

CAS products and
services in Korea

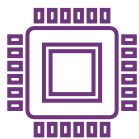
korea@acs-i.org

SciFinderⁿ Search Guide

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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

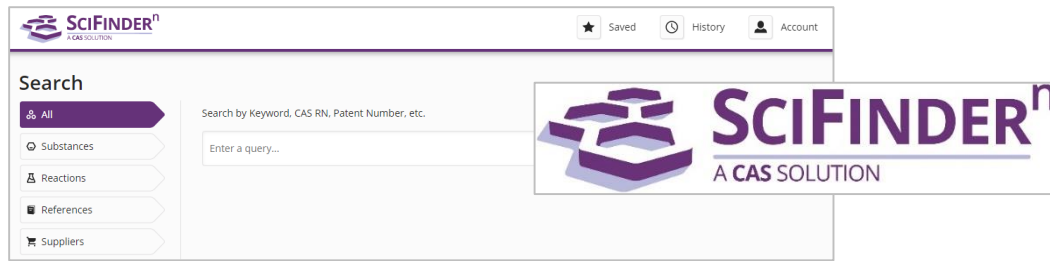
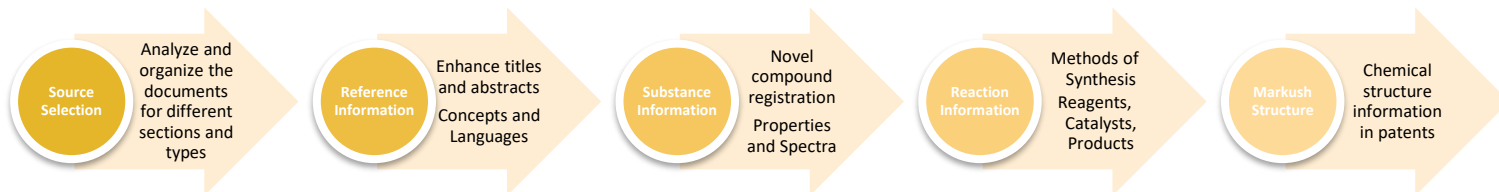
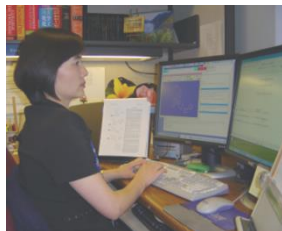
Big Data Infrastructure

Best in class search solutions like SciFinderⁿ, STNext and big data infrastructure to drive discoveries



SciFinderⁿ
A CAS SOLUTION

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




Create a SciFinderⁿ ID

1. Enter the university library website
2. Click “Databases” – Click “Overseas databases” * This may vary by university
3. Click SciFinderⁿ
4. Click the registration URL
(Starting with <https://scifinder.cas.org/registration/index.html?corpKey=>)

Create a SciFinderⁿ ID (Continued)

5. Registration link




SciFINDER[®]
A CAS SOLUTION

Welcome to User Registration for SciFinder[®]

Click Next to begin registration as a new user.

6. License Agreement



SciFINDER[®]
A CAS SOLUTION

License Agreement

SciFinder[®] is for Educational use ONLY.

Commercial use of your University account is strictly prohibited.

By clicking the Accept button, I agree to the terms below:

1. I am a current faculty, staff member or officially registered student of the University.
2. I will use SciFinder[®] ONLY for my own academic research.
3. I will not use SciFinder[®] for commercial research or for organizations other than my University.
4. I will not share my unique username and password with any other individual.
5. I will not use an automated script.
6. I may store no more than 5,000 records in electronic form at any one time.

Violations of these terms may result in your University losing SciFinder[®] access.

Contact your University's Key Contact for assistance or CAS Customer Care (help@cas.org) for commercial licensing information.

Create a SciFinderⁿ 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

The screenshot shows the SciFinder registration form with the following fields and values:

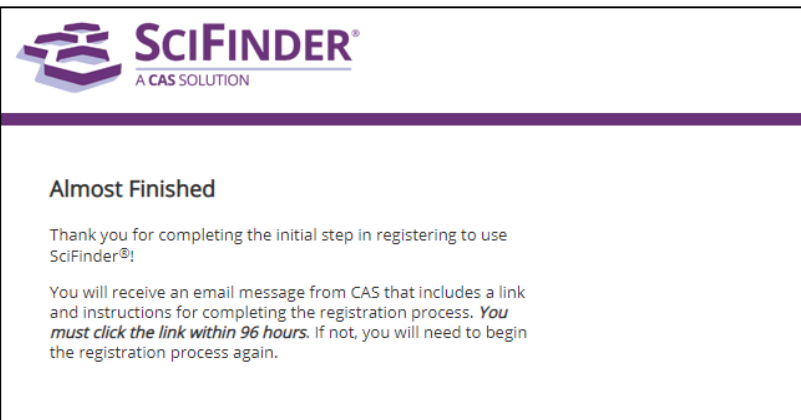
- Registration Information**
 - Please provide the following information:
(bold* = required)
- Contact Information**
 - First Name*: Sehee
 - Last Name*: Jung
 - Email*: sjung@abcuniv.ac.kr (highlighted with a red box)
 - Confirm Email*: sjung@abcuniv.ac.kr (highlighted with a red box)
 - Phone Number: (empty)
 - Fax Number: (empty)
 - Area of Research*: Select one Biochemistry (highlighted with a red box)
 - Job Title*: Select one Undergraduate (highlighted with a red box)
- Username and Password**
 - Username*: seheejung
 - Password*: ***** (highlighted with a red box)
 - Re-enter Password*: ***** (highlighted with a red box)

