CAS products and services in Korea

korea@acs-i.org

SciFinder^{n} Search Guide

SciFinder^{n}
A CAS SOLUTION

Contents

SciFinder^n
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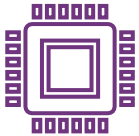
CAS, a division of the American Chemical Society (ACS)



CONTENT

Breadth and Depth Required

High-scale data ingesting across time, disciplines, and at an in-dept scientific level to fuel new breakthroughs

HISTORY

World's Largest Scientific Society

With more than 110 years of experience, CAS collects and analyzes the world's disclosed science to help advance discovery everyday

EXPERTISE

Context is Crucial

500+ expert scientists who know context, semantic linking and languages for insights beyond an algorithm

TECHNOLOGY

Big Data Infrastructure

Best in class search solutions like SciFinder^n, STNext and big data infrastructure to drive discoveries

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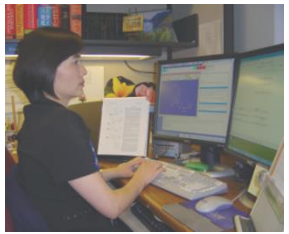
CAS expert scientists read the literature to extract, organize and connect the valuable details within.


Source Selection — Analyze and organize the documents for different sections and types

Reference Information — Enhance titles and abstracts; Concepts and Languages

Substance Information — Novel compound registration; Properties and Spectra

Reaction Information — Methods of Synthesis Reagents, Catalysts, Products

Markush Structure — Chemical structure information in patents

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Create a SciFinder^{n} ID

1. Enter the university library website

2. Click “Databases” – Click “Overseas databases” * This may vary by university

3. Click SciFinder^{n}

4. Click the registration URL
(Starting with https://scifinder.cas.org/registration/index.html?corpKey=)

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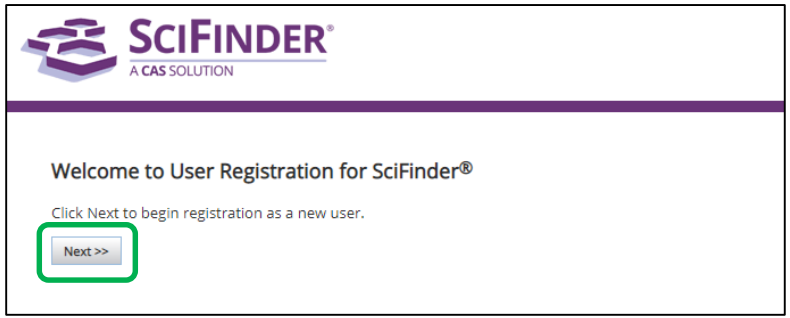
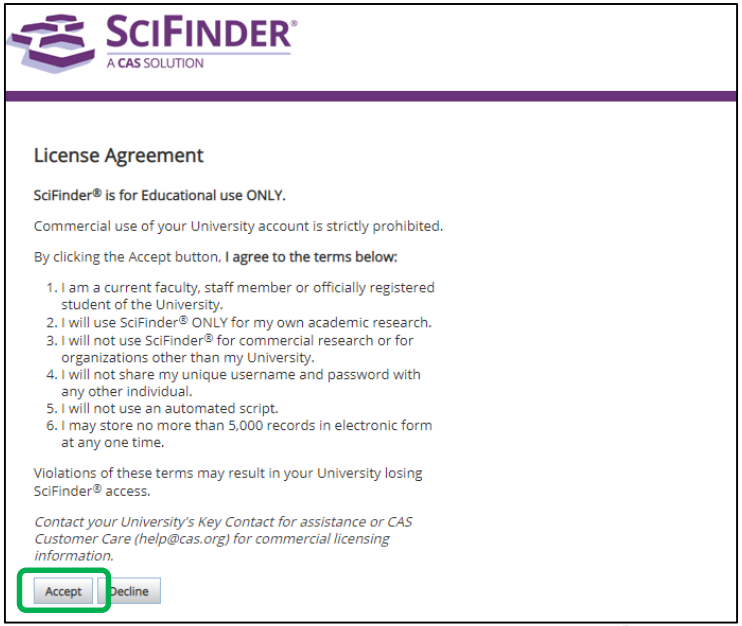
Create a SciFinder^{n} ID (Continued)

5. Registration link



6. License Agreement



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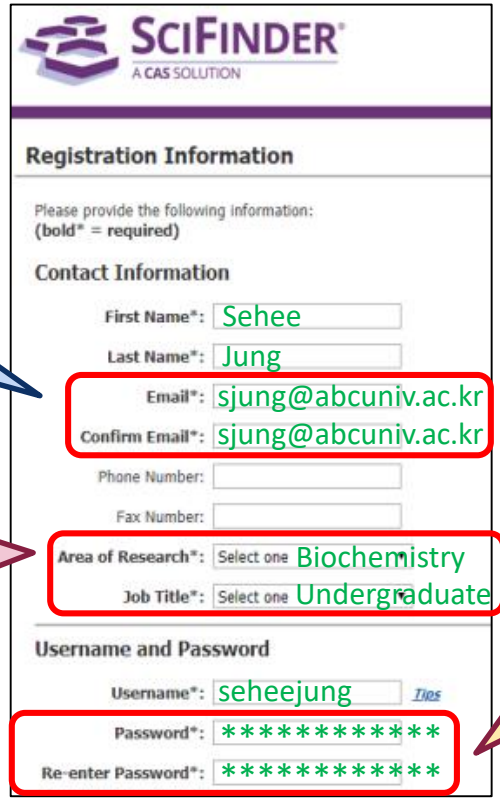
Create a SciFinder^n ID (Continued)

7. Registration Information example

※ **University email** must be used

(e.g sjung@abcuniv.ac.kr)

	Undergraduate	Masters/PhD
Area of Research	Choose your major (e.g Biochemistry)	Choose your major (e.g Nanotechnology)
Job Title	Undergraduate Student	Graduate Student/ Post Doc



3 from
Uppercase, Lowercase, Number and Symbols

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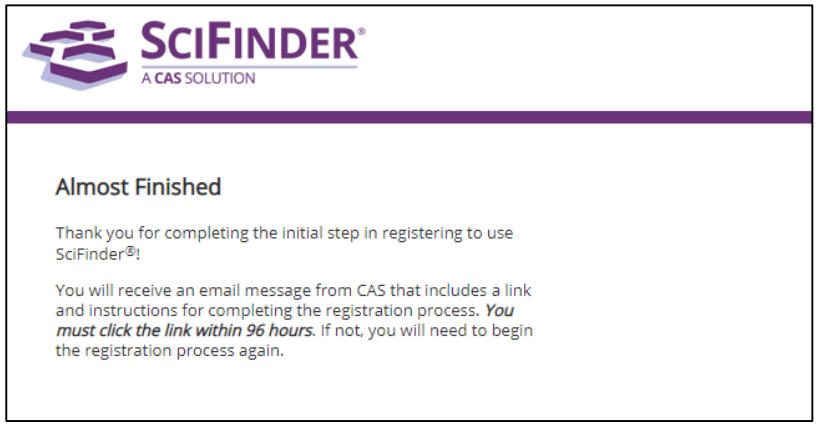
Create a SciFinder^n ID (Continued)

8. You will receive below message.



9. Log in to your university email.
(e.g sjung@abcuniv.ac.kr)

10. Find an email sent from CAS and click Registration Complete Link.

11. Now, you can search in SciFinder^n using your ID and Password.

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1. How to Start SciFinder^n

- www.scifinder-n.cas.org
- If you already have a SciFinder account, the same Username and Password can be used in SciFinder^n.
- Previously created Keep Me Posted can be migrated into SciFinder^n.
- Unlimited access to PATENTPAK® A CAS SOLUTION
- Unlimited access to METHODSNOW™ A CAS SOLUTION

SCIFINDER^n A CAS SOLUTION

1-1. Main Home page of SciFinder^{n}

Once you log in to SciFinder^{n}, choose a search option on the left.
(Click the logo to return to the home page)

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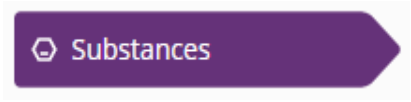
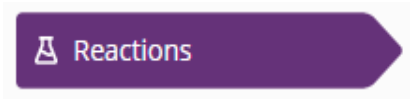
1-2. Choose a Search Option

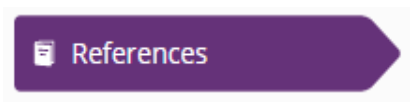
All finds substances, reactions, references and suppliers that match your query. You can enter keyword, research topic, document identifier, patent information, substance name, CAS Registry Number or draw/import a structure query.



Find **Substances** by substance name, CAS Registry Number and document identifier or chemical structure. Use **Advanced Search** to find substances by molecular formula, substance property, and experimental spectra.



