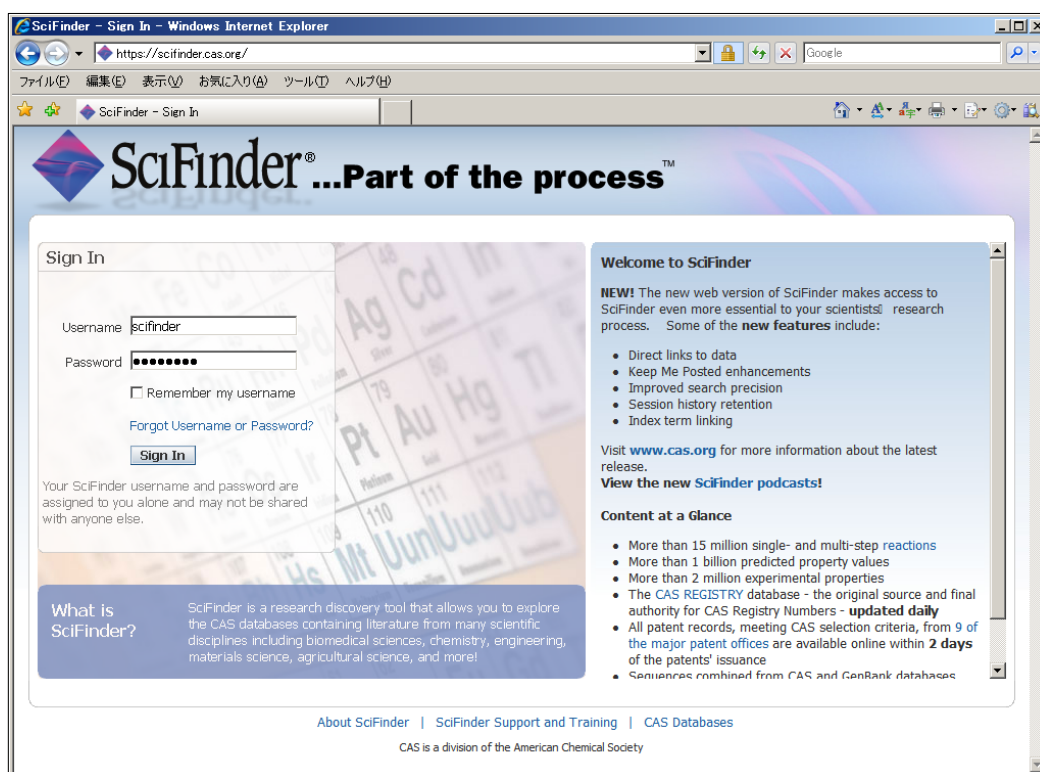


SciFinder (Web version) Presentation Material

January 2009 (Revised)



Note

- For personal research purposes only
- Over downloaded of data is prohibited



JAICI 社団法人 化学情報協会

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URL: www.jaici.or.jp

E-mail: support@jaici.or.jp

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Introducing SciFinder

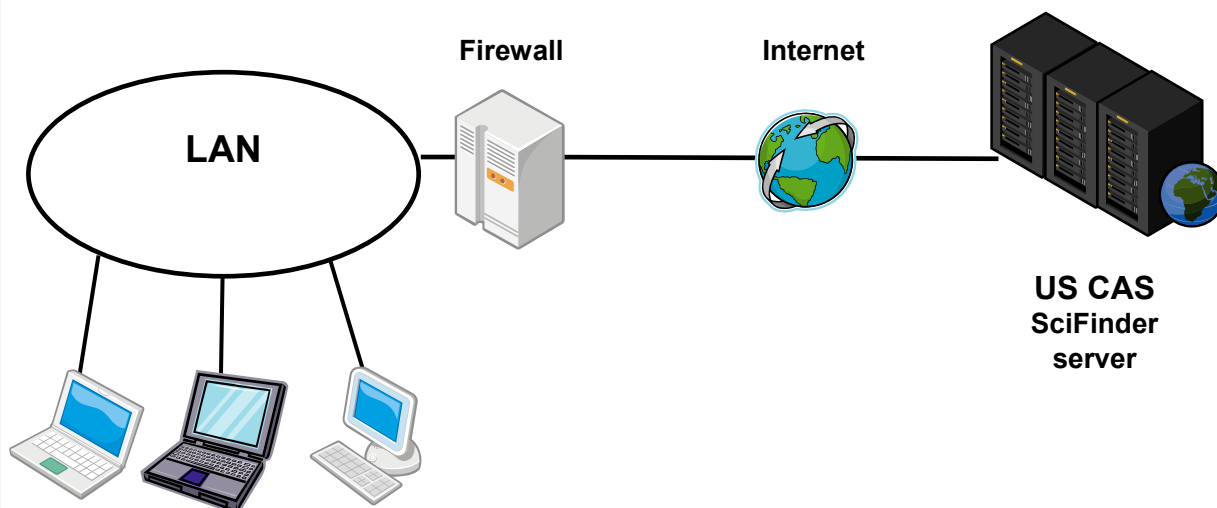
- ◆ SciFinder (Web version) is an online search service designed to provide scientific information focusing on chemistry such as medical, bioscience, physics, engineering necessary for scientists to use in their own research. Today, it is used as a leading edge and standard tool of research and development by researchers in enterprises, universities and research institute worldwide. Now, the Web version is released.



- ◆ With complete integration with CAS database, famous for its world's highest level of information volume, SciFinder can cover an extensive range of research. From its excellent interface, it can quickly extract the necessary information from a huge amount of information.

Usage Format

Researchers will access SciFinder using a browser from a PC that is connected to a local area network they use every day, and various processes will take place on the CAS SciFinder server through the Internet. Unlike previous SciFinder, Web version SciFinder does not require setting up such as software installation.



Information Provided by SciFinder

SciFinder can extract the necessary information from the following databases.

(As of June 2010)

Types of Information	Contents
Reference Information	More than 32 million reference information on essays and patents with abstracts since 1808 [CAplus File]*2
Chemical Substance Information	More than 54 million organic, inorganic chemical substances and more than 62 million proteins and nucleic acid information found in essays and patents since 1907. [REGISTRY File]*1
Organic Chemistry Reaction Data	Organic chemistry reaction information published in essays and patents since 1840 (24 million single step reactions and multi-steps reactions) [CASREACT File]
Reagents & Chemical Catalog	Catalog information of approximately 41 million reagents and chemicals from 1,100 types of catalog issued by 1,000 companies [CHEMCATS File]
Existing Chemical Substances Registry Data	Existing chemical substances registry and various regulatory information from Japan, US, EU, Canada, Korea, Australia, Switzerland, The Philippines, Israel, and New Zealand [CHEMLIST File]
Medical References Data	More than 18 million information on essays with abstracts since 1947 [MEDLINE File]

*1 Contains all chemical substances listed in the CA (Chemical Abstracts) Chemical Substance Index and all nucleic acid registered in GENBANK.

*2 Contains all reference listed in CA, and all articles from periodicals using CA as its information source (approximately 100 million journals) including approximately 19 million major journals whose essays contained little chemical elements since 1994. The information from these major journals can be look up using SciFinder within a week of its arrival at CAS.

In addition, concerning patents issued in major countries (Japan, the US, Germany, Great Britain, France, Russia, European Patents, Canada, PCT application), along with extensive listing of patents outside of CA contents, the bibliographic information and abstract can be searched after 2 days of announcement, and the index within 27 days (CA content patents only).

See the following sites for major journals that accepted publications (See also p 48).

<http://www.cas.org/expertise/cascontent/caplus/corejournals.html>

Information published from these 1,900 journals dominated approximately 50% of this database.

Record Samples

◆ Reference Details (CAplus File)

Link to Full Text

Bibliographical Information

Abstract

Index

Section Category → Page 49

Chemical Substance Index

Supplementary Terms

Link to the reference in the database

• Title
• Author
• Journal
• Institution

Reference Detail

Regio- and stereoselective hydroxylation of taxoids by filamentous fungi

Hu, Shanghui; Sun, Di-An; Tian, Xufang; Fang, Qicheng

Paclitaxel (Taxol), is one of the most promising chemotherapeutic agents developed for cancer treatment in past two decades. Microorganisms such as filamentous fungi are known to perform regio- and stereoselective hydroxylation of taxoids. Highly regio- and stereoselective hydroxylation at the 1 β and 9 α positions of the taxane skeleton by *Abisidia coerulea* was described. E.g., taxane I (R $_1$ = R $_9$ = H) was hydroxylated by incubation for 96 h in a culture of *A. coerulea* to give hydroxylated products I (R $_1$ = OH, R $_9$ = H) and I (R $_1$ = H, R $_9$ = OH) in yields of 58% and 8%, resp. Such hydroxylation reactions proceed readily for the taxadienes as substrates rather than taxoids having an oxetane ring. The presence of different oxygen substituents on the taxane nucleus, such as 5-acetoxy, has a significant effect on the selectivity and yield of the hydroxylation catalyzed by the microbial oxidases.