3 from
Uppercase, Lowercase,
Number and Symbols

Create a SciFinderⁿ 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.**

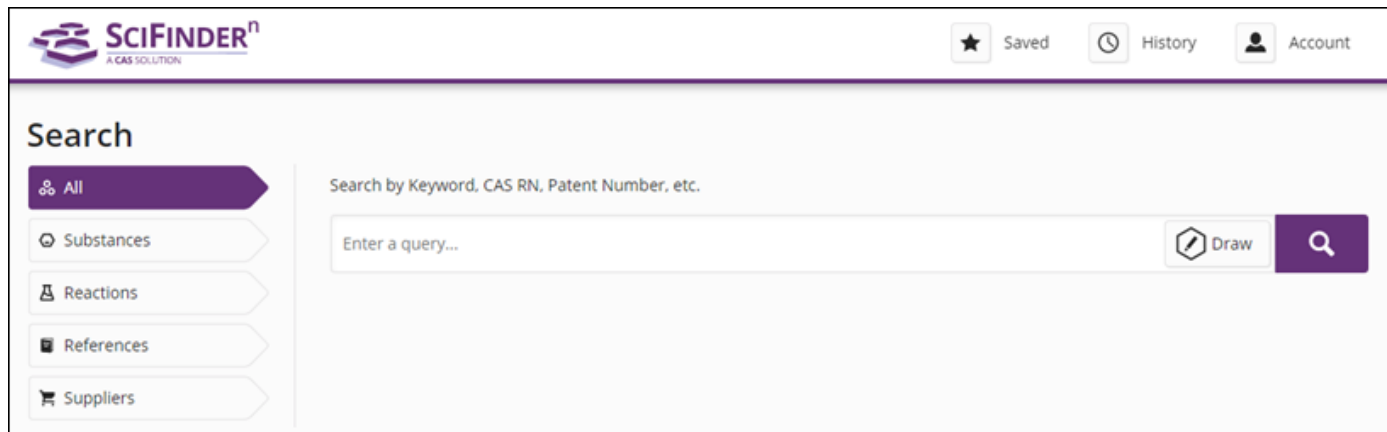
11. Now, you can search in SciFinderⁿ using your ID and Password.

1. How to Start SciFinderⁿ

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

1-1. Main Home page of SciFinderⁿ

Once you log in to SciFinderⁿ, choose a search option on the left.
(Click the logo to return to the home page)



1-2. Choose a Search Option



All

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.



Substances

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.



Reactions

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



References

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.



Suppliers

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



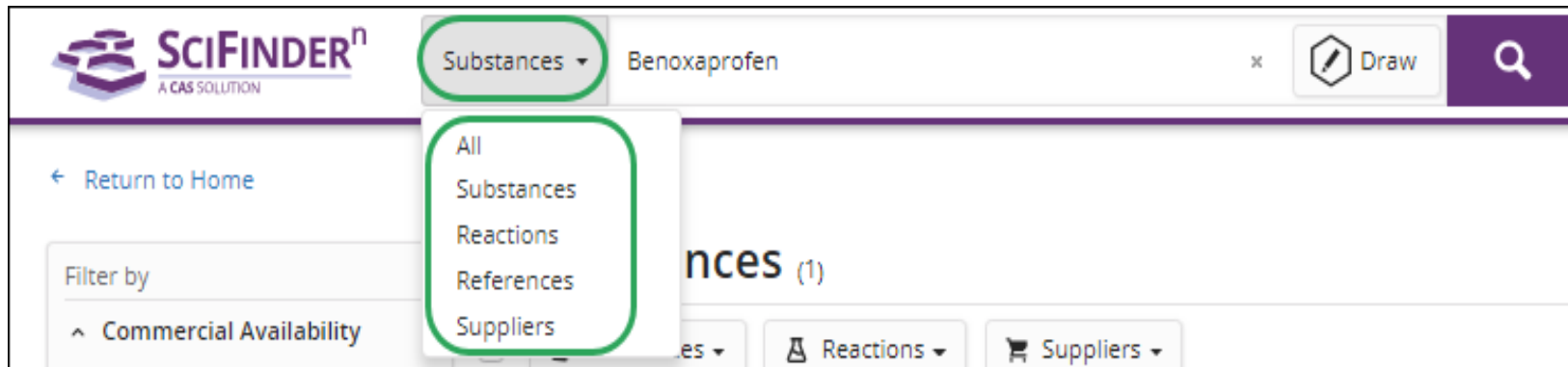
1-3. Enter a text query or click the Draw button to import/draw a structure query. Click the magnifying glass to submit the query.

Search by Keyword, CAS RN, Patent Number, etc.