Find **Reactions** by substance name, CAS Registry Number and document identifier or chemical structure that identifies a substance that participates in the reaction.



Find **References**에서는 by keyword, research topic, document identifier, patent information, substance name, CAS Registry Number or chemical structure. Use **Advanced Search**를 to search by author, journal or organization.

Find **Suppliers**에서는 by substance name or CAS Registry Number or chemical structure.

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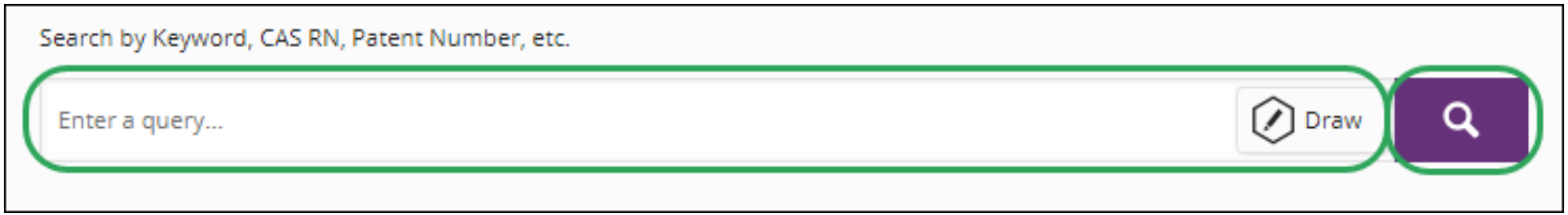
1-3. Enter a text query or click the Draw button to import/draw a structure query. Click the magnifying glass to submit the query.



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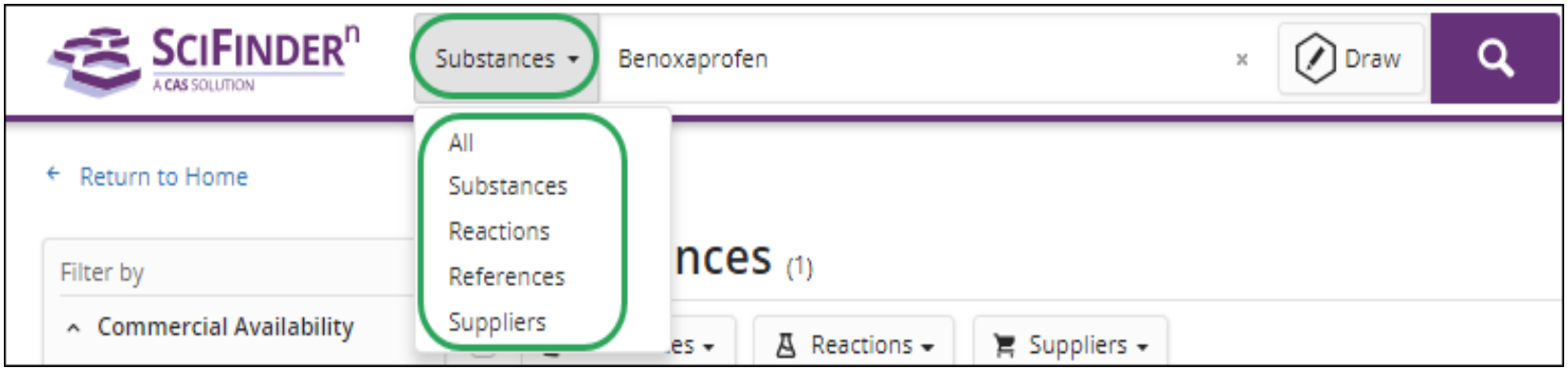
1-4. You can re-search by selecting the search type using the Drop-down button.



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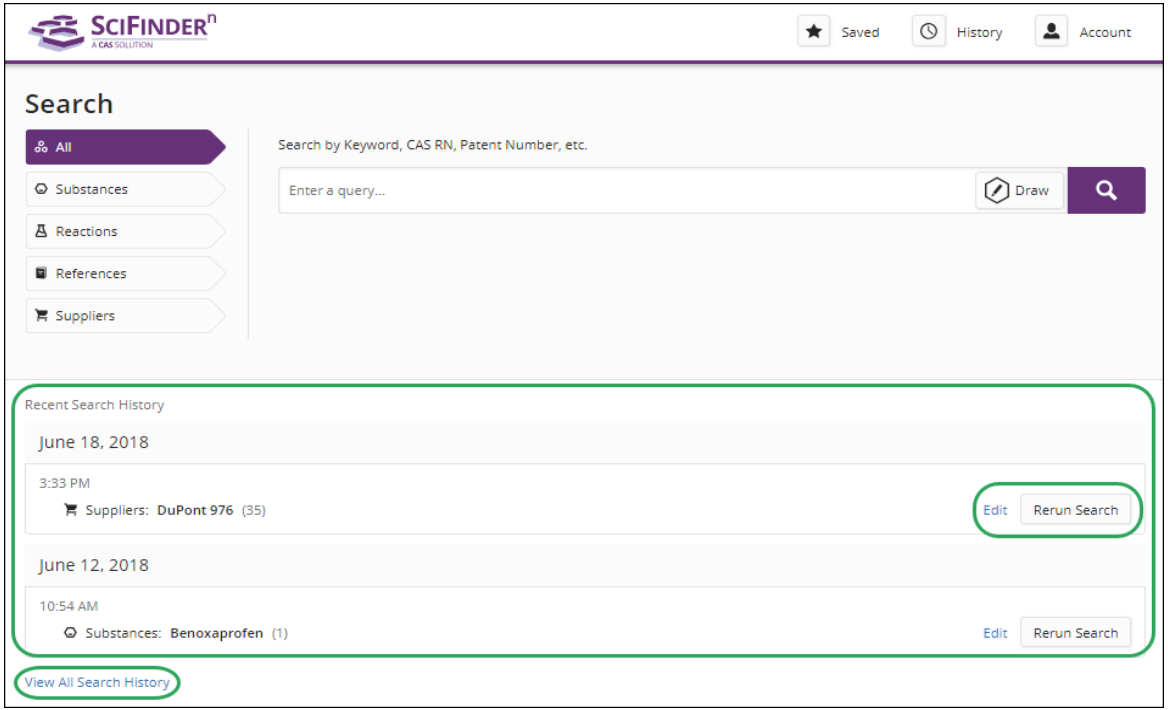
1-5. Click View All Search History to display your search history.



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2. Search References using Keywords

	<Example>
Research topic/Keyword/Concept	Analgesics
Chemical Name	Ibuprofen
CAS Registry Number	51146-57-7
Accession Number	1986:230471
PubMed ID Number	15980585
DOI	10.1093/nar/gki470
Patent Number	US4571400
Patent Application Number	US1984-682902

※ You may enter multiple numbers separated by a space, no commas or other punctuation. (2000-character limit)

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2-1. You can select from the list of autosuggestions or continue typing. Click the magnifying glass to submit the query.

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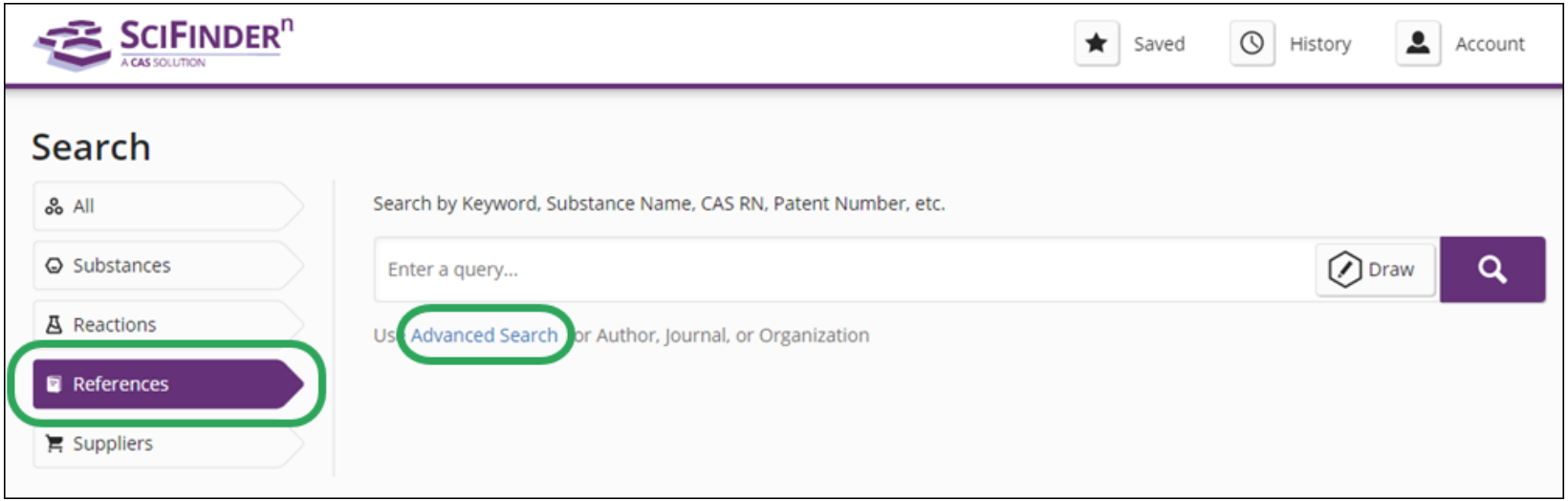
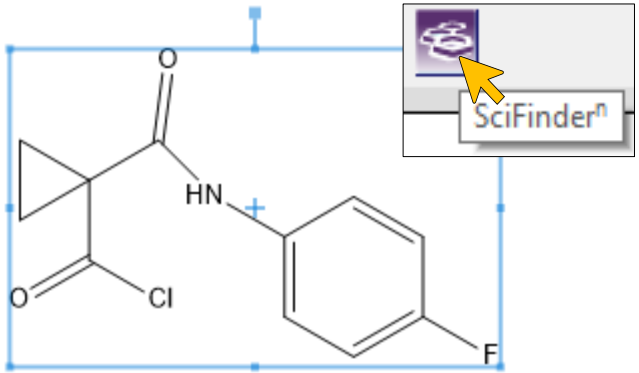
2-2. Select Advanced Search to search by authors, organizations or journal information.