Indexing

Terpenes and Terpenoids (Section 30-20)

Section cross-reference(s): 7, 10, 16

Concepts

Abisidia coerulea **Hydroxylation**

regio- and stereoselective hydroxylation of taxoids by the filamentous fungi *Abisidia coerulea*

Taxanes

regio- and stereoselective hydroxylation of taxoids by the filamentous fungi *Abisidia coerulea*

Biosynthetic preparation; Reactant; Biological study; Preparation; Reactant or reagent

Substances

119347-14-7
325780-61-8

non-reactive substrate for regio- and stereoselective hydroxylation by the filamentous fungi *Abisidia coerulea*

Biological study, unclassified; Biological study

148877-83-2P
153229-33-5P
243146-80-7P
458570-00-8P
458570-01-9P

regio- and stereoselective hydroxylation of taxoids by the filamentous fungi *Abisidia coerulea*

Biosynthetic preparation; Biological study; Preparation

33069-62-4P Taxol

regio- and stereoselective hydroxylation of taxoids by the filamentous fungi *Abisidia coerulea*

Preparation, unclassified; Preparation

27854-02-0
87193-98-4
156576-64-6
458569-99-8

regio- and stereoselective hydroxylation of taxoids by the filamentous fungi *Abisidia coerulea*

Reactant; Reactant or reagent

Supplementary Terms

taxoid regioselective stereoselective hydroxylation fungi *Abisidia coerulea*; oxidase *Abisidia coerulea* taxoid regioselective stereoselective hydroxylation

Citations

- 1) Wildung Koepp, A; J Biol Chem 1995, V270, P8686
- 2) Wildung, M; J Biol Chem 1996, V271, P9201
- 3) Hefner, R; Chem Biol 1996, V3, P479
- 4) Hu, S; Tetrahedron 1996, V52, P9739
- 5) Hu, S; Biocatal Biotransform 1997, V14, P241
- 6) Hu, S; Tetrahedron Lett 1997, V38, P2721
- 7) Hu, S; Chin Chem Lett 1998, V9, P39
- 8) Kingston, D; Prog Chem Org Nat Prod 1993, V61, P1
- 9) Appendino, G; Nat Prod Rep 1995, P349

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Record Samples

◆ Substance Details (REGISTRY File)

SciFinder - CAS Registry Number 58-08-2 - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/substance/substanceDetail.jsf?nav=00ABX0AAWF0ACF

SciFinder®

Welcome Taro Kagaku | Sign Out

Create Keep Me Posted Substance Identifier "58-08-2" > substances (1) > 58-08-2

Substance Detail

Get References Get Reactions Get Commercial Sources Get Regulatory Information

Link Save Print Export

CAS Registry Number: 58-08-2

Molecular formula: C8H10N4O2

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
Caffeine (8CI); 1,3,7-Trimethyl-2,6-dioxopurine; 1,3,7-Trimethylxanthine; 3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione; 7-Methyltheophylline; Alert-Pep; Caffeina; Caffedrine; Caffein; Cafipiel; DHCplus; Dasin; Diurex; Durvitan; Guaranine; Hycominine; Koffein; Mateina; Methyltheobromine; Miudol; NSC 5036; No-Doz; Phenal; Propoxyphene Compound 65; Refresh'n; SK 65 Compound; Shape Plus; Stay Alert; Stim; Synalgos; Thein; Theine; Tri-Aqua; Wigraine Component

Deleted CAS Registry Numbers: 71701-02-5; 95789-13-2

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

Listing by reference type

Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical study	✓	✓	✓	✓
Biological study	✓	✓	✓	✓
Combinatorial study		✓		
Formation, nonpreparative	✓	✓		✓
Miscellaneous	✓	✓		
Occurrence	✓	✓		✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓

Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(48)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(48)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(48)	
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(48)	

Experimental Properties: Biological Chemical Density Lipinski and Related Optical and Scattering Spectra Structure-related Thermal

Biological Properties	Value	Conditions	Notes	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 10	(2) CAS	
Half-Life (Biological)	See full text	1 of 5	(15) CAS	
LC50	See full text	1 of 2	(21) CAS	
LD50	See full text	1 of 2	(22) CAS	
Median Lethal Dose(LD50)	355 mg/kg	Organism: rat Route: oral	(25) APC	
Median Lethal Dose(LD50)	265 mg/kg	Organism: rat Route: subcutaneous	(26) CAS	

Spectra Properties

Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum	See spectrum		(3) WSS
Carbon-13 NMR Spectrum	See full text	1 of 2	(4) CAS
IR Absorption Spectrum	See spectrum		(17) AIST
IR Absorption Spectrum	See spectrum		(17) AIST
IR Absorption Spectrum	See full text	1 of 7	(18) CAS
IR Reflectance Spectrum	See full text	1 of 2	(19) CAS
IR Spectrum	See full text	1 of 3	
Mass Spectrum	See spectrum		

Properties citations

- (1) Rahman, M. Mizanur; Journal of Chromatography, A 2006, V1119(1-2), P105-114 CAPLUS
- (2) Jansson, Rasmus; Journal of Pharmaceutical Sciences 2008, V97(6), P2324-2339 CAPLUS
- (3) WSS: Spectral data were obtained from Wiley Subscription Services, Inc. (US)
- (4) Li, Ning; Tianran Chanwu Yanjiu Yu Kaifa 2003, V15(3), P208-211 CAPLUS
- (5) Lehmann, Christian W.; Chemistry--A European Journal 2007, V13(10), P2908-2911 CAPLUS
- (6) "Hazardous Substances Data Bank" data are provided by the National Library of Medicine (US)
- (7) Pozharskii, A. F.; Khimiya Geterotsiklicheskikh Soedinenii 1989, (2), P221-7 CAPLUS
- (8) Pinto, Susana S.; Journal of Chemical Thermodynamics 2006, V38(12), P1515-1522 CAPLUS

Link buttons (Next Page)

Substance name (CAS standard nomenclature, common name, etc.)

Reference literature tag

Numerical data

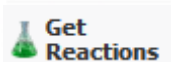
Spectrum display (Next Page)

Record Samples

【Link buttons】

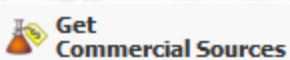


Link button to references → page 4



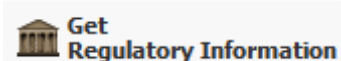
Link button to reactions → page 7

It is possible to search for reactions the substance involved in.



Link button to catalog information → page 8

It is possible to view the catalog information (supplier, price, unit packaging) immediately.



Link button to existing chemical substance registry and regulatory information → page 9

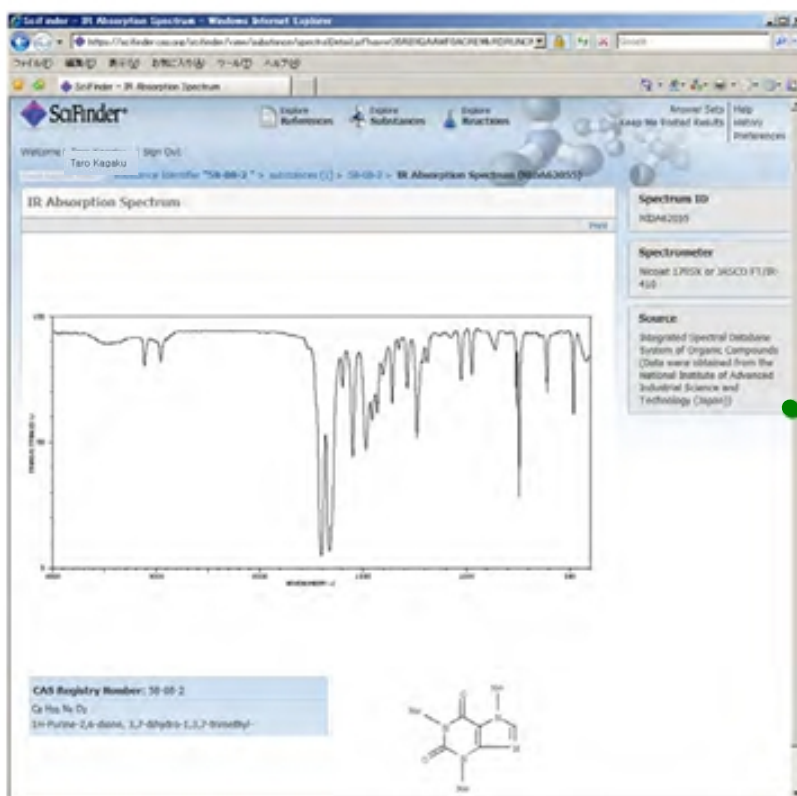
It is possible to view regulatory information in various countries or regions, and existing chemical substance registry information (such as Japan Chemical Council No., or EINECS No.) in either one of these countries - Japan, US, EU, Canada, Korea, Australia, Switzerland, The Philippines, Israel, Taiwan and New Zealand. However, the Registry information is limited to chemical substances assigned with CAS Registry Number, so with only this information, it is not possible to determine the substance listing in the Japanese and Korean Registry where there are many substances with general names.

【Spectrum Display】

Spectrum will be displayed by clicking the "See spectrum" in properties.