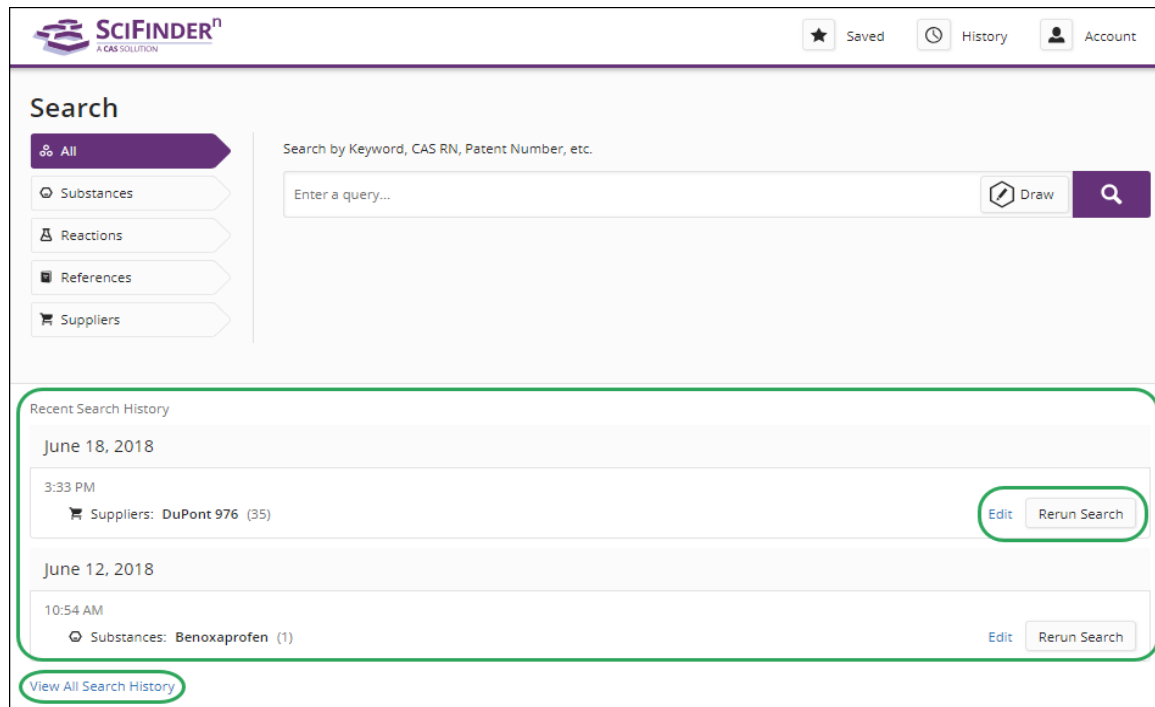
 Draw



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



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



The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Saved', 'History', and 'Account' are on the right. Below the header is a 'Search' section with a left-hand menu containing 'All' (selected), 'Substances', 'Reactions', 'References', and 'Suppliers'. The main search area includes a text input field with the placeholder 'Enter a query...', a 'Draw' button with a chemical structure icon, and a search button with a magnifying glass icon. Below the search bar is a 'Recent Search History' section, which is highlighted with a green border. This section lists two search entries: one from June 18, 2018, at 3:33 PM for 'Suppliers: DuPont 976 (35)', and another from June 12, 2018, at 10:54 AM for 'Substances: Benoxaprofen (1)'. Each entry has 'Edit' and 'Rerun Search' buttons. At the bottom left of the history section, there is a 'View All Search History' button, also highlighted with a green circle.

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)

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

Search

All Substances Reactions **References** Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

ibuprof

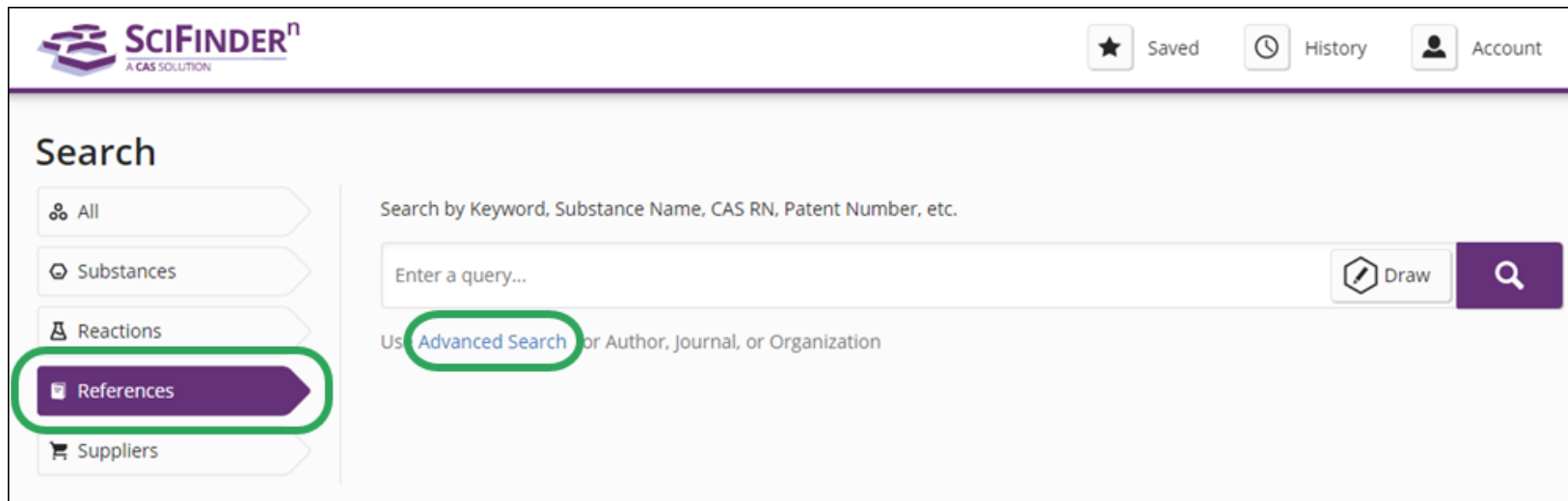
- ibuprofen
- Ibuprofenal
- Ibuprofen OH
- Ibuprofen COOH
- Ibuprofenamide
- Ibuprofen sodium

Author, Journal, or Organization

x Draw

Q

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



SCI FINDERⁿ
A CAS SOLUTION

★ Saved ⌚ History 👤 Account

Search

- All
- Substances
- Reactions
- References**
- Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

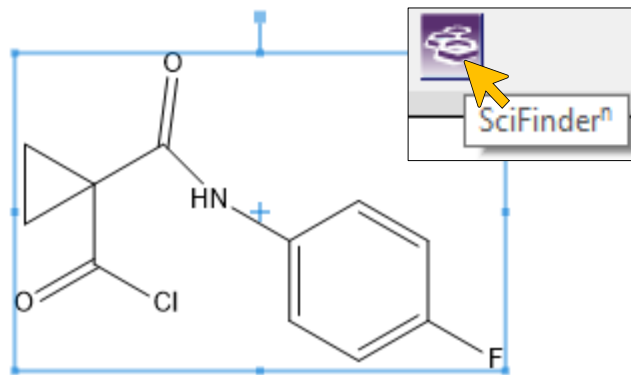
Enter a query...

