

All about CHEMISTRY

Quick Guide to SciFinder

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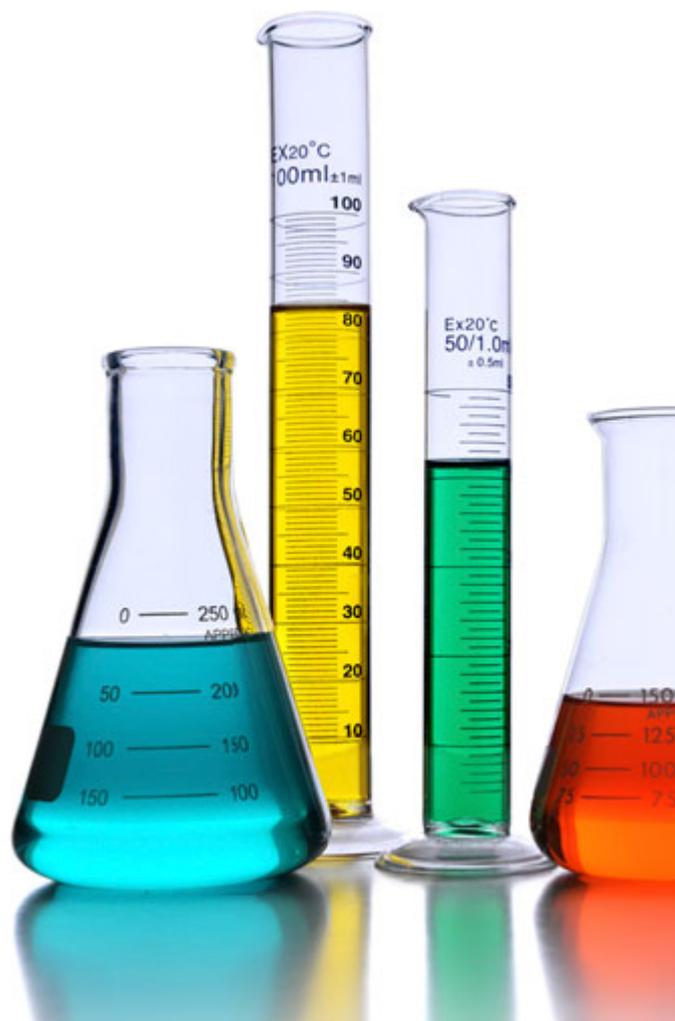


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SciFinder? Chemistry!

American Chemical Society에서 세계 화학 정보의 수집 및 조직을 담당하는 CAS(Chemical Abstracts Service) 분과에서 구축한 데이터베이스로, 화학 분야의 다양한 학술정보 (Journals, Patents, Commercial Chemical Sources, Dissertations, Books, Conference proceedings, Web sources)를 통합적으로 검색하고 이용 할 수 있는 사이트입니다.

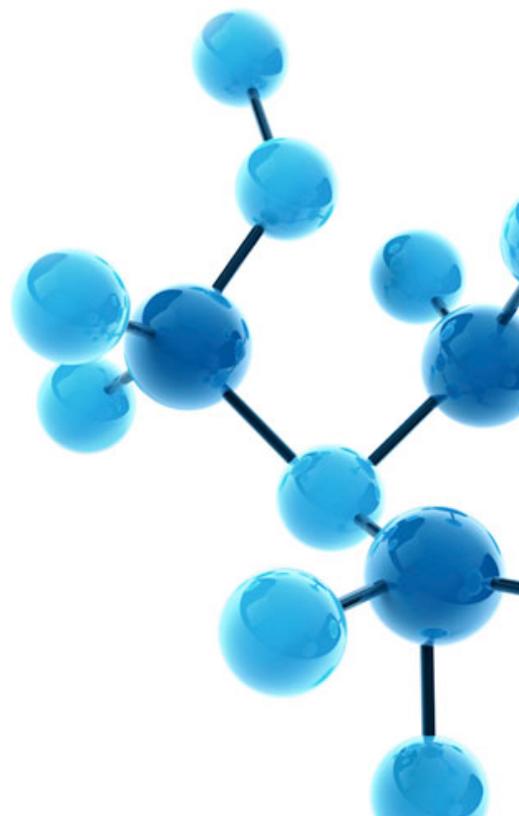


Databases of SciFinder – SciFinder에 수록된 콘텐츠

구분	데이터베이스	콘텐츠	검색 (Explore)
Reference DB	CA Plus	화학 분야 논문 및 특허 정보	References
	MEDLINE	의생명 분야 논문 정보	
Substance DB	CA Registry	화학 물질 정보	Substances
Reaction DB	CAS React	화학 반응 정보	Reactions
Specialized DB	CHEMLIST	화학 물질에 관한 통합적 정보	검색 결과에서 통합적으로 확인 가능
	CHEMCATS	구매 가능한 화학물질 정보	
	MARPAT	세계 특허 추출 Markush structure	Substances

For Whom? – 어떤 연구자에게 SciFinder가 필요한가?

- 화학 분야 연구 결과를 통합적으로 검색하고 싶은 연구자
- 화학 물질에 관한 정보를 얻고 싶은 연구자
- 물성 값을 기준으로 물질을 검색하고 싶은 연구자
- 화학 구조식으로 관련 연구 자료를 검색하고 싶은 연구자
- 화학 물질의 반응 결과를 알고 싶은 연구자
- 실험에 필요한 화학 물질의 합성 방법이나 구입 경로를 알고 싶
- 연구에 필요한 논문, 구조식 등 자료를 효과적으로 관리하고 싶



Sign in SciFinder – SciFinder 계정 만들기 및 접속하기

SciFinder에 수록된 자료들을 검색하고자 한다면 **개인 계정을 만든 후 로그인**해야 이용할 수 있습니다.

(1) SciFinder 계정 생성 사이트 접속: 도서관 홈페이지 > FIND > **Databases > SciFinder**

(2) **'Web Version User Registration'** 클릭

URL: <https://origin-scifinder.cas.org/registration/index.html?corpKey=335964D8X86F35055X19A1AFB318C1F24828>

(3) 웹사이트의 지시에 따라 계정 생성

* **e-Mail 주소: 반드시 UNIST 메일 주소 기입**

* 비밀번호: 영문 알파벳(대문자 또는 소문자), 숫자, 특수기호 포함 7-15자리로 구성

(4) UNIST e-Mail로 발송되는 계정 생성 확인 메일 수신, 링크 주소를 클릭하여 등록 확인

※전 소속기관에서 사용하던 계정은 사용 불가. UNIST e-Mail로 새로운 계정 생성 필요

(5) SciFinder 접속하기: 도서관 홈페이지 > FIND > Databases > SciFinder 또는

<http://scifinder.cas.org>



Sign In

Username

Password

NEW Remember me for two weeks unless I sign out
(Do not use on a shared computer)

Sign In

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

What is SciFinder?

SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.

News & Updates

Welcome to SciFinder

The New SciFinder is Here!

What do you think of our new look? See [What's New in SciFinder](#) to learn about our sleek new design and capabilities, and start exploring today!

Collaboration Helps Integrate SciFinder to Streamline Research Workflows

See how our collaboration with several customers, including Vertex Pharmaceuticals, helped them better integrate SciFinder to streamline research workflows.

Expanded Coverage of Chemical Reaction Information in SciFinder

Learn how our collaboration with Thieme Publishing Group will add hundreds of thousands of new experimental procedures to SciFinder for chemical reactions reported in SYNLETT and SYNTHESIS.

CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster

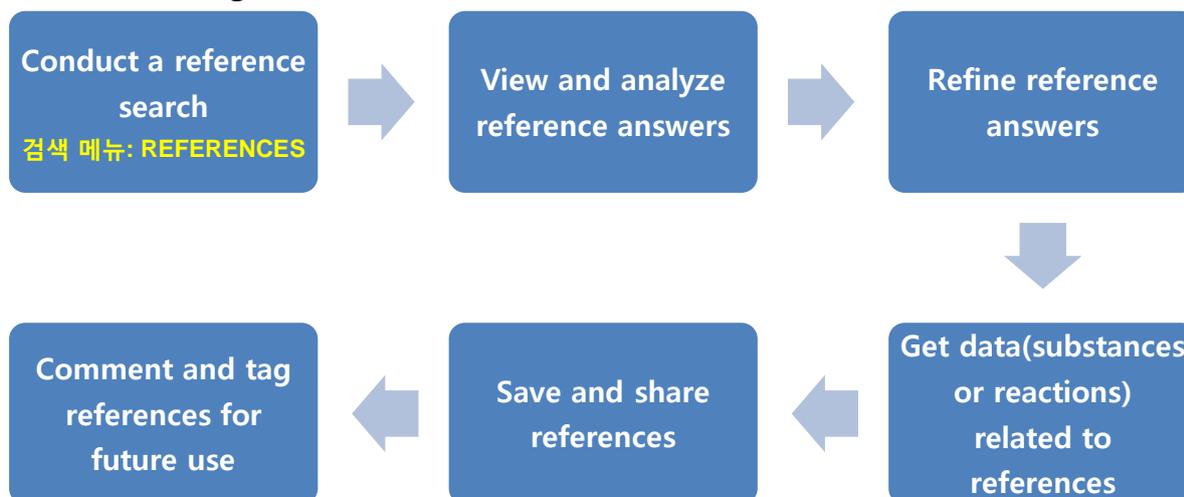
Thousands of new experimental procedures are being added to SciFinder for chemical reactions reported in 165 Springer chemistry journals from 1985 to the present. To learn more, see our [News Release](#).