3. Search References using Structures

- You can **draw** chemical structures in CAS Structure Editor or **import** an existing file (.mol, cxf)

- You can draw a chemical structure in ChemDraw ver 18.2 and click SciFinder^n button to link the search into SciFinder^n



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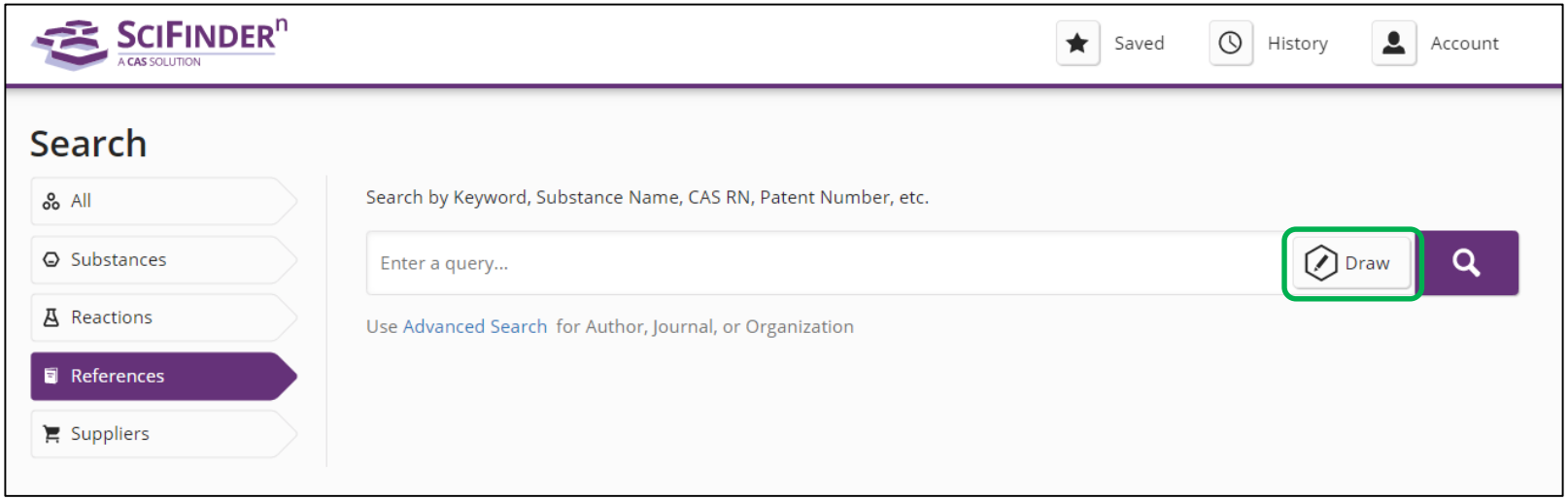
3-1. Click Draw button to open the Structure Editor.



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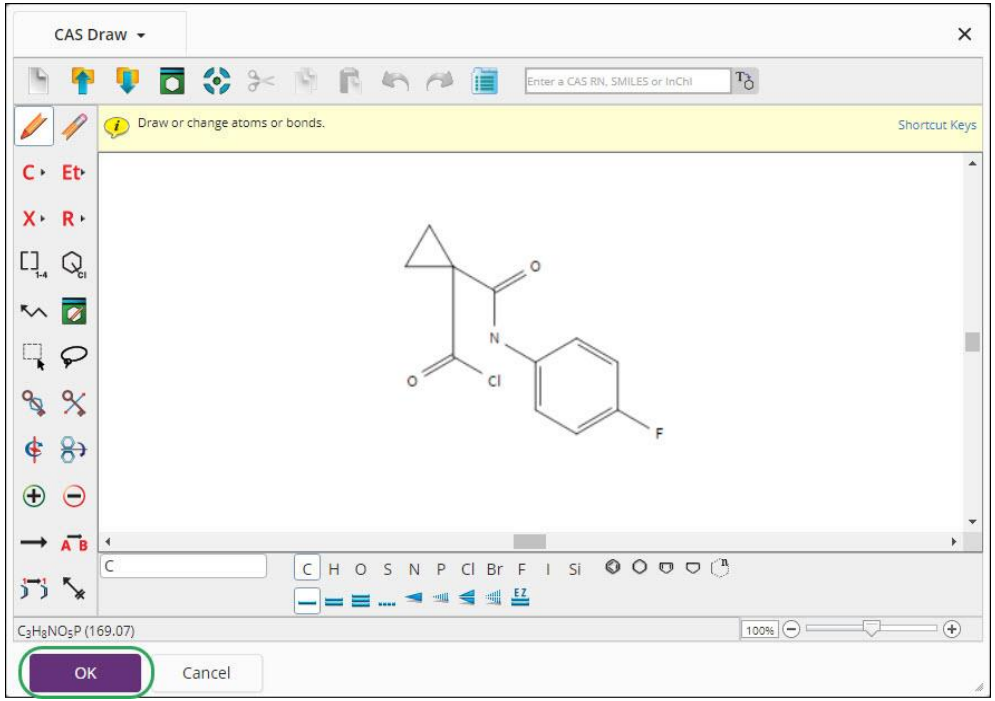
3-2. Once you finish drawing the structure, click the OK button.



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3-3. If needed, you can click Edit Drawing to return to the Structure Editor or Remove to delete the structure query.

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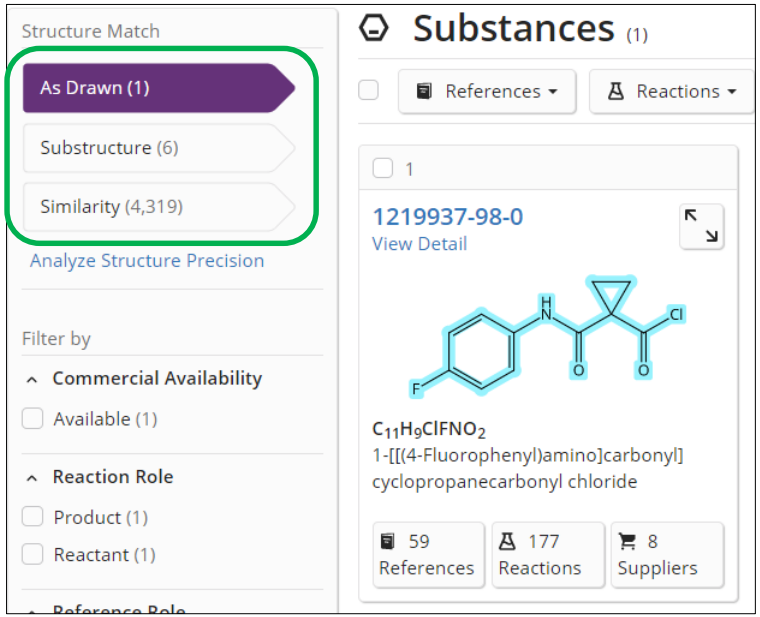
3-4. The structure match can be adjusted using As Drawn, Substructure and Similarity filters



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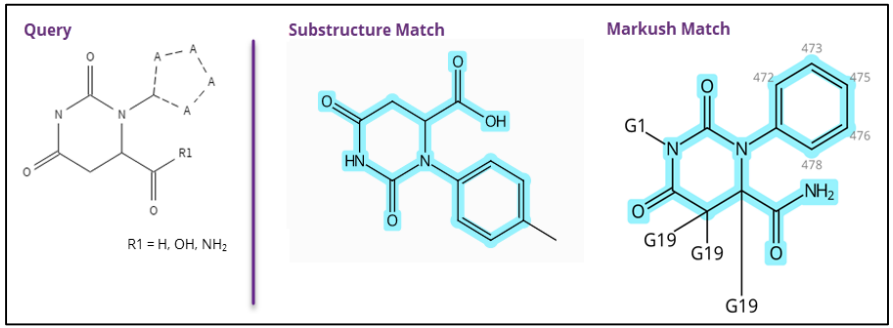
4. Search Patents using Markush Structures

- You can **Patent Markush** search to find patent references that contain structures (including generic structures) matching the structure query.

