

CAS 한국지사

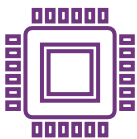
korea@acs-i.org

# SciFinder<sup>n</sup> 검색가이드

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# CAS, a division of the American Chemical Society (ACS)



## CONTENT

### Breadth and Depth Required

시간, 분야 및 심도 있는 대규모  
과학 데이터 수집

세계에서 가장 포괄적이고  
신뢰할 수 있는 과학 정보 제공



## HISTORY

### World's Largest Scientific Society

110년이 넘는 오랜 역사

CAS Registry Number® 부여

STNext®, SciFinder<sup>n</sup>과 같은  
데이터베이스 서비스를 제공



## EXPERTISE

### Context is Crucial

전문 과학자로 구성된 네트워크

전 세계 50여개 언어로 작성된  
문헌 검토

전 세계 과학 특허 및  
저널 콘텐츠를 선별하고 집계

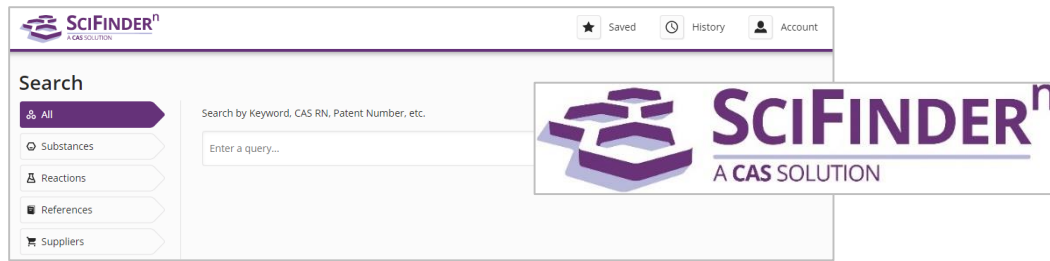
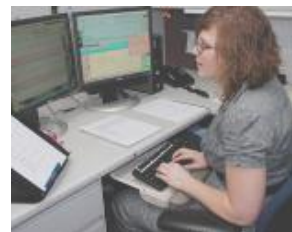
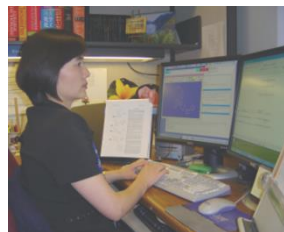


## TECHNOLOGY

### Big Data Infrastructure

SciFinder<sup>n</sup>과 같은  
검색 솔루션을 직접 제작하여  
과학 발전에 기여

# 사용자들이 쉽게 찾아볼 수 있도록 CAS의 과학자들이 문헌 내 정보를 직접 읽고 색인 합니다.



## SciFinder<sup>n</sup> 아이디 만들기

1. 도서관 홈페이지 접속

2. Database 선택 - 국외 Database (해외 데이터베이스) 선택

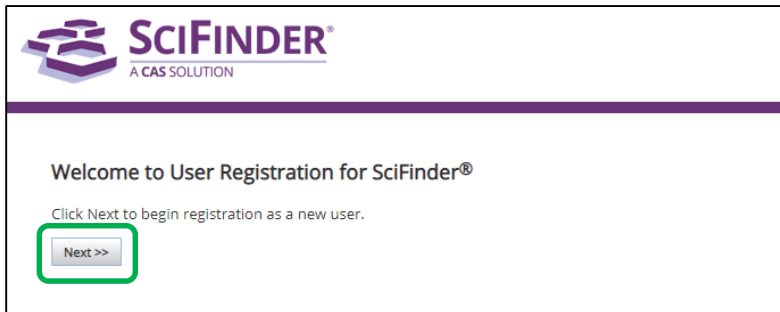
3. SciFinder<sup>n</sup> 선택

4. 이용자 등록 URL 선택

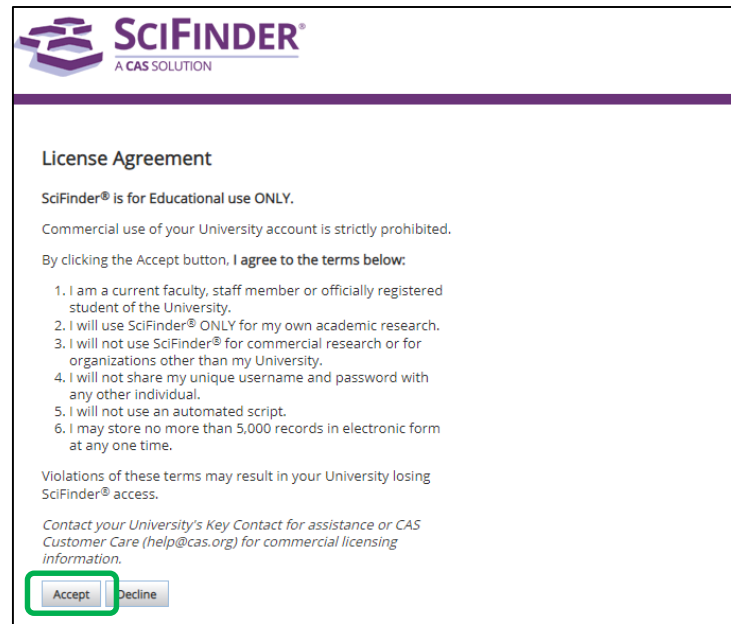
(<https://scifinder.cas.org/registration/index.html?corpKey=>로 시작되는 URL)

# SciFinder<sup>n</sup> 아이디 만들기 (Continued)

## 5. 계정 등록 사이트에 접속



## 6. 라이선스 조항 동의



# SciFinder<sup>n</sup> 아이디 만들기 (Continued)

## 7. 이용자 정보 등록 예시

※ 학교 계정 이메일 주소 사용 필수

(예: sjung@abcuniv.ac.kr)

	학부생	석/박사
Area of Research	학과 선택 (예: Biochemistry)	학과 선택 (예: Nanotechnology)
Job Title	Undergraduate Student	Graduate Student/ Post Doc

**Registration Information**

Please provide the following information:  
(bold\* = required)

**Contact Information**

First Name\*: Sehee  
Last Name\*: Jung  
Email\*: sjung@abcuniv.ac.kr  
Confirm Email\*: sjung@abcuniv.ac.kr  
Phone Number:   
Fax Number:   
Area of Research\*: Select one Biochemistry  
Job Title\*: Select one Undergraduate

**Username and Password**

Username\*: seheejung Dies  
Password\*: \*\*\*\*\*  
Re-enter Password\*: \*\*\*\*\*

대문자, 소문자, 숫자,  
기호문자 중  
3가지 사용

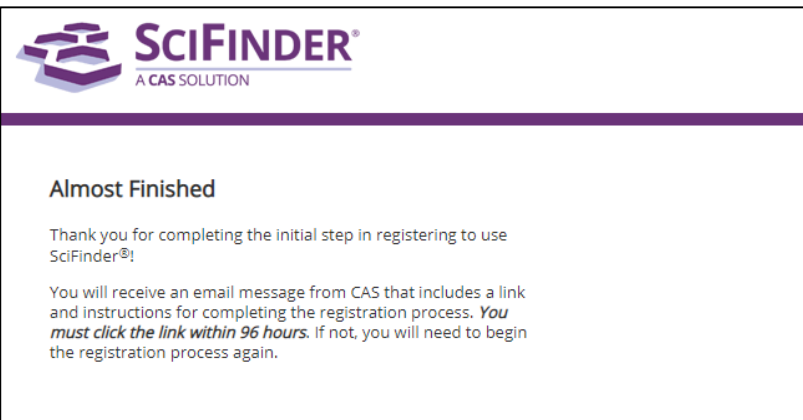


**SciFinder<sup>n</sup>**  
A CAS SOLUTION

## SciFinder<sup>n</sup> 아이디 만들기 (Continued)

8. 아래와 같은 페이지를 확인한 후

9. 등록 시 사용한 이메일로 로그인  
(예시: [sjung@abcuniv.ac.kr](mailto:sjung@abcuniv.ac.kr))