<Currently displayed spectrum values>

- ^1H -NMR
- ^{13}C -NMR
- ^{19}F -NMR
- ^{29}Si -NMR
- ^{31}P -NMR
- IR
- MASS
- Raman



Record Samples

◆ Chemical reaction information (CASREACT File)

SciFinder - Reaction Answer Set - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/reaction/reactionList.jsf?nav=r00ABXQ

Reaction Detail [Link](#)

Reaction 8: 5-Methyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide + MeI (Step 2.1) → 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide

1 R:Fe, R:AcOH, S:AcOH, 30 min, reflux
2 R:NaH, S:DMSO, 50 min, rt

NOTE: Reactants: 2, Reagents: 3, Solvents: 2, Steps: 2, Stages: 2

A Novel Method of Caffeine Synthesis from Uracil
By Zajac, Matthew A. et al
From Synthetic Communications, 33(19), 3291-3297; 2003

Reaction 9: 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide + MeI → 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide

R:NaH, S:DMSO, 50 min, rt

NOTE: Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1

A Novel Method of Caffeine Synthesis from Uracil
By Zajac, Matthew A. et al
From Synthetic Communications, 33(19), 3291-3297; 2003

Citations

【Intermediary steps display】

SciFinder - Reaction Detail - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/reaction/reactionDetail.jsf?nav=r00ABXQAAWF0ACRENjkwRUY5MID

Reaction Detail [Get Reference Detail](#) [Get Full Text](#)

Reaction 8: 5-Methyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide → 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide

R:Fe, R:AcOH, S:AcOH, 30 min, reflux

NOTE: Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages: 1

Reaction 9: 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide + MeI → 1,3,5-trimethyl-2-nitro-4-oxo-1,2,3,4-tetrahydropyrimidin-6-ylidenehydrazinecarboxamide

R:NaH, S:DMSO, 50 min, rt

NOTE: Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1

Source
A Novel Method of Caffeine Synthesis from Uracil
Zajac, Matthew A.; Zakrzewski, Anthony G.; Kowal, Mark G.; Narayan, Saraswathi Synthetic Communications Volume 33 Issue 19 Pages 3291-3297 Journal 2003

Company/Organization
Science Department
Villa Julie College
Stevenson, USA

Number of Steps
2

Citations

Record Samples

◆ Catalog Details (CHEMCATS File)

SciFinder - Commercial Sources - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/commercialSourceList.jsf?nav=00ABXQAAWF0ACRENJK5QUNG1

Welcome Taro Kagaku | Sign Out

Substance Identifier "58-08-2" > substances (1) > commercial sources (215)

Commercial Sources

215 Commercial Sources 0 Selected Keep Selected Remove Selected

Select All Deselect All Sort by: Catalog Name

133. **Fluka**
Sigma-Aldrich, 4 Sep 2008
Order Number: 84677, 1g, 5g
58-08-2 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
Link

134. **George Uhe Product List**
George Uhe Company, Inc., 15 Sep 2005
N/A
58-08-2 CAFFEINE
Link

135. **Hawk Chemical Product List**
Hawk Chemical Company, Inc., 1 Jan 2009
N/A
58-08-2 Caffeine
Link

136. **Interchim Intermediates**
Interchim, 18 Feb 2008
Order Number: UZI2284130, milligram quantities
58-08-2 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
Link

137. **Junsei Chemical Co. Product List**
Junsei Chemical Co., 10 May 2007
Order Number: 24015-0410, N/A
58-08-2 Caffeine anhydrous
Link

138. **Kanto Product List**
Kanto Chemical Co., Inc., 8 Aug 2006
Order Number: 07036-31, 25 g
58-08-2 Caffeine, anhydrous
Link

Analyze by: Catalog Name

Advanced Technology Product List 34

AccuStandard Chemical Reference Materials 27

VWR Chemical Catalog 7

Pfaltz & Bauer Chemicals

SciFinder - Commercial Source Detail - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/commercialSourceDetail.jsf?nav=00ABXQAAWF0ACRENJK5QUNG1

Welcome Taro Kagaku | Sign Out

Substance Identifier "58-08-2" > substances (1) > commercial sources (215) > Kanto Product List

Commercial Source Detail

Kanto Product List

8 Aug 2006

Order Number: 07036-31

Quantity: 25 g Price: 1200 YEN

CAS Registry Number: 58-08-2

Caffeine, anhydrous

Kanto Chemical Co., Inc.
11-5, Nihonbashi Honcho 3-chome, Chuo-ku
Tokyo, 103-0023
Japan
Phone: +81-3-3663-7631
Fax: +81-3-3667-8277
Email: reag-info@gms.kanto.co.jp
Web: http://www.kanto.co.jp

Kanto Chemical Co., Inc. International Business Department
Marusan bldg. 11-5, Nihonbashi Honcho 3-chome, Chuo-ku
Tokyo, 103-0023
Japan
Phone: +81-3-3667-6991
Fax: +81-3-3639-9435
Email: kanto-61@gms.kanto.co.jp
Web: http://www.kanto.co.jp

Chemical structure: CN1C=NC2=C1C(=O)N(C(=O)N2C)C

Price and Unit Packaging

Link Print **Export**

Download in Excel format

* Bulk display multiple substances is also available

Data upload to catalogs is free and available.
Contact our Information Technology Department at
TEL: 03-5978-3606.

CAS Registry Number	Chemical Name	Catalog Name	Company Name	Street Address	City	State or Province	Country	Quant
182-58-08-2	Caffeine	Fluka	Sigma-Aldrich	P O Box 14508	St. Louis	MO	USA	25g
191-58-08-2	Caffeine anhydrous	Junsei Chemical Co. Product List	Junsei Chemical Co.	4-16, 4-Chome, Nihonbashi-Honcho, Chuo-ku	Tokyo		Japan	N/A
192-58-08-2	Caffeine, anhydrous	Kanto Product List	Kanto Chemical Co., Inc.	11-5, Nihonbashi Honcho 3-chome, Chuo-ku	Tokyo		Japan	25 g
194-58-08-2	Caffeine	Kanto Product List	Kanto Chemical Co., Inc.	11-5, Nihonbashi Honcho 3-chome, Chuo-ku	Tokyo		Japan	500 g
273-58-08-2	1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-	SIGMA-ALDRICH	Sigma-Aldrich	P O Box 14508	St. Louis	MO	USA	N/A
282-58-08-2	Caffeine	TCI America Laboratory Chemicals	TCI America	9211 N. Harborgate Street	Portland	OR	USA	25g
284-58-08-2	Caffeine	TCI America Laboratory Chemicals	TOKYO CHEMICAL INDUSTRY CO.	TCI Bldg. 4-10-2, Nihonbashi-Honcho, Chuo-ku	Tokyo		Japan	25g
378-58-08-2	Caffeine	Wako Pure Chemicals Product List	Wako Pure Chemical Industries, Ltd.	1-2, Doshomachi 3-Chome	Chuo-ku	Osaka	Japan	25 g
379-58-08-2	Caffeine	Wako Pure Chemicals Product List	Wako Chemicals USA, Inc.	1600 Bellwood Road	Richmond	VA	USA	25 g
380-58-08-2	Caffeine	Wako Pure Chemicals Product List	Wako Chemicals GmbH	Nissanstrasse 2	Neuss		Germany	25 g
381-58-08-2	Caffeine	Waterstone Technology Product List	Waterstone Technology	12202 Hancock Street	Camel	IN	USA	N/A

* <http://www.jaici.or.jp/chemcats/chemcats.htm>

Record Samples

◆ Existing Chemical Substances Registry Details (CHEMLIST File)

SciFinder - Regulatory Information Detail - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/regulatoryListingDetail

Welcome | Taro Kagaku | Sign Out

Create Keep Me Posted Substance Identifier "87061-04-9" > substances (1) > 87061-04-9 > regulatory listing (1)

Regulatory Information Detail

CAS Registry Number: 87061-04-9

1,2-Propanediol, 3-[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]- (TSCA, DSL, AICS, ASIA-PAC, NZIoC)
 3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]propane-1,2-diol (English, French) (DSL, EINECS)
 3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]propan-1,2-diol (German) (EINECS)
 3-[[5-metil-2-(1-metiletil)ciclohexil]oxi]propano-1,2-diol (Spanish) (EINECS)
 3-(p-Menth-3-yloxy)-1,2-propanediol (ENCS)
 3-(1-Menthoxo)-1,2-propanediol
 TK 10

Chemical structure: CC1(C)CCCC(C1)OCC(O)CO

File Segment

ASIA-PACIFIC: ASIA-PAC
 AUSTRALIA: AICS
 CANADA: DSL
 EEC: EINECS
 JAPAN: ENCS
 NEW ZEALAND: NZIoC
 USA: FDA, TSCA

Confidentiality Status

Public

Regulatory List Number

EINECS No.: 289-296-2
 ENCS No.: 3-3857

Inventory Status

On TSCA Inventory
 July 2008 TSCA Inventory
 EPA Flags:
 P Commenced PMN
 On DSL
 Supplement to Canada Gazette, Part I, January 26, 1991
 On ENCS
 Japanese Gazette. Contained within class: Low Molecular Carbo-monocyclic Organic Compounds.
 On AICS
 Australian Inventory of Chemical Substances, June 1996 Ed
 On ASIA-PAC
 On NZIoC
 New Zealand Inventory of Chemicals, 2006

Regulatory Inventories

[U.S. EPA Regulations - TSCA](#)
[U.S. FDA Regulations](#)
[European Community Regulations](#)
[Asian and Pacific Rim Regulatory Lists and Data](#)

U.S. EPA Regulations - TSCA

Inventory Update Rule

<http://www.epa.gov/oppt/iur/index.htm> (2004).
 This chemical was reported under the TSCA Inventory Update Rule for the 2002 reporting period.

U.S. FDA Regulations

FDA Priority-Based Assessment of Food Additives

Priority-Based Assessment of Food Additives (PAFA) File, FDA Center for Food Safety and Applied Nutrition (CFSAN) (1998)
 Listed Name(s): 3-((L-Menthyl)oxy)propane-1,2-diol.