Watch Part 3 of Our Science in the News Podcast on Natural Product Chemistry



Reference Searching: 화학 분야 논문 및 특허 정보 통합 검색 (from CAS Plus)

Workflow for working with references



(1) Conduct a reference search: 원하는 검색 옵션으로 검색

① 검색 옵션

Option	Note
Research Topic	전치사 등으로 조합한 자연어로 표현된 검색어 입력 가능 (예) effect of antibiotic residues in dairy products *전치사는 검색 엔진이 검색어의 의미를 파악하는데 도움됨.
Author Name	논문의 저자명으로 검색, 저자의 성(last name)은 필수
Company Name	화학 물질 제조 회사 등
Document Identifier	논문에 부여된 다양한 고유 번호로 검색 가능 Accession number(SciFinder 데이터베이스에 등록된 논문 고유 번호, 연도별 논문 등록 순서), Document number, Patent number, PubMed ID number, Digital Object Identifier(DOI)
Journal	Journal name, Volume, Issue, Starting Page 등
Patent	Patent Number, Assignee Name, Inventor Last Name 등
Tags	자신이 논문에 부여한 custom key words로 검색

② Research Topic 검색 결과 선택

Preferences | SciFinder Help | Sign Out

SciFinder®

Welcome Yulee Kwon

Explore | Saved Searches | SciPlanner

Research Topic "antibacterial with coatings fo..."

REFERENCES ⓘ

Select All Deselect All

1 of 11 Research Topic Candidates Selected

		References
<input type="checkbox"/>	664 references were found containing all of the concepts "antibacterial", "coatings" and "textiles" closely associated with one another.	664
<input checked="" type="checkbox"/>	1815 references were found where all of the concepts "antibacterial", "coatings" and "textiles" were present anywhere in the reference.	1815
<input type="checkbox"/>	6934 references were found containing the two concepts "antibacterial" and "coatings" closely associated with one another.	6934
<input type="checkbox"/>	13162 references were found where the two concepts "antibacterial" and "coatings" were present anywhere in the reference.	13162
<input type="checkbox"/>	5325 references were found containing the two concepts "antibacterial" and "textiles" closely associated with one another.	5325
<input type="checkbox"/>	8076 references were found where the two concepts "antibacterial" and "textiles" were present anywhere in the reference.	8076
<input type="checkbox"/>	43080 references were found containing the two concepts "coatings" and "textiles" closely associated with one another.	43080
<input type="checkbox"/>	59693 references were found where the two concepts "coatings" and "textiles" were present anywhere in the reference.	59693
<input type="checkbox"/>	430113 references were found containing the concept "antibacterial".	430113
<input type="checkbox"/>	1746155 references were found containing the concept "coatings".	1746155
<input type="checkbox"/>	397280 references were found containing the concept "textiles".	397280

Get References

검색결과 후보(candidates) 중 추 후 검색 확장에 가장 유용한 결과는 검색어가 어느 필드에든지 포함되는 'anywhere in the reference' 후보임.

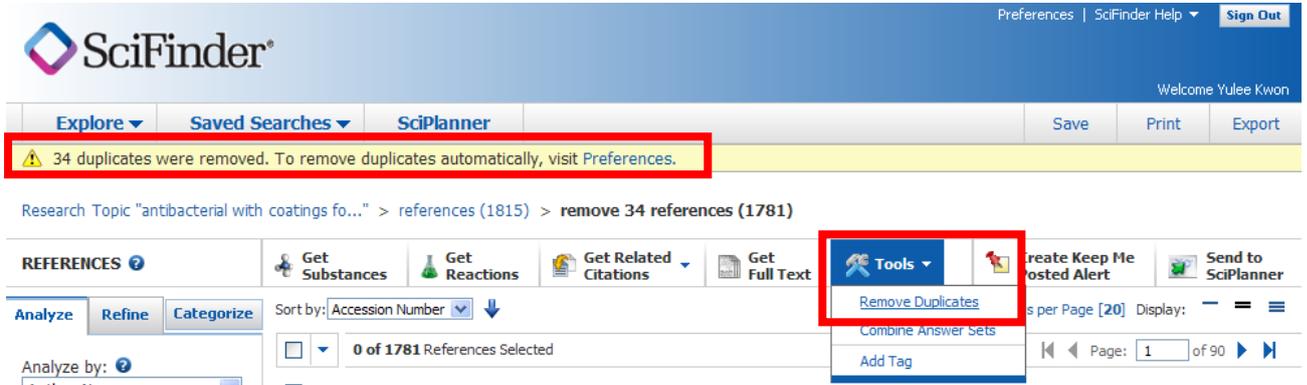
(A useful answer set for further exploration is often one which contains all of the concepts *anywhere in the reference*.)

(2) View and analyze reference answers: 검색 결과 중 원하는 자료 선택

① 검색 결과 중복 논문 삭제하기: Remove Duplicate

Reference Searching의 검색 결과는 SciFinder에 수록된 두 가지 문헌 데이터베이스인 'CAS Plus'와 'MEDLINE'에서 추출됩니다. 이 두 가지 데이터베이스에는 중복된 자료가 있으나 검색 결과에서 별도로 중복 데이터가 제거되지 않습니다. 그러므로 검색 결과에서 중복 데이터를 제거하고자 할 경우 별도의 과정이 필요합니다.

방법: 검색 결과 > Tools > **Remove Duplicate** (Preferences 메뉴에서 환경설정 가능)



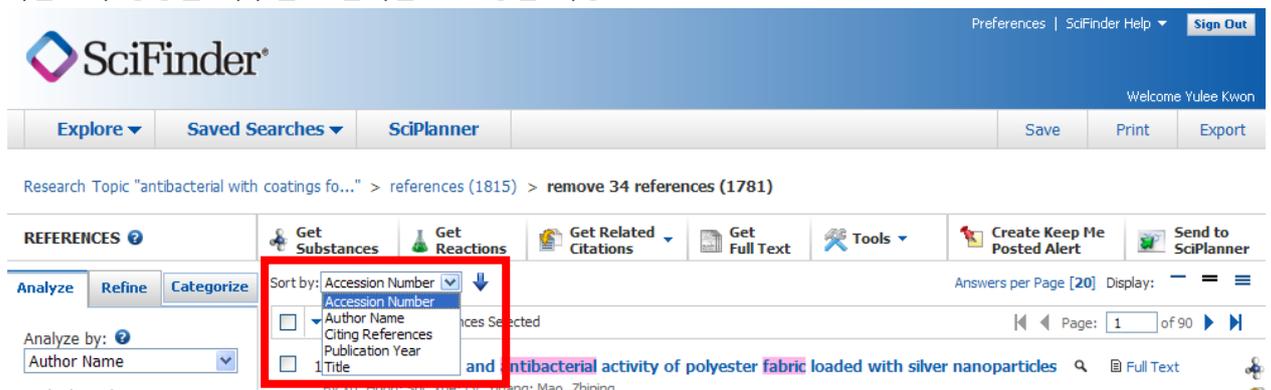
② 목적에 맞게 검색 결과 정렬하기: Sort by

검색 결과 화면에서 정렬 옵션을 활용하면 목적에 알맞은 자료를 더욱 쉽게 찾을 수 있습니다.

정렬 옵션 (기본: 최신순 정렬 – Accession Number 내림차순)

Accession Number	SciFinder 데이터베이스에 논문 정보가 입력된 순서대로 부여된 고유 번호 숫자가 클 수록 최신 논문임
Author Name	제 1 저자의 성(last name), 이름(first name) 순서로 정렬
Citing References	논문의 피인용 횟수를 기준으로 정렬
Publication Year	논문 출판년도 기준으로 정렬
Title	논문의 제목 알파벳 순으로 정렬

※ 화살표의 방향을 바꾸면 오름차순으로 정렬 가능



③ 검색 결과 필터링하여 보기: Analyze

원하는 정보 유형에 따라 검색 결과를 필터링하여 볼 수 있습니다. 검색 결과가 많을 때 문헌 수를 줄일 수 있는 좋은 방법입니다.

필터링 옵션

Author Name	문헌 저자명	Index Term	문헌이 색인된 용어 (통제어)
CAS Registry Number	CAS(SciFinder DB)에 등록된 물질 번호	CA Concept Heading	문헌이 색인된 주제어
CA Section Title	CAS에서 분류된 문헌의 주제분야	Journal Name	문헌(논문)이 수록된 학술지명
Company-Organization	문헌과 관련된 기업/조직	Language	문헌의 언어
Database	문헌이 색인된 DB CASPLUS: 화학/ MEDLINE: 의학	Publication Year	문헌의 출판년도
Document Type	문헌의 유형 (Patent, Journal Article 등)	Supplementary Terms	문헌의 주제를 나타낸 용어로 주로 저자가 사용한 용어

The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', 'SciPlanner', 'Save', and 'Print'. A yellow banner indicates '441 references with the CAS Registry Numbers 7440-22-4 are displayed' with 'Keep Analysis' and 'Clear Analysis' buttons. Below this, the search results are displayed for 'antibacterial with coatings fo...' (1781). The 'REFERENCES' section is active, and the 'Analyze' menu is open, showing various filter options like 'CAS Registry Number', 'Author Name', etc. The 'Show More' button at the bottom of the menu is highlighted. The search results list includes items like '5. Heat-insulating sock with sterilization and deodorization functions' and '7. Manufacture method of hydrophilic and antibacterial ultrafiltration membrane'.