10. CAS에서 도착한 가입완료 메일에서  
Registration Complete Link 버튼 클릭

11. 등록한 아이디와 비밀번호로  
SciFinder<sup>n</sup> 이용 가능

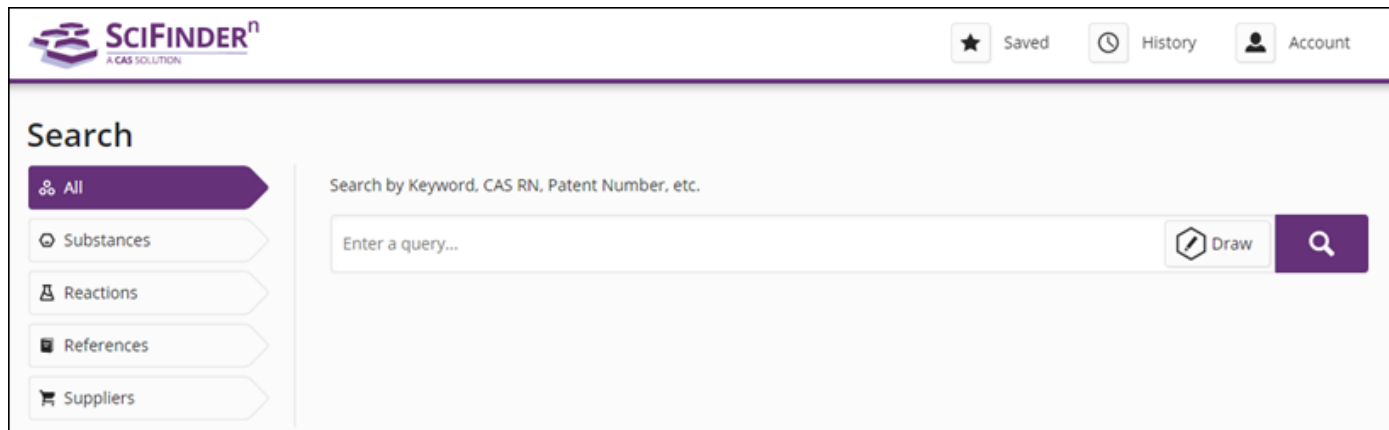


# 1. SciFinder<sup>n</sup> 시작하기

- [www.scifinder-n.cas.org](http://www.scifinder-n.cas.org)
- 기존 버전에서 사용하던 아이디와 비밀번호가 있을 경우 SciFinder<sup>n</sup>에서 그대로 이용 가능 (**동일 아이디/비번 사용**)
- 기존 버전에 설정한 Keep Me Posted를 SciFinder<sup>n</sup>으로 이동 가능 (Migration)
- 특허솔루션  PATENTPAK<sup>®</sup> A CAS SOLUTION 의 **무제한 사용** 가능
- 합성솔루션  METHODSNow<sup>™</sup> A CAS SOLUTION 의 **무제한 사용** 가능

## 1-1. SciFinder<sup>n</sup> 메인 홈페이지

SciFinder<sup>n</sup>에 로그인 후 홈페이지 왼쪽에 Search 옵션 선택 가능  
(로고를 선택하면 홈페이지로 이동)




The screenshot shows the SciFinder<sup>n</sup> main homepage. At the top left is the SciFinder<sup>n</sup> logo with the tagline "A CAS SOLUTION". To the right of the logo are three navigation icons: a star for "Saved", a clock for "History", and a person icon for "Account". Below the header is a "Search" section. On the left side of the search section, there is a vertical list of search categories: "All" (highlighted in purple), "Substances", "Reactions", "References", and "Suppliers". To the right of this list is a search input area with the text "Search by Keyword, CAS RN, Patent Number, etc." and a search box containing the placeholder text "Enter a query...". To the right of the search box are two buttons: a "Draw" button with a chemical structure icon and a search button with a magnifying glass icon.


## 1-2. 검색 종류 선택

 All


**All**에서는 물질, 반응식, 문헌, 판매처 모두를 검색. 검색어(키워드, DOI, 특허정보, 물질명, CAS Registry Number 등)를 넣거나 구조식 그리기

 Substances


**Substances**에서는 물질명, CAS Registry Number, 문헌 정보 (예: 특허번호) 또는 구조식을 검색  
**Advanced Search**에서는 Molecular formula, 물질 특성, 스펙트럼으로 검색

 Reactions

**Reactions**에서는 물질명, CAS Registry Number, 문헌정보 또는 구조식으로 반응식 검색

 References

**References**에서는 키워드, 문헌정보, 특허 정보, 물질명, CAS Registry Number 또는 구조식으로 문헌 검색  
저자, 저널 또는 기관으로 검색하기 위해서는 **Advanced Search**를 클릭

 Suppliers

**Suppliers**에서는 물질명, CAS Registry Number, 구조식으로 물질 판매처를 검색



## 1-3. 키워드를 넣거나 Draw 버튼을 통해 구조식을 그려 넣고, 돋보기 버튼으로 검색을 실행

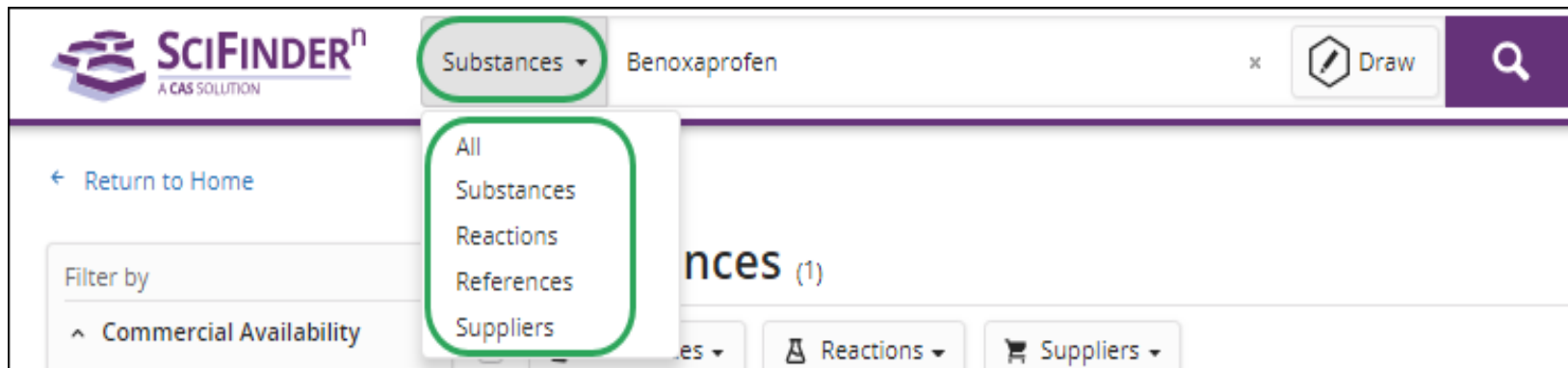
Search by Keyword, CAS RN, Patent Number, etc.