European Community Regulations

European Community Legislation

Official Journal of the European Union, No L 97 (05 Apr 2006).
 This substance is listed in Section 1, Annex I (Cosmetic Ingredients other than Perfume and Aromatic Raw Material) of Commission Directive 2006/257/EC, an amendment of Section 5a of Commission Directive 76/768/EEC which establishes the

CAS Registry Number

Chemical substance name

Regulatory List Number

Information in the Registry

Various countries Regulatory details

Record Samples

◆ Reference Details (MEDLINE File)

The screenshot shows a SciFinder record page for a study on urinary electrolytes in rats during spaceflight. The page is annotated with green boxes and lines to identify key components:

- Bibliographical information:** Points to the title, authors, and journal information on the right.
- Abstract:** Points to the summary text of the study.
- Index:** Points to the 'Indexing' section, which includes 'Concepts' (Check Tags: Male, Animals, Calcium: UR, urine, Creatinine: UR, urine, Electrolytes: UR, urine, Kidney: PH, physiology, Potassium: UR, urine, Rats, Inbred F344, Sodium: UR, urine, Water-Electrolyte Balance: PH, physiology) and 'Substances' (Registry Numbers: 60-27-5 (Creatinine), 7440-09-7 (Potassium), 7440-23-5 (Sodium), 7440-70-2 (Calcium); Chemical Names: Electrolytes).
- CAS Registry Number Index:** Points to the 'Registry Numbers' section.
- Index Term:** Points to the 'Supplementary Terms' section, which includes 'nasa center arc; nasa discipline regulatory physiology'.
- Source:** Points to the journal information on the right, including 'Journal of gravitational physiology', 'Volume 6', 'Issue 2', 'Pages 25-31', 'ISSN: 1077-9248', 'Journal Code: 9437868', and 'United States'.
- Company/Organization:** Points to the 'Life Science Division, NASA Ames Research Center, Moffett Field, CA 94035, USA'.
- Email:** Points to the email address 'cwade@mail.arc.nasa.gov'.
- Accession Number:** Points to the '2001661664' and 'PubMed ID: 11543083'.
- Language:** Points to the 'English' language indicator.
- Title, Author, Journal, Organization:** Points to the top right section of the record.

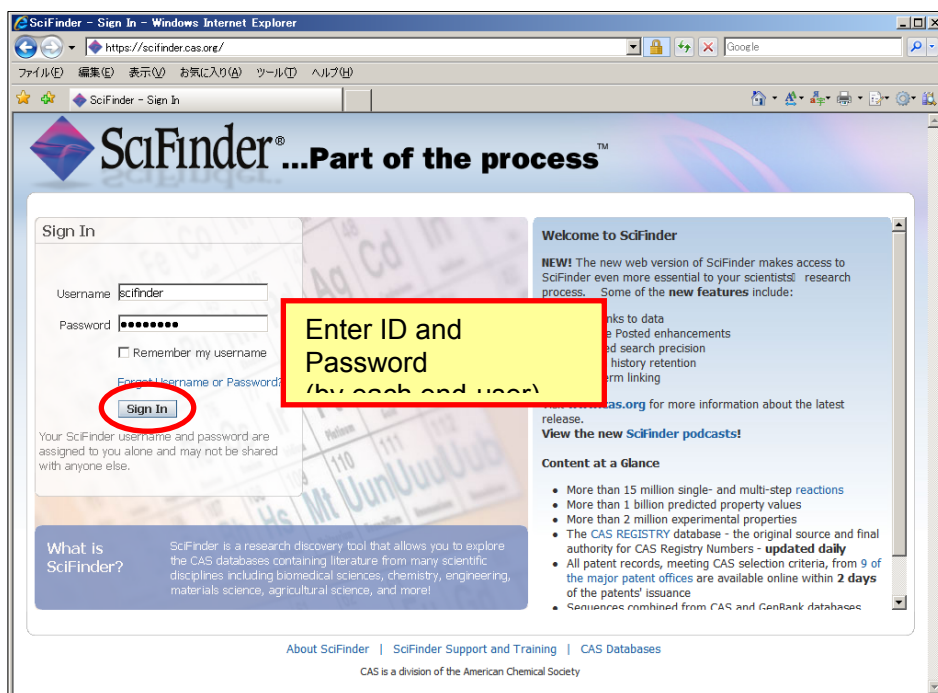
Copyright © 2008 American Chemical Society. All Rights Reserved

Accessing SciFinder

◆ Accessing SciFinder (Web version)

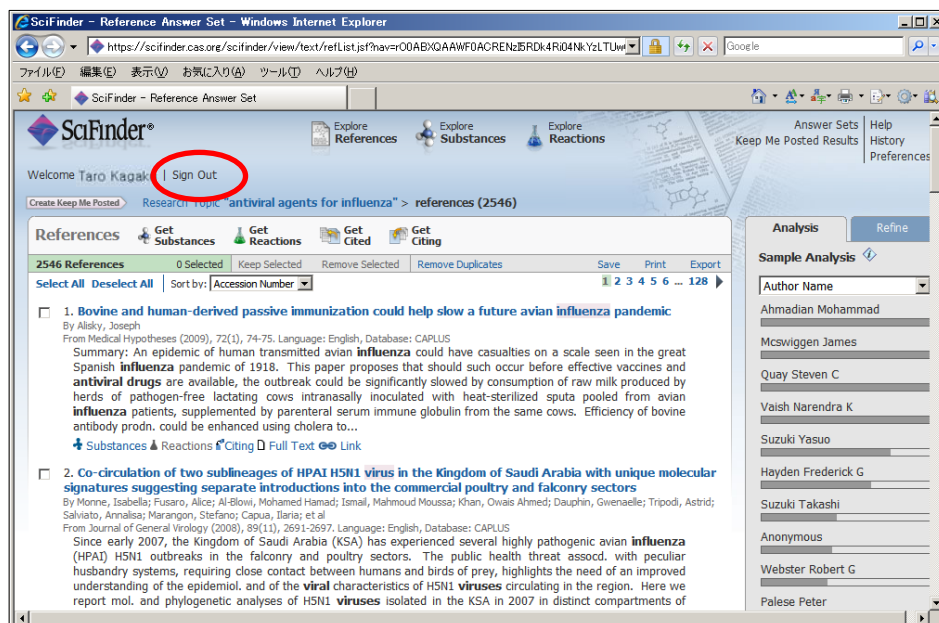
Access URL : <https://scifinder.cas.org>

Click the Sign in button after entering your ID password when prompted in the screen below. Contact your system administrator for ID and password. System requirements are listed on the last page of this document.



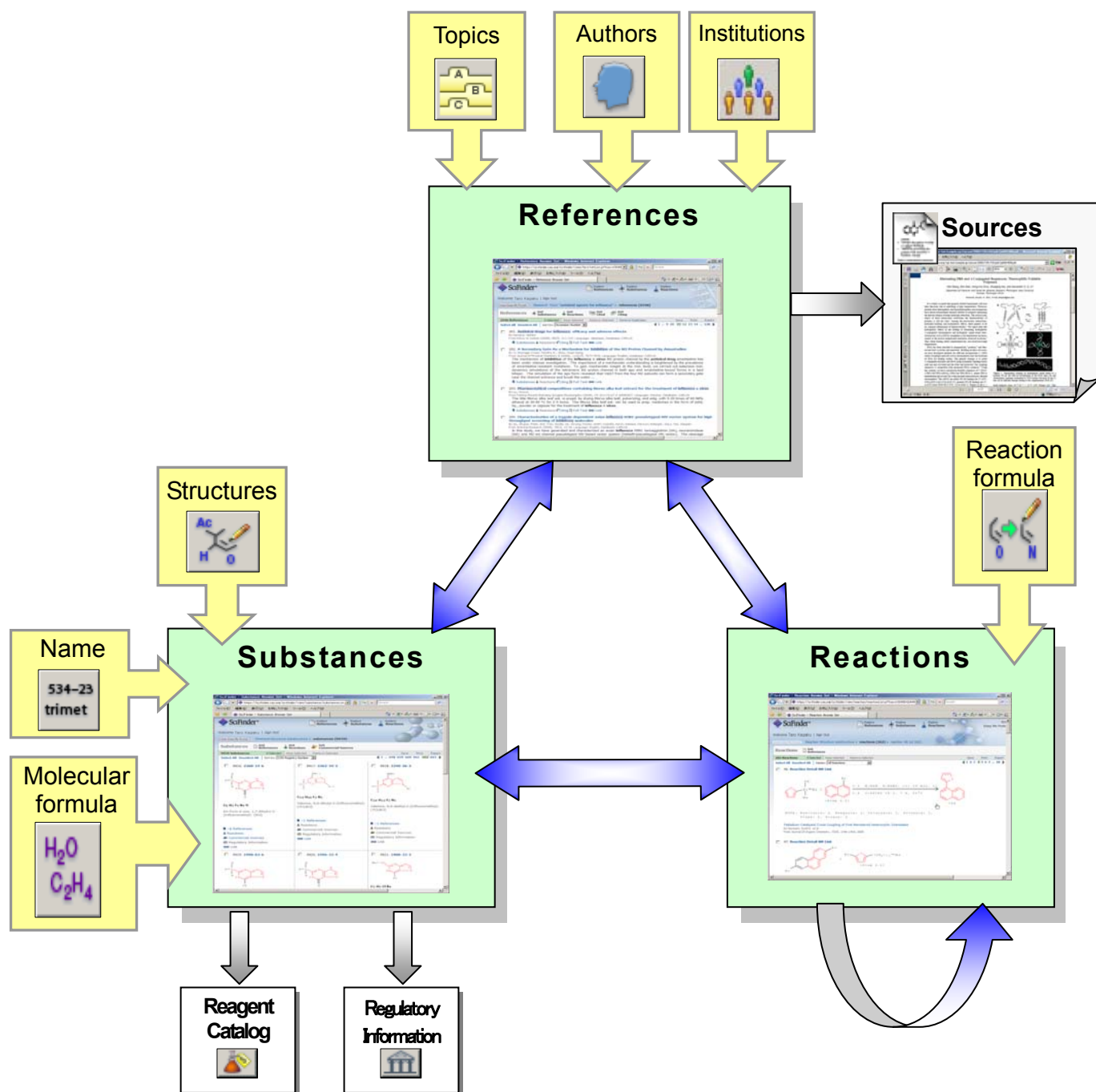
◆ Existing SciFinder (Web version)

Click "Sign Out" when you exit.