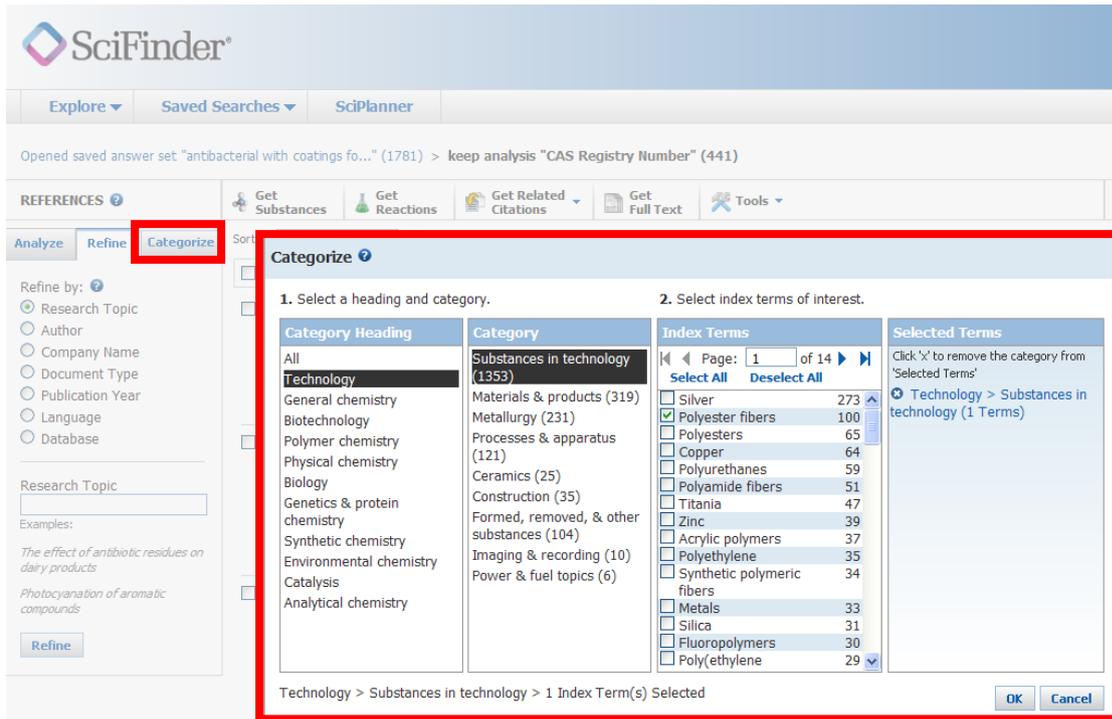
※ 검색 결과가 20,000건 이상일 경우에는 필터링이 불가함.

※ 두 개 이상의 옵션으로 필터링 하고자 할 경우? 'Show More' 메뉴 이용

※ 필터링 결과를 저장/삭제하고자 할 경우: 상단 'Keep Analysis'/'Clear Analysis' > Save 메뉴 이용 ('Saved Answer Sets'에서 확인 가능)

④ 주제 분야로 검색 결과 한정하기: Categorize

'Categorize' 메뉴를 이용하면 검색 결과 중 원하는 주제 분야의 자료만 추출하여 볼 수 있습니다.



(3) Refine reference answers: 검색 결과 축소하기

Analyze 방법 외에도 검색 결과를 축소하고 싶다면 'Refine' 기능으로 결과 내 검색을 할 수 있습니다.

Refine 옵션: Research Topic, Author, Company Name, Document Type, Publication Year 등



※ Analyze / Refine 결과 저장: 우측 상단 'Save' 메뉴 이용 ('Saved Answer Sets'에서 확인 가능)

※ 검색 결과 조합: 'Tools' > 'Combine Answer Sets'

또는 'Saved Searches' > 'Saved Answer Sets' > 'Combine Answer Sets'

(4) Get data related to references: 문헌 관련 자료

검색결과에서 자료의 물질 정보, 반응 정보, 인용/피인용 문헌 목록, 원문 등을 획득할 수 있습니다. 이 기능은 문헌 검색 외에 물질 검색 또는 반응 검색 결과에서도 동일하게 적용 가능한 기능입니다.

The screenshot shows the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', and 'Export'. Below this, a message indicates an opened saved answer set: "antibacterial with coatings fo..." (1781) > citing references (350). The main area is titled 'REFERENCES' and features a toolbar with buttons for 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', and 'Tools'. A red box highlights these four buttons. Below the toolbar, there are options for 'Analyze by:' (Document Type) and 'Sort by:' (Accession Number). A list of references is shown, with the first one selected: '1. The preparation and antibacterial activity of polyester fabric loaded with silver nanoparticles'. The abstract of this reference is visible on the right side of the page.

Full-text 이용

SciFinder는 문헌의 정보를 수록하고 있는 데이터베이스로, 원문(Full-text)는 제공하지 않고 원문에 접근할 수 있는 링크만 제공합니다. 원문을 이용하기 위해서는 제시된 링크를 통해 문헌의 사이트로 이동해야 합니다. 해당 사이트에서 원문이 보이지 않을 경우 (PDF파일 다운로드가 안 될 경우) 우리 도서관에서 이용 불가능한 자료로, 원문복사 서비스(Document Delivery Service)로 이용할 수 있습니다.

(5) Save and share references: 문헌 검색 결과 저장, 공유, 반출하기

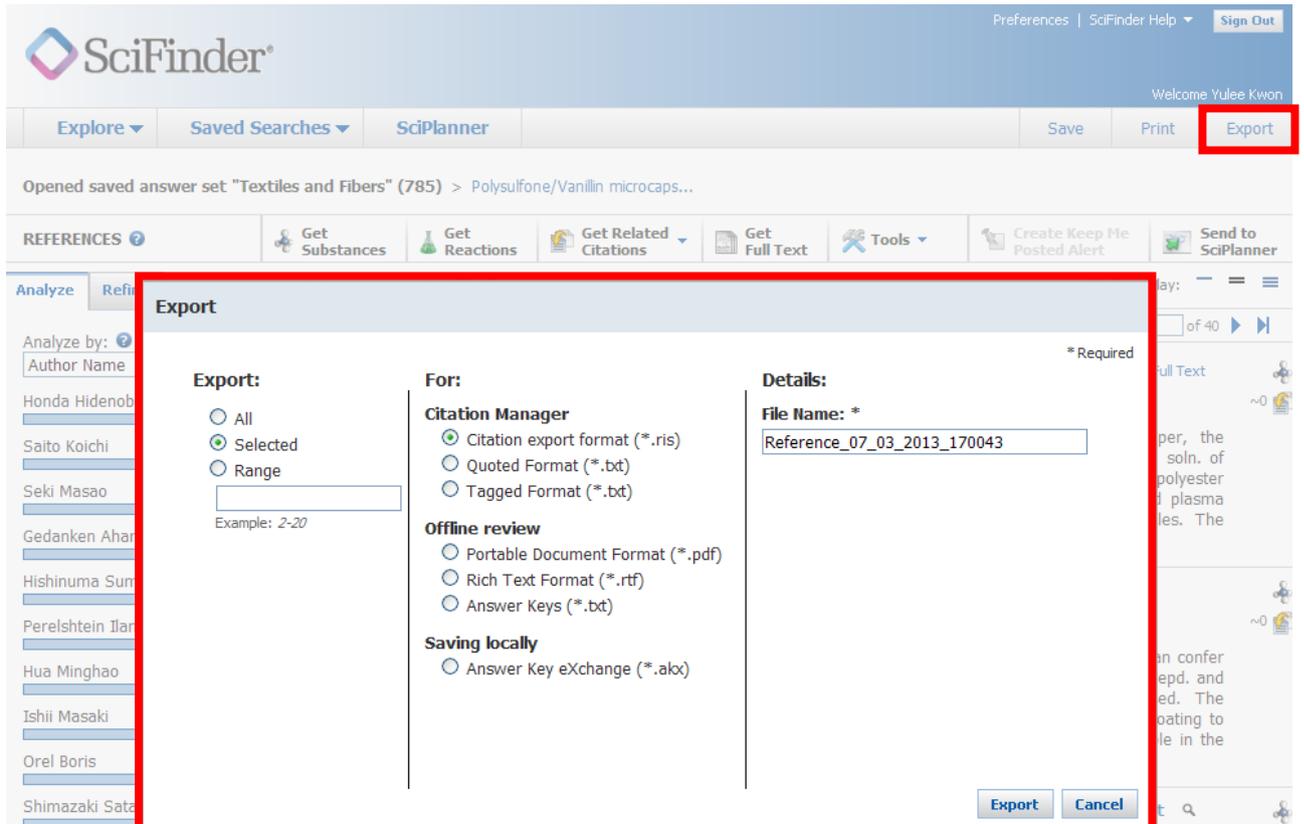
① Save the current answer set: 화면 상단 'Save' 메뉴를 활용하면 현재 검색 결과를 저장 할 수 있습니다.

The screenshot shows the SciFinder web interface with the 'Save' button in the top navigation bar highlighted in a red box. Below the navigation bar, a message indicates an opened saved answer set: "antibacterial with coatings fo..." (1781) > The preparation and antibacter... The main area is titled 'REFERENCES' and features a toolbar with buttons for 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', and 'Tools'. Below the toolbar, there are options for 'Analyze by:' (Document Type) and 'Sort by:' (Accession Number). A list of references is shown, with the first one selected. A dialog box titled 'Save This Answer Set' is open in the foreground, allowing the user to save the current search results. The dialog box has a 'Save:' section with two radio buttons: 'All answers' and 'Only selected answers'. There is also a 'Title:' field and a 'Description:' field. The 'OK' and 'Cancel' buttons are at the bottom of the dialog box.

- ② **Link:** 문의 상세 페이지 'Link' 메뉴로 현재 페이지 정보(URL)를 공동 연구자에게 전달 할 수 있습니다



- ③ **Export:** 문헌의 정보를 서지관리 프로그램 EndNote로 저장하거나, PDF 파일 등으로 저장할 수 있습니다.



※ 검색결과를 SciFinder가 아닌 개인 컴퓨터에 저장하기: 'Saving locally' - 'Answer Key eXchange' 이용
저장한 검색 결과 파일 열기: 메인화면 > 'Saved answer Sets' > 'Import'

④ Send to SciPlanner

'SciPlanner'란 SciFinder의 검색 결과(문헌 리스트, 물질 정보, 반응식)를 시각적으로 자유롭게 정리할 수 있는 작업 공간입니다. SciPlanner에서 정리한 자료들은 저장하고 다른 연구자들과 공유할 수 있습니다.