Enter a query...

 Draw



## 1-4. Drop-down 버튼을 통해 언제든지 검색 종류를 선택하여 새로운 검색을 실행 가능



The screenshot displays the SciFinder search interface. At the top left is the SciFinder logo with the text "A CAS SOLUTION". The search bar contains the text "Substances" (highlighted with a green box), "Benoxaprofen", a search icon, and a "Draw" button. A dropdown menu is open below the "Substances" button, listing "All", "Substances", "Reactions", "References", and "Suppliers" (all highlighted with a green box). Below the search bar, there is a "Return to Home" link and a "Filter by" section with "Commercial Availability" selected. The main content area shows "nces (1)" and several filter buttons: "Substances", "Reactions", and "Suppliers".

## 1-5. 홈페이지 하단 View All Search History를 클릭하면 모든 검색 히스토리 페이지 확인 가능

The screenshot displays the SciFinder search 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 bar with the text 'Search by Keyword, CAS RN, Patent Number, etc.' and a search input field containing 'Enter a query...'. To the left of the search bar is a sidebar with search filters: 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. Below the search bar is a 'Recent Search History' section, which is highlighted with a green border. This section contains two search entries: one from June 18, 2018 at 3:33 PM for 'Suppliers: DuPont 976 (35)' with 'Edit' and 'Rerun Search' buttons, and another from June 12, 2018 at 10:54 AM for 'Substances: Benoxaprofen (1)' with 'Edit' and 'Rerun Search' buttons. At the bottom left of the history section is a 'View All Search History' button, also highlighted with a green border.

## 2. 검색어로 문헌 검색하기

	<예시>
연구제목, 키워드, 콘셉트	Analgesics
물질명	Ibuprofen
CAS Registry Number	51146-57-7
문헌 등록 번호	1986:230471
PubMed ID Number	15980585
DOI	10.1093/nar/gki470
특허번호	US4571400
특허 출원번호	US1984-682902

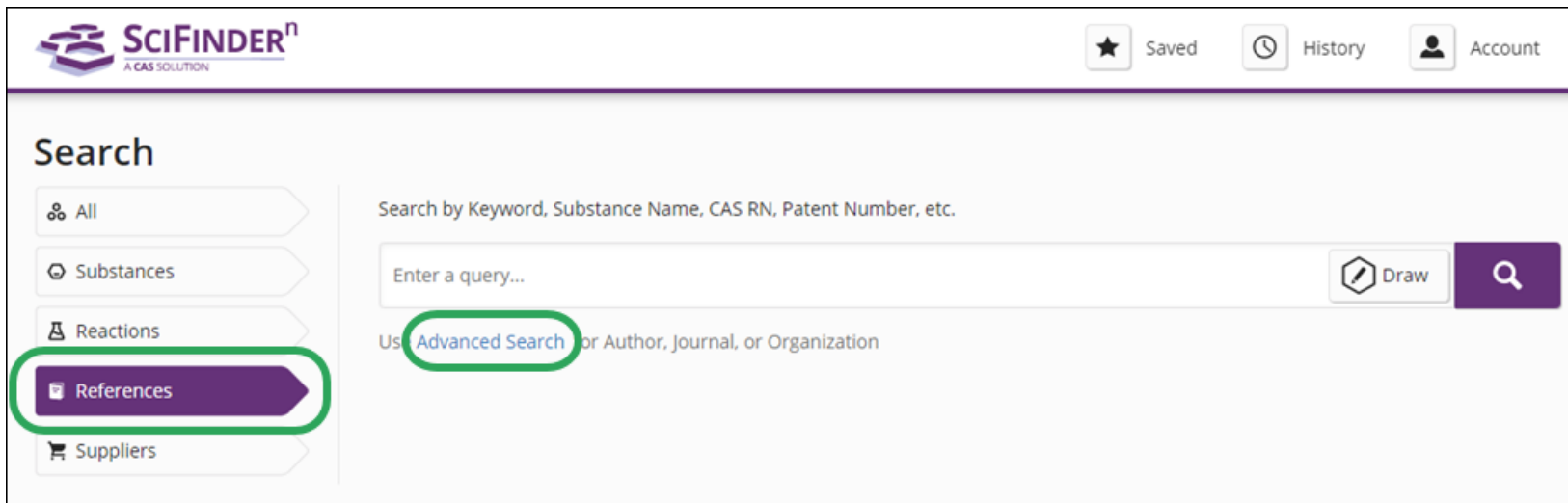
※ 띄어쓰기를 통해 여러 개의 특허번호 입력 가능 (2000-character limit)

## 2-1. 텍스트의 자동완성 기능으로 선택 또는 직접 타이핑 후 검색 실행

The screenshot displays the SciFinder search interface. On the left, a 'Search' sidebar contains navigation buttons for 'All', 'Substances', 'Reactions', 'References' (highlighted in purple), and 'Suppliers'. The main search area features a text input field with the text 'ibuprof' and a dropdown menu of suggestions: 'ibuprofen', 'ibuprofenal', 'Ibuprofen OH', 'Ibuprofen COOH', 'Ibuprofenamide', and 'Ibuprofen sodium'. The dropdown menu is highlighted with a green border. Above the search bar, the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' is visible. To the right of the search bar, there is a 'Draw' button and a search icon.



## 2-2. Advanced Search를 클릭하면 저자, 회사/연구기관, 저널정보로 검색 가능



SCI FINDER<sup>n</sup>  
A CAS SOLUTION

★ Saved    ⌚ History    👤 Account

### Search

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

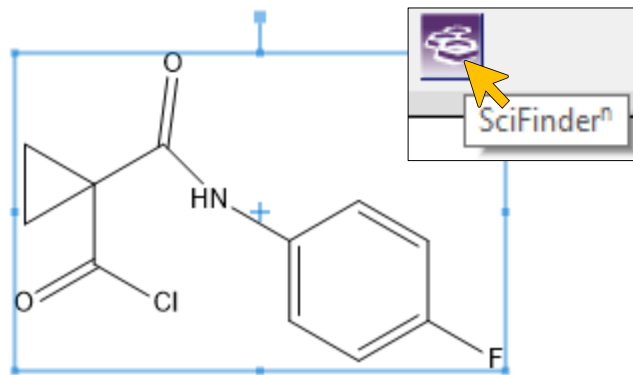
Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query... Draw 🔍

