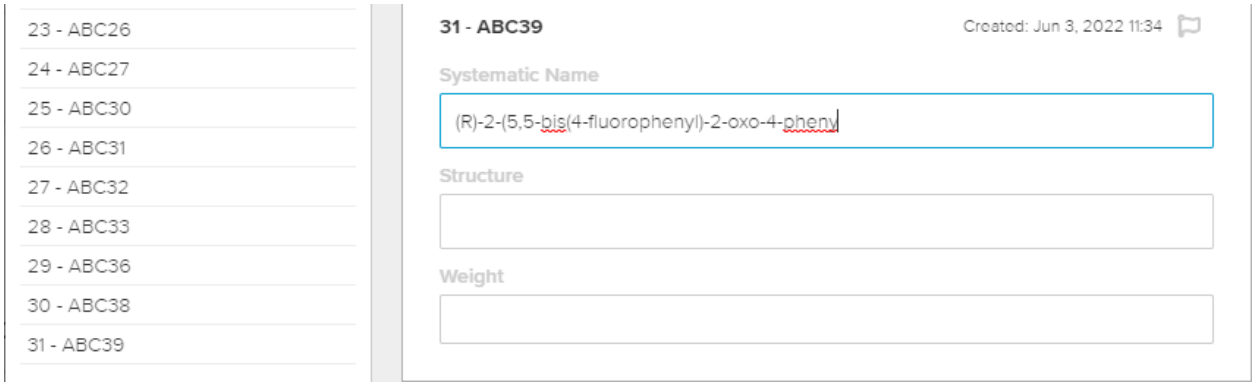


2. Enter an internal reference ID for the compound and click the Save button.



➢ Your compound will be numbered automatically and added at the end of your compound list.

3. Type or copy and paste to fill in additional compound data in the fields provided.

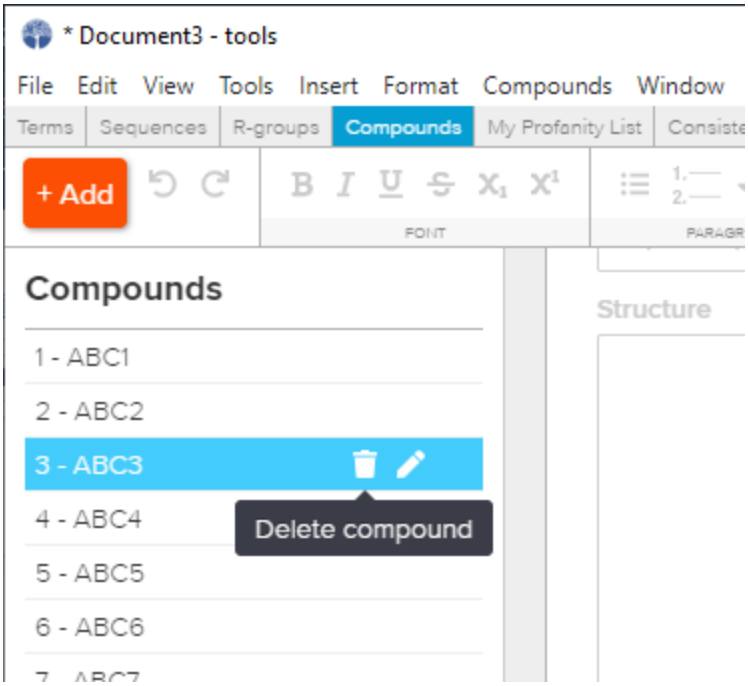


➢ JPEG, PNG, or SVG images can be pasted into the Structure field, or molecular drawings can be added as described in the drawing support sections below.

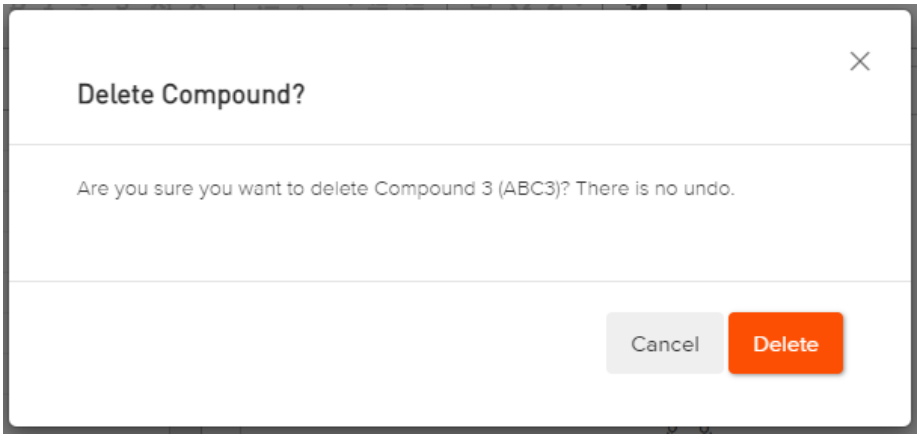
Deleting a Compound

1. Open the Rowan Compounds Manager from the Tools menu and locate the compound you want to delete in the left-hand list.

2. Click the trash bin icon to delete the compound.



3. Click the Delete button in the resulting dialog.

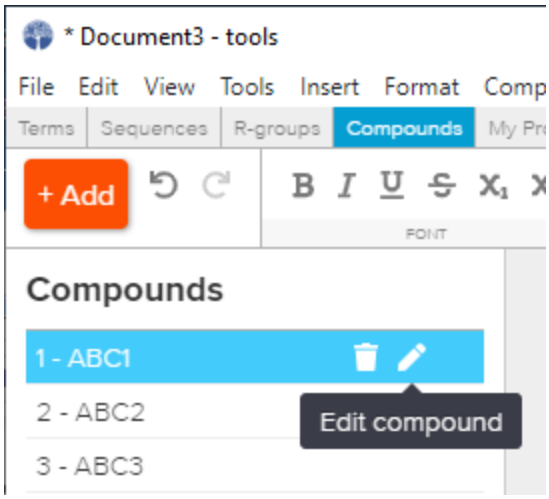


➢ Compounds later in the list will be automatically renumbered to preserve continuous compound numbering.

Editing a Compound

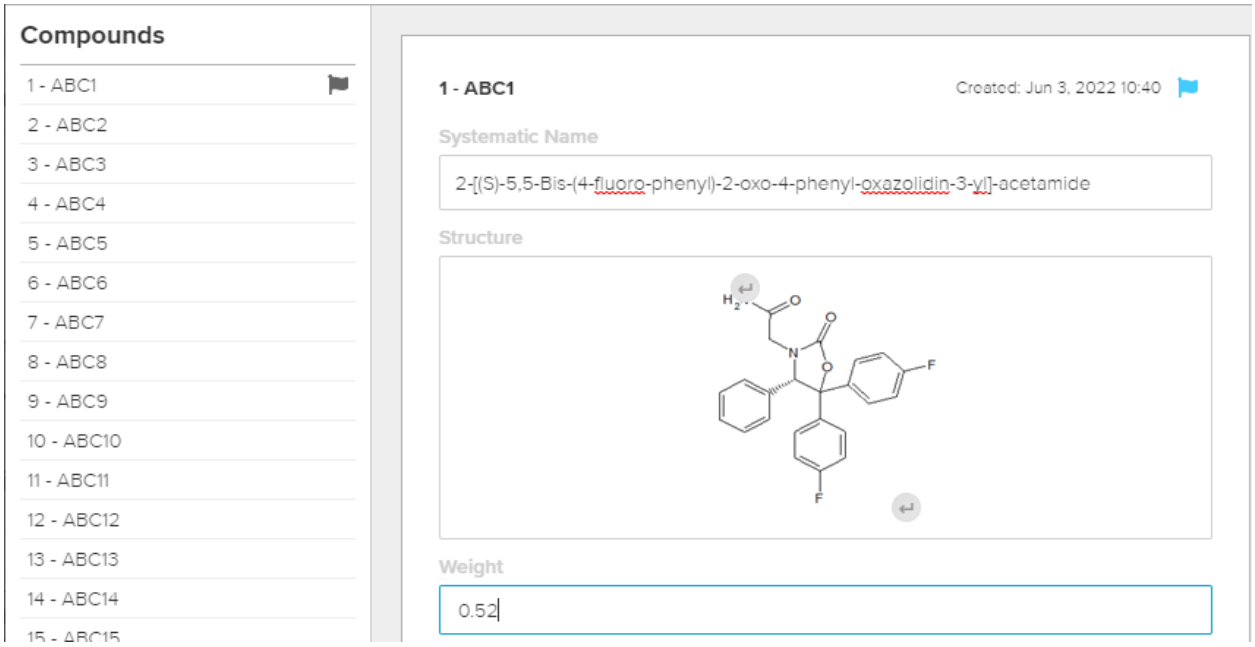
1. Open the Rowan Compounds Manager from the Tools menu and locate the compound you want to edit in the left-hand list.

2. Click the pencil icon to edit the Internal Reference ID.



3. Modify the reference ID as desired, and click the Save button.

4. Type or copy and paste directly in the fields provided to the right to edit other compound details. Click the flag icon to the upper right to identify a lead compound.



➢ Flags for lead compounds are an internal Rowan feature. No data related to flags is included in exported files.

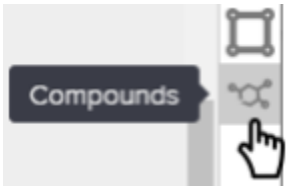
Inserting Compound Information into an Application

1. To insert a compound number or a systematic name begin typing what you want to insert, then select the correct option from the dropdown menu offered.