The screenshot shows the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' (highlighted with a red box). Below this, a message indicates 'Opened saved answer set "Textiles and Fibers" (785)'. A toolbar contains several action buttons: 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner' (highlighted with a red box). On the left, there is an 'Analyze' sidebar with a table of author names and counts:

Author Name	Count
Honda Hidenobu	9
Saito Koichi	8
Seki Masao	8
Gedanken Aharon	7

The main content area displays a list of references. The first reference is selected and expanded, showing the title '1. The preparation and antibacterial activity of polyester fabric loaded with silver nanoparticles' and a brief abstract.

The screenshot shows the SciPlanner workspace interface. The title bar reads 'SciPlanner_06_26_2013_111136'. The workspace contains a chemical reaction scheme. The reactant is a naphthalene derivative with a methoxy group (MeO) and a hydroxymethyl group (CH₂-OH). The reaction is labeled with '1' and shows the formation of a silver nanoparticle (represented by a yellow and red cluster) on the surface of the naphthalene ring. The product is the same naphthalene derivative with the silver nanoparticle attached to the hydroxyl group. On the right side, there is a 'Clear Reactions' button and a list of reaction schemes.

※ 작성한 SciPlanner PDF 파일로 저장하기: 'Workspace' > 'Export'

(6) Comment and tag references for future use: 나만의 용어로 문헌 찾기

① 문헌에 나만의 코멘트 / 태그 입력하기

검색으로 찾은 문헌에 나만의 메모를 기록하고 싶다면 문헌의 상세 페이지 하단에 있는 'Add Comment' 기능을 이용하면 됩니다. 그리고 문헌에 기억하기 쉬운 용어로 태그를 입력 해 두면 나중에 내가 입력한 메모와 필요한 문헌을 쉽게 찾을 수 있습니다.

The screenshot shows the SciFinder interface for a reference titled "1. The preparation and antibacterial activity of polyester fabric loaded with silver nanoparticles". The page includes a navigation bar with "Explore", "Saved Searches", "SciPlanner", and "Link". Below the title, there are buttons for "Get Related Citations" and "Get Full Text". A red box highlights the "Add Comment" section, which contains a text input field and a "0 Tags | Edit Tags" link. The comment box is currently empty and has a maximum character limit of 1024 characters per comment and 50 comments per reference.

② 나만의 태그로 문헌 찾기

SciFinder 검색 메뉴 중 'References > Tag'로 이동하면 자신이 입력한 태그 별로 문헌을 볼 수 있습니다.

The screenshot shows the SciFinder interface for the "References > Tag" view. The page title is "Explore Tag 'textiles' > references (1)". The left sidebar shows a list of search criteria, with "Tags" highlighted in red. The main content area shows a "REFERENCES: TAGS" section with a red box around it. The text inside the box says "Click a tag to retrieve references associated with that tag." and lists the tag "textiles" with a small 'T' icon next to it.

Reference Detail: 문헌 검색 결과 상세 페이지

*상세 페이지에서 확인할 수 있는 정보

- ① 문헌의 초록 전문
- ② 문헌의 서지 정보 (수록된 학술지 정보, 출판년도 등 - **Source**)
- ③ 문헌과 관련된 특허정보 (특허 자료일 경우 - **Patent information**)
- ④ 문헌이 색인된 section 정보 (**Indexing** - CA Section)
- ⑤ 문헌의 일반적인 주제 분야 (**Concepts**)
- ⑥ 문헌의 내용을 표현하는 비 통제된 저자가 부여한 키워드 (**Supplementary terms**)
- ⑦ 문헌에 포함된 물질정보 (**Substances**)
- ⑧ 문헌에 인용된 자료 목록 (**Citations**)


Preferences | SciFinder Help | Sign Out

Explore ▾
Saved Searches ▾
SciPlanner
Link
Save
Print
Export

Opened saved answer set "antibacterial with coatings fo..." (1781) > **Nanosilver: A nanoparticle in m...**

REFERENCE DETAIL ⓘ
Get Substances
Get Related Citations
Get Full Text
Send to SciPlanner

Return
Previous | Next

1. Nanosilver: A nanoparticle in medical application

By: Chen, X.; Schluessener, H. J.

A review. Nanotechnol. is a most promising field for generating new applications in medicine. However, only few nanoproducts are currently in use for medical purposes. A most prominent nanoproduct is nanosilver. Nanosilver particles are generally smaller than 100 nm and contain 20-15,000 silver atoms. At nanoscale, silver exhibits remarkably unusual phys., chem. and biol. properties. Due to its strong antibacterial activity, nanosilver coatings are used on various textiles but as well as coatings on certain implants. Further, nanosilver is used for treatment of wounds and burns or as a contraceptive and marketed as a water disinfectant and room spray. Thus, use of nanosilver is becoming more and more widespread in medicine and related applications and due to increasing exposure toxicol. and environmental issues need to be raised. In sharp contrast to the attention paid to new applications of nanosilver, few studies provide only scant insights into the interaction of nanosilver particle with the human body after entering via different portals. Biodistribution, organ accumulation, degradn., possible adverse effects and toxicity are only slowly recognized and this review is focusing on major questions assocd. with the increased medical use of nanosilver and related nanomaterials.

Indexing

Pharmaceuticals (Section63-0)

Section cross-reference(s): 48

Concepts

Biocompatibility Human
Nanoparticles Pharmacokinetics

nanoproduct in medical application

Substances

7440-22-4 Silver, biological studies 🔍

nanoproduct in medical application

Adverse effect, including toxicity; Pharmacokinetics; Therapeutic use; Biological study; Uses

Supplementary Terms

review silver nanoparticle toxicity pharmacokinetics

Citations

Ahn, M; Respir Res 2005, 13, 34
 Alfaro-Moreno, E; Curr Opin Pulm Med 2007, 13, 98
 Alimonti, M; J Biochem 2003, 134, 43 🔍
 Andre, N; Science 2005, 6, 804

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Toxicology Letters
 Volume176
 Issue1
 Pages1-12
 Journal; General Review
 2008
 CODEN:TOLED5
 ISSN:0378-4274
 DOI:10.1016/j.toxlet.2007.10.00

COMPANY/ORGANIZATION

Institute of Brain Research
 University of Tuebingen
 Tuebingen, Germany D-72076

ACCESSION NUMBER

2007:1443074
 CAN148:151576
 CAPLUS

PUBLISHER

Elsevier B.V.

LANGUAGE

English

Tip for future references! Keep Me Posted (KMP) Alerts

관심 있는 키워드 또는 분야에서 새롭게 발표되는 문헌들의 정보를 자동으로 안내 받고 싶다면, 'Keep Me Posted(KMP) Alert' 기능을 이용하면 됩니다. 이 기능을 설정 해 놓으면 SciFinder 에서 별도의 검색 없이 최신 연구 결과를 확인하거나 e-Mail 로 문헌 정보를 확인 할 수 있습니다.

(1) Keep Me Posted (KMP) Alerts 설정하기

- ① SciFinder 에서 문헌 검색 결과 화면에서 'Create Keep Me Posted Alert' 메뉴 선택

The screenshot shows the SciFinder search results page for the topic "effect of plant flavonoids on ...". The interface includes a top navigation bar with "SciFinder" logo, "Preferences", "SciFinder Help", and "Sign Out". Below the navigation bar are tabs for "Explore", "Saved Searches", and "SciPlanner", along with "Save", "Print", and "Export" buttons. A yellow warning banner indicates "26 duplicates were automatically removed." The main content area shows the search topic and "references (91)". A toolbar contains buttons for "Get Substances", "Get Reactions", "Get Related Citations", "Get Full Text", "Tools", and "Create Keep Me Posted Alert" (highlighted in red). There is also a "Send to SciPlanner" button. Below the toolbar, there are options to "Analyze", "Refine", and "Categorize" results, with a "Sort by: Accession Number" dropdown and "Answers per Page [20]" and "Display:" settings. A list of references is shown, with the first one selected: "1. Doxorubicin cardiotoxicity and cardiac function improvement after stem cell therapy diagnosed by strain echocardiography".

- ② Alert 서비스의 제목, 발송 주기(week/month) 선택 후 생성

The screenshot shows the "Create Keep Me Posted Profile" form. It includes a warning banner: "Some steps cannot be included in this profile." The form has several sections: "Title: *" (required), "Description:" (with a character count of 1024 remaining), "Duration" (Expires On: Jul 03, 2014, with a "Change" link), and "Frequency" (Send updates once every "Week", with an option to "Exclude previously retrieved references."). A "Search:" section shows the current search topic: "effect of plant flavonoids on heart disease" and the "Candidates Selected:" criteria: "References which contain the two concepts 'plant flavonoids' and 'heart disease' anywhere in the reference". "Create" and "Cancel" buttons are at the bottom.

- ③ 'Keep Me Posted Alert' e-Mail 로 받기 설정: 'Preferences' 메뉴에서 설정

The screenshot shows the "Preferences" page in SciFinder. The "Keep Me Posted Notification" section is highlighted in a red box. It contains a checked checkbox for "Receive e-mail notification of Keep Me Posted results" and a note: "Please ensure that CAS has your current e-mail address. Visit myCAS to add or change your address."