- A Markush search differs from a substructure search in that it matches the structure query against generic structures found in patents. The result is a list of patent references.



※ A Markush structure is a representation of chemical structure used to indicate a group of related chemical compounds and are commonly found in chemistry texts and patent claims.

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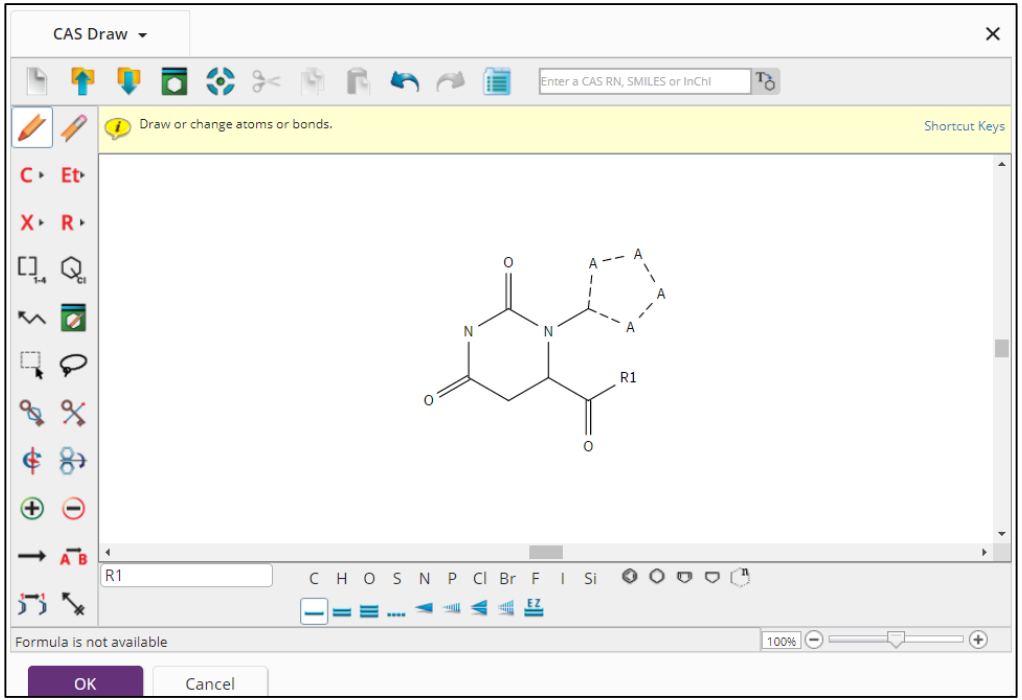
4-1. Click the Substance search type and Draw the query in the Structure Editor.



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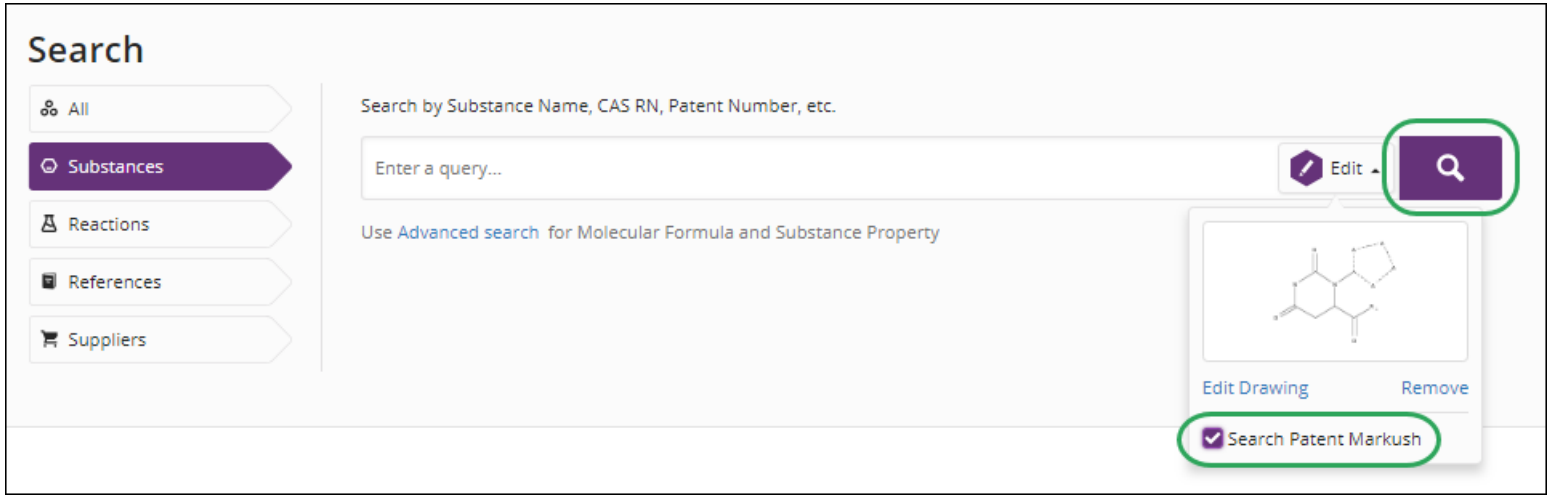
4-2. Check the box for Search Patent Markush and submit the query by clicking the magnifying glass.



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5. Search Substances using Keywords

		<Example>
Substance Name		Benoxaprofen, methyl ethyl ketone
CAS Registry Number		51146-57-7, 51146577
Document Identifier	Patent Number	US4571400
	Accession Number	1986:230471
	PubMed ID Number	15980585
	CAS Accession Number (CAN)	148:486341

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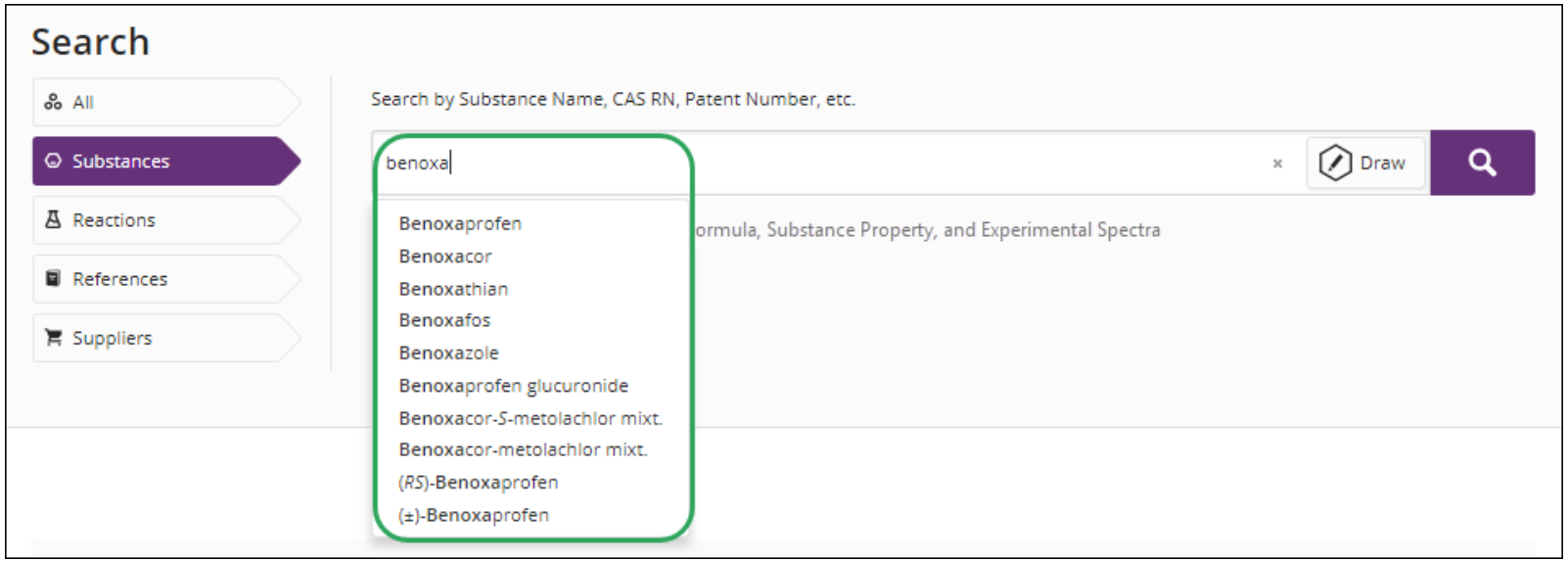
5-1. You can select the keywords appeared in the autosuggestion or continue typing. Submit the query.