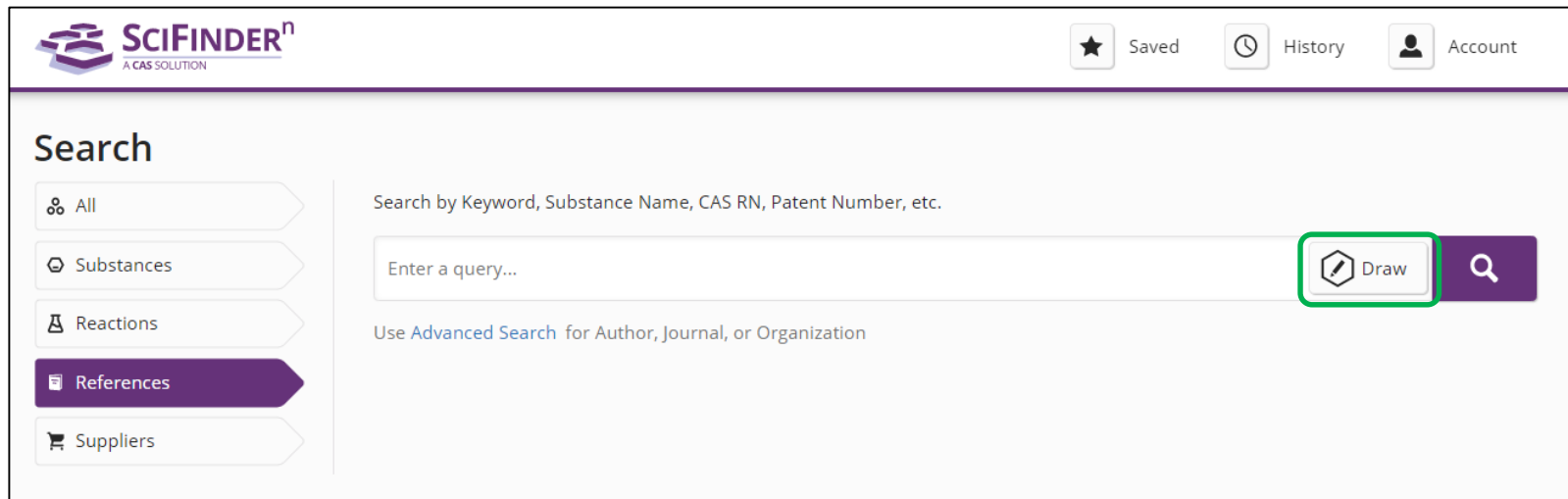
Use [Advanced Search](#) for Author, Journal, or Organization

### 3. 구조식으로 문헌 검색하기

- CAS Structure Editor에서 직접 구조를 그리거나 구조식 파일을 업로드(.mol, .cxf 파일 가능) 하여 물질 검색
- ChemDraw ver 18.2 에서 구조를 그린 후 상단 SciFinder<sup>n</sup>버튼을 클릭하면 SciFinder<sup>n</sup>으로 검색이 연결됨

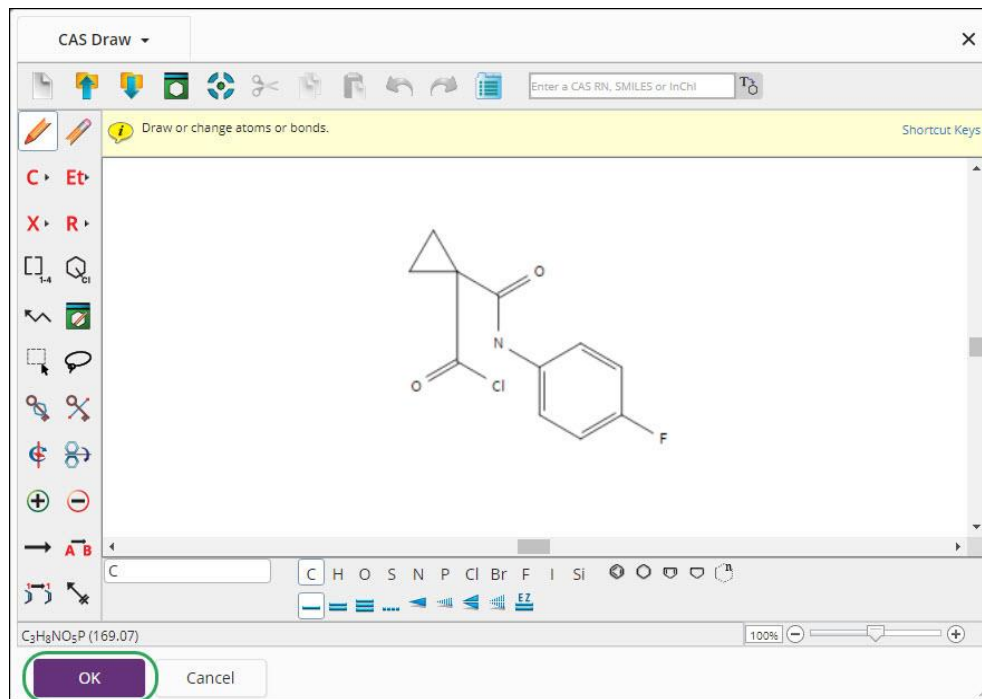


## 3-1. Draw 버튼을 클릭하여 Structure Editor 열기



The screenshot displays the SciFinder search page. At the top left is the SciFinder logo with the text "A CAS SOLUTION". To the right are navigation icons for "Saved", "History", and "Account". Below the logo is a "Search" section with a vertical list of filters: "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 with a pencil icon, which is highlighted with a green rectangular box, and a search button with a magnifying glass icon. Below the input field, it says "Use [Advanced Search](#) for Author, Journal, or Organization".

## 3-2. 구조식 그리기가 완료되면 OK 버튼으로 검색 실행



### 3-3. Edit Drawing 버튼을 클릭하면 구조식 수정이 가능하고, Remove 버튼을 클릭하면 삭제 가능

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

Enter a query...

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



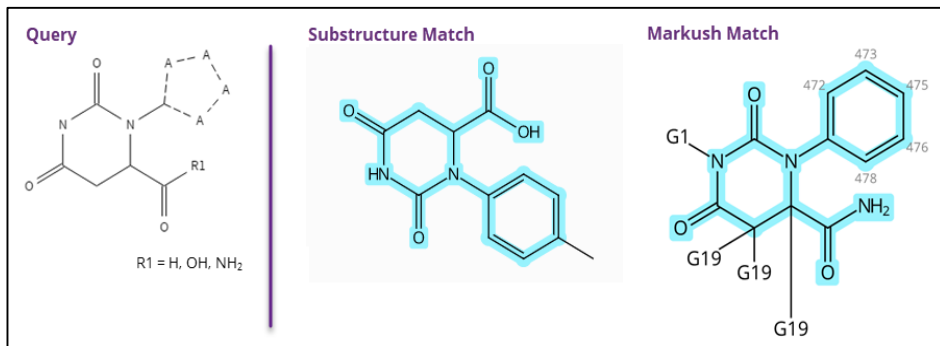
The screenshot shows the SciFinder search interface. At the top, there is a search bar with the placeholder text "Enter a query...". To the right of the search bar is an "Edit" button with a pencil icon and a search button with a magnifying glass icon. Below the search bar, there is a link that says "Use [Advanced search](#) for Author, Journal, or Organization". In the center, there is a chemical structure of a complex organic molecule. Below the structure are two buttons: "Edit Drawing" and "Remove".

### 3-4. 검색된 구조는 완전일치 (As Drawn), 부분일치 (Substructure), 유사구조 (Similarity) 필터를 통해 검색 범위 조절 가능

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)', 'Substructure (6)', and 'Similarity (4,319)'. Below this, there are sections for 'Analyze Structure Precision' and 'Filter by', which includes 'Commercial Availability' (Available (1)), 'Reaction Role' (Product (1), Reactant (1)), and 'Reference Role'. The main search results area on the right is titled 'Substances (1)'. It shows a search result for '1219937-98-0' with a 'View Detail' link. The chemical structure is displayed, and the name is '1-[[4-Fluorophenyl]amino]carbonyl cyclopropanecarbonyl chloride'. The molecular formula is  $C_{11}H_9ClFNO_2$ . Below the structure, there are three buttons: 'References' (59), 'Reactions' (177), and 'Suppliers' (8).