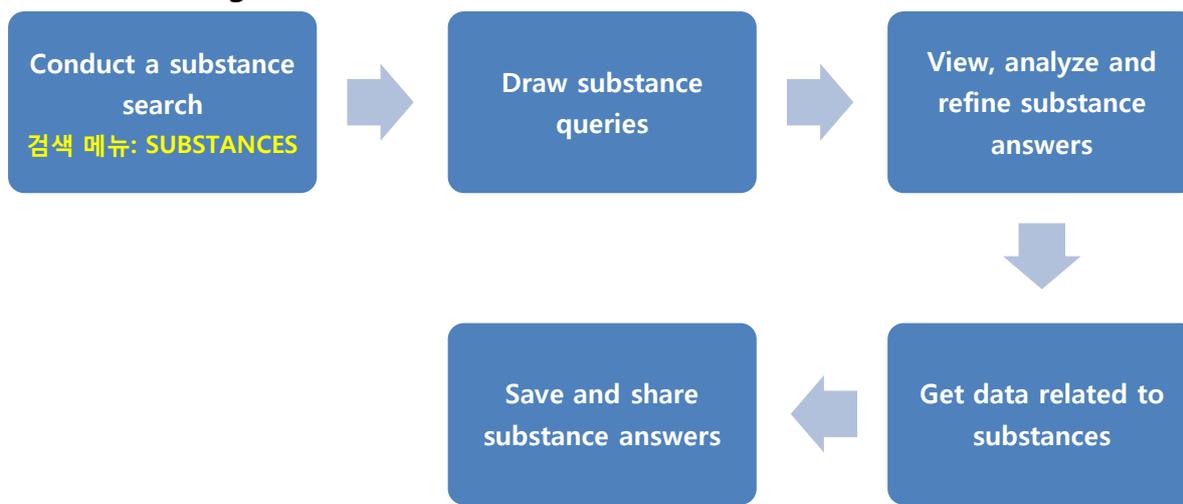
- (2) Keep Me Posted Alerts 내역 보기: 메인 화면 또는 'Saved Searches' 내 'Keep Me Posted' 메뉴에서 확인

Substance Searching: 화학 물질 정보 검색 (from CA Registry)

Tutorial: Introduction to Substance Searching ([Click](#))

- Search by substance identifier
- Search using a structure query
- View, analyze, and refine your research results
- Retrieve commercial sources
- Save an answer set
- Create a Keep Me Posted alert

Workflow for working with substances



(1) Conduct a substance search: 원하는 검색 옵션으로 검색

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Yulee Kwon

Explore | Saved Searches | SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Import CXF

Search

Advanced Search

SAVED ANSWER SETS

Textiles and Fibers

antibacterial with coatings for textiles

View All | Import

KEEP ME POSTED

plant flavonoids

No results

View All

Option	Note						
<p>Chemical Structure</p>	<p>물질의 화학 구조식을 그려서 해당 구조식이 포함된 문헌을 검색 <u>Exact Structure, Substructure, Similarity</u> 옵션으로 검색 가능</p> <p>*검색 제한자</p> <table border="1" data-bbox="395 427 1497 613"> <thead> <tr> <th data-bbox="395 427 628 472">Characteristics</th> <td data-bbox="628 427 1497 472">Single component, Commercially available, Included in references</td> </tr> <tr> <th data-bbox="395 472 628 566">Classes</th> <td data-bbox="628 472 1497 566">Alloys, Coordination compounds, Incompletely defined, Mixtures, Polymers, Organic and others</td> </tr> <tr> <th data-bbox="395 566 628 613">Studies</th> <td data-bbox="628 566 1497 613">Analytical, Biological, Preparation, Reactant or reagent</td> </tr> </thead> </table>	Characteristics	Single component, Commercially available, Included in references	Classes	Alloys, Coordination compounds, Incompletely defined, Mixtures, Polymers, Organic and others	Studies	Analytical, Biological, Preparation, Reactant or reagent
Characteristics	Single component, Commercially available, Included in references						
Classes	Alloys, Coordination compounds, Incompletely defined, Mixtures, Polymers, Organic and others						
Studies	Analytical, Biological, Preparation, Reactant or reagent						
<p>Markush</p>	<p>Markush structure가 포함된 특허 문헌 검색</p>						
<p>Molecular Formula</p>	<p>분자식을 입력하여 검색</p> <p><TIPS for entering molecular formula queries></p> <ul style="list-style-type: none"> ■ To avoid ambiguity: <ul style="list-style-type: none"> ➢ Capitalize only the first character of a multiple-character symbol, as in Ca, Fe ➢ Include a space between an element symbol/count and the next element symbol, as in C21 H26 N2 S2 ■ It is not necessary to specify an element count of 1, as in C O2 ■ In a multi-component formula: <ul style="list-style-type: none"> ➢ Use a period surrounded by spaces to separate components, as in C4 H11 N O3 . C2 H4 O2 ➢ Use parentheses to nest component formulas, as in (C15 H10 N2 O2 . C6 H14 O3 . 3(C3 H6 O . C2 H4 O)x)x ➢ Use parentheses to enclose a portion of formula representing a structural repeating unit, and follow it with a numeric repetition n, as in (C2 H3)n C14 H13 N4 O2 ■ A component formula can be preceded with: <ul style="list-style-type: none"> ➢ an integer coefficient, as in C2 H4 O2 . 3 H2 O . Na ➢ a fractional coefficient, as in C2 H4 O2 . 1/2 Ca ➢ the unknown coefficient x, as in (C8 H8 O3 S)x . (C8 H8 O3 S)x . x H3 N . x K ■ A monomer-based polymer formula can be: <ul style="list-style-type: none"> ➢ a single-component homopolymer enclosed by parentheses and followed by either a numeric repetition or x, as in (C2 H3)x ➢ a multi-component formula enclosed by parentheses and followed by either a numeric repetition or x, as in (C2 H4 . C Br F3)x 						

Property

물질의 물리적 성질값을 이용한 물질 검색

*검색 옵션

Experimental property definitions (Click)	Predicted property definitions (Click)
<ul style="list-style-type: none"> ➤ Boiling point ➤ Density ➤ Electrical Conductance ➤ Electric Conductivity ➤ Electric Resistance ➤ Electric Resistivity ➤ Glass Transition Temperature ➤ IR (Infrared) Spectra ➤ Magnetic Moment ➤ Mass Spectra ➤ Median Lethal Dose (LD50) ➤ Melting Point ➤ NMR Spectra ➤ Optical Rotatory Power ➤ Raman Spectra ➤ Refractive Index ➤ Tensile Strength 	<ul style="list-style-type: none"> ➤ Bioconcentration Factor ➤ Boiling point ➤ Density ➤ Enthalpy of Vaporization ➤ Flash Point ➤ Freely Rotatable Bonds ➤ Hydrogen acceptors ➤ Hydrogen donors ➤ Hydrogen donors/acceptors sum ➤ Koc (Organic Carbon Adsorption Coefficient) ➤ logD ➤ Mass Intrinsic Solubility ➤ Mass Solubility ➤ Molar Intrinsic Solubility ➤ Molar Volume ➤ Molecular Weight ➤ NMR Spectra ➤ pKa ➤ Polar Surface Area ➤ Vapor Pressure

*아래 성질들은 정해진 소수점 자리로 반올림되어 검색됨.

Boiling Point: 1	Density: 3	Enthalpy of Vaporization: 2
Flash Point: 1	logD: 2	logP: 3
Molar Volume: 1	Molecular Weight: 2	pKa: 2

Substance Identifier

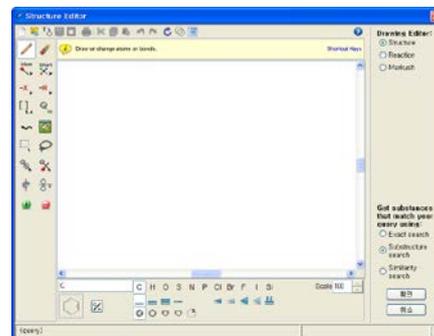
물질에 부여된 고유 인식어로 검색

* 검색 가능 항목: CAS Registry Number, Chemical name, simple chemical names, Trade names, Abbreviations, Common names.

(2) Draw substance queries: 구조식 그리기

Introduction to the SciFinder Drawing Editor ([Click](#))

- Draw structures using a variety of tools
- Use templates and keyboard shortcuts to speed drawing
- Draw a simple reaction query



(3) View, analyze and refine substance answers: 물질 검색 결과 중 원하는 자료 찾기

① 목적에 맞게 검색 결과 정렬하기: Sort by

검색 결과 화면에서 정렬 옵션을 활용하면 목적에 알맞은 자료를 더욱 쉽게 찾을 수 있습니다.

정렬 옵션 (기본: 검색의 정확도 – Relevance 내림차순)

Relevance	검색 결과의 정확도를 기준으로 정렬
CAS Registry Number	CAS (SciFinder 데이터베이스)에 등록된 물질의 고유 번호를 기준으로 정렬
Number of References	검색된 물질과 관련된 문헌의 수로 정렬
Molecular Weight	예상되는 분자의 무게에 따라 정렬 (Predicted molecular weight value)
Molecular Formula	엘리먼트 개수에 따라 정렬 (Element count)

Chemical Structure exact > substances (350)

Sort by: Relevance

- Relevance
- CAS Registry Number
- Number of References
- Molecular Weight
- Molecular Formula

1. Substance Detail
74-11-3
~5580

2. Substance Detail
3686-66-6
(Component: 74-11-3)
~169

3. Substance Detail
4641-33-2
~183

② 검색 결과 필터링하여 보기: Analyze

원하는 정보 유형에 따라 검색 결과를 필터링하여 볼 수 있습니다. 검색 결과가 많을 때 문헌 수를 줄일 수 있는 좋은 방법입니다.