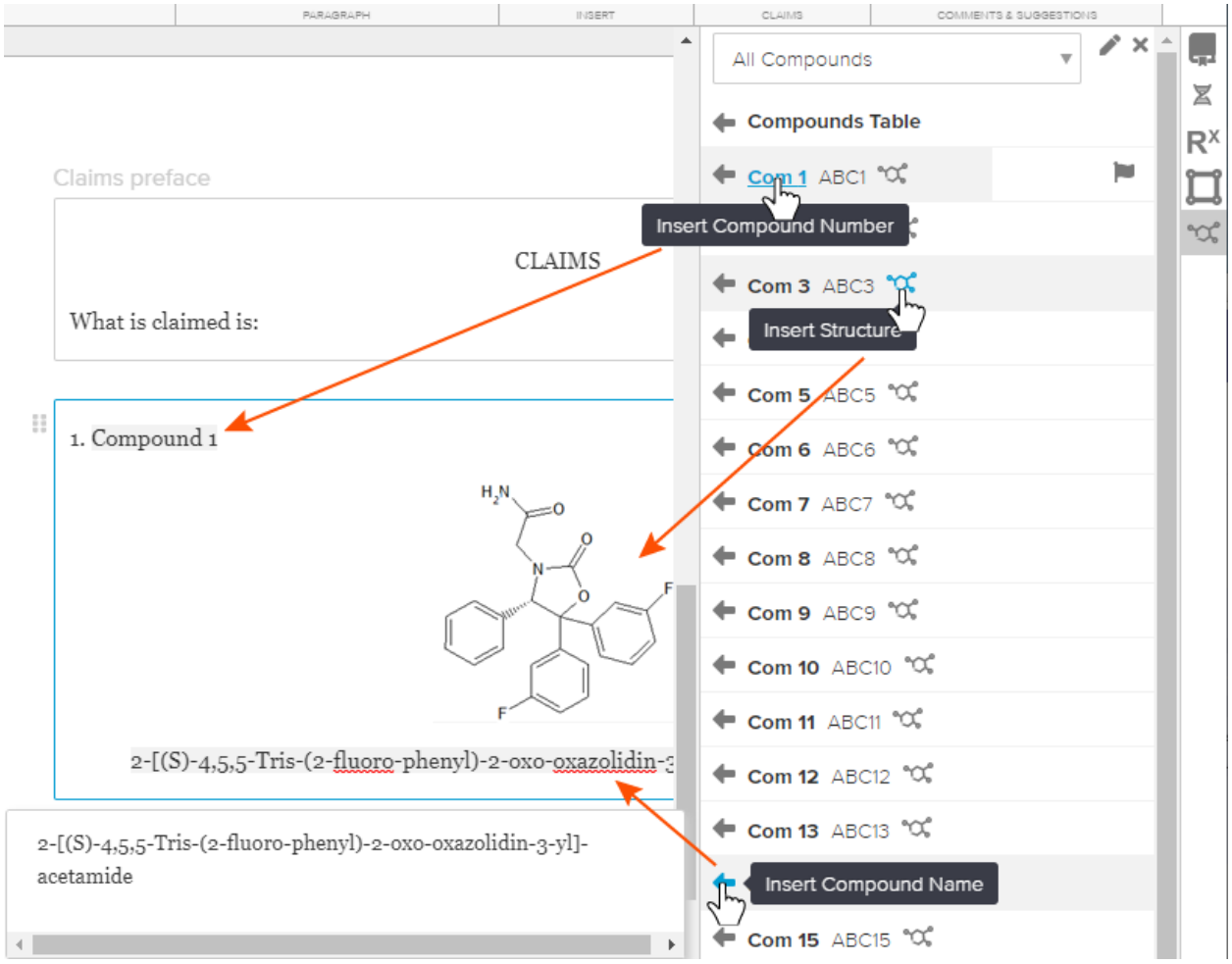
FIG. 1

FIG. 2

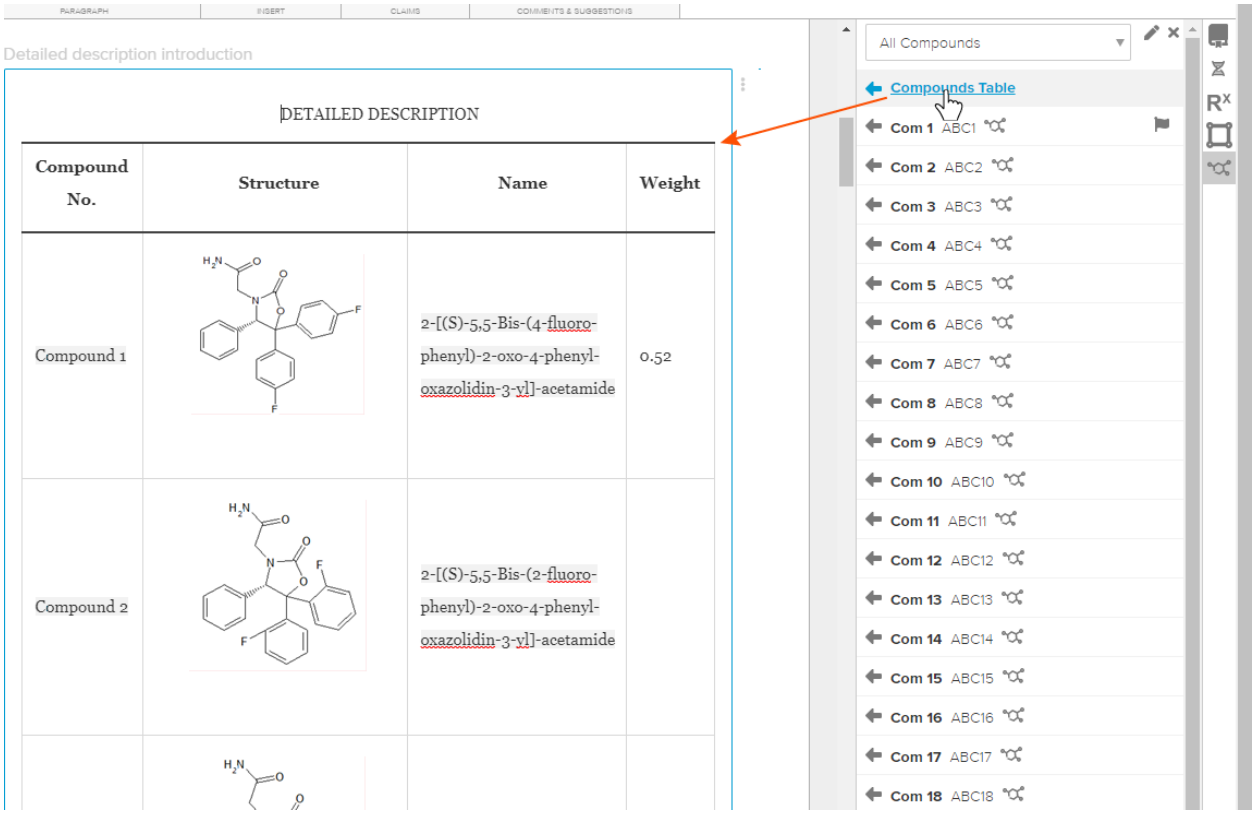
2. Alternatively, click the compound symbol to the right of the Rowan Patents main drafting window to open the compounds panel.



3. To insert compound data from the panel, place your cursor where you want to insert the data, and click the datum for the compound you want to insert.



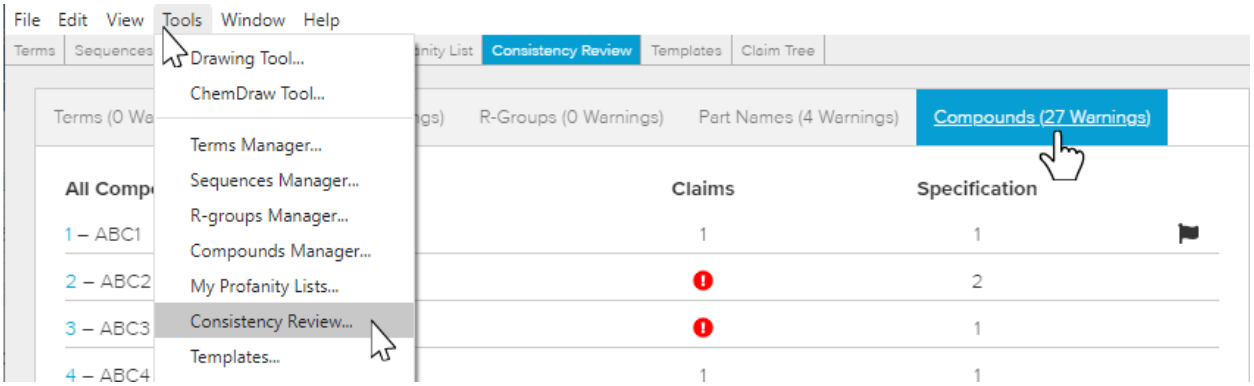
4. To insert a table of all compounds, place your cursor at your desired table location and click the Compound Table option.



➢ The compounds table does not sync to the Compound Manager, and will need to be re-inserted if compounds are further modified.

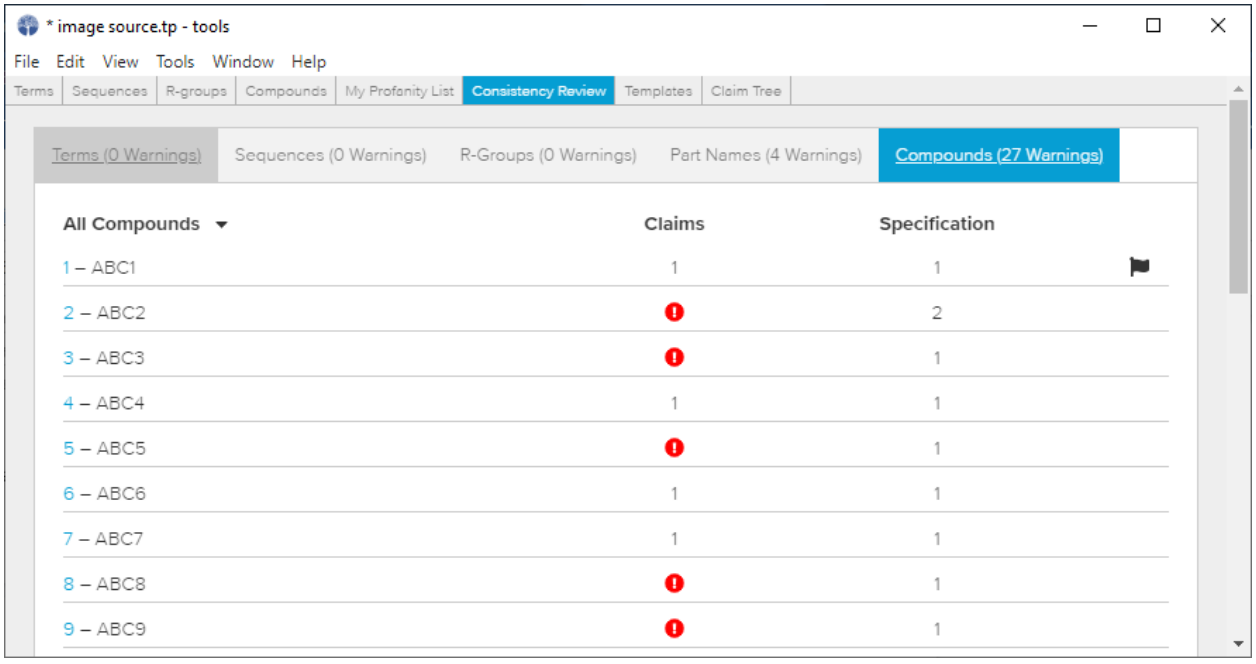
Consistency Review

1. Select “Consistency Review” under the Tools Menu and click the “Compounds” tab.



2. Review each compound and its data for adequacy/accuracy and flagging.

3. Confirm each group/description occurs in the claims and spec as needed.

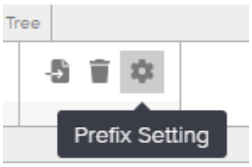


➢ Warning icons indicate elements missing from claims and specification. Where elements do not need to appear, warnings may be ignored; warning data is not included in export files.

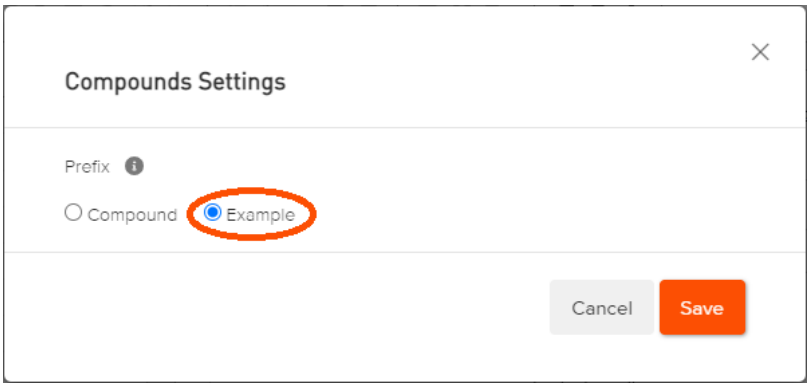
Changing the “Compounds” Prefix to “Examples”

1. Open the Compounds Manager.

2. Click the Prefix Setting icon.

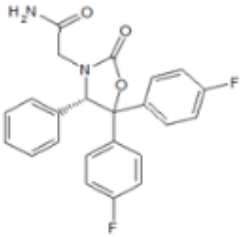
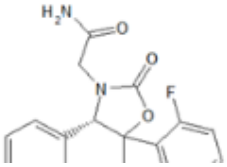


3. Select the “Example” option from the dialog.



4. Click the Save button.

5. The word shown in front of the sequential number will be updated. For example, instances of Compound 1 will switch to Example 1.

