Searching SciFinder
Registry File

1. What subjects and publication types are included in the database?
   Reactions from journal articles and patents.

2. What are the coverage dates?
   Registry File is 1957 to the present.

3. What Boolean or Proximity operators are used by the database?
   You can use Analyze/Refine.

4. If truncation is allowed then what symbols are used?
   None.

5. If wildcards are allowed then what symbols are used?
   None.

6. How do you search for a phrase?
   None.

7. Is it possible to group words from the same concept?
   None.

8. Any unique features?
   Atom to Atom mapping.
   Variable point of attachment.
   Variable groups.
SciFinder
Structure & Reaction Searching

EXPLORE – Substances – Chemical Structure – Non-Java – Click to Edit

Fusing Rings, Changing Bonds, Changing Atoms

1. Draw the structure. Select the Structure button.

* You will use the Cyclohexane, Cyclopentane from and the pencil and maybe the Eraser.

* You will use the Bonds Palette and atoms from the Common Atoms Palette.

Click the OK button.
(This transfers the structure from the drawing editor to SciFinder.)

A. Search all the search types Exact Structure, Substructure, Similarity (75 - ≥ 99). Record the number of results and look at the answers to figure.

Help: Click the breadcrumb trail Chemical Structure exact > substances (36) to go back.

B. Place the search types in their proper relation to one another given the answers above.

_________________________ > __________________________ > __________________________

C. What is the difference between Exact and Substructure?

Exact – no substitution is allowed, in other words, just what you drew.
Substructure – exact search answers + substitution is allowed, in other words, any hydrogen can be replaced by another element.
Using Shortcuts

Use either Selection Tool or the Lasso to select the entire structure from the previous question then press the delete key to delete the structure.

2. Draw the structure.

You will use the Shortcut menu (i.e., structure shortcuts).

A. **Substructure** search.

How many did you get? ________________

2,000+? You forgot the Me but you had the two N.

875-925? You forgot to add the two N but you have the single Me.

450-500? Way to go!

275-325? You forgot to add the two N and you added an extra Me.

The C at the terminal end of the ketone is just a carbon. Methyl was not implied. By assigning that C as a methyl you prevented substitution at that point. When it is just a C the system can assign three hydrogens, or two hydrogens and one other element (like a carbon chain), or 1 hydrogen and two other elements.

100-150? You added an extra Me.

The C at the terminal end of the ketone is just a carbon. Methyl was not implied. By assigning that C as a methyl you prevented substitution at that point. When it is just a C the system can assign three hydrogens, or two hydrogens and one other element (like a carbon chain), or 1 hydrogen and two other elements.
Preventing Substitution and Preventing Ring Fusion

3. Draw the structure.

\[
\text{\begin{tikzpicture}
  \begin{scope}[thick]
    \draw (0,0) circle (1cm);
    \draw (0,0) -- (90:2cm);
    \draw (0,0) -- (210:2cm);
    \draw (0,0) -- (330:2cm);
    \draw (0,0) -- (90:1cm);
    \draw (0,0) -- (210:1cm);
    \draw (0,0) -- (330:1cm);
    \draw (0,0) -- (90:0.5cm);
    \draw (0,0) -- (210:0.5cm);
    \draw (0,0) -- (330:0.5cm);
  \end{scope}
  \end{tikzpicture}}
\]

A. **Substructure** search. How many substances did you get? ______________
(You should get 119,000 – 124,000)

B. Look at the first 50 substances. Identify one atom on the structure you drew having a lot of substitution (Deuterium is not substitution).

Preventing substitution: Click on the Lock Atoms tool then click on the atom you identified.

On which ring is the identified atom? 5-member 6-member
At which position is the identified atom? ortho meta para

Redo **substructure** search. How many substances did you get? ______________
(You should get <65,000)

Is this: More Same Less as your first search?

C. Let’s prevent ring fusion on the ring not containing the atom in the previous question. Preventing ring fusion: Click on the Lock Ring Fusion or Formation tool then click on the desired ring.