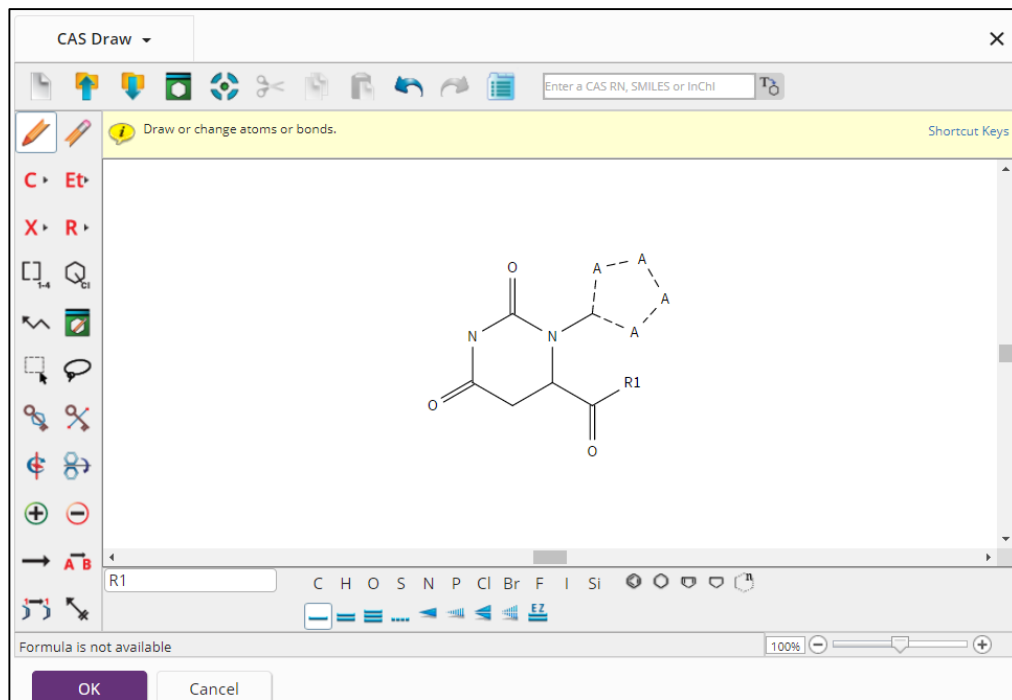
## 4. 특허 마쿠시 문헌 검색하기

- **Patent Markush** 검색으로 마쿠시 구조(Markush Structure)를 가진 특허 검색 가능
- 마쿠시 검색은 단순 물질 구조 검색과 다르게 특허 내 **Generic Structure**를 검색



※ Markush 구조는 관련 화합물 그룹을 나타내는 데 사용되는 구조로, 화학 텍스트 및 특허 청구에 일반적으로 사용됨

## 4-1. Substance 검색을 선택하고 Structure Editor에서 구조식 그리기





## 4-2. Search Patent Markush 버튼을 클릭한 후 검색 실행

The screenshot displays the SciFinder search interface. On the left, a sidebar titled 'Search' contains navigation buttons for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Substances' button is highlighted in purple. The main search area features a search bar with the placeholder text 'Enter a query...' and a search icon. Below the search bar, there is a link for 'Advanced search' and a note about molecular formula and substance property. A dropdown menu is open, showing a chemical structure and options for 'Edit Drawing', 'Remove', and 'Search Patent Markush'. The 'Search Patent Markush' button is highlighted with a green circle.

## 5. 키워드로 물질 검색하기

<예시>

<b>물질명</b>	Benoxaprofen, methyl ethyl ketone
<b>CAS Registry Number</b>	51146-57-7, 51146577
<b>특허번호</b>	US4571400
<b>Document Identifier</b>	Accession Number 1986:230471
	PubMed ID Number 15980585
	CAS Accession Number (CAN) 148:486341

## 5-1. 자동완성 기능으로 생성된 키워드를 선택하거나 직접 키워드를 완성한 후 검색 버튼 클릭

The screenshot displays the SciFinder search interface. On the left, a sidebar titled "Search" contains navigation buttons for "All", "Substances", "Reactions", "References", and "Suppliers". The "Substances" button is highlighted in purple. The main search area has a header "Search by Substance Name, CAS RN, Patent Number, etc." and a search input field containing the text "benoxa". A dropdown menu is open below the input field, listing several search suggestions: "Benoxaprofen", "Benoxacor", "Benoxathian", "Benoxafos", "Benoxazole", "Benoxaprofen glucuronide", "Benoxacor-S-metolachlor mixt.", "Benoxacor-metolachlor mixt.", "(R5)-Benoxaprofen", and "(±)-Benoxaprofen". The dropdown menu is enclosed in a green rounded rectangle. To the right of the search input field, there are icons for "Draw" and a search button (magnifying glass).

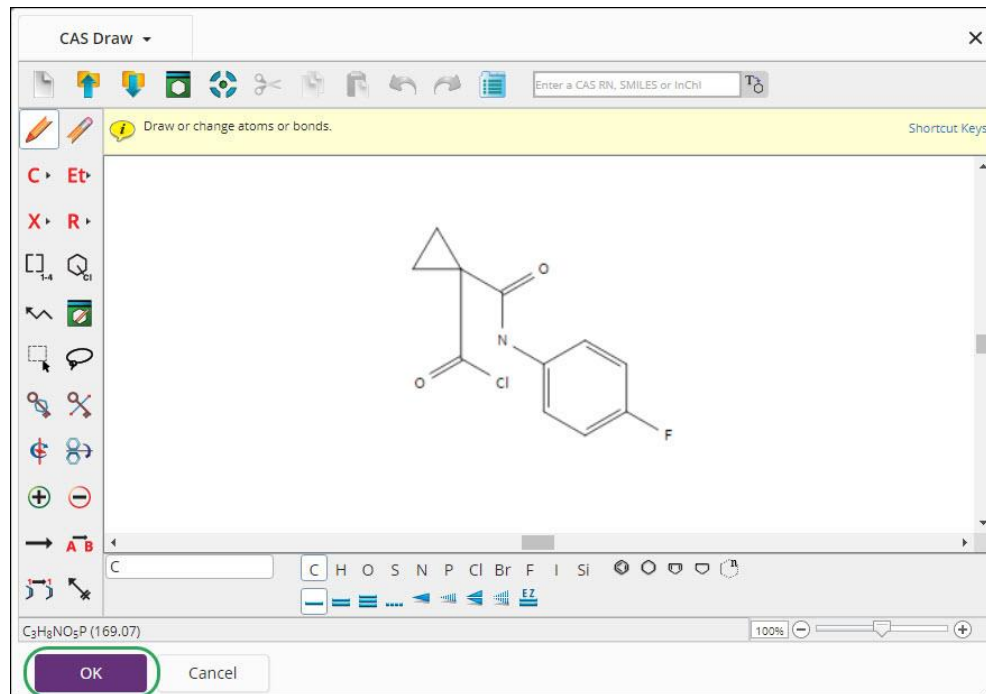
## 6. 구조식으로 물질 검색하기

- **CAS Structure Editor**에 직접 그리거나 구조식 파일(.mol, .cxf 파일)을 업로드하여 구조식으로 물질 검색 가능
- 특허의 Markush 구조식 검색은 “4. 특허 마쿠시 문헌 검색하기” 참고 (4)

## 6-1. Draw 버튼을 클릭하여 Structure Editor 열기

The screenshot shows the SciFinder search page. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. To the right are navigation buttons for 'Saved', 'History', and 'Account'. Below the logo is a 'Search' section with a list of filters: 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Suppliers' button is highlighted with a green rounded rectangle. To the right of the filters is a search input field with the placeholder text 'Enter a query...'. Above the input field is the text 'Search by Substance Name, CAS RN, etc.'. To the right of the input field is a 'Draw' button with a chemical structure icon, also highlighted with a green rounded rectangle. A magnifying glass icon is to the right of the 'Draw' button.