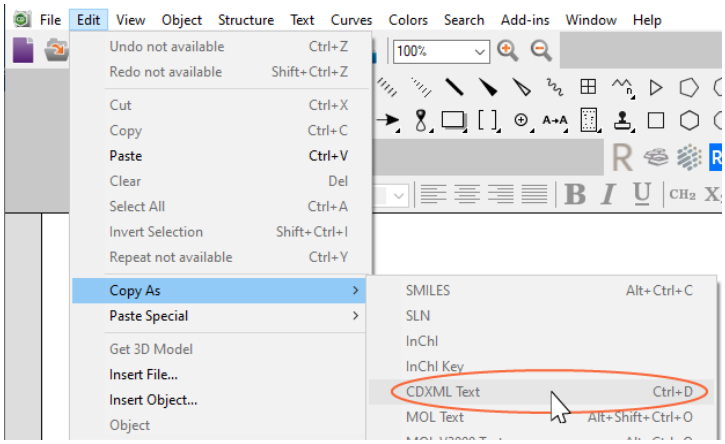
Compound No.	Structure	Name	Weight
Example 1		2-[(S)-5,5-Bis-(4-fluoro-phenyl)-2-oxo-4-phenyl-oxazolidin-3-yl]-acetamide	
Example 2		2-[(S)-5,5-Bis-(2-fluoro-phenyl)-2-oxo-4-phenyl-	

ChemDraw Drawing Support

Adding Molecule Drawings from the ChemDraw Application

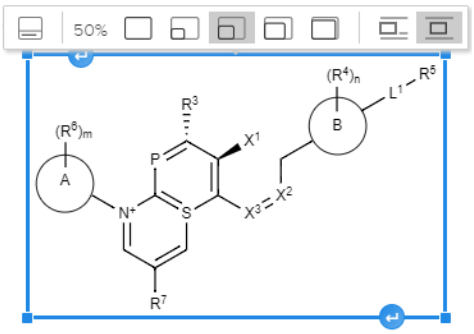
1. Open a ChemDraw file in the ChemDraw application and select the molecule(s) you wish to import using the lasso tool or Select All command.

2. Copy the molecule(s) as CDXML text using Ctrl+D or Cmd-D, or the menu option below.



3. Place your cursor in the Rowan drafting window where you wish to add the copied molecule(s).

4. Paste the copied molecule data at your cursor location.

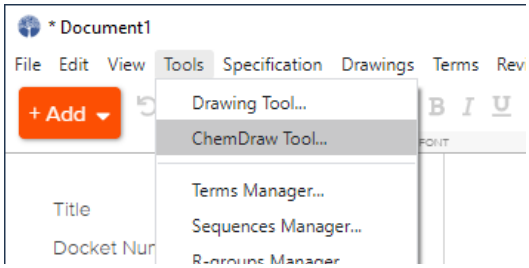


➢ The molecule(s) will be displayed on screen in .svg format but may be edited as described below.

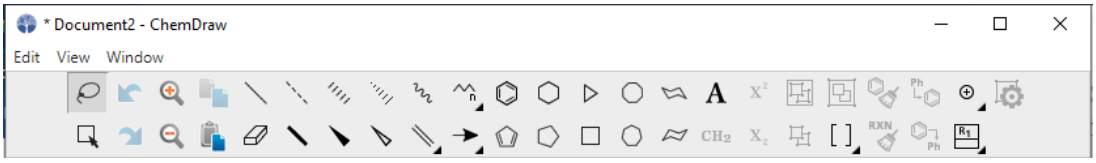
Adding Molecule Drawings using the Integrated ChemDraw Tool

1. Place your cursor in the Rowan main drafting window where you wish to add your molecule drawing(s).

2. Open the Rowan integrated ChemDraw tool from the Tools menu.

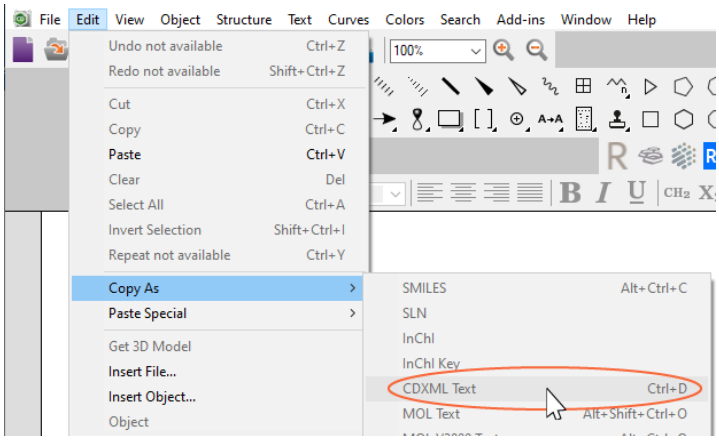


3. Use the tools provided to draw your desired molecule(s).

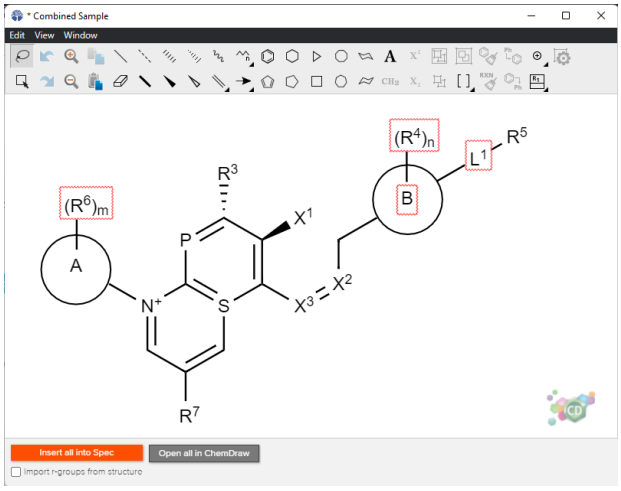


OR

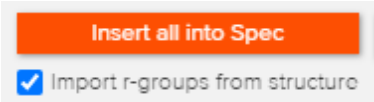
4. Copy molecules in the ChemDraw application as CDXML text using Ctrl+D or Cmd-D, or the menu option below, then paste the copied data into the integrated ChemDraw tool.



5. To insert your molecule(s) into your application, click the Insert all into Spec button provided at the lower left-hand corner of the window.

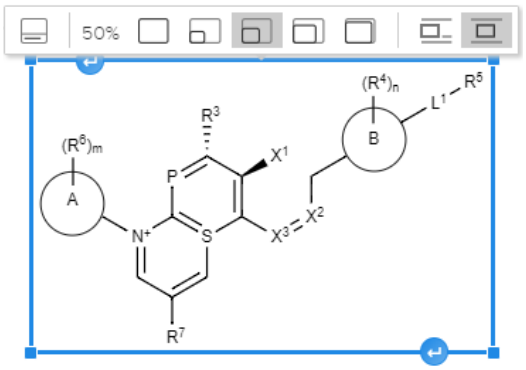


➢ A checkbox is provided allowing you to instruct the tool to detect Markush groups as drawings are inserted into your application.



➢ Detected and imported Markush groups may be edited as described below.

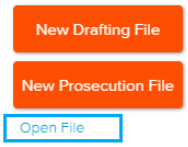
6. The molecule(s) will be displayed on screen in .svg format, but may be edited as described below.



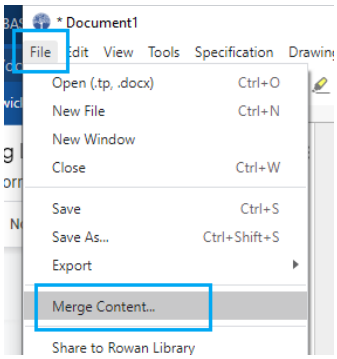
Adding ChemDraw Drawings from a Word Document

There are **three ways** to import ChemDraw drawings contained in a Word file:

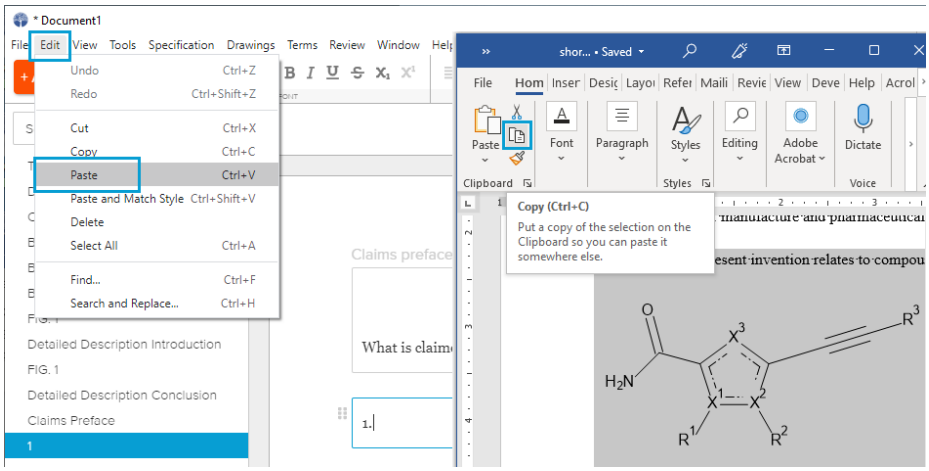
A. Open the Word file containing ChemDraw drawings in Rowan drafting



B. Merge the Word file containing ChemDraw drawings into a Rowan .tp file



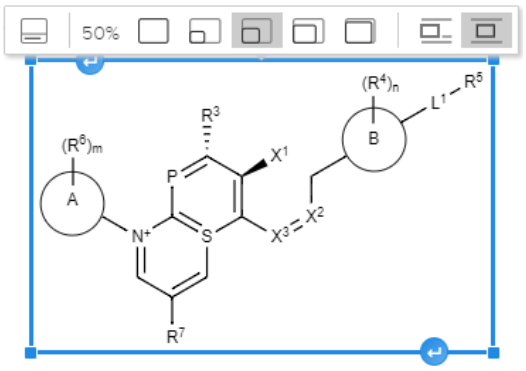
C. Copy one or more ChemDraw drawings (and additional Word text if desired) from Word the Word file and paste them into a Rowan drafting text field



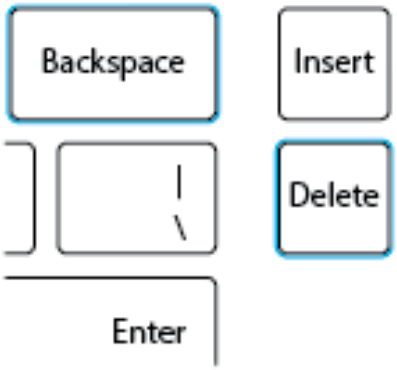
➢ The molecule(s) will be displayed on screen in .svg format, but may be edited as described below.