필터링 옵션

Bioactivity Indicators	사전 정의된 약 260가지의 보드를 참고하고 대생물 작용 조건으로 결과를 축소 CAS Registry의 물질 정보와 CA Plus에 수록된 문헌정보 간에 연결된 refers to a predefined set of approximately 260 broad and narrow bioactivity terms for which relationships have been identified between CAS REGISTRY substances and CAplus documents
Commercial Availability	상업적으로 구입 가능한 물질 정보
Elements	물질에 표현된 화학 성분
Reaction Availability	반응식이 있는 물질 정보
Substance Role	문헌 속에 표현된 물질의 역할 정보 (예: Adverse Effect, Biological Study, Preparation)
Target Indicators	protein, enzyme, 그 외 target 용어 refers to a predefined set of approximately 5800 protein, enzyme, and other target terms for which relationships have been identified between CAS REGISTRY substances and CAplus documents

The screenshot shows the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, the search path is 'Chemical Structure exact > substances (350)'. The main content area is titled 'SUBSTANCES' and includes buttons for 'Get References', 'Get Reactions', 'Get Commercial Sources', and 'Tools'. A 'Sort by: Relevance' dropdown is visible. On the left, a red box highlights the 'Analyze' filter menu, which lists options: 'Substance Role', 'Bioactivity Indicators', 'Commercial Availability', 'Elements', 'Reaction Availability', 'Substance Role', and 'Target Indicators'. Below the menu, a 'Reactant or Reagent' filter is set to '64'. The search results show two entries: '1. Substance Detail 74-11-3' with ~5580 results and '2. Substance Detail 3686-66-6 (Component: 74-11-3)' with ~169 results. Both entries include chemical structures of 4-chlorobenzoic acid.

③ 검색 결과 축소하기: Refine

Analyze 방법 외에도 검색 결과를 축소하고 싶다면 'Refine' 기능으로 결과 내 검색을 할 수 있습니다.

Opened saved answer set "substance searching" (350)

Substances: 0 of 350 Substances Selected

Sort by: Relevance

Answers per Page [15] View: [Icons]

Page: 1 of 24

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

1. Substance Detail 74-11-3 (~5582)

2. Substance Detail 3686-66-6 (Component: 74-11-3) (~169)

3. Substance Detail 4641-33-2 (~183)

Refine 옵션

Chemical Structure	검색한 화학 구조식을 수정하여 재 검색
Isotope-Containing	동위 원소 (isotope)가 포함된 물질을 함께 검색 할 지 여부 선택
Metal-Containing	금속이 포함된 물질을 함께 검색 할 지 여부 선택
Commercial Availability	상업적으로 구입 가능하거나 불가능한 물질 여부 선택
Property Availability	Any property / Any predicted property / Any experimental property / Any selected experimental property 중에서 선택하여 검색 결과 제한
Property Value	Experimental / Predicted property 중 원하는 성질 값을 입력하여 재 검색 상세 내용: Refine by property value (Click)
Reference Availability	관련 문헌이 있는 검색 결과로 제한
Atom Attachment	물질 구조식에서 원하는 위치에 다른 원자를 붙였을 때 어떠한 검색 결과가 나오는지 확인 가능 (상세 내용: Refine by atom attachment, Click)

Refine by Atom Attachment

1. Click an atom to display the attachments present at that site. 2. Select attachment(s) of interest.

Substructure

Atom Attachments

Select All Deselect All

- H or None 5
- C 1986
- S 10
- Other 4
- A - Any (not H) 1996
- Cb - Carbocycle 1955
- Hy - Heterocycle 21
- Q - Any (not C,H) 10
- Ak - Alkyl chain 6

? = S,Hy

Refine Cancel

(4) Get data related to substance: 물질과 관련된 추가 정보 얻기

검색결과에서 물질과 관련된 문헌정보, 반응 정보, 물질 구입 정보, 규제 정보를 얻을 수 있습니다.

The screenshot shows the SciFinder interface with the following elements:

- Header: SciFinder logo, Preferences, SciFinder Help, Sign Out, Welcome Yulee Kwon.
- Navigation: Explore, Saved Searches, SciPlanner, Save, Print, Export.
- Search Results: Opened saved answer set "substance searching" (350).
- Substances Section:
 - Buttons: Get References, Get Reactions, Get Commercial Sources (highlighted in red), Tools.
 - Sort by: Relevance.
 - Answers per Page: [15]. View: [Grid/Text/Map].
 - 0 of 350 Substances Selected.
 - Three Substance Detail cards:
 - 1. Substance Detail 74-11-3: Benzoic acid, 4-chloro- (C₇H₅ClO₂). ~558 references. Includes a red box around the 'Get Commercial Sources' icon.
 - 2. Substance Detail 3686-66-6 (Component: 74-11-3): Benzoic acid, 4-chloro-, sodium salt (1:1) (C₇H₅ClO₂ · Na). ~169 references.
 - 3. Substance Detail 4641-33-2: Benzoic acid, 4-chloro-, ion(1-) (C₇H₄ClO₂). ~183 references.
- Analyze/Refine sidebar:
 - Analyze by: Substance Role.
 - Preparation: 234
 - Properties: 154
 - Uses: 87
 - Reactant or Reagent: 64
 - Process: 52
 - Biological Study: 47
 - Analytical Study: 16
 - Formation, Nonpreparative: 13

Tip for commercial sources

실험에 활용할 물질을 구입하고 싶다면, SciFinder 검색 결과에서 'Get Commercial Sources' 메뉴를 클릭하면 해당 물질의 구입처와 가격 등을 알 수 있습니다.

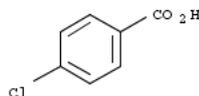
1. 3B Scientific Corporation Product List

Catalog Information

Catalog Publication Date: 12 Jul 2012
 Order Number: 383-035854
 Purity: 98%
 Quantity: 5,000g, Price: \$500

Substance Information

CAS Registry Number: 74-11-3
 CAS Index Name: Benzoic acid, 4-chloro-
 Chemical Name: 4-Chlorobenzoic acid



Catalog Suppliers

Below are the contributing supplier(s) to this catalog.

Supplier Name	Address	Contact Information	Status
3B Scientific Corporation	1840 Industrial Drive, Suite 160 Libertyville, IL 60048 USA	Phone: 847-281-9822 Fax: 847-281-9855 Email: sales@3bsc.com Web: http://www.3bsc.com	Unclassified

(5) Save and share substance answers: 검색 결과 물질 정보 저장 및 공유하기

- ① 추 후 검색 결과를 활용하기 위하여 SciFinder 내에 나의 검색 결과를 저장하기 (Save 메뉴)
 - ② 서지 관리 프로그램인 EndNote로 반출하고 PDF 파일로 저장하기 (Export 메뉴)
 - ③ 검색 결과를 인쇄 (Print 메뉴)하고 시각적인 작업 공간인 SciPlanner로 보내기
- ※ 간략한 이용 방법은 'Reference Searching'에 소개된 내용을 참고하시기 바랍니다.

Substance Detail: 물질 검색 결과 상세 페이지

*상세 페이지에서 확인할 수 있는 정보

- ① 물질에 대한 기본 정보 (CAS Registry Number, molecular formula, chemical names, chemical structure)
- ② 물질과 관련된 문헌 정보와 문헌에 나타난 해당 물질의 역할 (References, CAS Role)
- ③ Bioactivity Indicators
- ④ Target Indicators
- ⑤ Predicted Properties: Biological, Chemical, Density, Lipinski and Related, Spectra, Structure-related, Thermal properties
- ⑥ Experimental Properties: Biological, Chemical, Density, Flow and Diffusion, Interface, Lipinski and Related, Optical and Scattering, Spectra, Structure-related, Thermal properties

Preferences | SciFinder Help ▾ [Sign Out](#)
Welcome Yulee Kwon

Explore ▾
Saved Searches ▾
SciPlanner
Link
Save
Print
Export

Opened saved answer set "substance searching" (350) > 74-11-3

SUBSTANCE DETAIL ⓘ

Get References
 Get Reactions
 Get Commercial Sources
 Get Regulatory Information

Send to SciPlanner

Return
◀ Previous | Next ▶

1.

CAS Registry Number: 74-11-3

C₇ H₅ Cl O₂

Benzoic acid, 4-chloro-

Benzoic acid, p-chloro- (7CI,8CI); 4-CBA; 4-Chlorobenzoic acid; Mycosid; NSC 143358; NSC 32738; NSC 8444; p-Carboxychlorobenzene; p-Chlorbenzoic acid; p-Chlorobenzoic acid

Source of Registration: CA

~5,587 References

Document Types: Conference, Dissertation, Journal, Patent, Preprint, Report

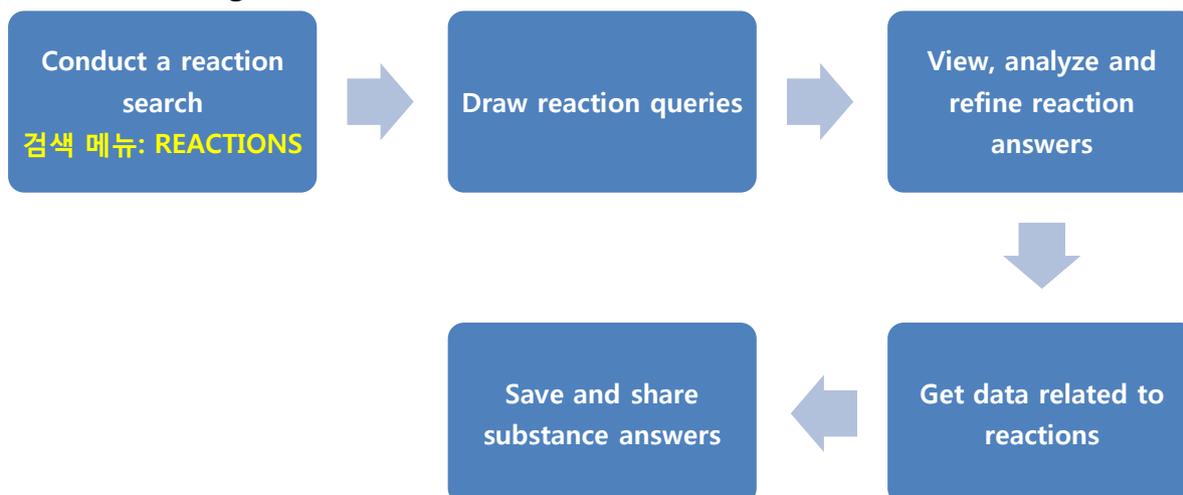
CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓		✓
Biological Study	✓	✓	✓	✓
Combinatorial Study	✓	✓		
Formation, Nonpreparative	✓	✓		✓
Miscellaneous	✓	✓		
Occurrence	✓	✓		
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			