Redo **substructure** search. How many substances did you get? ______________
(You should get <60,000)

Is this: More Same Less as your second search?
Using Variables and R-Groups

4. Draw the structure.

You will use the Variable \(-X\) and Define R-groups \(=R\) icons.

\[
\begin{align*}
\text{R}_1 &= \text{N, S, O} \\
\text{R-Group hint:} \\
1. & \text{Click the Define R-groups } =R \text{ icon,} \\
2. & \text{Select the Atoms option} \\
3. & \text{Click the desired atoms then click the Close button – you just defined R1} \\
4. & \text{In the structure click the atom to be the R1}
\end{align*}
\]

\text{Anytime the structure has a variable you will not be able to perform an exact search.}

\text{Anytime the structure has a variable you will not be able to perform a similarity search.}

A. \textbf{Substructure} search. How many substances did you get? ________________

(You should get 225-275)
Variable point of attachment

5. Draw the structure with a variable point of attachment for the Me at one of two nodes on the ring.

You will use the Variable Attachment Position (VAP) icon. After drawing the structure, click Me somewhere to the right of the structure before clicking the VAP icon. Click on the VAP icon, then click on that Me and drag to the point of attachment on the ring and release.

\[
R_1 = 0, S
\]

A. **Substructure** search.

How many substances did you get? _______________

0 – 50    Didn’t use Variable Attachment Position tool

125 – 175 Way to go
6. Draw the structures in the reaction.

You will use the Reaction Arrow icon and the Structure Template menu – steroid submenu.

Click the OK button.
(This transfers the structure from the drawing editor to SciFinder.)

A. Reaction – **Allow variability only as specified.**
What is the yield of this reaction? ______

*(Assignment Hint: This is the reaction option <Allow variability only as specified> you will select for the questions on the assignment.)*

B. Reaction – **Substructure.**
How many reactions have more than one step? ____________
(Hint: Use Analysis or Refine to answer this.)
(You should get 100-150)
EXPLORE – Reactions – Reaction Structure – Non-Java – Click to Edit

Retrosynthesis & SciPlanner

7. Find the reaction path with the highest yield.

You have a reactant/reagent and a product but you don’t know if it is one, two, three, or more steps. You will use the Repeating Group tool. Once the tool has been selected, two boxes will appear in the upper right corner of the editor.

$$R_1 = \text{Br, OH}$$

A. Reaction Search – **Allow variability only as specified.**

How many reactions? ________________

If there are zero then do part B.

B. Use SciPlanner to show the reaction path.

1: You are going to work backwards – this is known as retrosynthesis. Draw the product and a reaction arrow but don’t put anything on the left side of the equation.

2: Reaction Search – Allow variability only as specified.

3: Sort by: Product Yield

4: Look at the reactants/reagents in the answer set to see which ones look like they will get you to the original reactant/reagent and meet any search limitations like percent yield. When you find one click the check box next to that reaction.

Then click (upper right corner of page)

5: Place your cursor on the intermediate reactant/reagent and select the More Options icon then click on the Get reactions where substance is a product link.

6: Did you get your original reactant/reagent? If yes, then you are done. If no, then repeat steps 3 and 4.

7: Click on the SciPlanner icon (upper left corner of page)

8: Drag and drop reactions onto your workspace, if it hasn’t already been done.

9: To make one path out of many identify a substance that appears in two paths, clicking on one of them will put a red box around the substance. Then drag the red boxed substance over the other identical substance. Now you have combined two reaction paths into one.
**EXPLORE – Reactions – Reaction Structure – Non-Java – Click to Edit**

**Atom to Atom mapping and Marking bonds to be formed or cleaved**

You are looking for a particular set of reactions. You want the bond with the double lines to be formed and you want the Sulfur in the reactant to be the Sulfur in the product.

8. Draw the structures in the reaction with the given criteria mentioned in the previous paragraph.

Use the Mark bonds to be formed or broken tool and the Map atoms in a reaction tool.

![Diagram of atom mapping example]

**A. Reaction Search – Substructure.**

How many reactions did you get? ____________

Zero – Do a substructures of more complex structures search

40-60 – Way to go!

300-400 – Forgot to do atom to atom mapping of the Sulfur.

The Sulfur in the reactant/reagent role is not the same Sulfur in the product. Use the Atom Mapping tool and click on the S in both the reactant/reagent and product and redo the search.

1,000+ – Forgot to mark the reaction site.
More Practice Problems:

9. Draw the structure.

\[
\begin{align*}
\text{R1} &= \text{any element} \\
\text{R2} &= \text{any element except Hydrogen}
\end{align*}
\]

No substitution allowed on the ring and the ring is isolated

A. How many structures do you find?

B. How many reactions have this structure as a product?

10. Find a pathway for the following reaction. How many one-step reactions are there?

\[
\begin{align*}
\text{R1} = \text{any element} \\
\text{R2} = \text{any element except Hydrogen}
\end{align*}
\]

11. The following reaction has an R group containing four (4) fragments for the reactant. The product can have free sites or substitution at two atoms C* and N*. How many reactions do you find that have a yield between 70% and 79%?

\[
\begin{align*}
\text{R1} = \text{any element} \\
\text{R2} = \text{any element except Hydrogen}
\end{align*}
\]