SciFinder search overview

◆ SciFinder Search overall image



* As at December 2008, array search and journal table of content browsing cannot be used.

SciFinder search overview

◆ SciFinder search initial screen:

- You can find the required information on chemical substances, essays and patents for your research in SciFinder.
- First, select search object (references, substances and reactions).

【Reference search initial screen】

SciFinder - Explore References - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/textExplore.jsf

SciFinder - Explore References

Welcome Taro Kagaku | Sign Out

Explore References

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Search

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Publication Year(s)

Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

☐ Biography ☐ Dissertation ☐ Patent

☐ Book ☐ Editorial ☐ Preprint

☐ Clinical Trial ☐ Historical ☐ Report

☐ Commentary ☐ Journal ☐ Review

☐ Conference ☐ Letter

Language(s)

☐ Chinese ☐ German ☐ Polish

☐ English ☐ Italian ☐ Russian

☐ French ☐ Japanese ☐ Spanish

Author Name

Last * First Middle

Company Name

Examples:
Minnesota Mining and Manufacturing
DuPont

Answer Sets

Keep Me Posted Results

20081021REAsample
SSM sample
Similarity sample
influenza references
sample
CAlus1
REGstr1
ref1
Autosaved Substance Set

View All

Import

Keep Me Posted Results

antiviral agents from SFweb
Nov 22, 2008 (48)
Nov 15, 2008 (43)
Nov 08, 2008 (38)

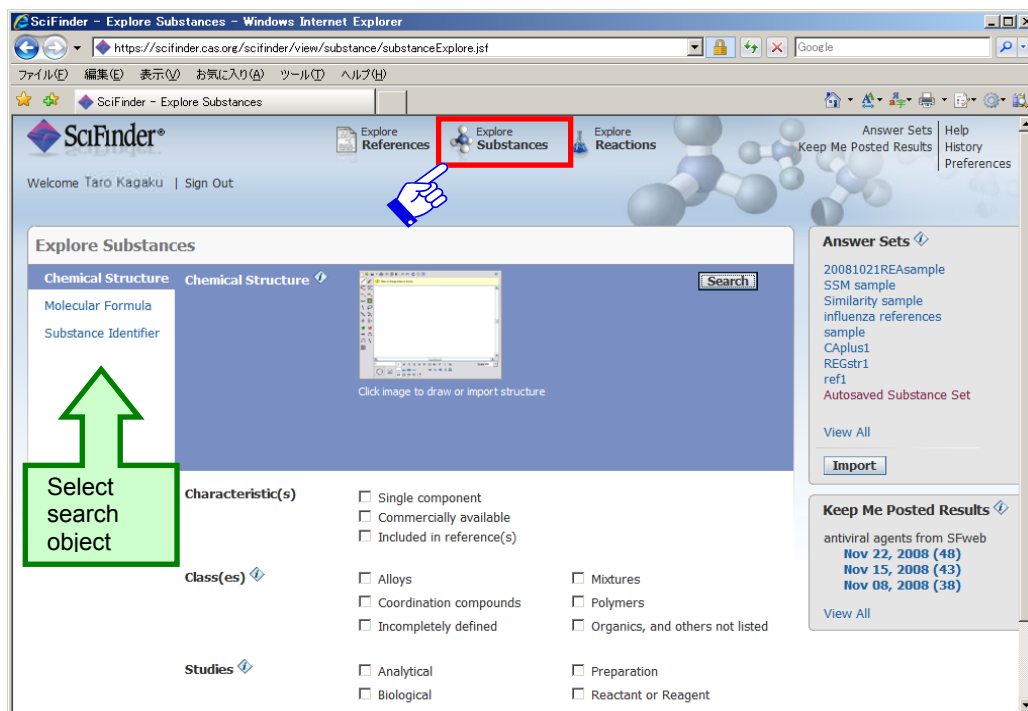
View All

Reference search object

- | | | |
|-----------------------|-------------------------------------|-------------|
| • Research Topic | → Search research topics (keywords) | P.15 |
| • Author Name | → Search authors | P.37 |
| • Company Name | → Search companies (universities) | P.38 |
| • Document Identifier | → Search patent numbers | |
| • Journal | → Search from reference information | P.38 |
| • Patent | → Search from patent information | |

SciFinder search overview

【Chemical substance search initial screen】



Substance search objects

- Chemical Structure → Chemical structure
- Molecular Formula → Molecular formula
- Substance Identifier → Chemical substance name, CAS Registry Number

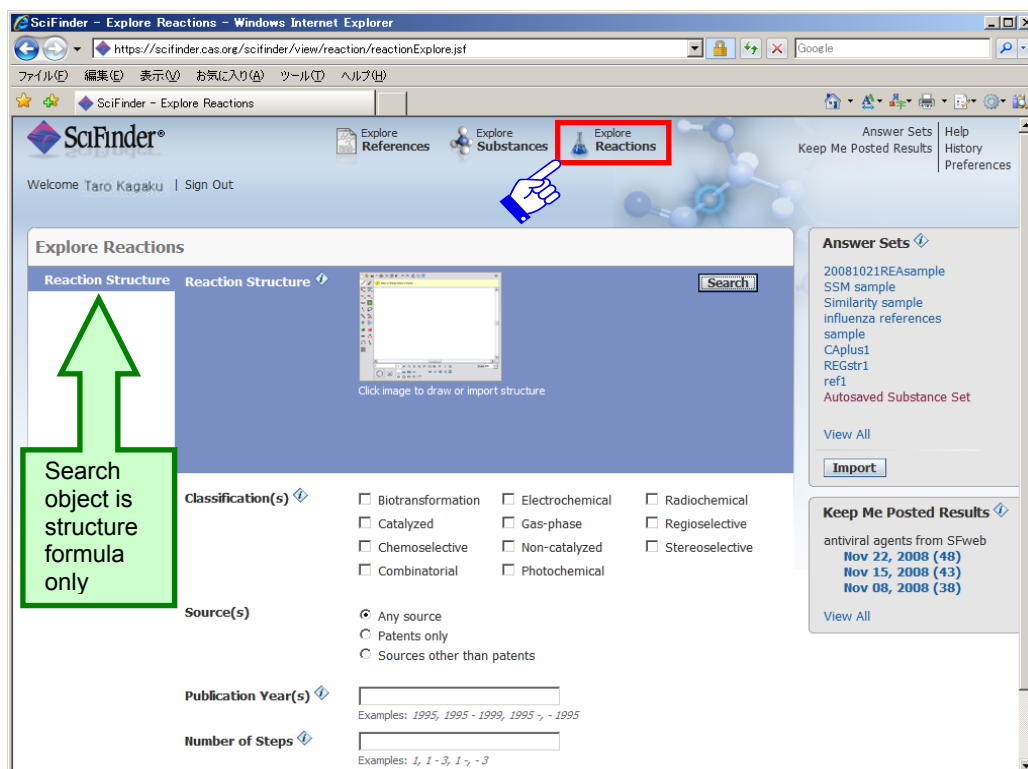
P.27

P.26

P.24

【Chemical reaction search initial screen】

P.32



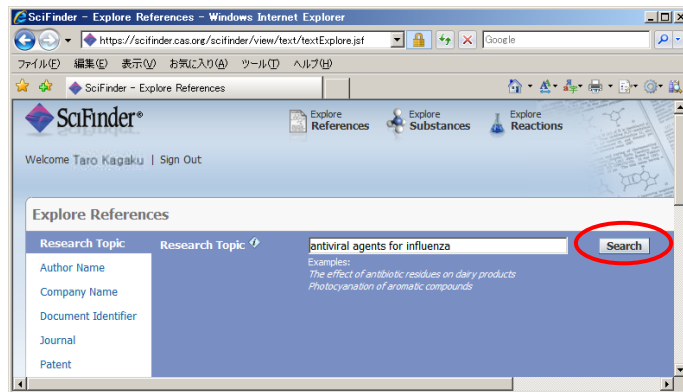
Research Topic Search



◆ Research topic search (keywords) <CPlus file, MEDLINE File>

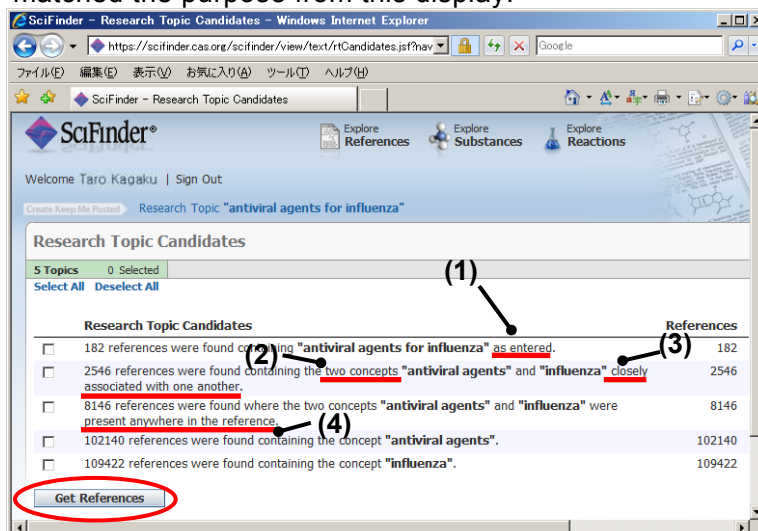
- The look cup can be done by just entering appropriate English phrase expressing the search topic.

- ① Enter the relevant keywords in English. In this example, we are searching for "**Antiviral agents for influenza**".