SciFinder^n
A CAS SOLUTION

6. Search Substances using Structures

- You can **draw** chemical structures in CAS Structure Editor or **import** an existing file (.mol, cxf)

- Markush structure search for patents can be found in “4. *Search Patents using Markush Structures”. (숫자)*

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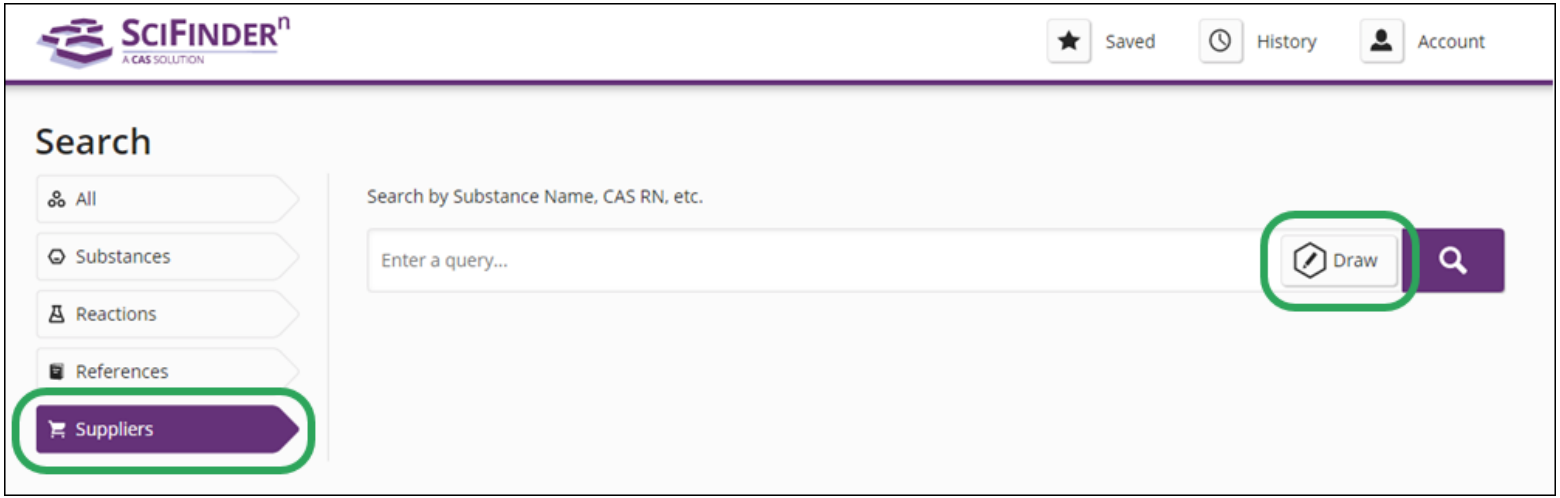
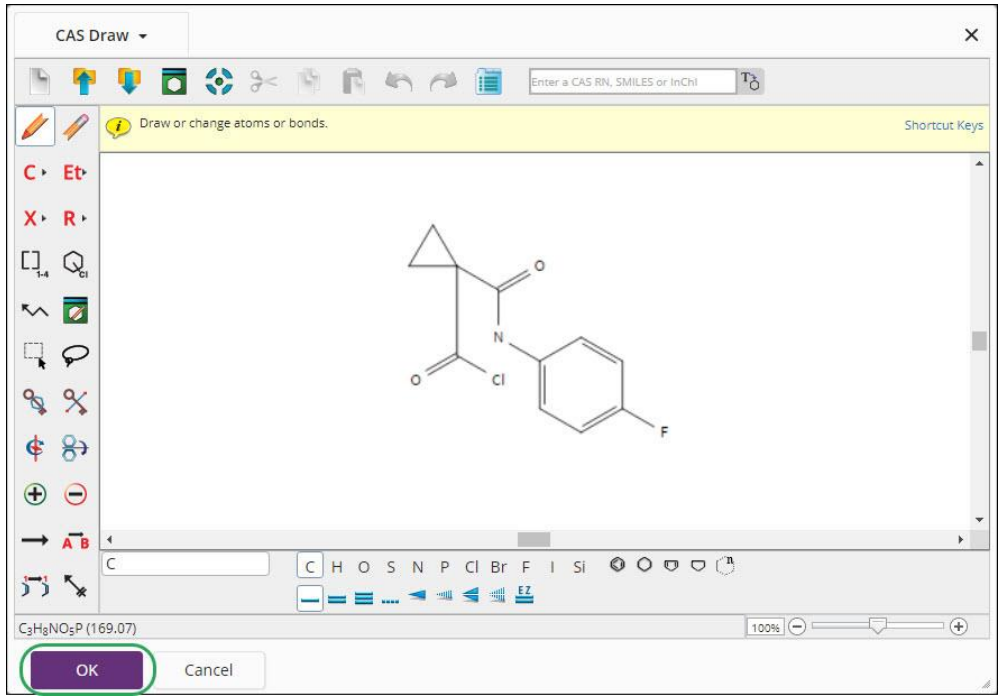
6-1. Open the Structure Editor by clicking the Draw button.



SciFinder n
A CAS SOLUTION

6-2. When the structure query is complete, click the OK button.



SciFinder^n
A CAS SOLUTION

6-3. If needed, you can click Edit Drawing to return to the Structure Editor or Remove to delete the structure query.

SciFinder^n
A CAS SOLUTION

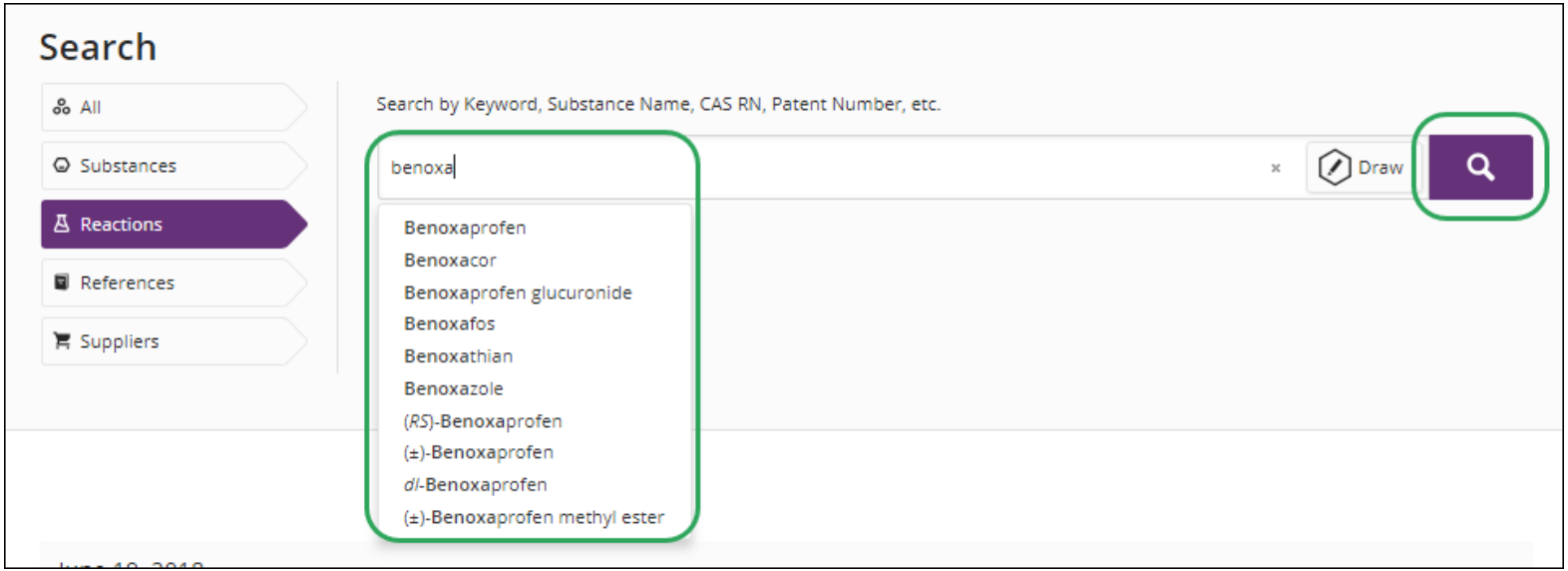
7. Search Reactions using Keywords

※ The text query must match the identifier in the results exactly. SciFindern will not match a partial name of number.