Use **Advanced Search** for Author, Journal, or Organization

Draw

3. Search References using Structures

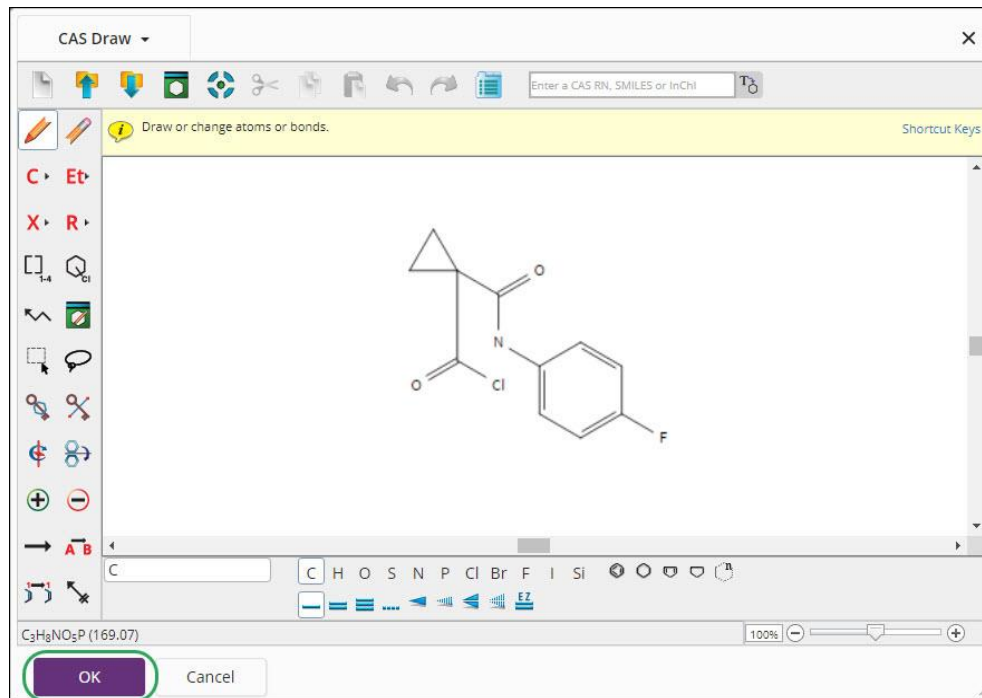
- You can **draw** chemical structures in CAS Structure Editor or **import** an existing file (.mol, cxf)
- You can draw a chemical structure in ChemDraw ver 18.2 and click SciFinderⁿ button to link the search into SciFinderⁿ



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

The screenshot shows the SciFinder^n search interface. At the top, the SciFinder^n logo is on the left, and navigation links for 'Saved', 'History', and 'Account' are on the right. Below the header, the 'Search' section features a left-hand menu with options: 'All', 'Substances', 'Reactions', 'References' (highlighted in purple), and 'Suppliers'. The main search area contains the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' and a search input field with the placeholder 'Enter a query...'. To the right of the input field is a 'Draw' button, which is highlighted with a green rectangular box. The 'Draw' button has a chemical structure icon and the text 'Draw'. A magnifying glass icon is located to the right of the 'Draw' button. Below the search input field, there is a link that says 'Use [Advanced Search](#) for Author, Journal, or Organization'.

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



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

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced search](#) for Author, Journal, or Organization

 Edit 



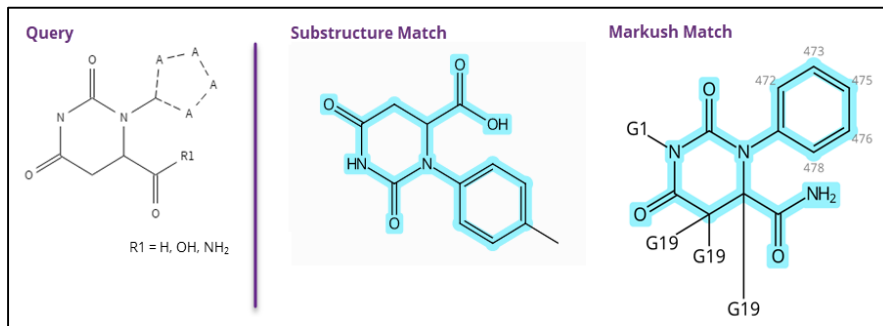
[Edit Drawing](#) [Remove](#)

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

The screenshot displays the SciFinder search results interface. On the left, the 'Structure Match' section is highlighted with a green box, showing three filter options: 'As Drawn (1)' (selected), 'Substructure (6)', and 'Similarity (4,319)'. Below this, the 'Filter by' section includes 'Commercial Availability' (with 'Available (1)' selected) and 'Reaction Role' (with 'Product (1)' and 'Reactant (1)' listed). The main search results pane on the right shows 'Substances (1)' with a 'References' dropdown. The first result is '1219937-98-0', with a 'View Detail' link and a chemical structure of 1-[[4-fluorophenyl]amino]cyclopropanecarbonyl chloride. The structure is a cyclopropane ring with a carbonyl group and a chlorine atom, attached to a 4-fluorophenylamino group. Below the structure, the molecular formula C11H9ClFNO2 and the name '1-[[4-Fluorophenyl]amino]cyclopropanecarbonyl chloride' are shown. At the bottom of the result card, there are three buttons: 'References' (59), 'Reactions' (177), and 'Suppliers' (8).

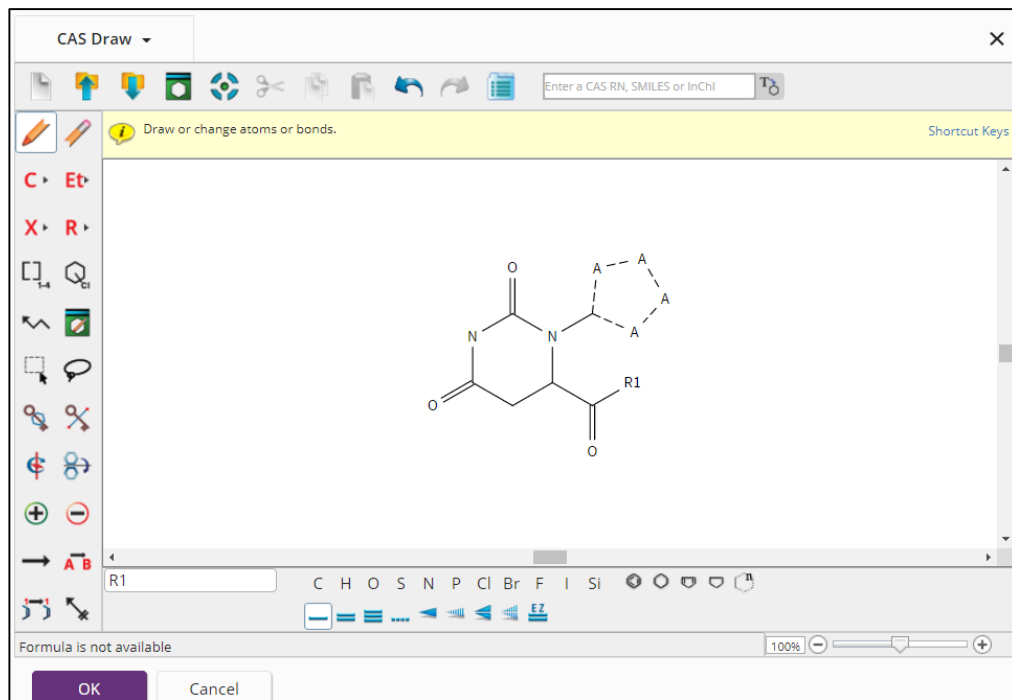
4. Search Patents using Markush Structures

- 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.