Reaction Searching: 화학 반응식을 통한 자료 검색 (from CA React)

Tutorials

Title	Contents	Link
Introduction to Reaction Searching	<ul style="list-style-type: none">➤ Search by reaction structure➤ Group reactions by transformation and by document➤ Sort, analyze, and refine the reaction answer set➤ View Experimental procedures➤ Get commercial sources for a reaction participant➤ Save a reaction answer set	Click
Introduction to the SciFinder Drawing Editor	<ul style="list-style-type: none">➤ Draw structures using a variety of tools➤ Use templates and keyboard shortcuts to speed drawing➤ Draw a simple reaction query	Click
Draw Reactions	<ul style="list-style-type: none">➤ Draw reactions by assigning reaction roles to structures➤ Increase precision by specifying the bonds that change during the reaction (reaction sites) or by mapping the atoms between reactants and products➤ Use functional groups to represent classes of compounds involved in the reaction	Click
Plan a Synthesis Project	<ul style="list-style-type: none">➤ Send substances, reactions, and references to SciPlanner➤ Initiate searches from within SciPlanner➤ Merge reactions into a synthetic plan➤ Display reaction information➤ Export and import a SciPlanner project	Click

Workflow for working with substances



(1) Conduct a reaction search: 검색 옵션 선택

SciFinder®

Explore | Saved Searches | SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REACTIONS: REACTION STRUCTURE

Click to Edit

Search Type:

- Allow variability only as specified
- Substructure

Import CXF

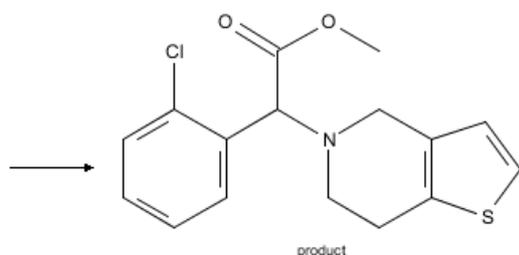
Search

Advanced Search | Always Show

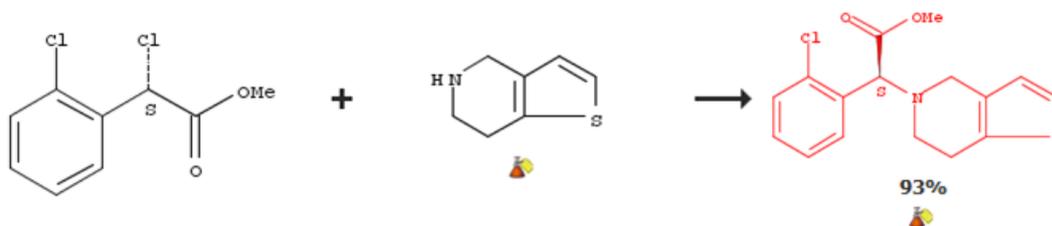
- 반응 구조식으로 검색: 반응물질(reactants), 시약(reagents), 화학물질의 구조식과 매치되는 반응 검색
- 검색 결과 제한: Solvents, Non-participating Functional Groups, Number of Steps, Classifications, Sources, Publication Years
- 검색 옵션

Variable only at the specified positions:	Substances must match the structure query exactly, except where variability is specifically defined through the use of query features such as variable atom types (e.g., X = any halogen) or R-groups.
Substructures of more complex structures	Substances include the structure query embedded within a more complex structure, with substitution allowed at all locations except where specifically blocked by query features such as Lock Atom

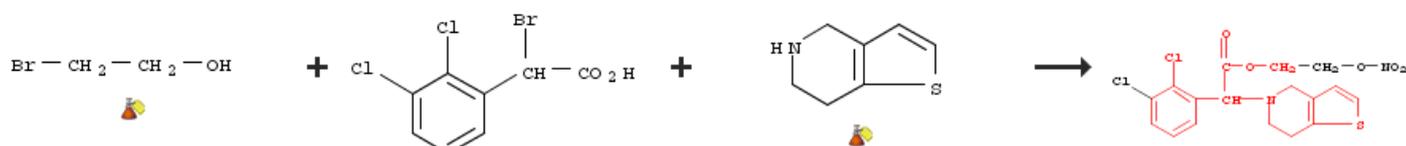
Example reaction query



Variable only at the specified positions result



Substructures of more complex structures result



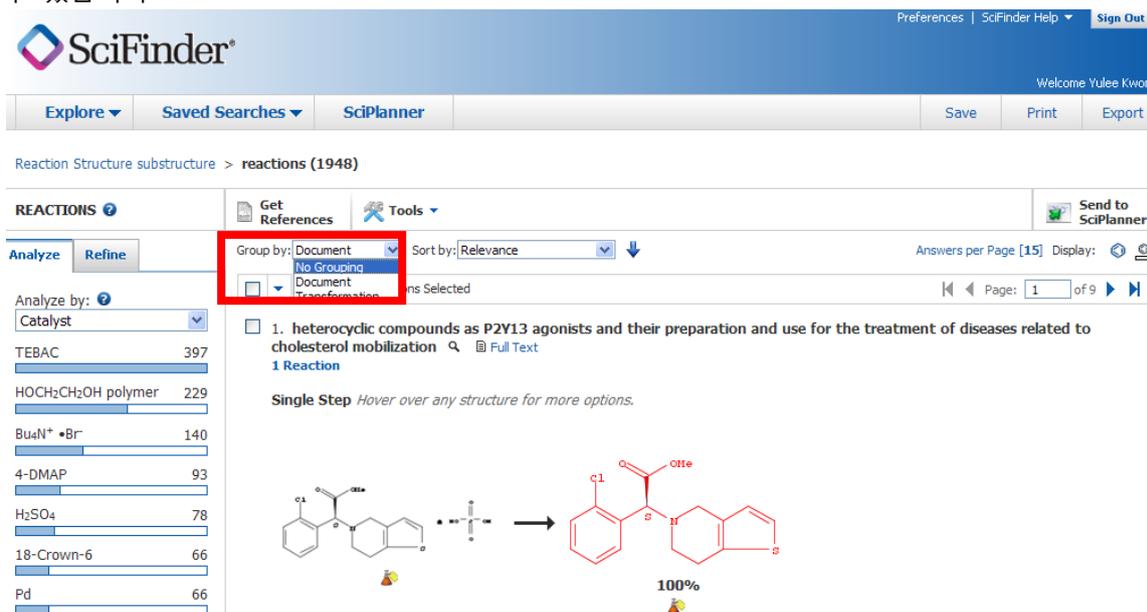
(2) Draw reaction queries: Reaction query tool을 활용하여 화학 반응식 그리기

How to	Note
Draw a reaction query 	물질의 화학 구조식을 그린 후 반응 물질을 Reaction arrow tool  로 표시하여 검색식을 생성. 검색식 생성 시 'product, reactant, reagent, reactant/reagent, any role' 등 각각의 반응 역할을 지정할 수 있음. Draw the substances and then indicate reactants and products by drawing the reaction arrow  . Alternatively, you can individually assign reaction roles (product, reactant, reagent, reactant/reagent, any role) to each substance
Specify reaction roles 	Reaction Role Tool  을 이용하여 역할을 지정하거나 수정 가능 Use the Reaction Role Tool  to assign or change the role of a substance.
Map atom pairs 	반응물질 또는 결과물에 나타난 특정한 원자의 쌍을 지정하여 검색 You can focus the reaction search by specifying corresponding pairs of atoms present in the reactant and product.
Mark reaction sites 	반응 지점을 표시하여 검색 You can focus the reaction search by marking bonds that are changed (broken, formed, or change bond order) in the reaction.
Specify a substance by functional group 	특정 구조를 그리는 대신 functional group을 활용하여 반응물질, 시약 또는 결과물 등을 대신할 수 있음. Instead of drawing a specific structure, you can represent a reactant, reagent, or product by its functional group (e.g., Acyclic Ketone).

(3) View, analyze and refine reaction answers: 반응 검색 결과 중 원하는 자료 찾기

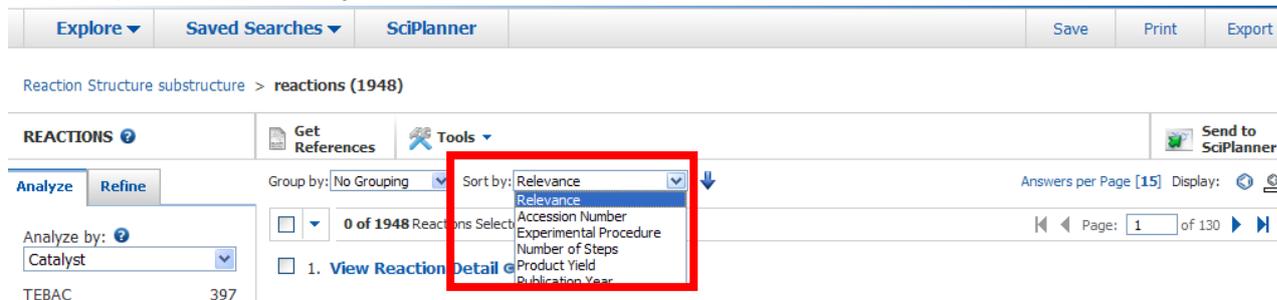
① 반응 검색 결과 그룹화 하기: Group by

검색 결과를 Transformation(변화 유형별) 또는 Document(반응이 수록된 문헌별)로 구분하여 그룹화 할 수 있습니다.