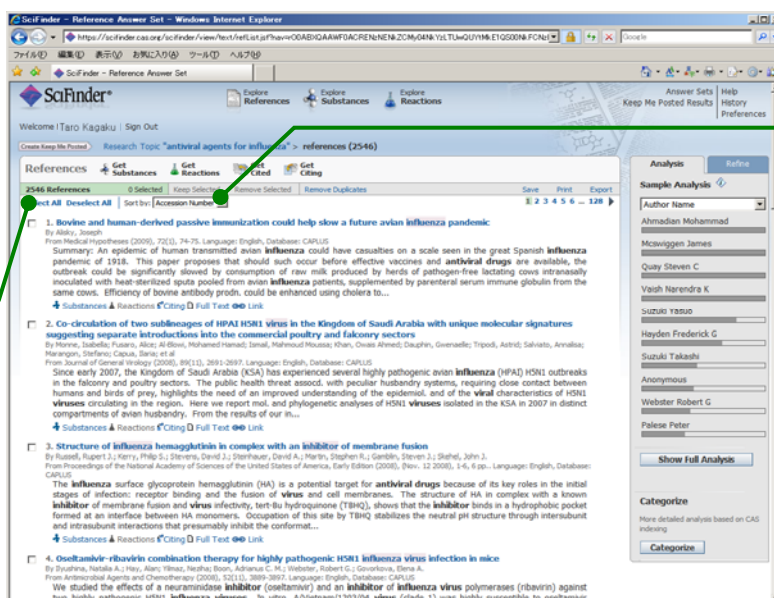
- * Not case sensitive.
- * Other than preposition, AND, OR and NOT can be used as keywords conjunction.
- * Do not use "?" or "*" symbols in queries

- ② The number of results is displayed according to a number of search formulas, from high relevancy search formula to open search formula. Select the search formula that matched the purpose from this display.



- (1) "antiviral agents" and "influenza" are lined up with a space between them
- (2) Taking into accounts synonyms, different word forms (discrepancies due to part of speech, singular, plural, etc.) abbreviation, and difference in American and British spelling.
- (3) Within the same sentence (In the title, in abstract sentences, in the same index, within the range of supplementary term separated by semicolon)
- (4) Within the same record (Title, abstract, index, supplementary terms)

- ③ Once the "Get References" button is clicked, the relevant reference list is displayed.



Click to sort

Accession Number
Accession Number
Author Name
Publication Year
Title

Number of hits

☐ Click the title to display detailed information on abstract and such.

You can remove duplicate references by clicking here (Less than 10,000 items)

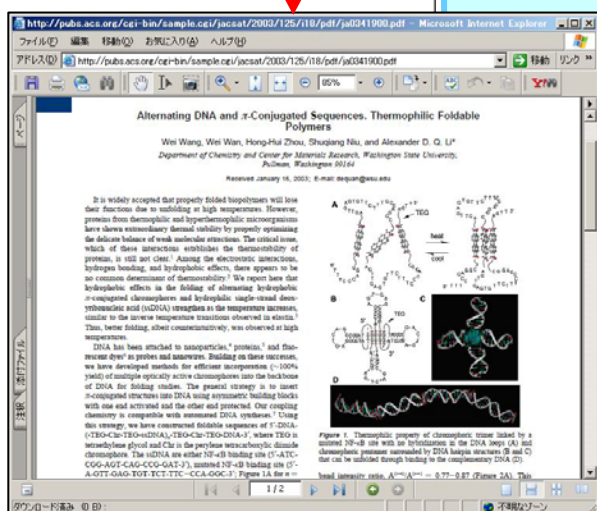
If you click the CAS Registry Number in the reference, the substance details will be displayed

Linking to Original Reference

- When you click the Full text (document) link button in the acquired literature list, the following will be available to you via ChemPort.
 - Essays published in approximately 7,400 journals delivered in digital journal published by major technical publishers (360 publishers) such as American Chemical Society, Royal Science College, Academic Press, Elsevier, and Wiley are available free of charge for digital journal subscribers only in HTML and PDF format. The latest list of publishers linked her can be verified at ChemPort home page (<http://chemport.cas.org/>).
 - Even if you are not a subscriber, you can access essays in journals published by 14 publishers such as ACS, RSC, Springer-Verlag, and Karger by paying its individual fee (Pay-per-view). In this case, the fee will be invoiced in the following month (Only for industrial version).
 - For a part of journal and patent detailed description, you can view the full text directly without going through ChemPort Connection screen.



There are cases where it is displayed directly



*Links where charges apply will not be displayed in university version

Linking to Original Reference

- From the US Patent and Trademark Office (USPTO, <http://www.uspto.gov/>, HTML and TIFF format), European Patent Office (EPO, esp@cenet, PDF format), Japan Patent Office, Korea Patent and Information Institute, Chinese Patent Office (State Intellectual Property Office, SIPO) home page, you can view patent details from the US, Japan, Switzerland, Germany, EP, France, the UK, PCT, Korea and China free of charge.
- MicroPatent's Global TOPS Subscribers will be able to view the whole document of patent details provided by MicroPatent free of charge.
- — A portion of patent details can be viewed for a certain fee (Pay-per-view). In this case, the charge will be invoiced in the following month (industrial version only).

The image displays two screenshots of patent search interfaces. The top screenshot shows the SciFinder 'Reference Answer Set' for a search on 'Cosmetic and pharmaceutical foam'. A yellow callout bubble points to the 'Full Text' link. The bottom screenshot shows the ChemPort 'Cosmetic and pharmaceutical foam' page, with green callout boxes highlighting various links and services.

SciFinder - Reference Answer Set - Windows Internet Explorer

15. **Cosmetic and pharmaceutical foam**
By Tamarkin, Dov; Friedman, Doron; Eini, Meir
From PCT Int. Appl. (2004), WO 2004/037225 A2 20040506. Language: English, Database: CAPLUS
The invention relates to an alc-free **cosmetic or pharmaceutical foam** carrier comprising water, a hydrophobic solvent, a **foam** adjuvant agent, a surface-active agent and a water gelling agent. The **cosmetic or pharmaceutical foam** carrier does not contain any oil-sol. **pharmaceutical and cosmetic** agents. For example, a vegetable oil-based **foam** carrier contains 40, water 48.5, stearyl alc. 0.8, sucrose ester 5.70 0....
+ Substances ▲ Reactions ◀ Citing ◀ Full Text ◀ Link

ChemPort CONNECTION

Cosmetic and pharmaceutical foam.
PCT Int. Appl. (2004), 76 pp. CODEN:PIXXD2; WO2004037225

- 書誌情報をメールで送る
- Esp@cenet
- Homepage

全文を表示したい場合は、次のオプションをご利用ください

- 指定サイトに接続
 - 化学情報 所蔵特許
- Web 上の原報サービス
 - ✓ esp@cenet ヨーロッパの特許庁 (EPO) での特許明細書表示
 - ✓ = 認証済み
- 有料の原報サービス
 - 原報のダウンロード
 - 原報複写注文

There are cases where it is displayed

esp@cenet original document view - Windows Internet Explorer

European Patent Office

Quick Search
Advanced Search
Number Search
Last result list
My patents list
Classification Search
Get assistance
Quick Help

COSMETIC AND PHARMACEUTICAL FOAM

Bibliographic data Description Claims Mosais Original document

(19) World Intellectual Property Organization International Bureau

(43) International Publication Date 6 May 2004 (06.05.2004) PCT

(10) International Publication Number WO 2004/037225 A2

(51) International Patent Classification: A61K 9/00

(21) International Application Number: PCT/JP2003/005527

(22) International Filing Date 24 October 2003 (24.10.2003)

(23) Filing Language: English

(24) Publication Language: English

(30) Priority Date: 25 October 2002 (25.10.2002) JP 2002-354079 A

(71) Applicant (for all designated States except US): FOAMEN LTD, 11, 2 Harbord Street, 74104 New Zone (IL)

(72) Inventor: and

(73) Inventor/Applicant (for US only): TAMARKIN, Dov

At esp@cenet the PDF document will be displayed when you click the "Original Documents" tab.

*Links where charges apply will not be displayed in university version

Reference Result Restrict and Analyze Function

■ A function that restrict and analyze search result (Analyze/Refine)

- After analyzing result list of references acquired by various searches based on 12 types of data, if necessary, the list can be restricted to these 12 types of data or refined to 7 types of perspectives.

Analyzing function

Refine search

Analysis **Refine**

Sample Analysis

Author Name

Ahmadian Mohammad

Mcswiggen James

Quay Steven C

Vaish Narendra K

Suzuki Yasuo

Hayden Frederick G

Suzuki Takashi

Anonymous

Webster Robert G

Palese Peter

Show Full Analysis

Categorize

More detailed analysis based on CAS indexing

Categorize

Refine by:

☒ Research Topic

☐ Author Name

☐ Company Name

☐ Document Type

☐ Publication Year

☐ Language

☐ Database

Research Topic:

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

Click to select perspective

Author Name

Author Name

CAS Registry Number

CA Section Title

Company/Organization

Database

Document Type

Index Term

CA Concept Heading

Journal Name

Language

Publication Year

Supplementary Terms

CA Section

Click to go to full analysis (See next page)

Categorize function (See page 21)

Restrict and Analyze References Results Function

Sample analysis

Full analysis

It is possible to click and select display of relevant items

Sample Analysis

Author Name

Ahmadian Mohammad

Mcswiggen James

Quay Steven C

Vaish Narendra K

Suzuki Yasuo

Hayden Frederick G

Suzuki Takashi

Anonymous

Webster Robert G

Palese Peter

Show Full Analysis

Analyze by:

Author Name

Click bar to view only those references within the current answer set

Mcswiggen James 80

Ahmadian Mohammad 79

Quay Steven C 79

Vaish Narendra K 79

Hayden Frederick G 50

Suzuki Yasuo 46

Anonymous 33

Webster Robert G 31

Sidwell Robert W 25

Suzuki Takashi 25

Show More

Analysis - Author Name

Only 500 Authors are displayed.