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



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

Search

All

Substances

Reactions

References

Suppliers

Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced search](#) for Molecular Formula and Substance Property

Edit

[Edit Drawing](#) [Remove](#)

☒ Search Patent Markush

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

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

Search

All
Substances
Reactions
References
Suppliers

Search by Substance Name, CAS RN, Patent Number, etc.

benoxa

- Benoxaprofen
- Benoxacor
- Benoxathian
- Benoxafos
- Benoxazole
- Benoxaprofen glucuronide
- Benoxacor-S-metolachlor mixt.
- Benoxacor-metolachlor mixt.
- (R)-Benoxaprofen
- (±)-Benoxaprofen

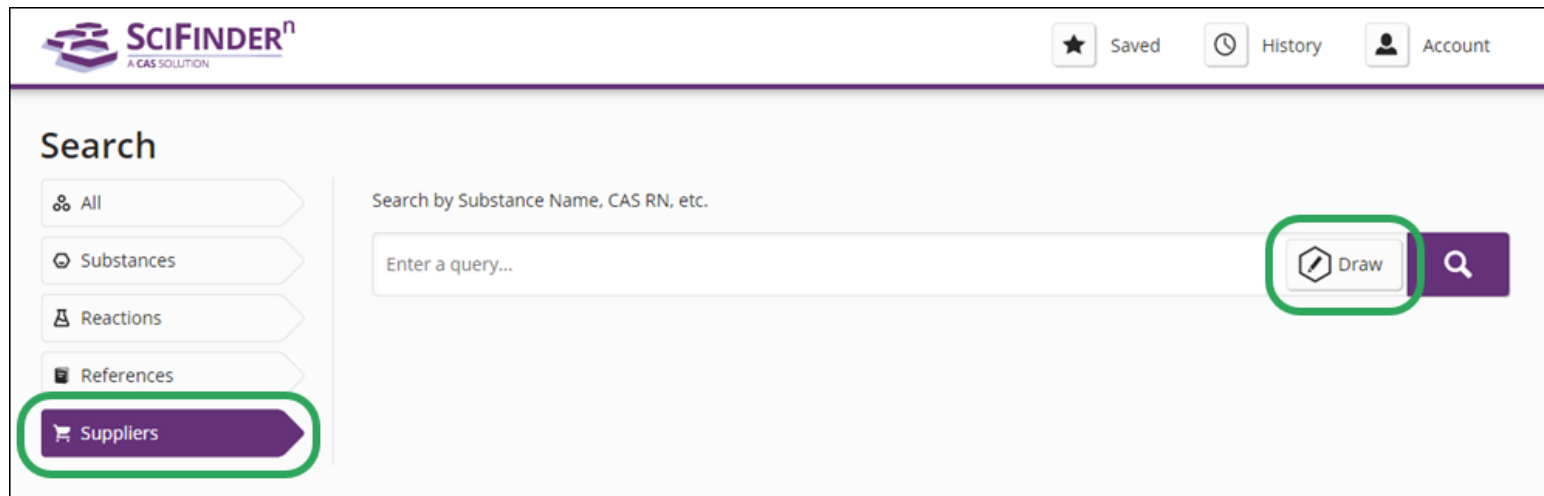
Formula, Substance Property, and Experimental Spectra

Draw

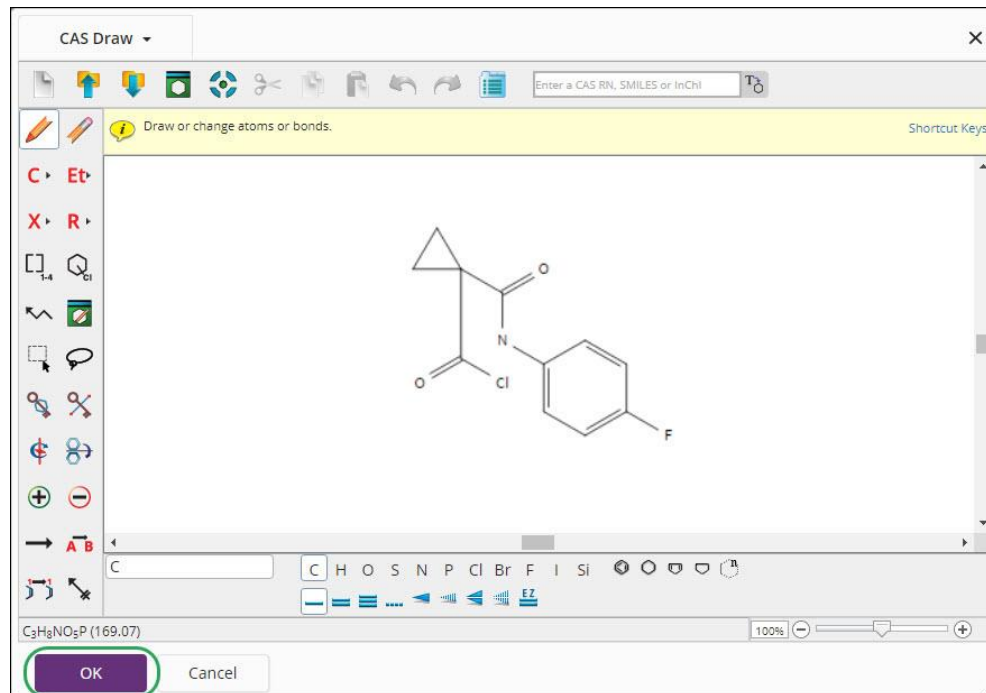
6. Search Substances using Structures

- 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)

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



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




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

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced search](#) for Author, Journal, or Organization

 Edit 



[Edit Drawing](#) [Remove](#)