Deleting a ChemDraw Molecule Drawing

1. Click the molecule drawing you want to delete to select it.

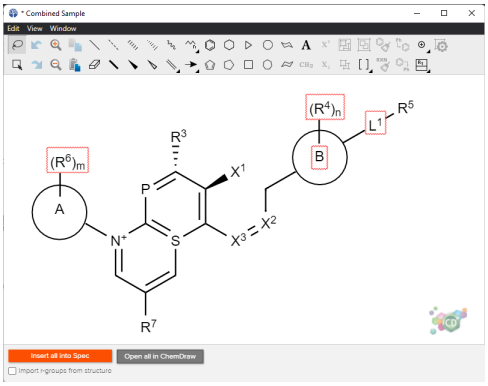


2. Press your keyboard's Backspace or Delete key to delete the drawing.

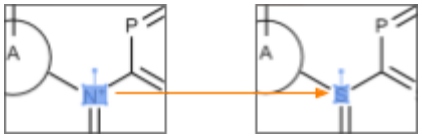


Editing a ChemDraw Molecule Drawing

1. Double-click a molecule drawing in your Rowan file specification or claims to open an inline instance of the ChemDraw tool.

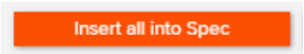


2. Edit the molecule drawing as desired.

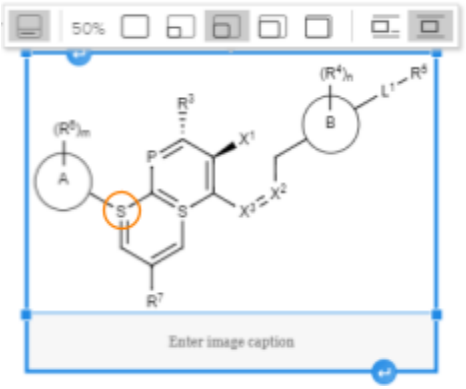


3. Deselect all elements so the entire molecule is inserted (not one selected element).

4. Click the “Insert all into Spec” button or copy and paste your updated drawing to insert your updates into your spec or claims.



5. The molecule will be updated in the main drafting window.

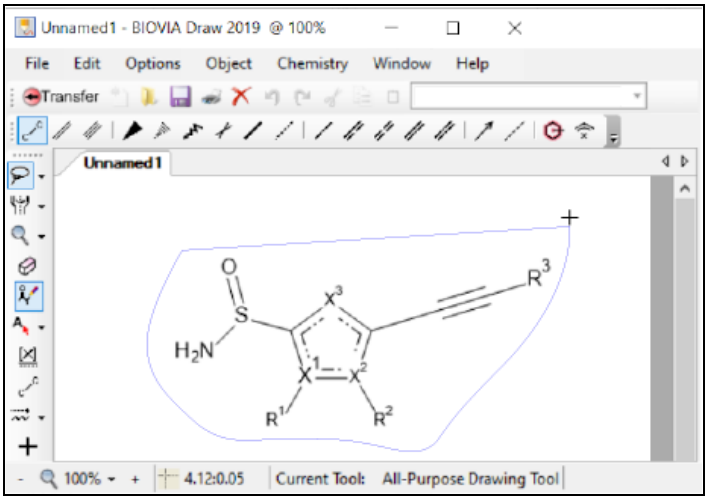


BIOVIA Draw Drawing Support

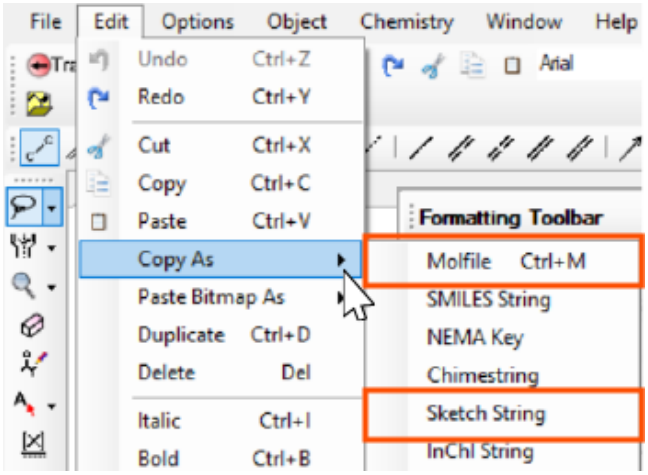
➢ BIOVIA Draw support is limited to BIOVIA Draw 2019 or later, for Windows.

Adding Molecule Drawings from the BIOVIA Draw Application

1. Open a BIOVIA Draw file in the BIOVIA Draw application and select the molecule(s) you wish to import.



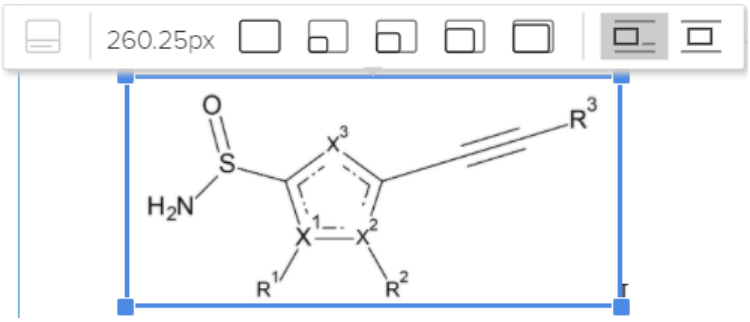
2. Copy the molecule(s) using the Edit > Copy As > Sketch String or Molfile (Ctrl+M) menu options.



➢ BIOVIA Draw molecular drawing data must be MOL/RXN compliant for Molfile data to display correctly. Refer to BIOVIA support documentation for more information.

3. Place the cursor where you want to paste the molecules within the main drafting window.

4. Use Ctrl+V/Cmd-V or the Paste menu option to paste the molecule(s) at your cursor location.

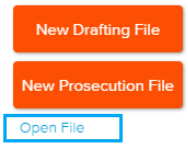


➢ The molecule(s) will be displayed on screen in .png format, but may be edited as described below.

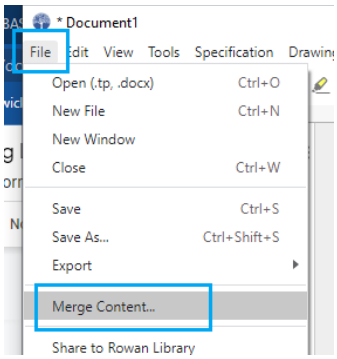
Adding BIOVIA Drawings from a Word Document

There are **three ways** to import BIOVIA Draw drawings contained in a Word file:

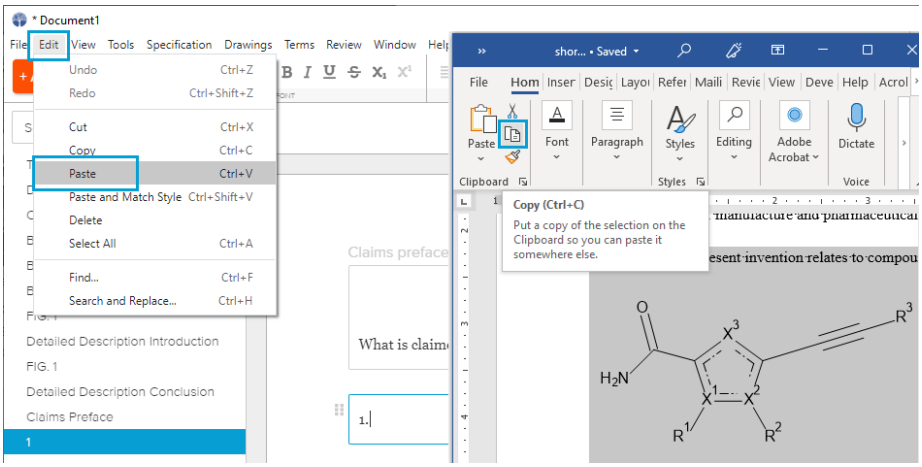
A. Open the Word file containing BIOVIA Draw drawings in Rowan drafting



B. Merge the Word file containing BIOVIA Draw drawings into a Rowan .tp file



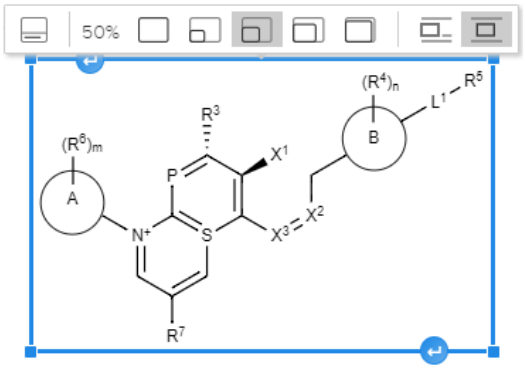
C. Copy one or more BIOVIA Draw drawings (and additional Word text if desired) from Word the Word file and paste them into a Rowan drafting text field



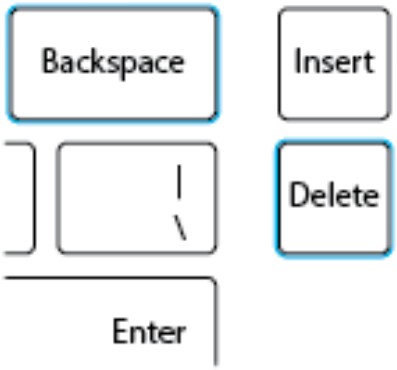
➢ The molecule(s) will be displayed on screen in .png format, but may be edited as described below.

Deleting a BIOVIA Draw Molecule Drawing

1. Click the molecule drawing you want to delete to select it.

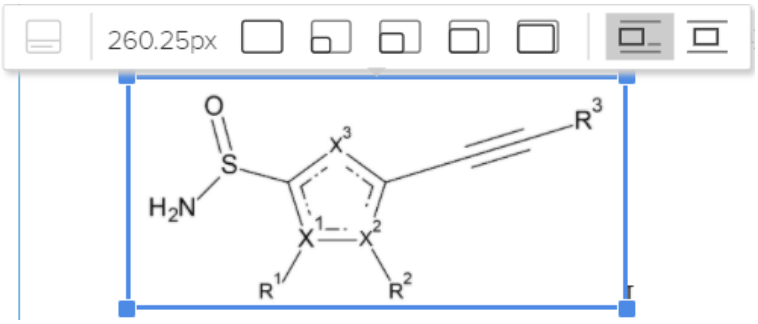


2. Press your keyboard's Backspace or Delete key to delete the drawing.

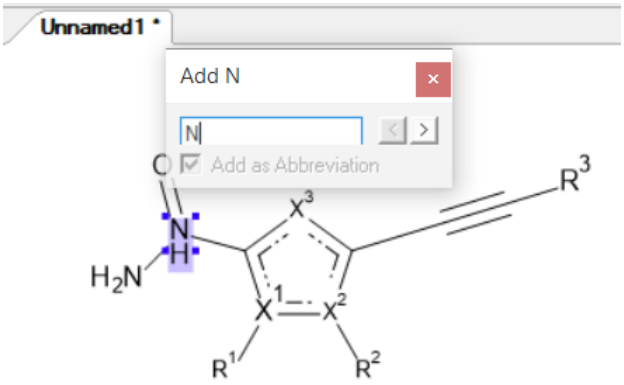


Editing a BIOVIA Draw Molecule Drawing

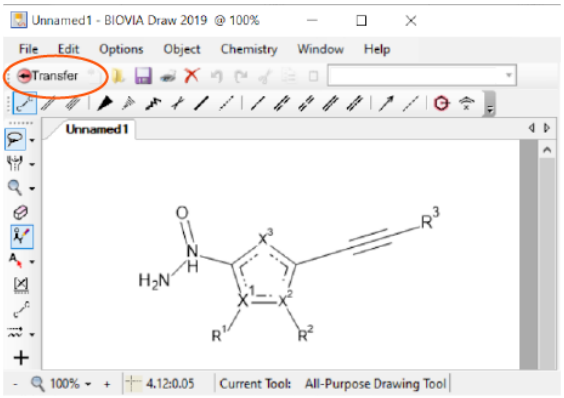
1. Double click the compound from within the specification. This action opens an instance of BIOVIA Draw.