## 6-2. 구조식 그리기가 완료되면 OK 버튼으로 검색 실행

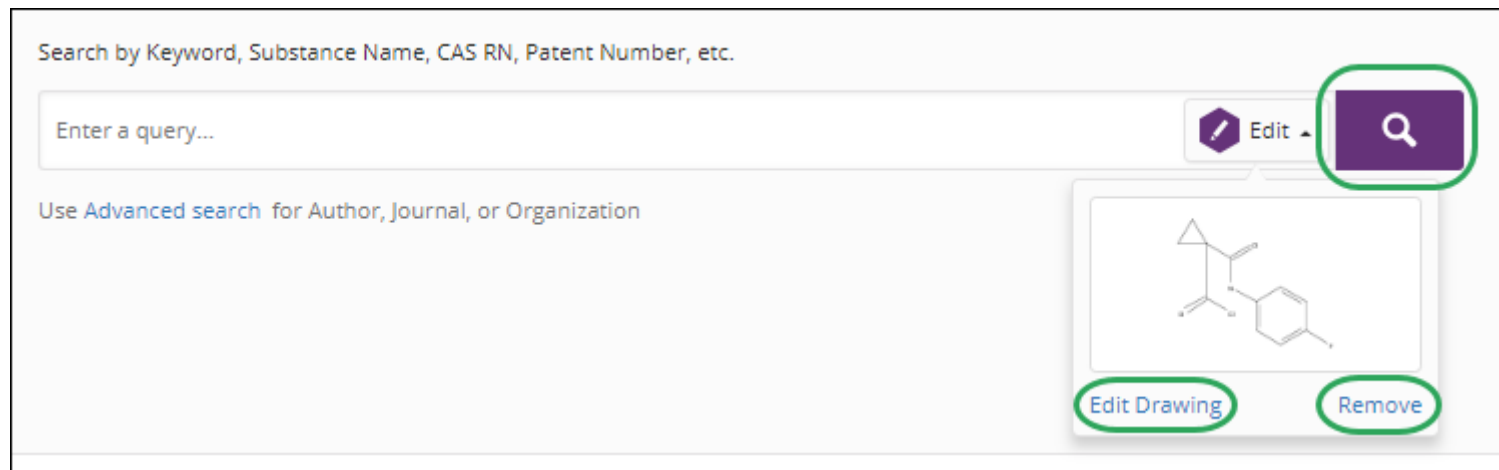


## 6-3. Edit Drawing 버튼을 클릭하여 수정하거나 Remove 버튼을 클릭하여 삭제 가능

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

Enter a query...

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



The screenshot displays the SciFinder search interface. At the top, there is a search bar with the placeholder text "Enter a query...". To the right of the search bar is a purple search button with a magnifying glass icon. Below the search bar, there is a link for "Advanced search" and a note about searching by Author, Journal, or Organization. On the right side, there is a preview of a chemical structure. Below the structure are two buttons: "Edit Drawing" and "Remove".

## 7. 키워드로 반응식 검색하기

※ 정확한 키워드를 통해서만 검색이 가능하고, 물질명이나 번호의 일부만 작성하면 검색 불가함

<예시>

<b>물질명</b>	Benoxaprofen, methyl ethyl ketone
<b>CAS Registry Number</b>	51146-57-7, 51146577
<b>특허번호</b>	US4571400
<b>Document Identifier</b>	Accession Number 1986:230471
	PubMed ID Number 15980585
	CAS Accession Number (CAN) 148:486341



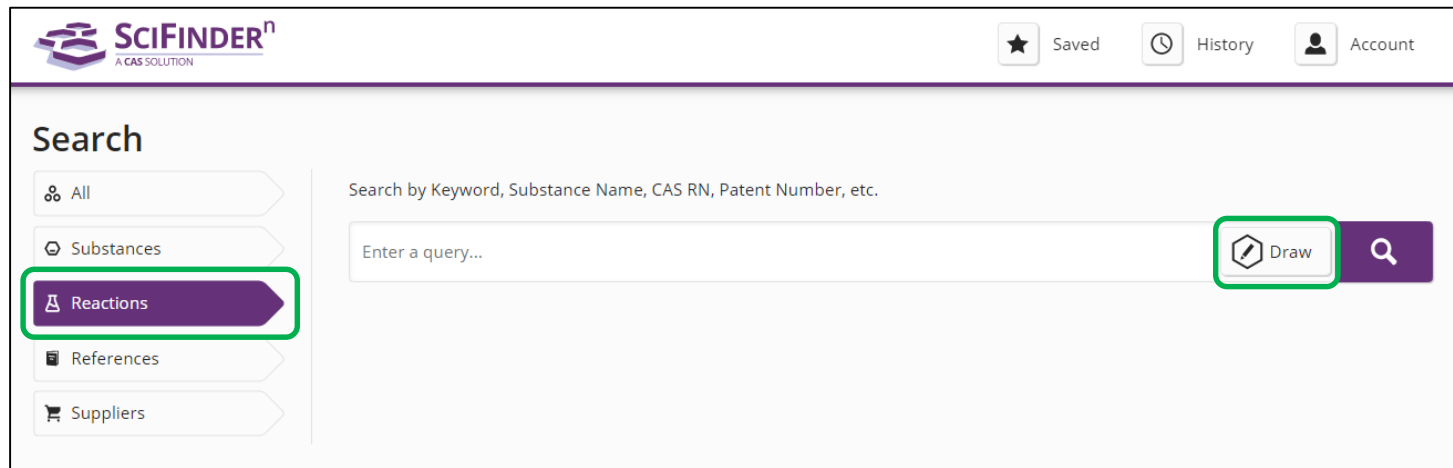
## 7-1. 자동 완성된 키워드를 선택하거나 직접 작성한 키워드로 반응식 검색 가능

The screenshot displays the SciFinder search interface. On the left, there is a 'Search' sidebar with navigation buttons for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Reactions' button is highlighted in purple. The main search area features a search bar with the text 'benoxa' and a dropdown menu of suggestions. The suggestions are: Benoxaprofen, Benoxacor, Benoxaprofen glucuronide, Benoxafos, Benoxathian, Benoxazole, (R)-Benoxaprofen, (±)-Benoxaprofen, d,l-Benoxaprofen, and (±)-Benoxaprofen methyl ester. To the right of the search bar, there is a 'Draw' button and a search icon (magnifying glass) which is circled in green. Above the search bar, the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' is visible.