1 Selected Sort by: Frequency

Select bars to view only those references within the current answer set.

☐ Mcswiggen James 80

☐ Ahmadian Mohammad 79

☐ Quay Steven C 79

☐ Vaish Narendra K 79

☐ Hayden Frederick G 50

☒ Suzuki Yasuo 46

☐ Anonymous 33

☐ Webster Robert G 31

☐ Sidwell Robert W 25

☐ Suzuki Takashi 25

Apply **Cancel**

Checked item selection display

SciFinder®

Welcome Taro Kagaku | Sign Out

Create Keep Me Posted Research Topic "antiviral agents for influenza" > references (2567)

References

2567 References 0 Selected Keep Selected Remove Selected Remove Duplicates Save Print Export

46 references with Author Name Suzuki Yasuo are displayed

Select All **Deselect All** Sort by: Accession Number

Keep Analysis

Analysis **Refine**

Analyze by: Author Name

Click bar to view only those references within the current answer set

Mcswiggen James 80

Ahmadian Mohammad 79

Quay Steven C 79

Vaish Narendra K 79

Hayden Frederick G 50

Suzuki Yasuo 46

Anonymous 33

Webster Robert G 31

Sidwell Robert W 25

Suzuki Takashi 25

Show More

42. Limited inhibitory effects of oseltamivir and zanamivir on human sialidases

By Hata, Kikuo; Koseki, Koichi; Yamaguchi, Kazunori; Moriya, Setsuko; Suzuki, Yasuo; Yingsakmongkol, Sangchai; Hirai, Go; Sodeoka, Mikio; von Itzstein, Mark; Miyagi, Taisaku

From Antimicrobial Agents and Chemotherapy (2008), 52(10), 3484-3491. Language: English, Database: CAPLUS

Oseltamivir (Tamiflu) and zanamivir (Relenza), two extensively used clin. effective anti-influenza drugs, are viral sialidase (also known as neuraminidase) inhibitors that prevent the release of progeny virions and thereby limit the spread of infection. Recently mortalities and neuropsychiatric events have been reported with the use of oseltamivir, esp. in pediatric cases in Japan, suggesting that these drugs might also inhibit endogenous enzymes involved in sialic acid metab., including sialidase, sialyltransferase, and CMP-synthase, in addn. to their inhibitory effects on the viral sialidase...

165. Sialyl α(2→3) lactose clusters using carboxilane dendrimer core scaffolds as influenza hemagglutinin blockers

By Oka, Hiroyuki; Onaga, Tomotsune; Koyama, Tetsuo; Guo, Chao-Tan; Suzuki, Yasuo; Esumi, Yasuaki; Hatano, Ken; Terunuma, Daiyo; Matsuo, Koji

From Bioorganic & Medicinal Chemistry Letters (2008), 18(15), 4405-4408. Language: English, Database: CAPLUS

An efficient synthesis of a series of carboxilane dendrimers uniformly functionalized with sialyl α(2→3) lactose (Neu5Ac(2→3)Galβ(1→4)Glcβ(1→3)GlcNAc) moieties was accomplished. The results of a preliminary study on biol. responses against influenza virus hemagglutinin, using the sialyl lactose clusters showed unique biol. activities on the basis of the structure-activity relationship according to the carboxilane scaffolds.

207. In vitro inhibition of human influenza A virus infection by fruit-juice concentrate of Japanese plum (Prunus mume SIEB. et ZUCC)

By Yingsakmongkol, Sangchai; Miyamoto, Daisai; Sriwattajaroen, Nongkui; Fujita, Kinie; Matsumoto, Kosai; Jampangern, Wipawee; Hiramatsu, Hiroaki; Guo, Chao-Tan; Sawada, Toshiko; Takahashi, Tadanobu; et al

From Biological & Pharmaceutical Bulletin (2008), 31(3), 511-515. Language: English, Database: CAPLUS

Hints

After selection display of checked items, to perform further analysis or refining, create a list using "Keep Analysis".

System limitation information

- Maximum analysis data is 20,000 hits
- Sample analysis is not displayed in a list of less than 1,000 hits
- In full analysis detailed display, a maximum of 500 items will be displayed in frequency sorting

Restrict and Analyze Reference Results Function

■ Categorize Function

- Indexed terms and chemical substances can be analyzed for reference hit list acquired from various searches.

The screenshot shows the 'Categorize' window with the following components and annotations:

- ① Select the category you want to analyze:** Points to the 'Category' column where 'Substances in medicine' is selected.
- ② Select the terms:** Points to the 'Index Terms' column where several terms are checked.
- Main Category:** Points to the 'Category Heading' column where 'Biotechnology' is selected.
- The list of selected terms:** Points to the 'Selected Terms' column showing a list of terms like Zanamivir, Amantadine, etc.
- Refine/Cancel buttons:** Located at the bottom right of the window.

Biotechnology > Substances in medicine > 6 Selected

♣ System limitation information

- Maximum data included in the analysis will be 15,000

*See Help for Category definition.

The screenshot shows the 'SciFinder - Help' window in Internet Explorer. The 'Contents' sidebar on the left lists various topics, with 'Science Categories' highlighted. The main content area is titled 'Science Categories' and includes the following information:

- Science Categories:** Science categories are groups of **index terms** with common attributes. Categories may consist of general subjects or registered substances. Examples include:
 - Anatomical parts of animals
 - Substances used in agriculture
 - Pollutants
- Categories and Index Terms:** Choose any of these science category headings to view its member categories and index terms.

A table is provided for selecting categories:

All	Analytical chemistry	Biology
Biotechnology	Catalysis	Environmental chemistry
General chemistry	Genetics & protein chemistry	Physical chemistry
Polymer chemistry	Synthetic chemistry	Technology

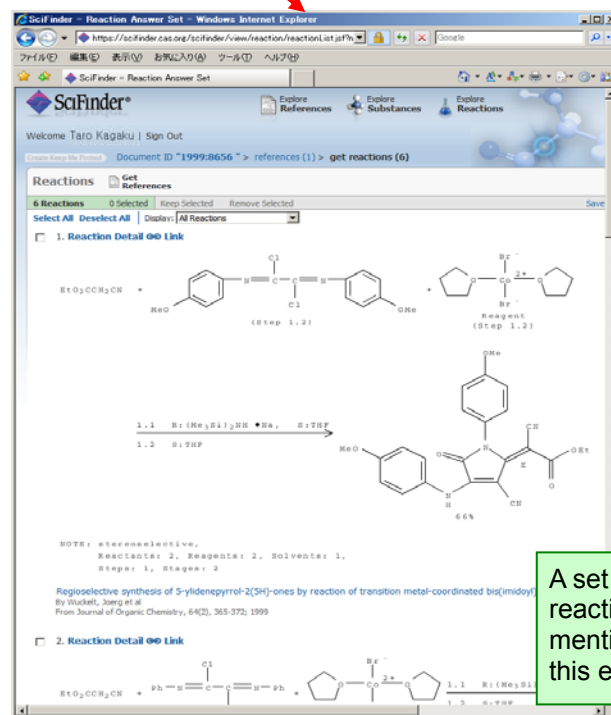
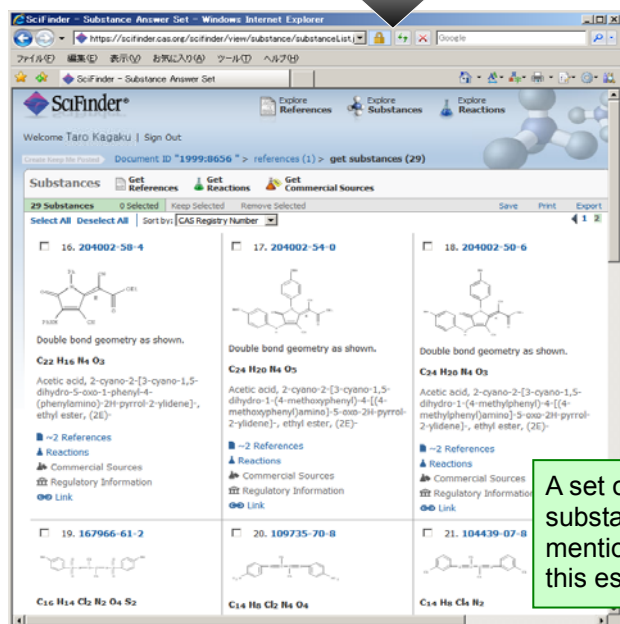
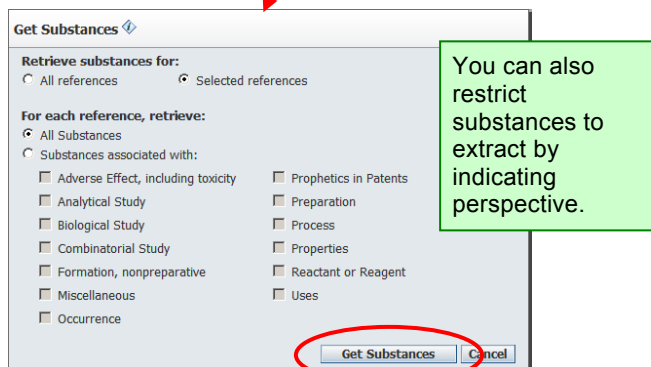
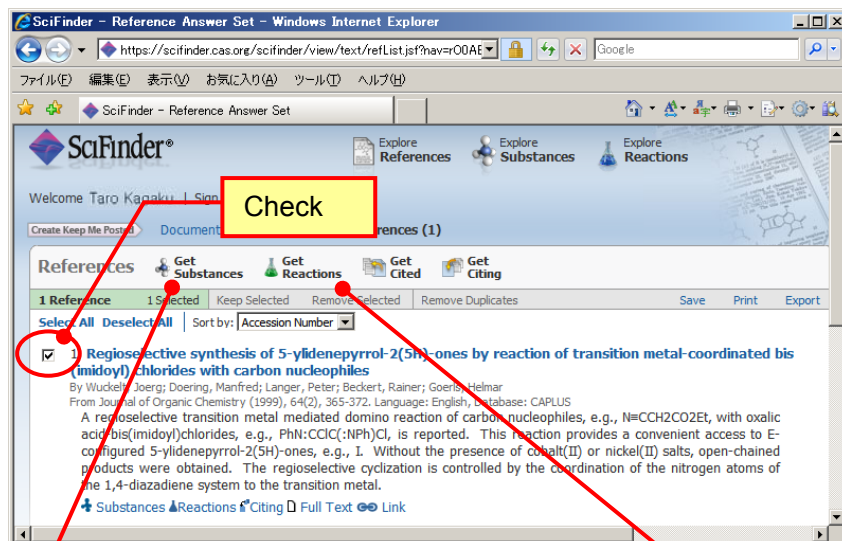
An annotation 'Click item that you want to verify' points to the 'Genetics & protein chemistry' item in the table.