2. Edit the molecule drawing as desired.



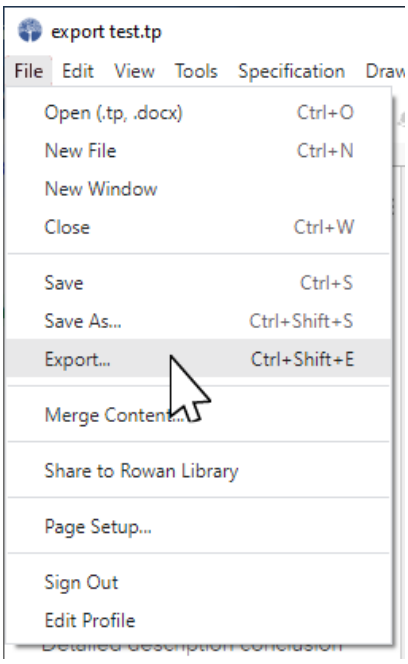
3. When finished, click the transfer button in the top left corner of the window.



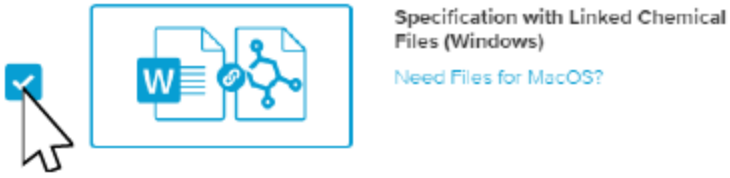
4. The updated version of the molecule will be inserted in the main drafting window.

Word File Export with Editable Molecule Drawings

1. Select Export > Spec and Claims (DOCX) from the Rowan drafting Files menu.

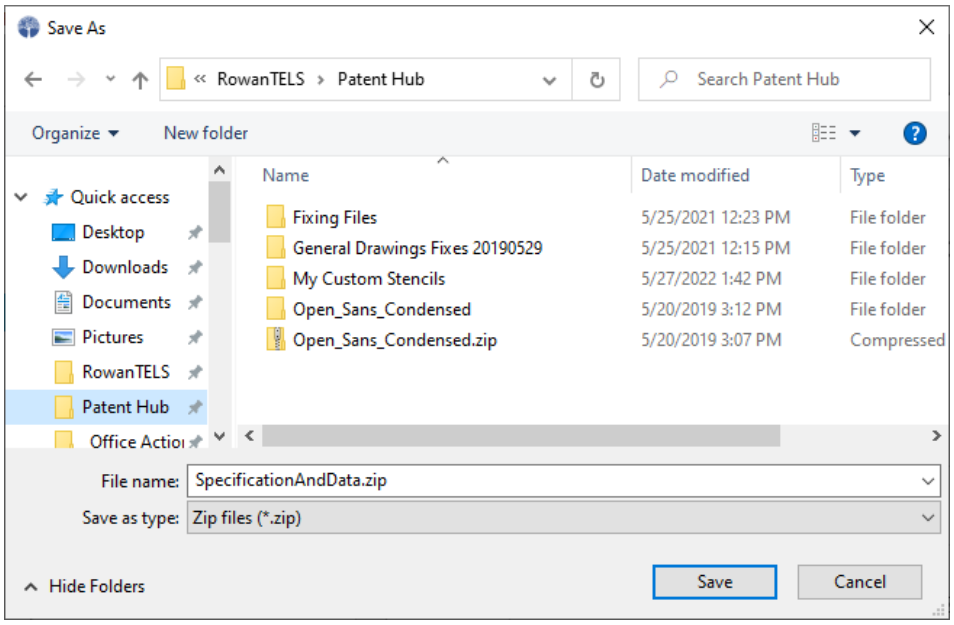


2. Click the Specification with Linked Chemical Files option.

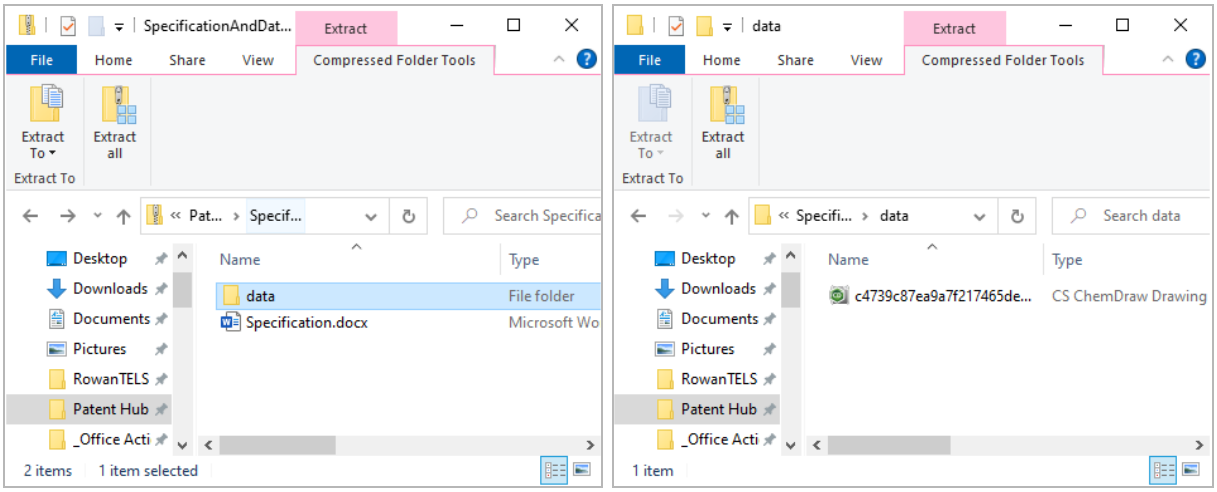


➢ Windows and MacOS users will need different export formats, and can change what will be exported by toggling the “Need Files for” option.

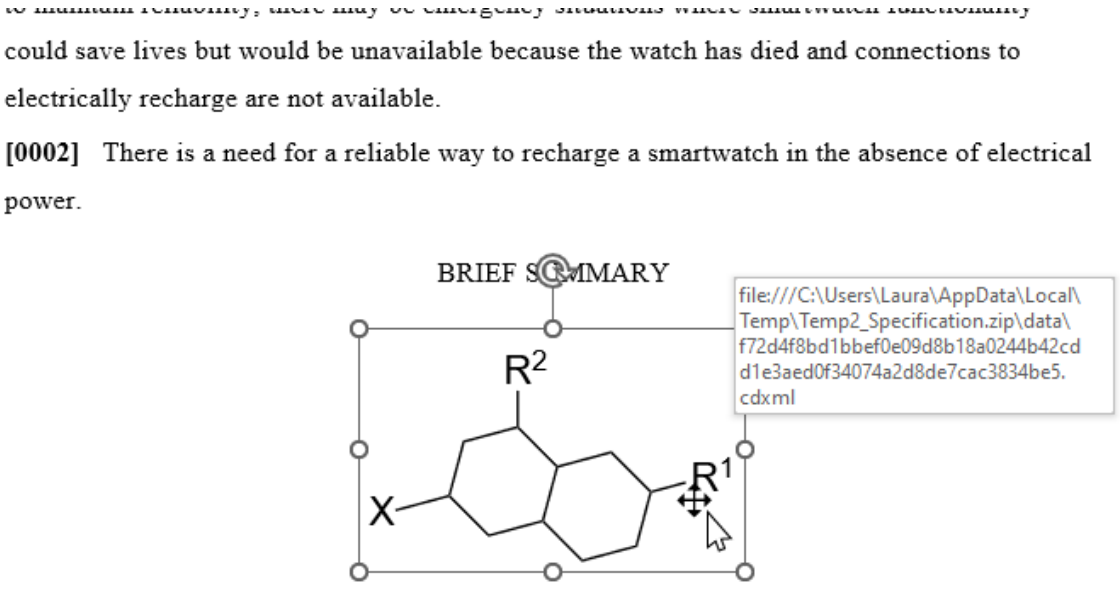
3. Click the Export button and complete the Save dialog.



4. A .zip file will be saved containing a Word .docx file including molecule images that are linked to editable molecule data in a molecule drawing application data file.



5. The .docx file exported will contain the linked images:



Note: A clean file exported with linked data will NOT be suitable for filing with the patent office. For a fileable copy, export a Clean file without the Linked Chemical Files option selected.

Markush Group Management

Adding Markush Groups from Molecular Drawings

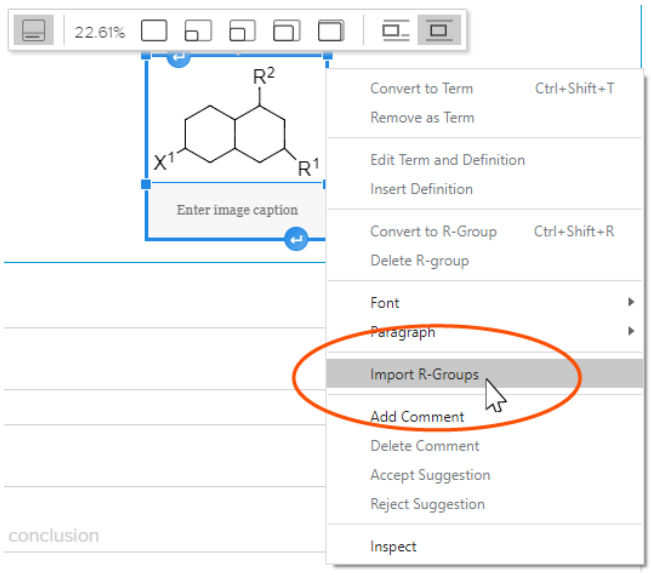
1. Locate the editable molecule drawing within your specification.

   ➢ Markush groups cannot be detected from non-editable molecule images, such as inserted PNGs, JPEGs, or SVGs.

   ➢ BIOVIA Draw molecular drawing data must be MOL/RXN compliant for Markush group recognition. Refer to BIOVIA support documentation for more information.

2. Right-click the molecule drawing to open the context menu.

3. Select the Import R-Groups option, underneath the Font and Paragraph sections.

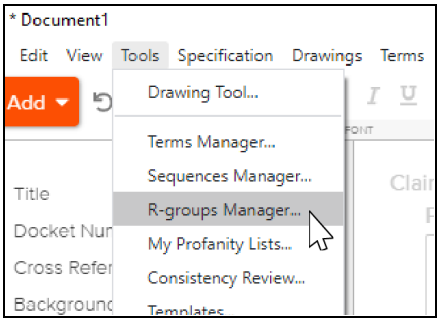


4. Labels in the molecule drawing will be examined, and detected Markush groups will be added to the R-groups Manager. R-groups that already appear in application text will be tagged as data objects and maintained consistent with changes in the Manager.