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

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

Search

All Substances Reactions References Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

benoxa

- Benoxaprofen
- Benoxacor
- Benoxaprofen glucuronide
- Benoxafos
- Benoxathian
- Benoxazole
- (*RS*)-Benoxaprofen
- (\pm)-Benoxaprofen
- dl*-Benoxaprofen
- (\pm)-Benoxaprofen methyl ester

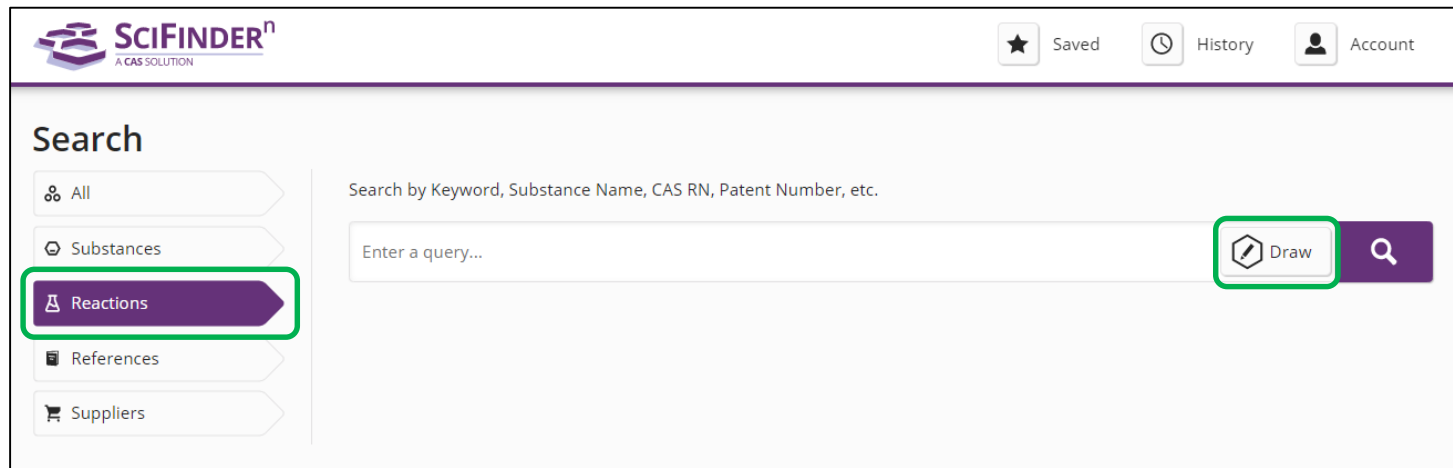
Draw

Search

8. Search Reactions using Structures

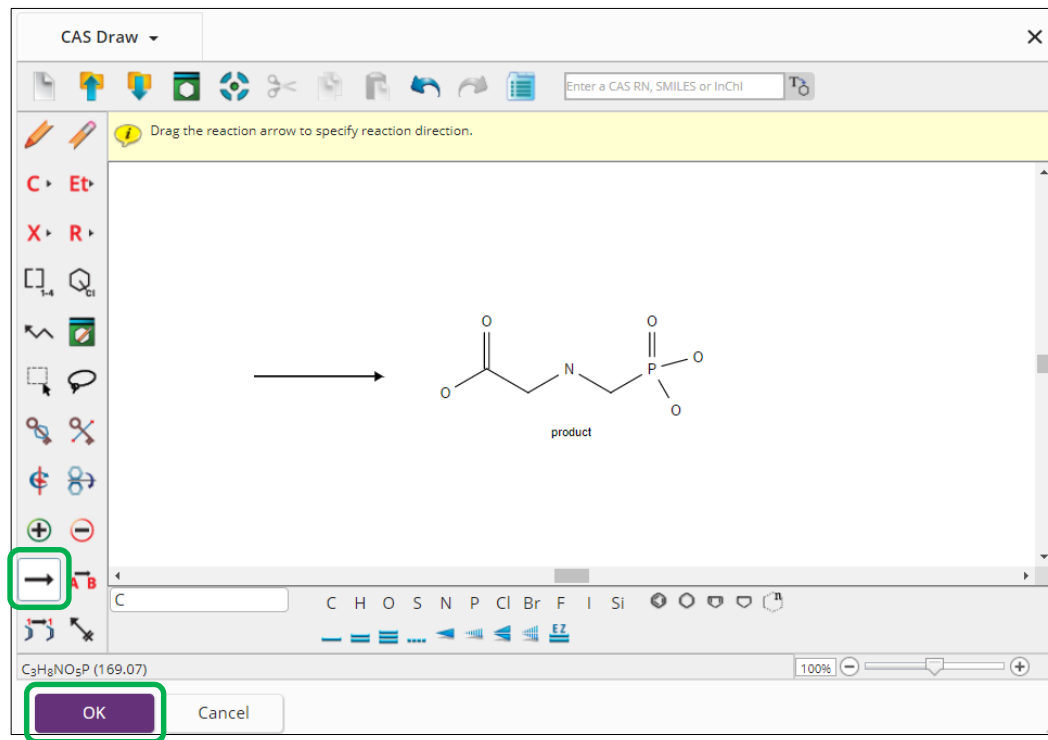
- You can search reactions by drawing Reactants AND/OR Products.
- **Existing files (.mol, .cxf files)** can be uploaded.