## 8. 구조식으로 반응식 검색하기

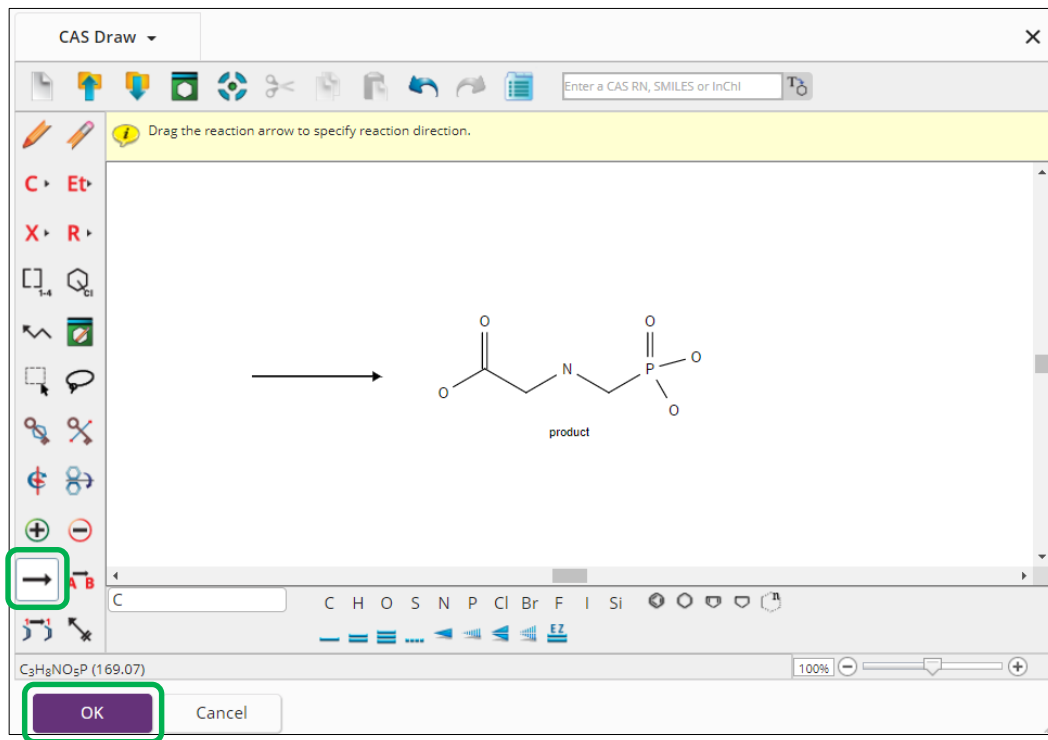
- 반응식의 Reactants AND/OR Products를 그려 검색할 수 있음
- 구조식 파일(.mol, .cxf 파일) 업로드 가능

## 8-1. Draw 버튼을 클릭하여 Structure Editor 열기

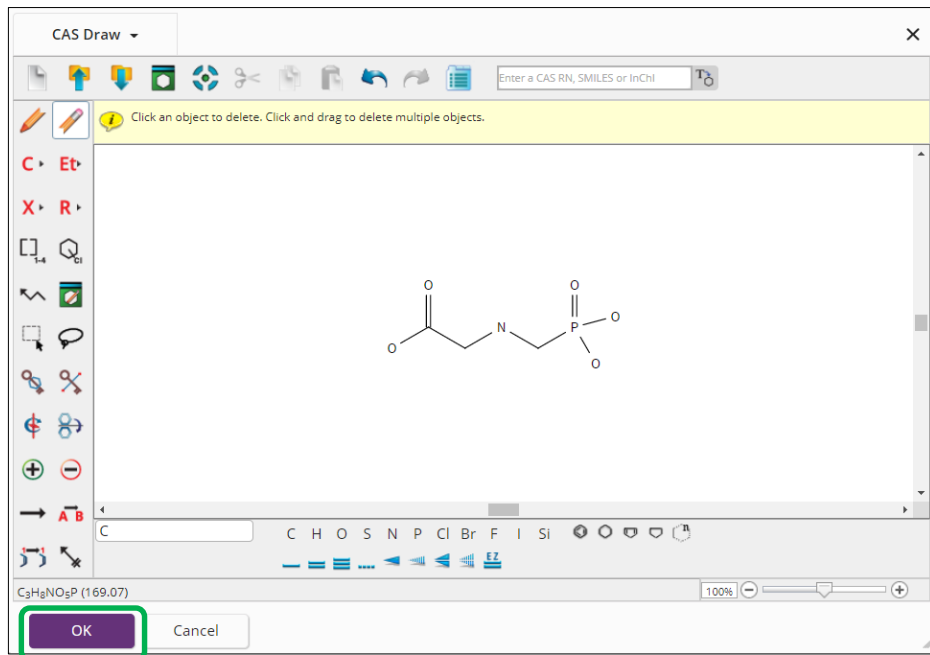


The screenshot displays the SciFinder search page. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. To the right are navigation buttons for 'Saved', 'History', and 'Account'. Below the logo is a 'Search' section with a list of filters: 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Reactions' filter is highlighted with a green border. To the right of the filters is a search input field with the placeholder text 'Enter a query...'. A 'Draw' button, featuring a chemical structure icon and the text 'Draw', is highlighted with a green border. A magnifying glass icon is located to the right of the 'Draw' button. Above the search input field, the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' is displayed.

## 8.2 반응물을 그리고 Reactant 또는 Product로 설정한 후 검색 실행



## 8.3 반응물을 그리고 OK 버튼을 클릭하여 검색 실행



물질의 반응식 내에서의 역할을 따로 설정하지 않고 검색을 실행하면 결과 필터에서 선택이 가능합니다.

(8.4)

## 8.4 필터를 통해 화합물의 구조매치와 역할 선택

The screenshot displays the SciFinder interface for a reaction search. The top navigation bar includes the SciFinder logo, a search input field with the text "Enter a query...", and utility icons for Edit, Search, Favorites, History, and Profile. Below the navigation bar, a "Return to Home" link is visible. The main content area is titled "Reactions (657)" and includes a "View Expanded" dropdown. On the left, a "Structure Match" sidebar shows two filter options: "As Drawn (657)" (highlighted with a green border) and "Substructure (2,066)". Below this, a "Filter by" section contains two sub-sections: "Substance Role" with radio buttons for Product (569), Reactant (206), and Reagent (10); and "Yield" with radio buttons for 90-100% (149), 80-89% (61), and 70-79% (35). The main reaction area shows "Scheme 1 (115 Reactions) View All". It features a chemical reaction diagram where the reactant is a phosphonate derivative and the product is N-phosphonate methyl glycine. The reaction is labeled with "Steps: 1" and "Yield: 99-100%". Below the diagram are two "Suppliers" buttons: "Suppliers (39)" and "Suppliers (78)". At the bottom, a "Reaction Summary" table provides details:

Reaction Summary		Research progress in catalysts for producing N-phosphonate methyl glycine by air(oxygen) catalytic oxidation	
Reagents	Oxygen	Steps:	1
Catalysts	-	Yield:	100%

Additional information includes a "View Reference Detail" link and the citation "By: Chen, Dan; et al".