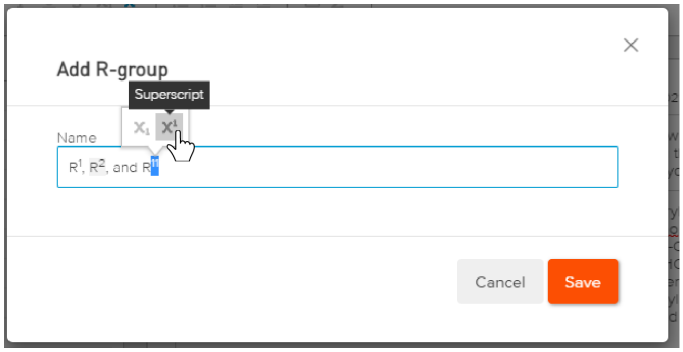
   ➢ If labels match groups that already exist, they will be omitted from the import.

Adding an Individual Markush Group

1. Open the R-groups Manager under the Tools menu and click the +Add button.



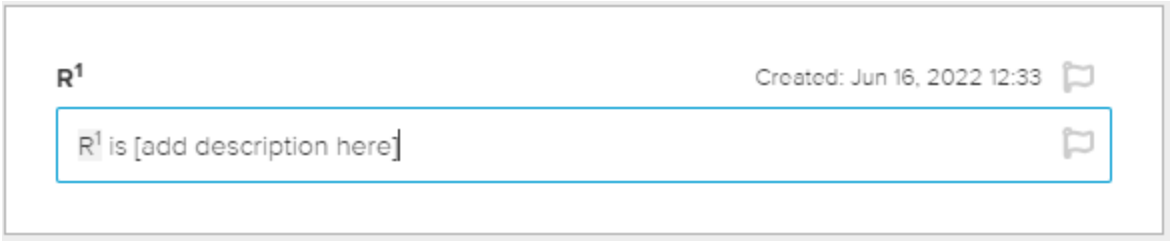
2. Enter your group name or a set of group names (X^3; R^1, R^2, and R^3, etc.) and click Save.



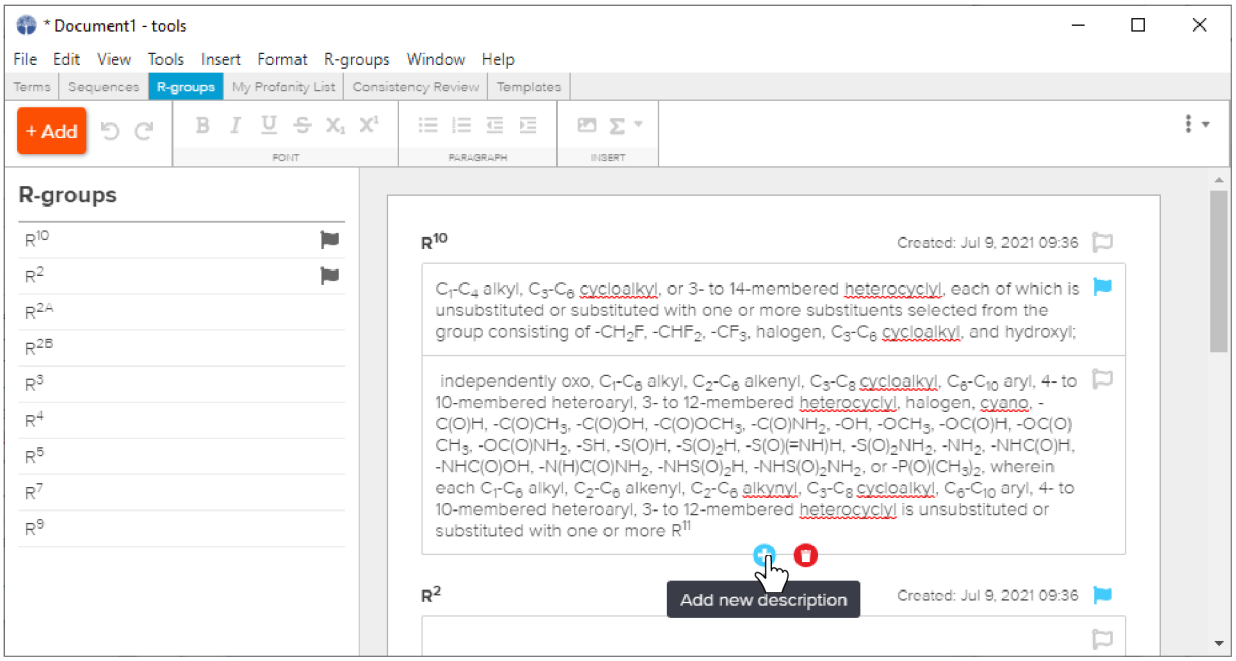
➢ Ctrl+Shift+= turns superscript style on/off. Ctrl+= toggles subscript style. Sub/superscript styles can also be applied to selected characters using toolbar or popup controls where provided.

➢ Existing R-groups included in sets will be individually tagged and will reflect name updates wherever used.

3. Enter description(s) for your R-group or other variable in the description field(s) provided.



4. Add and remove description fields using controls below the description field.



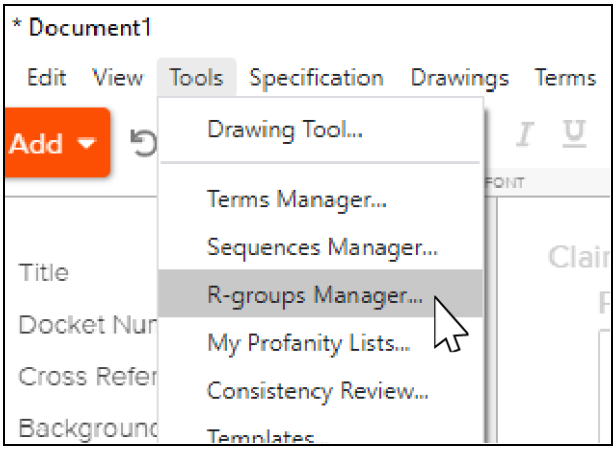
5. Flag lead Markush groups and key definitions by clicking the flag icon next to the name in the left-hand list. Click the flag again to unflag.

   ➢ Flags for lead groups and definitions are an internal Rowan feature. No data related to flags is included in exported files.

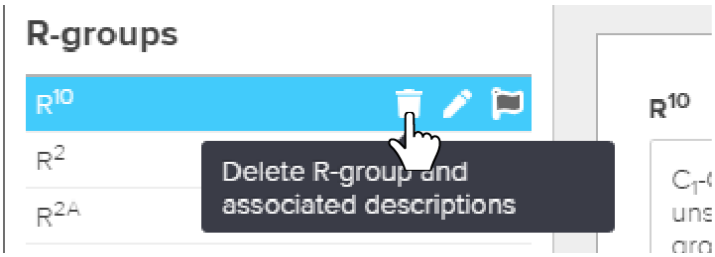
   ➢ R-groups that already appear in application text will be tagged as data objects and maintained consistent with changes in the Manager.

Deleting a Markush Group

1. Open the R-groups Manager under the Tools menu.

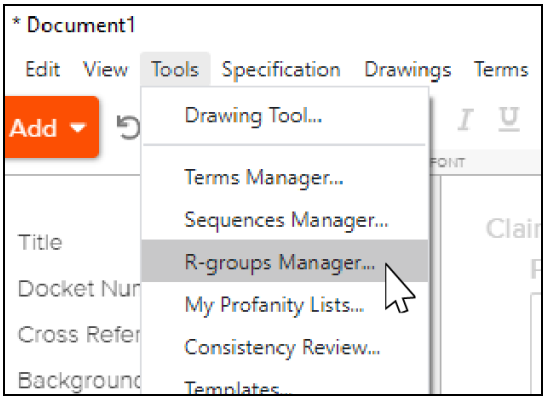


2. Click the trash bin icon next to the left-hand listing for group you wish to delete. All descriptions associated with the name will also be deleted.

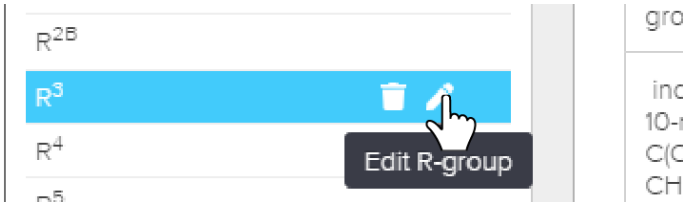


Editing a Markush Group

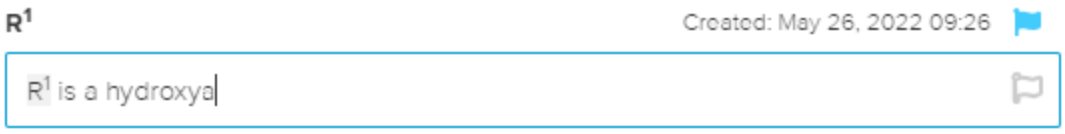
1. Open the R-groups Manager under the Tools menu.



2. Click the pencil icon next to the left-hand listing for the group you wish to edit.

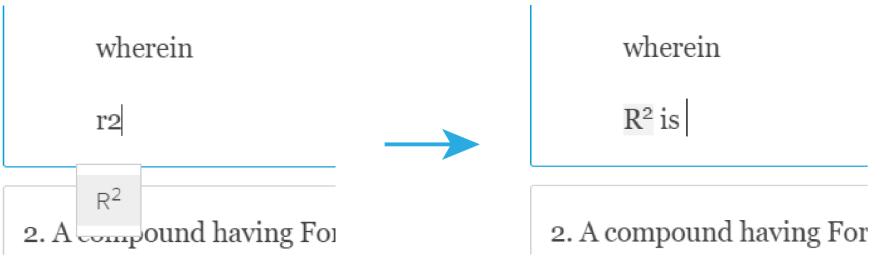


3. Edit Markush group definitions directly in the field(s) provided in the R-groups Manager.



Inserting Markush Group Information into an Application

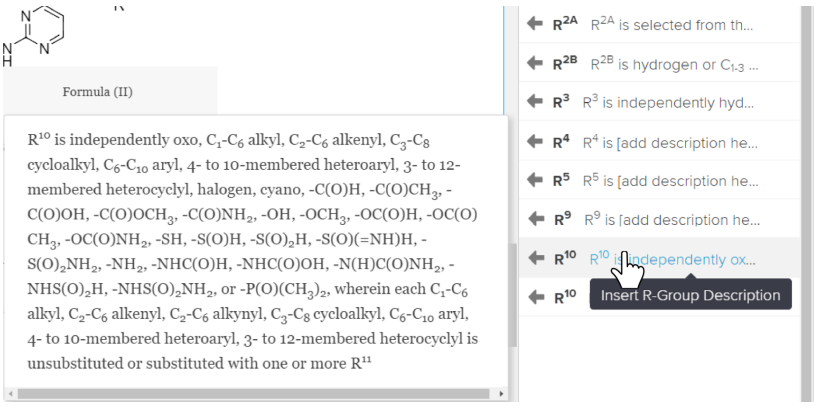
As you type, defined R-groups will autocomplete as tagged objects once you type a space after the R-group name, or can be selected from a dropdown list offered as you type.