		<Example>
Substance Name		Benoxaprofen, methyl ethyl ketone
CAS Registry Number		51146-57-7, 51146577
Document Identifier	Patent Number	US4571400
	Accession Number	1986:230471
	PubMed ID Number	15980585
	CAS Accession Number (CAN)	148:486341

SciFinder^n
A CAS SOLUTION

7-1. You can select the keywords appeared in the autosuggestion or continue typing. Submit the query.



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A CAS SOLUTION

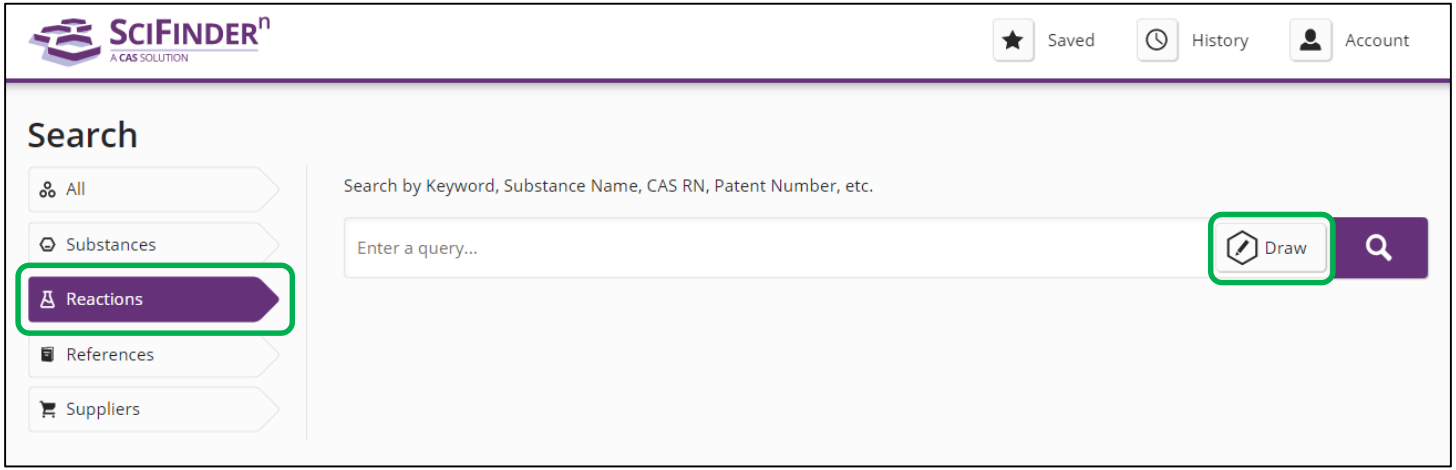
8. Search Reactions using Structures

- You can search reactions by drawing Reactants AND/OR Products.

- **Existing files (.mol, .cxf files)** can be uploaded.

SciFinder^n
A CAS SOLUTION

8-1. Click the Draw button to open the Structure Editor.



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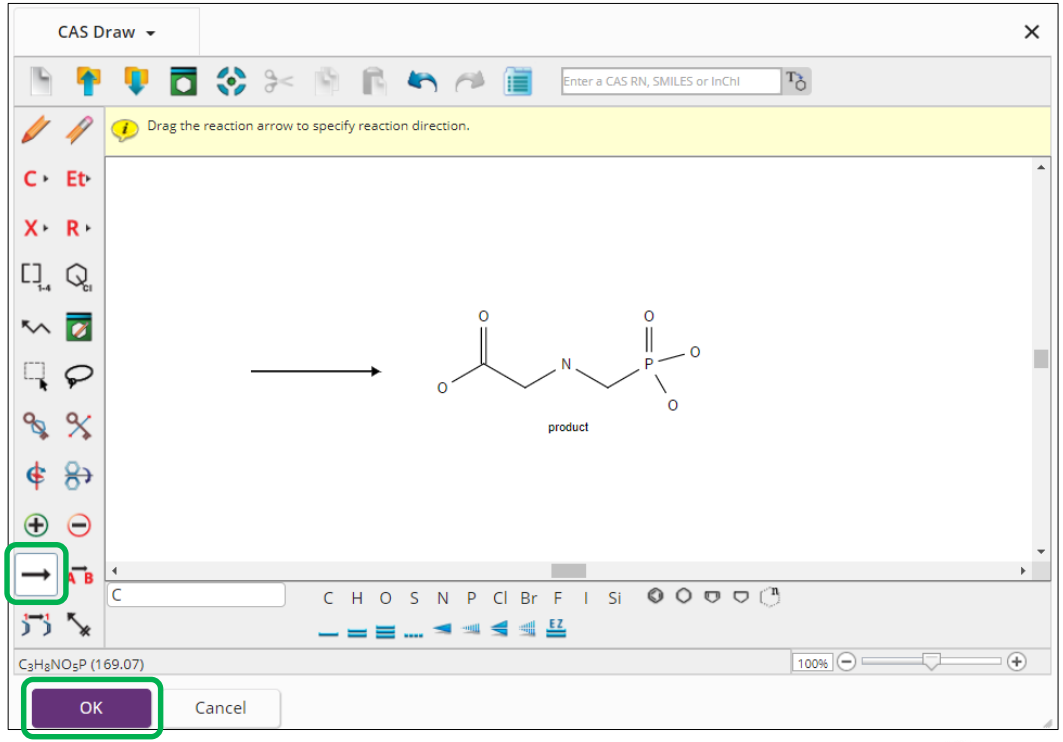
8.2 Draw a substance and select it as a Reactant or a Product. Click OK.



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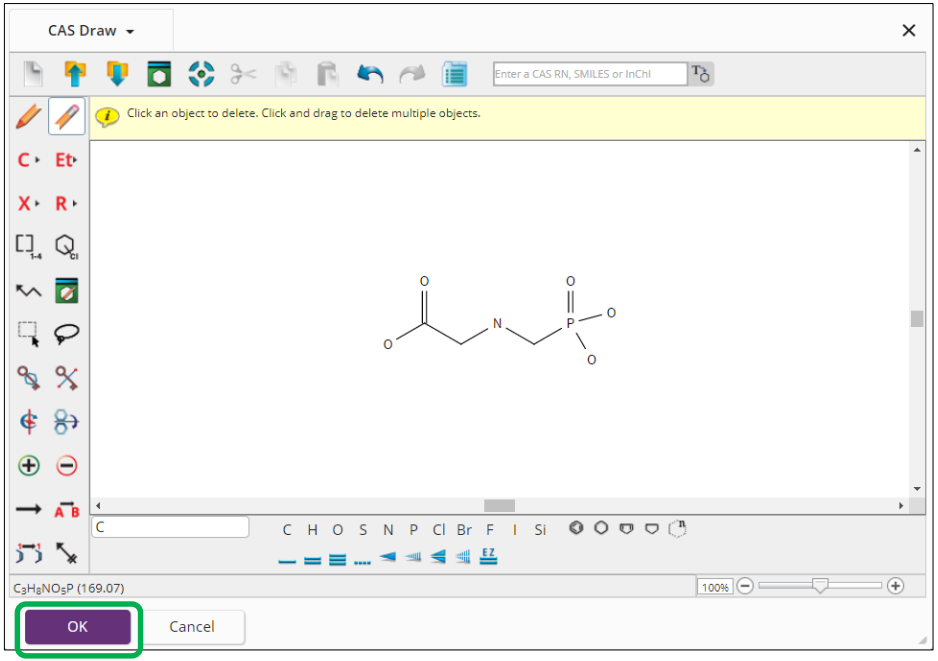
A CAS SOLUTION

8.3 OR you can draw a substance and select OK (without adding the reaction role).



If the reaction role is not selected for the drawn/imported substance, its role can be selected on the results page in the filter. (8.4)