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

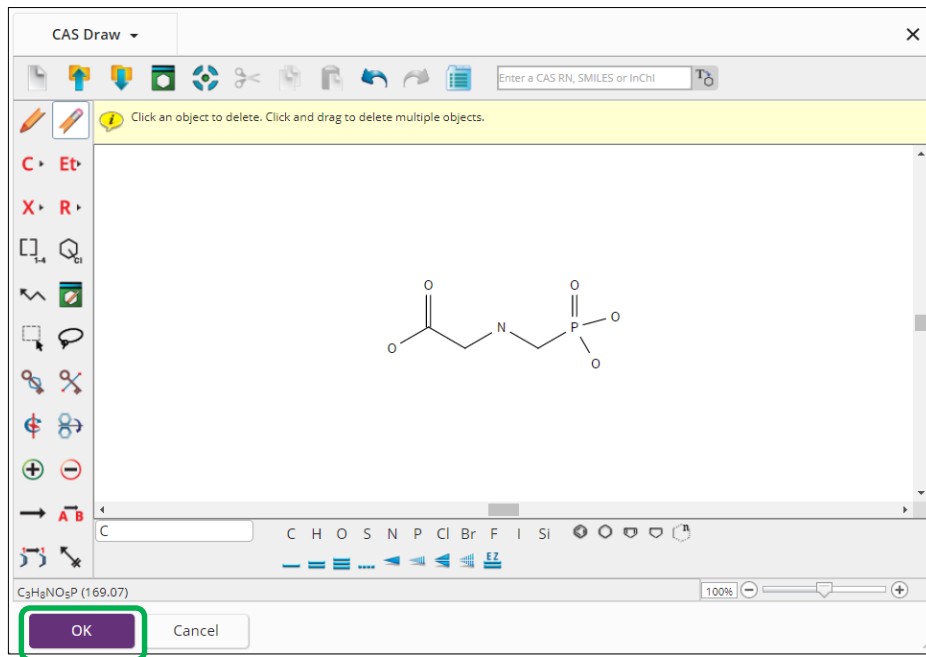


The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo with the tagline "A CAS SOLUTION". To the right are navigation links for "Saved", "History", and "Account". The main section is titled "Search" and includes a sidebar with filters: "All", "Substances", "Reactions" (highlighted with a green box), "References", and "Suppliers". The main search area contains the text "Search by Keyword, Substance Name, CAS RN, Patent Number, etc." and a search input field with the placeholder "Enter a query...". To the right of the input field is a "Draw" button (highlighted with a green box) featuring a chemical structure icon, and a search button with a magnifying glass icon.

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



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](#))

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

SciFINDERⁿ
A CAS SOLUTION

Reactions

Edit

[Return to Home](#)

Structure Match

As Drawn (657)

Substructure (2,066)

Filter by

Substance Role

☐ Product (569)

☐ Reactant (206)

☐ Reagent (10)

Yield

☐ 90-100% (149)

☐ 80-89% (61)

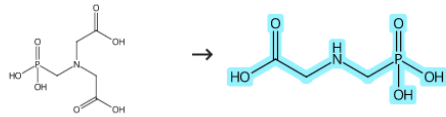
☐ 70-79% (35)

Reactions (657) View Expanded

☐ References

Save

Scheme 1 (115 Reactions) View All



Steps: 1
Yield: 99-100%

Suppliers (39) Suppliers (78)

☐ Reaction Summary

Reagents	Oxygen	Steps: 1
Catalysts	-	Yield: 100%

Research progress in catalysts for producing N-phosphonomethyl glycine by air(oxygen) catalytic oxidation
[View Reference Detail](#)
By: Chen, Dan; et al

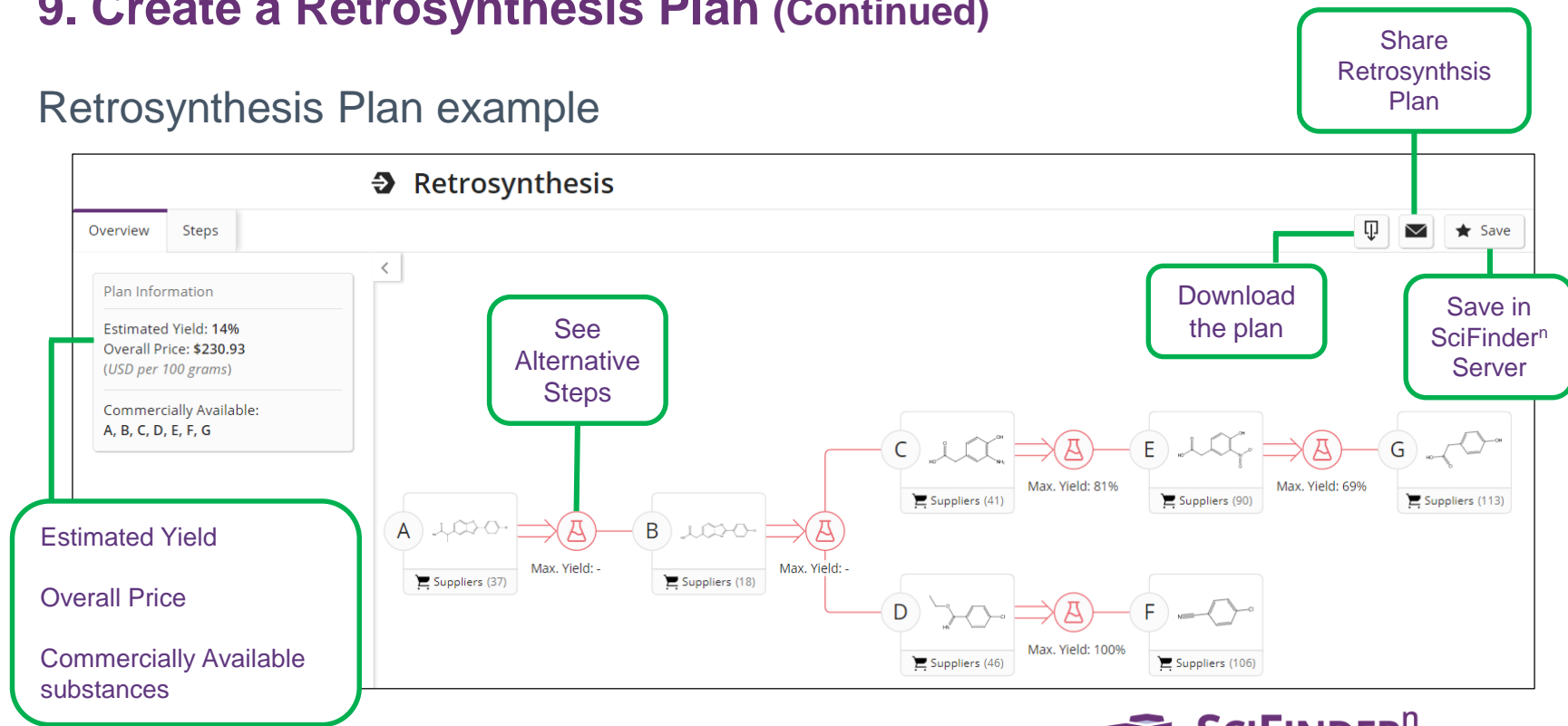
9. Create a Retrosynthesis Plan

- 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 SciFinderⁿ
 - 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.