To use the R-groups sidebar instead of typing:

1. Expand the R-groups panel in the right-hand sidebar by clicking the icon on the right side of the drafting window.

2. Click the arrow or description. Your description text will insert at your cursor location.

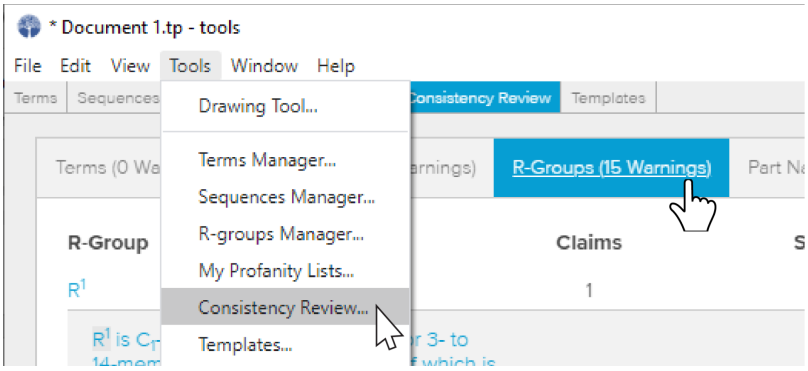


➢ Clicking the “R#” label will insert that label as a tagged object at your cursor location.

➢ Multiple descriptions for one R-group are shown as separate entries in this panel.

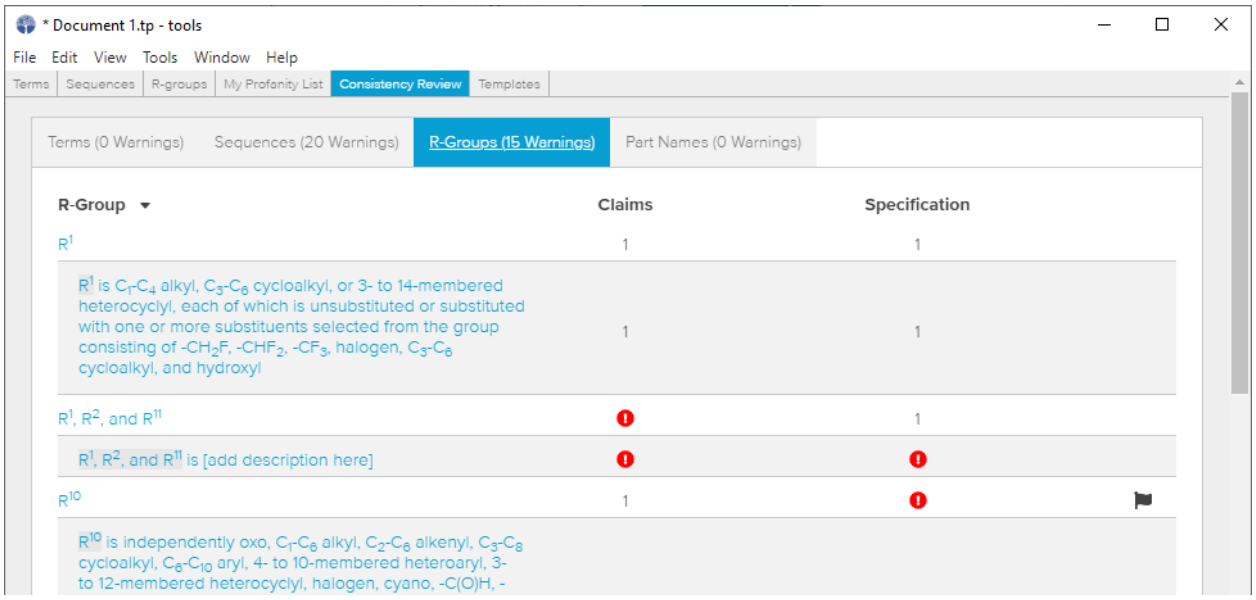
Consistency Review

1. Select “Consistency Review” under the Tools Menu and click the “R-Groups” tab.



2. Review each R group and descriptions for adequacy/accuracy and flagging.

3. Confirm each group/description occurs in the claims and spec as needed.

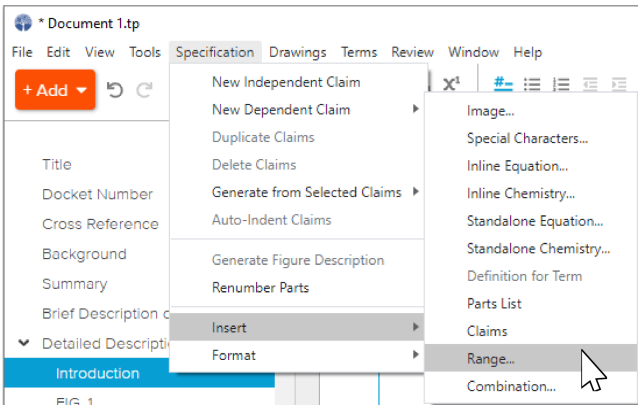


➢ Warning icons indicate elements missing from claims and specification. Where elements do not need to appear, warnings may be ignored; warning data is not included in export files.

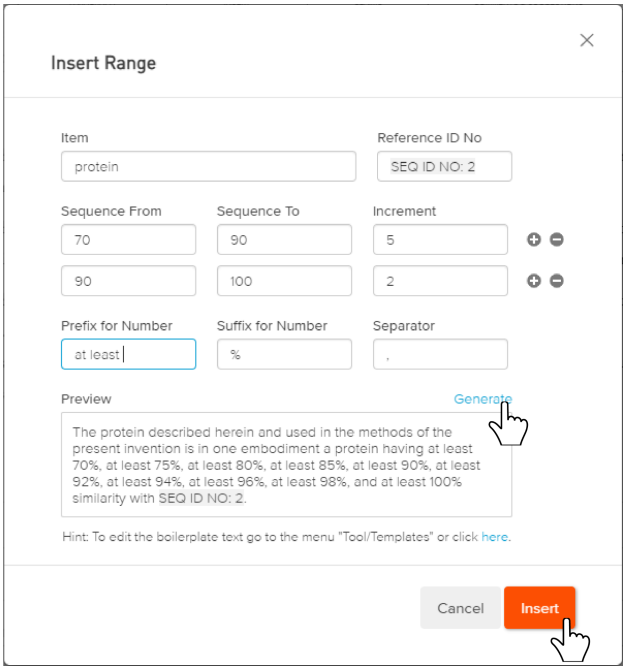
Ranges and Combinations

Inserting Number Ranges

1. Select “Insert” and “Range…” from the Specification menu in the main drafting window.

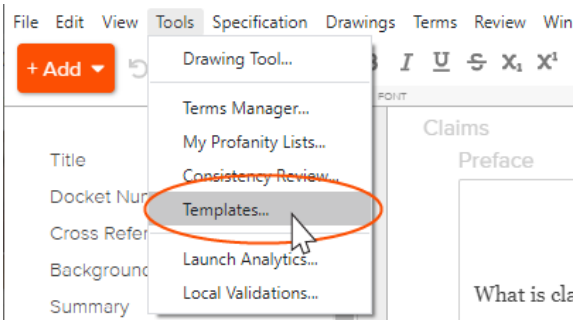


2. Enter the desired parameters. Click Generate to view a preview. Click Insert to place the range(s) created at your cursor location.

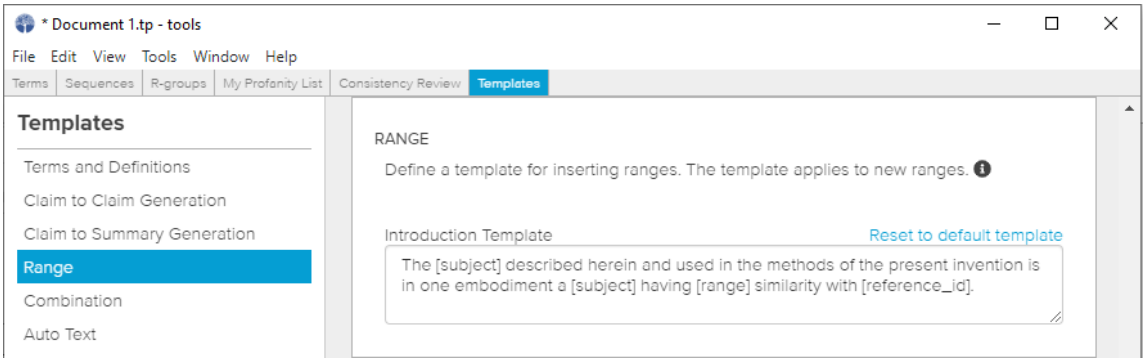


➢ The text generated for preview can be directly edited in the preview field if desired before inserting.

3. To modify the template used to construct the text containing the ranges you create, select “Templates” from the Tools menu.



4. Scroll down to the Range section (or click the Range listing in the left-hand sidebar), and make the desired changes to your template.

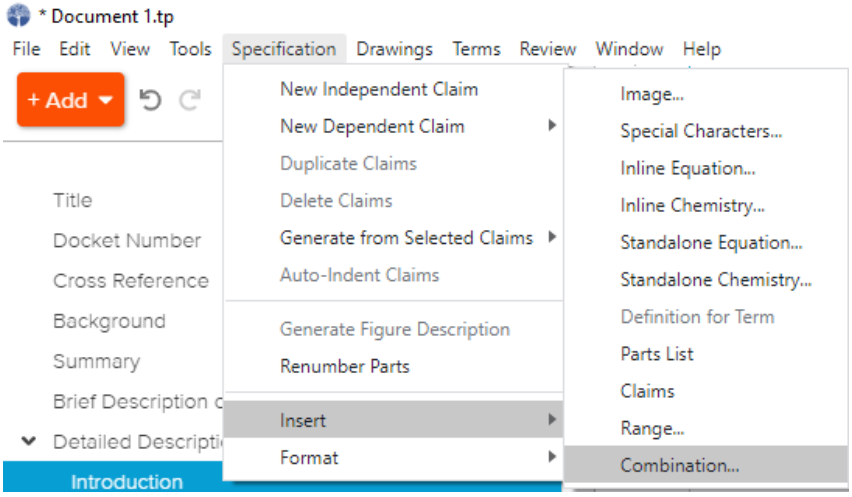


➢ Modified template text will be stored as part of your user set up. Changes made in one application will be reflected across newly inserted ranges in all applications.