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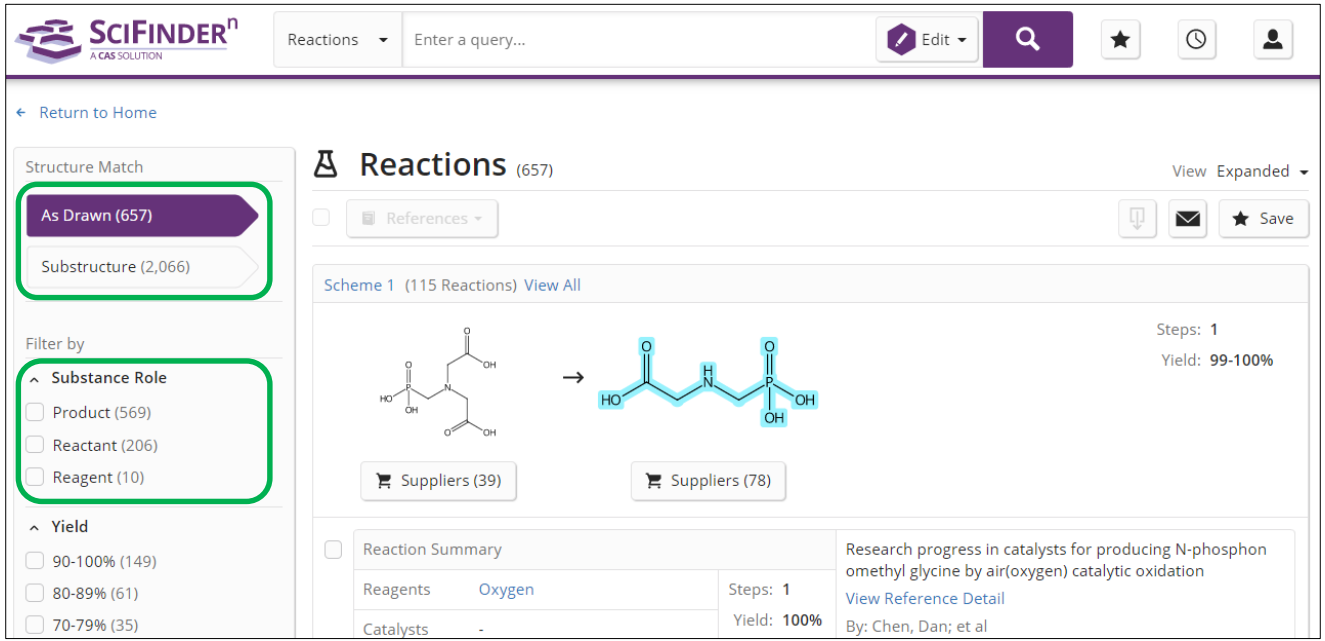
8.4 Choose the Structure Match and Substance Role in the filter.



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9. Create a Retrosynthesis Plan

- Based on the experimental reaction data that CAS possesses and newly formed rules, the retrosynthesis for target molecules can be generated with an intuitive design.

- There are two ways to create a retrosynthesis plan for a substance in SciFinder^n

    1) From the **Reactions Search Page** (9-1)

    2) From a **Substance Window** (9-2)

※ Retrosynthesis plan expires 90 days after the date they are first generated.

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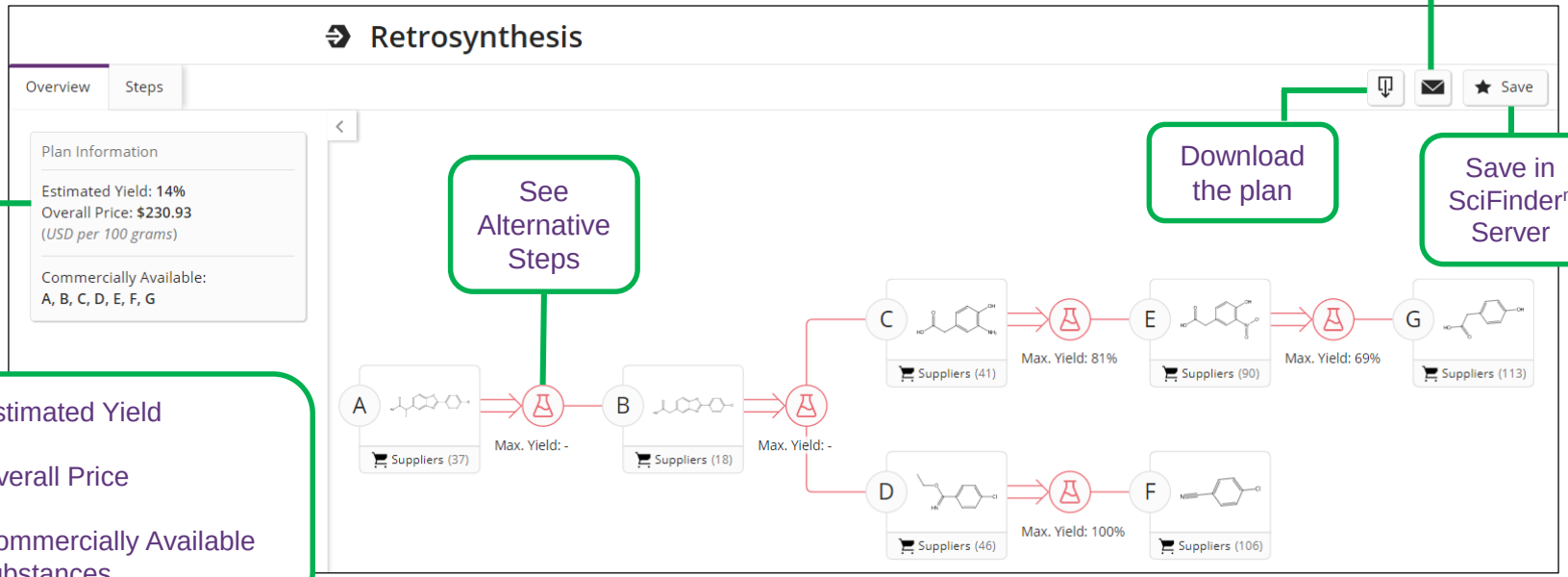
9. Create a Retrosynthesis Plan (Continued)

Retrosynthesis Plan example



Share Retrosynthsis Plan

Download the plan

Save in SciFinder^n Server

See Alternative Steps

Estimated Yield

Overall Price

Commercially Available substances

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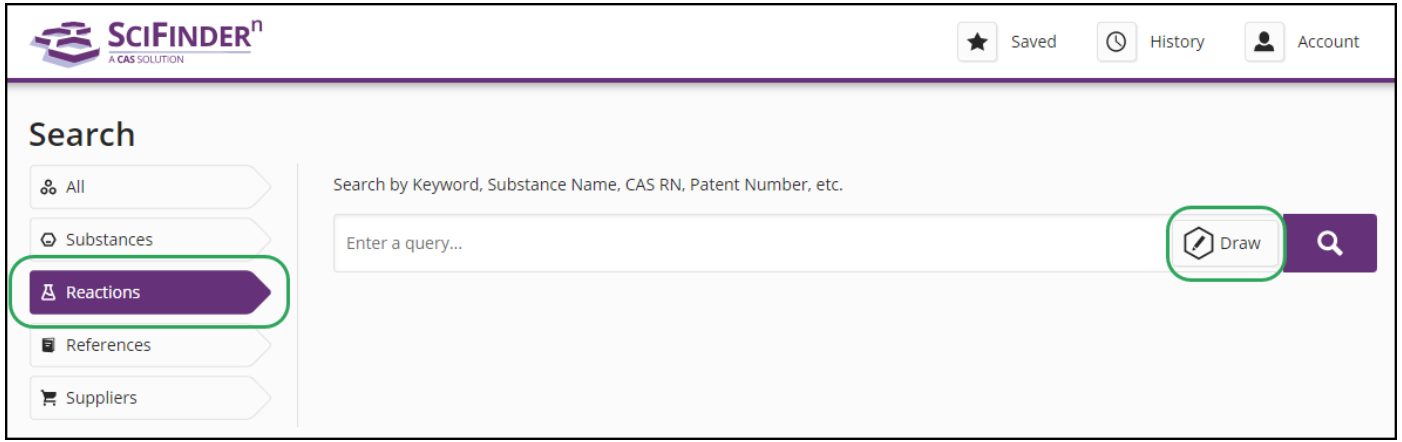
9-1. From the Reactions Search Page

- On the Search page, click the Reactions search type, and then click the **Draw** button.



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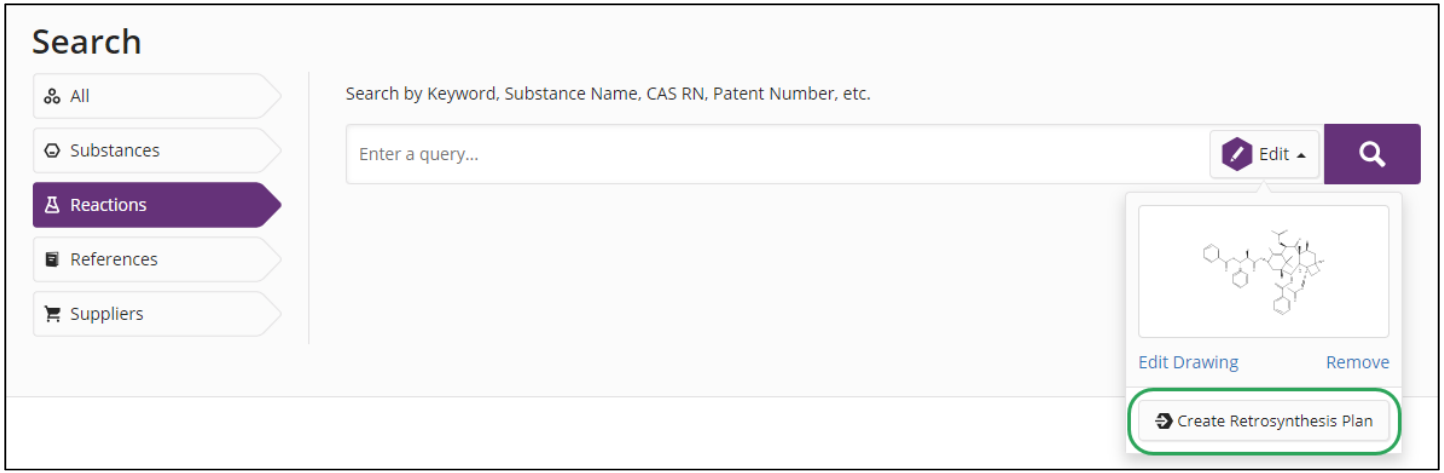
9-1. From the Reactions Search Page (Continued)

- After drawing or importing a structure, click the **Create Retrosynthesis Plan** button.