## 9. Retrosynthesis Plan 설계하기

- CAS가 보유한 Experimental Reaction 정보와 새로 고안된 Rule을 기반으로 표적 화합물에 대한 역합성 분석을 수행 및 직관적인 합성 계획 설계
- Retrosynthesis Plan은 아래 두가지 방법으로 설계 가능
  - 1) **Reactions Search Page**에서 시작하기 ([9-1](#))
  - 2) **Substance Window**에서 시작하기 ([9-2](#))

※ Retrosynthesis plan은 90일 후에 자동으로 삭제됨

# 9. Retrosynthesis Plan 설계하기 (Continued)

## Retrosynthesis Plan 예시

Retrosynthesis

Overview Steps

Plan Information

- Estimated Yield: 14%
- Overall Price: \$230.93 (USD per 100 grams)
- Commercially Available: A, B, C, D, E, F, G

예측 수율  
예상 가격  
구매가능한 물질

다른 실험방법 살펴보기

다운로드

SciFinder<sup>n</sup> 서버 내에 저장

현 페이지 링크를 이메일로 전달

A: Suppliers (37) Max. Yield: -

B: Suppliers (18) Max. Yield: -

C: Suppliers (41) Max. Yield: 81%

D: Suppliers (46) Max. Yield: 100%

E: Suppliers (90) Max. Yield: 69%

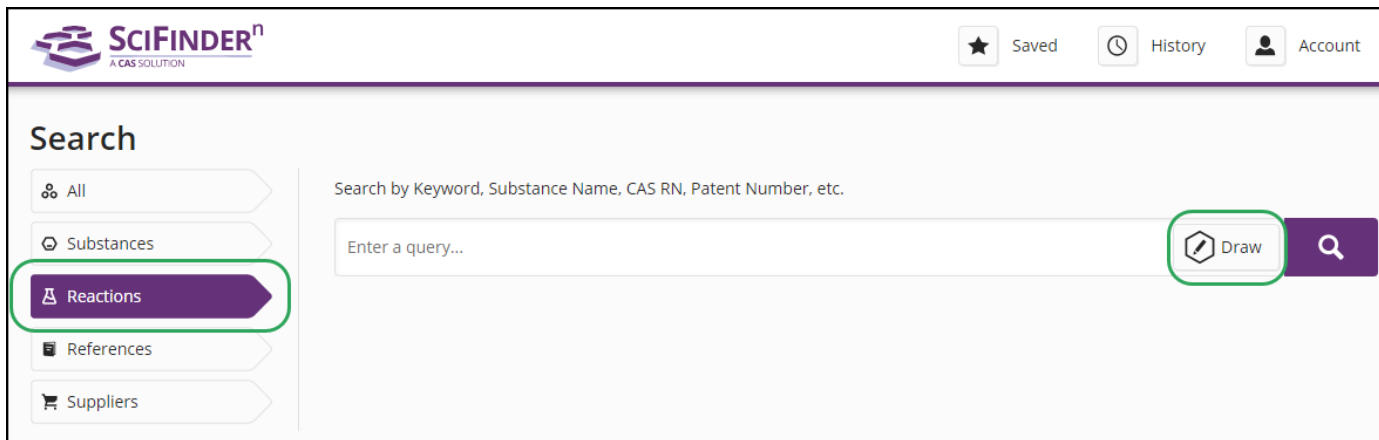
F: Suppliers (106)

G: Suppliers (113)



## 9-1. Reactions Search Page에서 시작하기

- Search 페이지에서 Reactions 검색 방법을 선택한 후 **Draw** 버튼을 클릭



The screenshot shows the SciFinder interface. At the top left is the SciFinder logo with the tagline 'A CAS SOLUTION'. On the top right, there are three icons: a star for 'Saved', a clock for 'History', and a person icon for 'Account'. Below the header is a 'Search' section. On the left, there is a vertical list of search methods: 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Reactions' option is highlighted with a purple arrow and a green circle. To the right of this list is a search input area with the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' and a text box containing 'Enter a query...'. To the right of the text box is a 'Draw' button with a chemical structure icon and a magnifying glass icon, both highlighted with green circles.

## 9-1. Reactions Search Page에서 시작하기 (Continued)

- 구조식을 그리거나 업로드한 후, **Create Retrosynthesis Plan** 버튼을 클릭

**Search**

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

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

Enter a query...

Edit

Chemical structure drawing

Edit Drawing Remove

**Create Retrosynthesis Plan**

## 9-1. Reactions Search Page에서 시작하기 (Continued)

- Retrosynthesis 설계에 문제가 있을 경우 에러 메시지가 나타남
- “**Plan in progress...**” 메시지가 나올 경우 OK를 클릭하여 홈페이지로 이동

### 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

## 9-1. Reactions Search Page에서 시작하기 (Continued)

- “Welcome to your retrosynthesis plan” 메시지가 나오면 **OK** 버튼을 클릭하여 Retrosynthesis Plan page로 이동

**Welcome to your retrosynthesis plan.**

SciFinder<sup>n</sup> 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.

Don't show me this again.

## 9-2. Substance Window에서 시작하기

- 물질 구조 이미지를 클릭하면 Substance Window가 열림
- 해당 물질의 Retrosynthesis설계가 가능한 경우 Create Retrosynthesis Plan 버튼이 활성화 됨
- **Create Retrosynthesis Plan** 버튼 클릭

51234-28-7  
View Detail

CC(C)C(=O)Oc1ccc2oc(cc2c1)C3=CC=C(C=C3)Cl

C<sub>16</sub>H<sub>12</sub>ClNO<sub>3</sub>  
Benoxaprofen

1,012 References   28 Reactions

CAS RN  
51234-28-7  
View Detail

CAS Name  
Benoxaprofen

Substance Detail

Reactions (28)

Synthesize (23)

**Create Retrosynthesis Plan**

References (1,005)

Suppliers (33)

Edit Structure   -   Reset   +   ↕

## 9-2. Substance Window에서 시작하기 (Continued)

- “Plan in progress...” 메시지가 나올 경우 **OK**를 클릭하여 홈페이지로 이동

### 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. Substance Window에서 시작하기 (Continued)

- “Welcome to your retrosynthesis plan” 메시지가 나오면 **OK**버튼을 클릭하여 Retrosynthesis Plan page로 이동

### Welcome to your retrosynthesis plan.

SciFinder<sup>n</sup> 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.

# Structure Drawing Editor 기능 세부설명

마디(Nodes)와 결합(Bonds)을 표현		그려진 구조식에서 마디나 결합을 지움
그린 구조식의 특정 마디에 특정 원자를 배치		구조식에 Shortcut을 삽입
Variable (X Menu) Tool		구조식에 R-Group (최대 20개) 생성
0 ~ 20 개까지, 노드, 링, 체인의 반복을 표시		Ring 구조 물질의 여러 위치에 치환체 결합 표시
1 ~ 30개 범위 내의 원자를 나타낼 수 있는 체인을 그림		미리 등록된 템플릿에서 원하는 구조 선택
마디, 결합, 구조식의 일부 또는 전체를 선택		그려진 구조식을 선택할 때 이용
특정 Ring/Chain에 추가적인 Ring 생성을 방지		선택한 Atom에 추가 Substitution이 일어나지 않도록 방지
구조식의 일부를 선택한 축을 중심으로 시계/반시계 방향으로 회전		구조식의 일부를 선택한 축을 중심으로 수직/수평 방향으로 회전
마디에 양전하를 표현		마디에 음전하를 표현
구조식에 대한 역할을 자동으로 구분		물질의 Role 표시 (Reactant, Reagent, Product 등)
반응물과 결과물의 원자쌍을 동일한 숫자로 표시하여 구분		본드 Breaking 또는 forming 표시



# CAS 한국지사

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Get further help on how to use  
[SciFinder<sup>n</sup>](#)