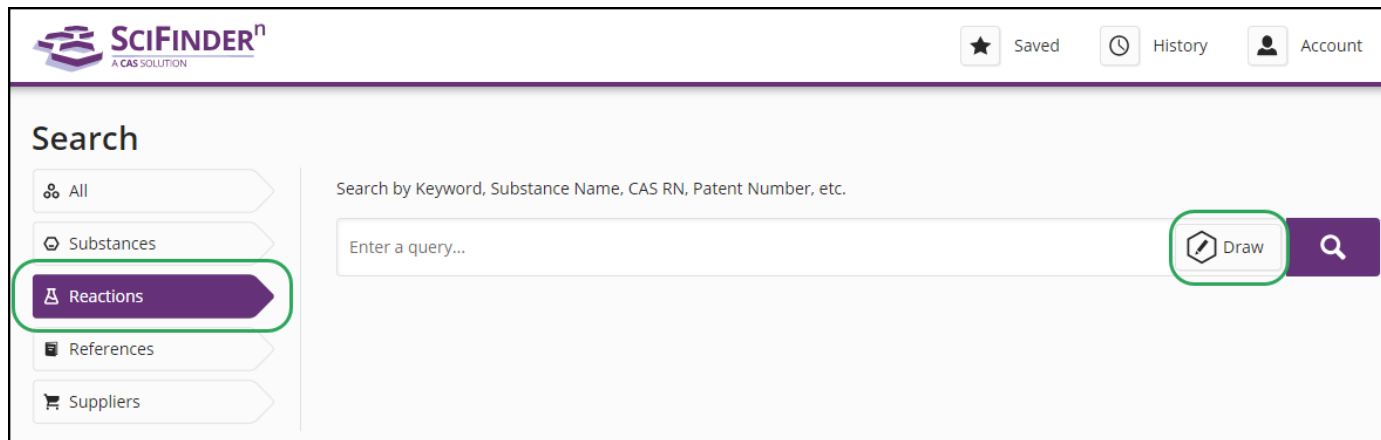
9. Create a Retrosynthesis Plan (Continued)

Retrosynthesis Plan example



9-1. From the Reactions Search Page

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



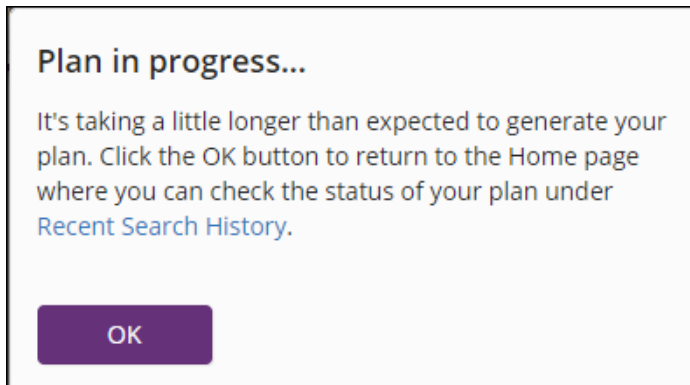
9-1. From the Reactions Search Page (Continued)

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

The screenshot displays the SciFinder search interface. On the left, a 'Search' sidebar contains navigation buttons: 'All', 'Substances', 'Reactions' (highlighted in purple), 'References', and 'Suppliers'. The main area features a search bar with the placeholder text 'Enter a query...' and a label 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.'. To the right of the search bar is an 'Edit' button and a search icon. Below the search bar, a chemical structure is shown within a preview window. Below the structure are two buttons: 'Edit Drawing' and 'Remove'. At the bottom right, a button labeled 'Create Retrosynthesis Plan' is highlighted with a green rounded rectangle.

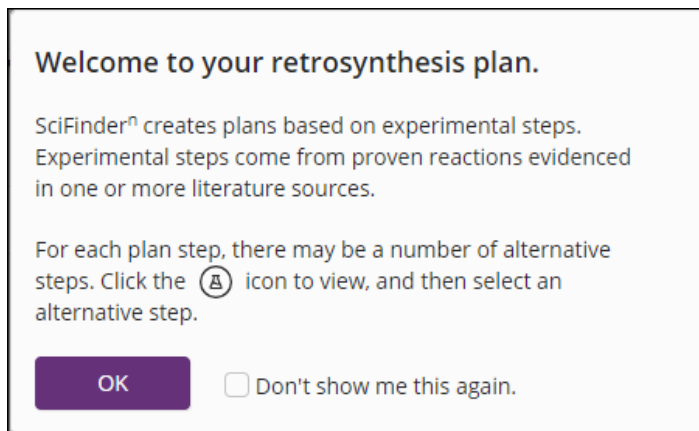
9-1. From the Reactions Search Page (Continued)

- 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.



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.



9-2. From a Substance Window

- Clicking a substance structure image in SciFinderⁿ 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.

The image shows a transition from a search result snippet to a full Substance Window. In the top-left snippet, a chemical structure of Benoxaprofen is shown with a yellow arrow pointing to it. Below the structure, the text reads "51234-28-7", "View Detail", "C₁₆H₁₂ClNO₃", "Benoxaprofen", "1,012 References", and "28 Reactions". A large yellow arrow points from this snippet to the main Substance Window on the right. The Substance Window has a title bar with "CAS RN 51234-28-7", "View Detail", and "CAS Name Benoxaprofen". It features a large chemical structure of Benoxaprofen on the right. On the left, a sidebar contains a list of options: "Substance Detail", "Reactions (28)", "Synthesize (23)", "Create Retrosynthesis Plan" (which is highlighted with a green circle), "References (1,005)", and "Suppliers (33)". At the bottom right of the window are buttons for "Edit Structure", "Reset", and a download icon.

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.

Plan in progress...

It's taking a little longer than expected to generate your plan. Click the OK button to return to the Home page where you can check the status of your plan under [Recent Search History](#).


OK

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.

Welcome to your retrosynthesis plan.























SciFinderⁿ creates plans based on experimental steps. Experimental steps come from proven reactions evidenced in one or more literature sources.

For each plan step, there may be a number of alternative steps. Click the  icon to view, and then select an alternative step.

OK

☐ Don't show me this again.

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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