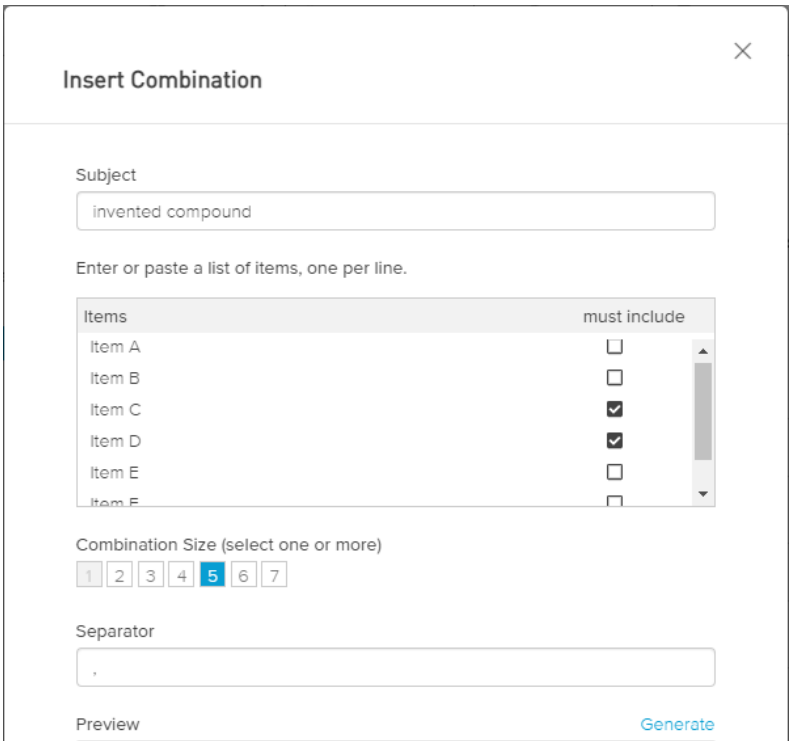
➢ Ranges that have already been inserted will not be updated by template changes.

Inserting Combinations of Items

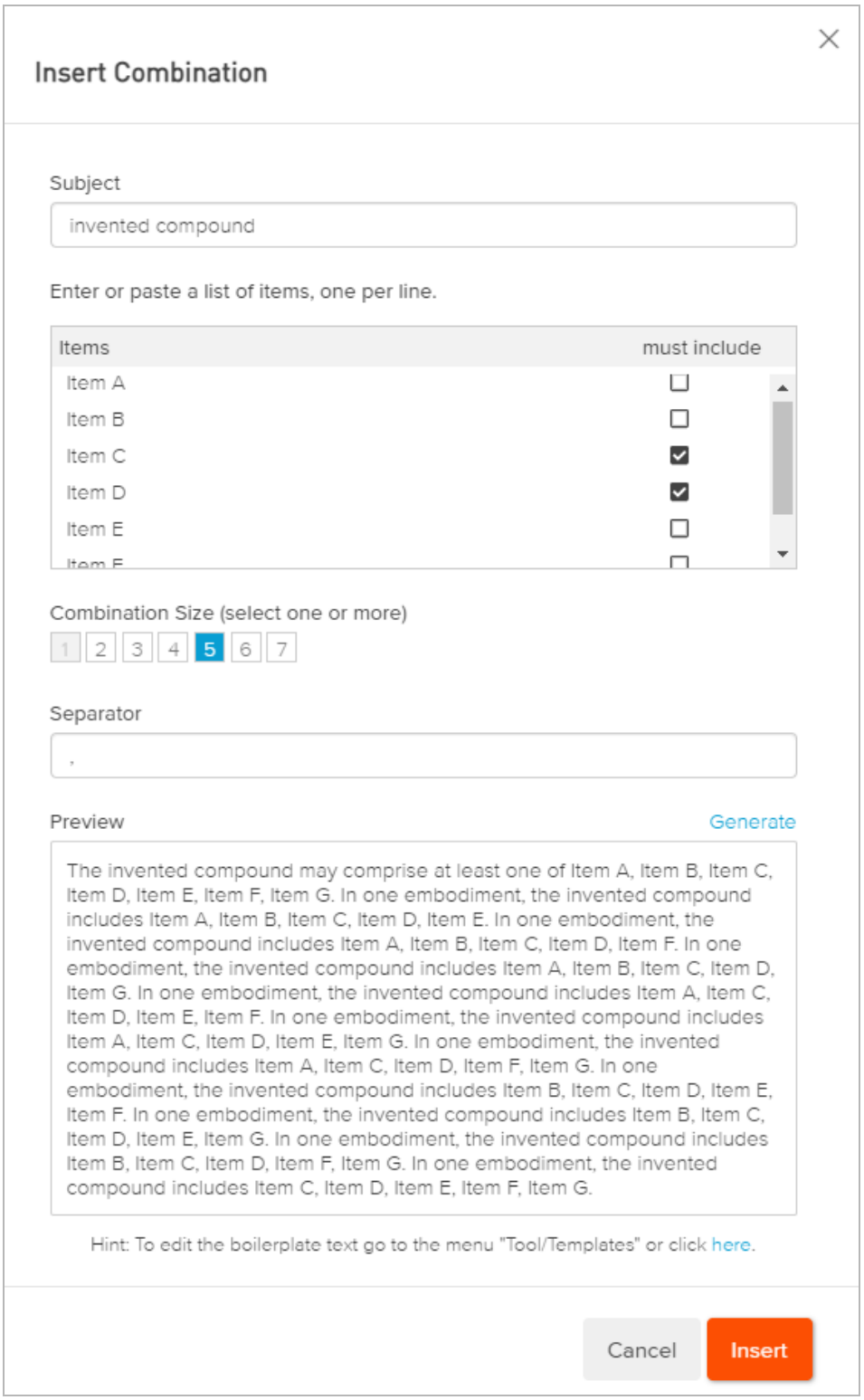
1. To create and insert a set of combinations of items, select “Insert” and “Combination…” from the Specification menu in the main drafting window.



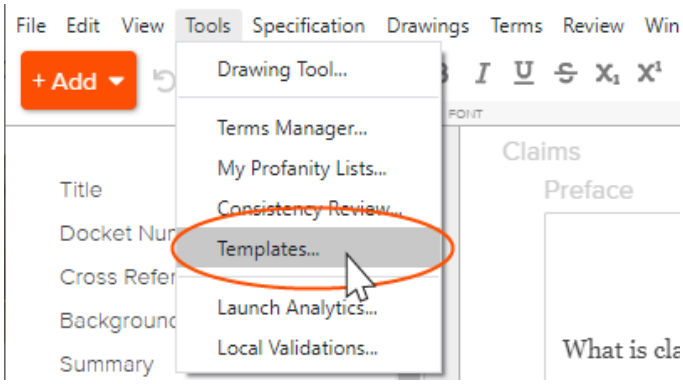
2. Include a subject comprising the combined items, include a list of items, define the parameters of your desired combinations, and click Generate to see a text preview.



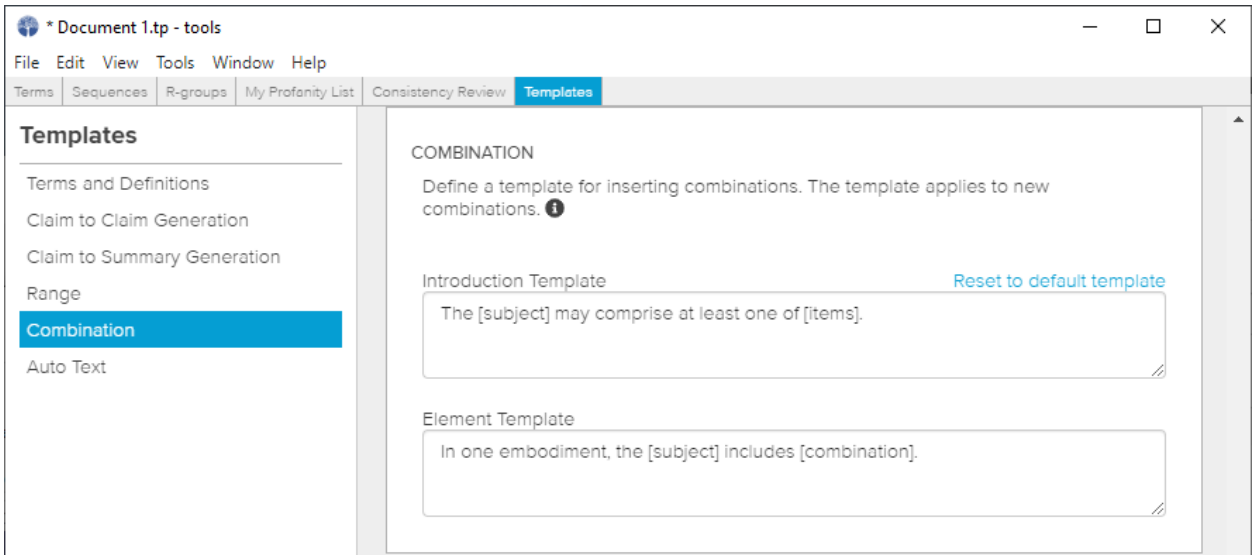
3. Review your text preview, and click Insert to place the generated text at your cursor location.



4. To modify the template used to construct the text containing the combinations you create, select “Templates” from the Tools menu.



5. Scroll down to the Combination section (or click the Combination listing in the left-hand sidebar), and make the desired changes to your template.



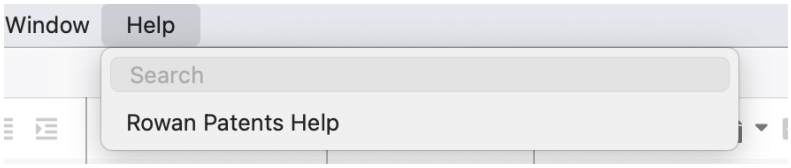
➢ Modified template text will be stored as part of your user set up. Changes made in one application will be reflected across newly inserted combinations in all applications.

➢ Combinations that have already been inserted will not be updated by template changes.

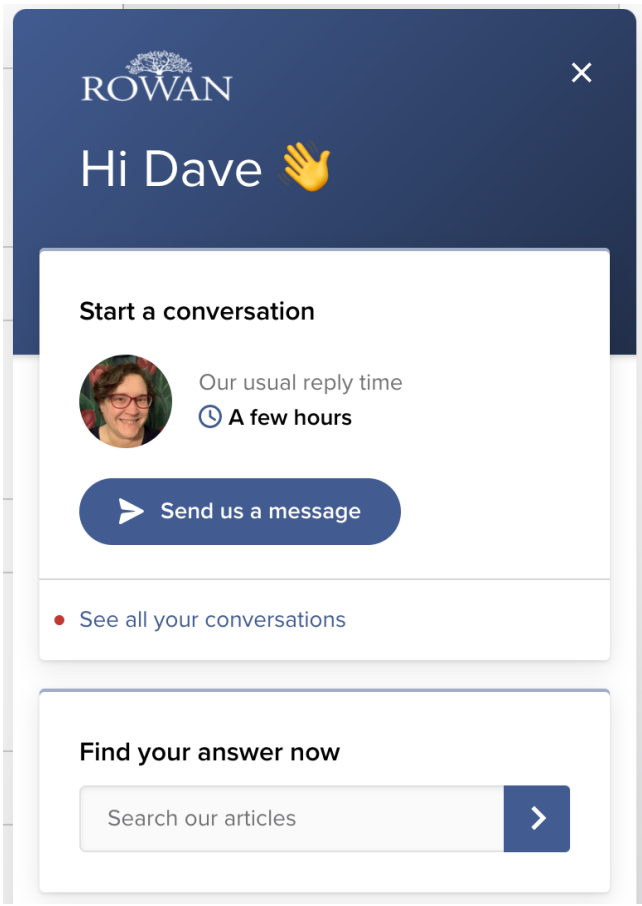
Support and Feedback

You can use our in-tool Help interface to search or browse our support articles or contact us with questions and feedback.

1. Click on the Help menu item and select Rowan Patents Help...



2. This invokes a panel in which you can send us a message, or search for answers in our support articles.



➢ Several Rowan product team members monitor the chat and will respond at least by the next business day, and typically within a couple of hours.