The screenshot shows the SciFinder interface. At the top, there is a navigation bar with 'SciFinder' logo, 'Preferences | SciFinder Help', and 'Sign Out'. Below this is a secondary bar with 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', and 'Export'. The main content area shows 'Reaction Structure substructure > reactions (1948)'. On the left, there is a 'REACTIONS' section with 'Analyze' and 'Refine' tabs. The 'Analyze by:' dropdown is set to 'Catalyst'. A list of catalysts with their counts is shown: TEBAC (397), HOCH₂CH₂OH polymer (229), Bu₄N⁺•Br⁻ (140), 4-DMAP (93), H₂SO₄ (78), 18-Crown-6 (66), and Pd (66). In the center, the 'Group by:' dropdown menu is open, showing options: 'Document', 'No Grouping', 'Document', and 'Transformation'. The 'Document' option is highlighted. The 'Sort by:' dropdown is set to 'Relevance'. Below the search results, there is a list of results. The first result is '1. heterocyclic compounds as P2Y₁₃ agonists and their preparation and use for the treatment of diseases related to cholesterol mobilization'. It shows a chemical reaction scheme with a 100% yield. The reaction involves a heterocyclic compound reacting with a reagent to form a product.

② 검색 결과 정렬하기: Sort by

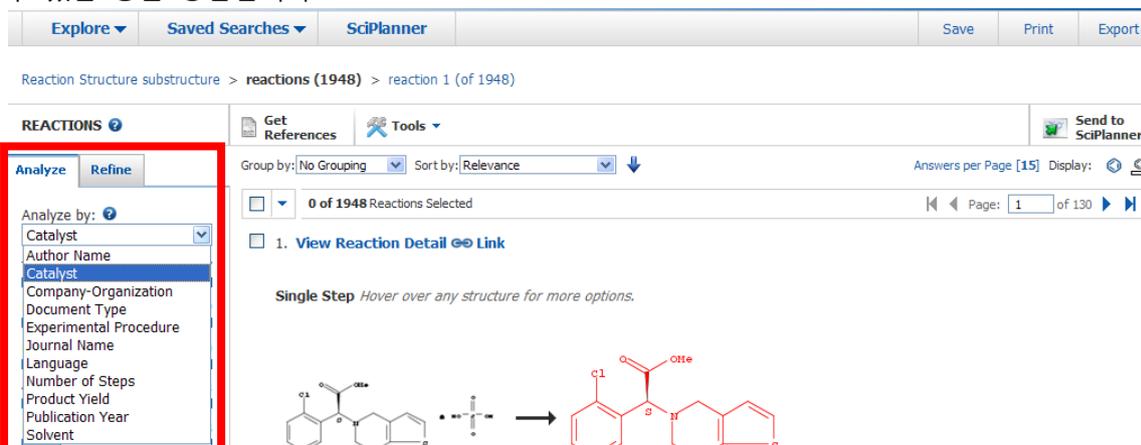


*정렬 옵션 (기본: 검색의 정확도 - Relevance 내림차순)

Relevance	검색 결과의 정확도를 기준으로 정렬
Accession Number	SciFinder 데이터베이스에 논문 정보가 입력된 순서대로 부여된 고유 번호 숫자가 클 수록 최신 논문임
Experimental Procedure	실험 절차 유무에 따른 정렬, 검색 결과에서 실험 방법 확인 가능
Number of Steps	반응의 단계에 따른 정렬
Product Yield	산출량에 따른 정렬
Publication Year	반응식이 수록된 문헌의 출판 년도
Similarity	반응식의 유사도에 따른 정렬

③ 검색 결과 필터링하여 보기: Analyze

원하는 정보 유형에 따라 검색 결과를 필터링하여 볼 수 있습니다. 검색 결과가 많을 때 문헌 수를 줄일 수 있는 좋은 방법입니다.



*필터링 옵션

Bibliographic data	Author Name	문헌 저자명
	Company - Organization	문헌과 관련된 기업/조직
	Document Type	문헌의 유형 (Patent, Journal Article 등)
	Journal Name	문헌(논문)이 수록된 학술지명
	Language	문헌의 언어
	Publication Year	문헌의 출판 년도
Reaction data	Catalyst	반응에 사용된 촉매
	Experimental Procedure	실험 방법 유무 (실험 방법 확인하기)
	Number of Steps	반응에 필요한 단계 수 (최소 단계 반응 검색)
	Product Yield	물질 산출량 (%)
	Solvent	반응에 사용된 용제

④ 검색 결과 축소하기: Refine

* Refine 옵션

Reaction Structure	Reaction editor에서 반응식을 수정(반응지점 표시 등)하여 검색
Product Yield	산출량의 최대 및 최소 범위(%)를 입력하여 검색 결과 축소
Number of Steps	반응 단계의 범위를 입력하여 검색 결과 축소 하이픈(-)을 이용하여 조정이 가능한 범위 입력 가능 (예) '-3': 3단계 또는 그 이하 단계
Reaction Classification	반응 유형 선택 가능 유형: Biotransformation, Catalyzed, Chemoselective, Combinatorial, Electrochemical, Gas-phase, Non-catalyzed, Photochemical, Radiochemical, Regioselective, Stereoselective
Excluding Reaction Classification	제외할 반응 유형 선택
Non-participating functional groups	반응에 포함되지 않고 반응 후 반드시 나타나야 할 functional group을 지정하여 검색 결과 축소

(4) Get data related to reactions

검색결과에서 물질과 관련된 문헌정보, 반응 정보, 물질 구입 정보, 규제 정보를 얻을 수 있습니다

(5) Save and share reactions answers: 검색 결과 반응 정보 저장 및 공유하기

- ① 추 후 검색 결과를 활용하기 위하여 SciFinder 내에 나의 검색 결과를 저장하기 (Save 메뉴)
- ② 서지 관리 프로그램인 EndNote로 반출하고 PDF 파일로 저장하기 (Export 메뉴)
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※ 간략한 이용 방법은 'Reference Searching'에 소개된 내용을 참고하시기 바랍니다.

Reaction Detail: 물질 검색 결과 상세 페이지

*상세 페이지에서 확인할 수 있는 정보

- ① 반응 정보가 수록된 문헌의 정보 (Sources)
- ② 반응 물질의 구입 가능 여부
- ③ Stages, Notes, Transformation
- ④ 실험 방법

Preferences | SciFinder Help | Sign Out

Welcome Yulee Kwon

Explore | Saved Searches | SciPlanner | Link | Save | Print | Export

Opened saved answer set "searching reactions" (1948) > reaction 5 (of 1948)

REACTION DETAIL | Get Reference Detail | Get Full Text | Send to SciPlanner

Return | Previous | Next

5. Single Step *Hover over any structure for more options.*

Reaction scheme showing the synthesis of a clopidogrel derivative. The reactant is a substituted benzimidazole with a chlorine atom and a methyl ester group. It reacts with sodium bicarbonate in water and t-butyl methyl ether to form a thioether-linked product.

Stages	Notes	Yield
1.1 R:NaHCO ₃ , S:H ₂ O, S:t-BuOMe, 30 min, rt	Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1 Transformation: 1. Formation of Acids, Bases, Salts and Hybrid Inorganic Organic Materials	100%

Experimental Procedure

To a solution of clopidogrel hydrosulfate (97.7 g, 233 mmol) in DIUF water (1 L) was added sodium bicarbonate (39.1 g, 466 mmol) in small portions. After mixing, t-butyl methyl ether (1 L) was added and the solution stirred for 30 minutes. The layers were separated and the aqueous layer was extracted a second time with t-butyl methyl ether (300 mL). The organic layers were combined, washed with brine (500 mL), and dried over sodium sulfate. After filtration, the t-butyl methyl ether was removed under reduced pressure. The remaining clopidogrel (yellow oil, 77.82 g, 104% yield) was dried under high vacuum at room temperature for 18 hours until most of the t-butyl methyl ether was removed.

SOURCE

Preparation of amino acid derivatives with high therapeutic index
Chandran, V. Ravi
Assignee Signature R&D Holdings, LLC, USA
2006

PATENT INFORMATION

Oct 26, 2006
US 20060241017
A1

NUMBER OF STEPS

1

SciFinder Training Materials

아래 사이트를 방문하시면 SciFinder 데이터베이스의 검색 방법을 익힐 수 있는 다양한 학습 자료를 이용할 수 있습니다.

SciFinder Training (<http://www.cas.org/training/scifinder>)

New – Need –to-know Videos

Structure Searching	<ul style="list-style-type: none"> ● Input Structures Using the Drawing Editor ● Search for Chemical Compounds Using a Structure Search ● Find Property Data, Regulatory Information, Commercial Availability, Bioactivity and Synthesis Information
Reaction Searching	<ul style="list-style-type: none"> ● Search for Specific Reactions for Reaction Type ● Use SciPlanner to Plan a Synthesis Project
Reference Searching	<ul style="list-style-type: none"> ● Search for a Specific Topic ● Search by Author Name
General Topics	<ul style="list-style-type: none"> ● Save and Combine Search Results ● Find Competitive Intelligence Information and Stay Up to Date on New Developments
Special Topics	
Polymers	<ul style="list-style-type: none"> ● Get Started Searching for Polymers and Oligomers ● Search for Polymer Substances ● Search for Polymer Reactions ● Search for Hybrid and Post-treated Polymers
Patents	<ul style="list-style-type: none"> ● Patent Coverage and Patent Information in SciFinder ● How Can a Markush Structure Search Help you in Your Research? ● Patent Family Information and How It Can Aid Your Research ● Finding Competitive Intelligence Information inSciFinder

NOTE 😊

All about CHEMISTRY

Quick Guide to SciFinder

화학 전문 데이터베이스 SciFinder 이용 가이드

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