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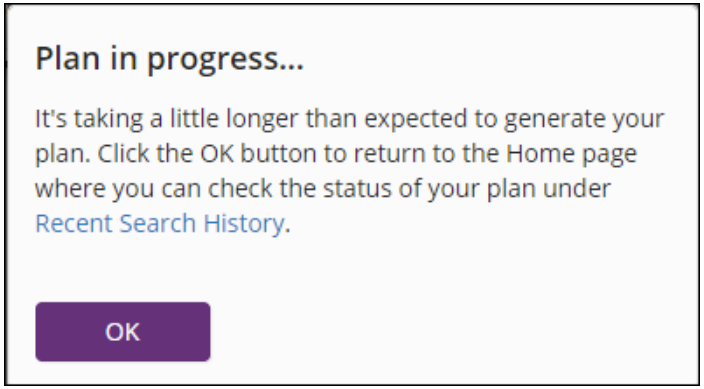
9-1. From the Reactions Search Page (Continued)

- If there is a problem with the structure submitted for retrosynthesis, you will receive an error message.
- "**Plan in progress…**" message tells you that your plan may take some time. Click OK button to return to the Home page.



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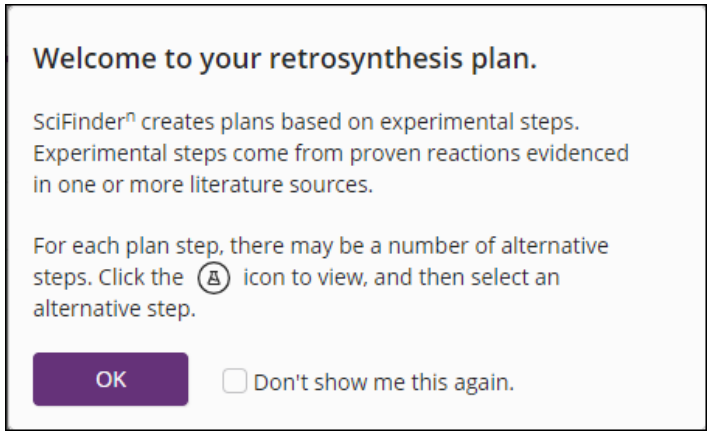
9-1. From the Reactions Search Page (Continued)

- **“Welcome to your retrosynthesis plan**” message welcomes you to your retrosynthesis plan. Click the OK button to view your plan on the Retrosynthesis Plan page.



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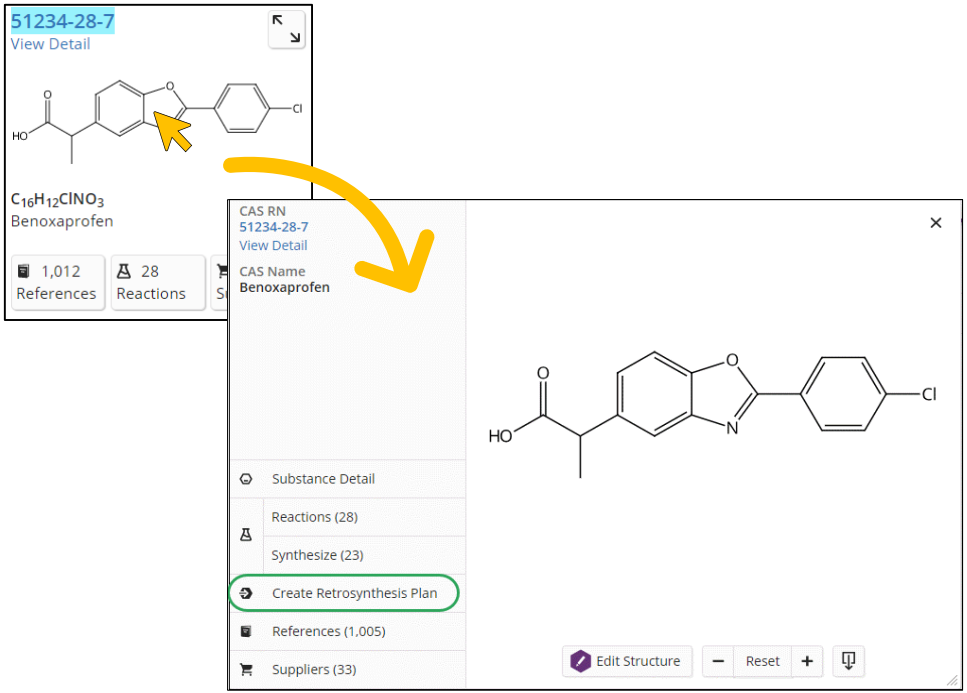
9-2. From a Substance Window

- Clicking a substance structure image in SciFinder^n opens the **Substance Window.**
- If retrosynthesis is available for the substance, you have the option to create a plan.
- Click the **Create Retrosynthesis Plan** button to proceed.



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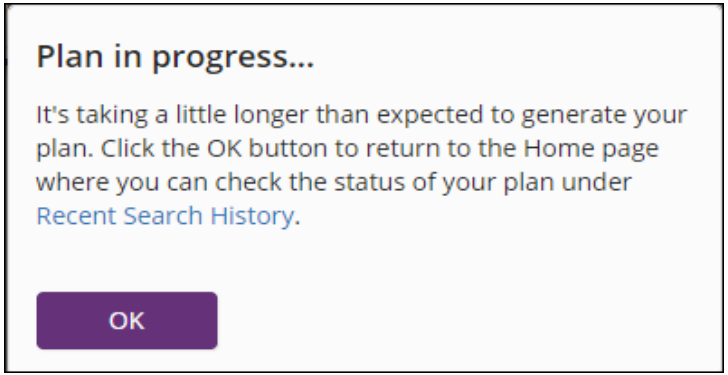
9-2. From a Substance Window (Continued)

- "**Plan in progress…**" message tells you that your plan may take some time. Click OK button to return to the Home page.



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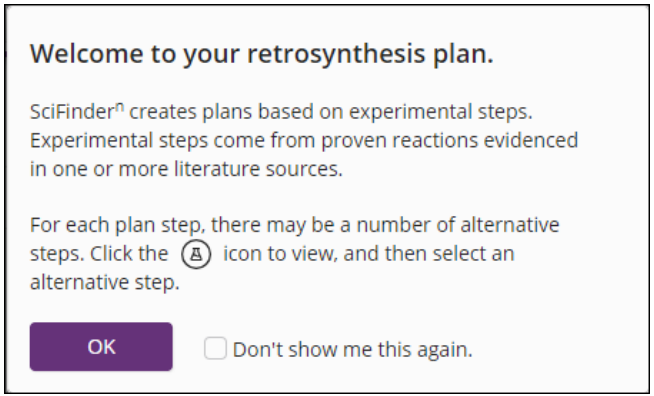
9-2. From a Substance Window (Continued)

- **“Welcome to your retrosynthesis plan**” message welcomes you to your retrosynthesis plan. Click the OK button to view your plan on the Retrosynthesis Plan page.



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Features in Structure Drawing Editor

Draw atoms and bonds

Delete atoms and bonds

Select the atom from the periodic table

Use a shortcut to represent a functional group

Variable (X Menu) Tool

Define a list of allowed substituent at an atom site

Repeating group tool specifying an atom or group that can be repeated within a structure

Specify multiple positions on a ring system where a substituent can attach

Quickly draw a chain of single bonds

Draw a predefined structure

Select atoms and bonds by drawing a rectangle around them

Select atoms, bonds, and structures by drawing a free-hand shape around them

Prevent ring formation in substructure and reaction search queries

Block substitution at an atom site in substructure and reaction search queries

Rotate a structure clockwise or anticlockwise

Invert a structure horizontally or vertically

Add positive charges to an atom

Add negative charges to an atom

Draw a reaction arrow by clicking or dragging the cursor in the drawing area

Click a substance and assign reaction roles (product, reactant, reagent, reactant/reagent, any role)

Specify corresponding atoms between reactants and products

Specify bonds that change in the course of the reaction

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