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Last modified: 11/15/2008 08:10:52

Extracting related information from reference results

■ Related information extracting function

- Allowing you to extract related substances and reaction information from references.

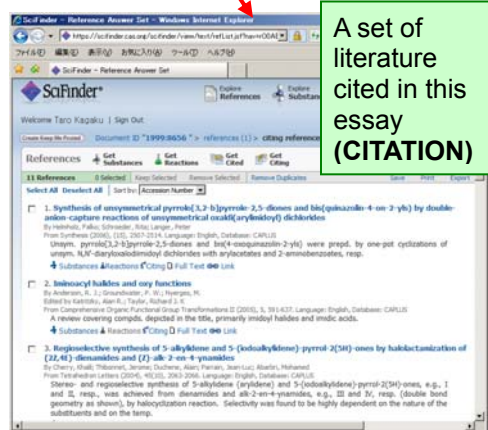
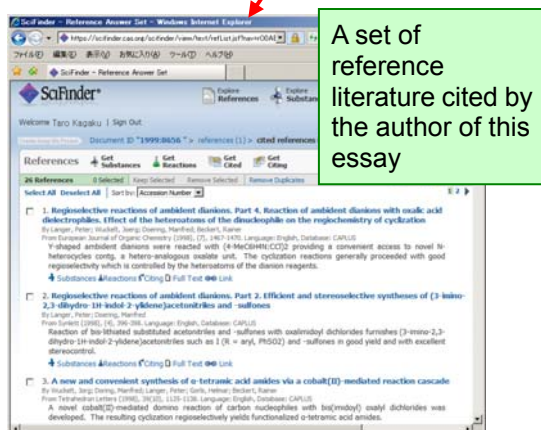
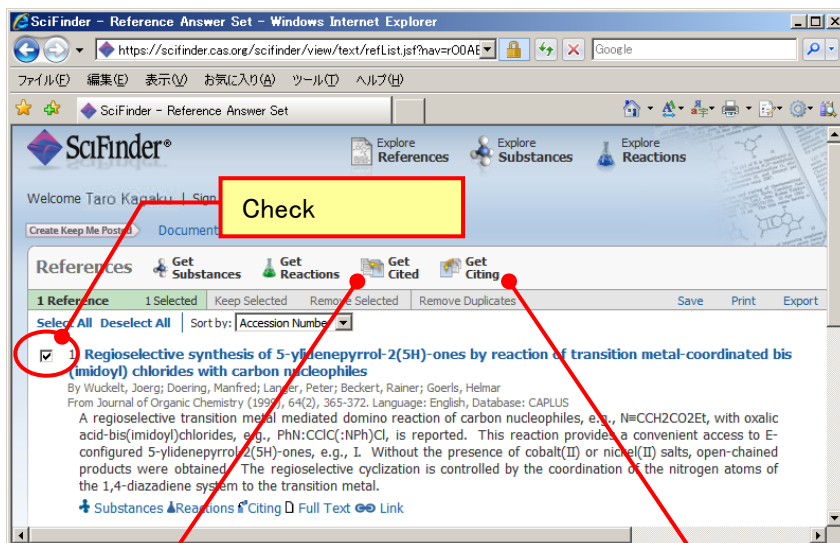


♣ System limitation information

- The maximum number of item in creating substance and reaction lists are 1,000
- Maximum results for citation information search is 500 hits

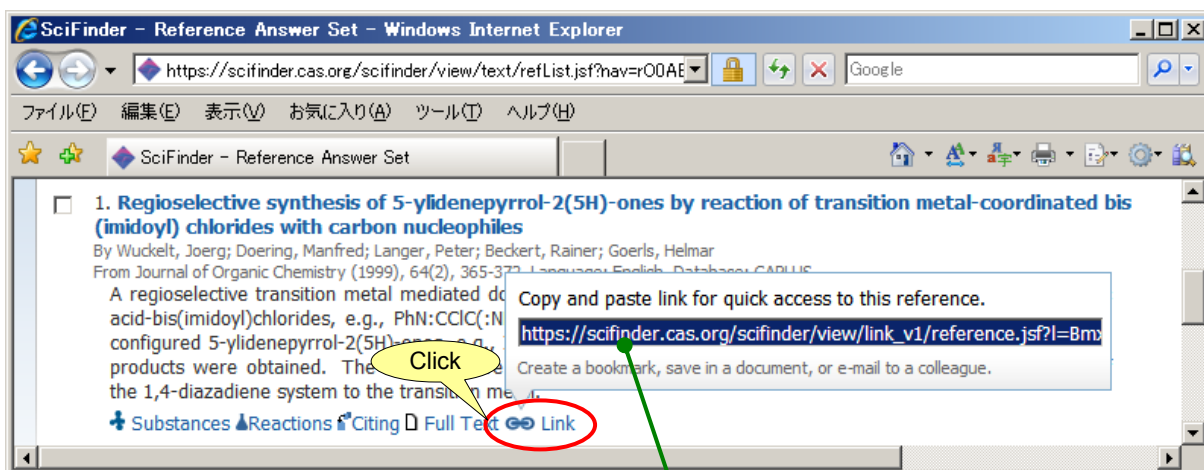
Extracting related information from reference results

- You can search for citation information of the reference being studied.



Information sharing function (Link function)

- You can share the reference being studied with other users using the URL assigned to each record.

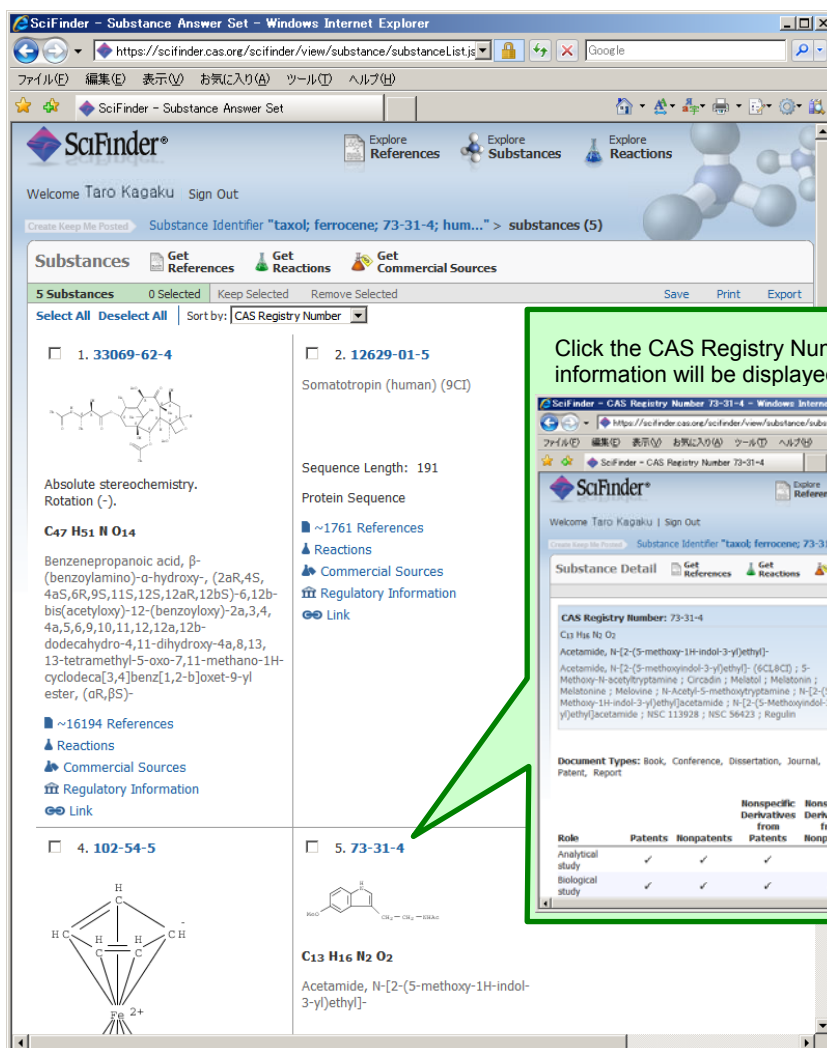
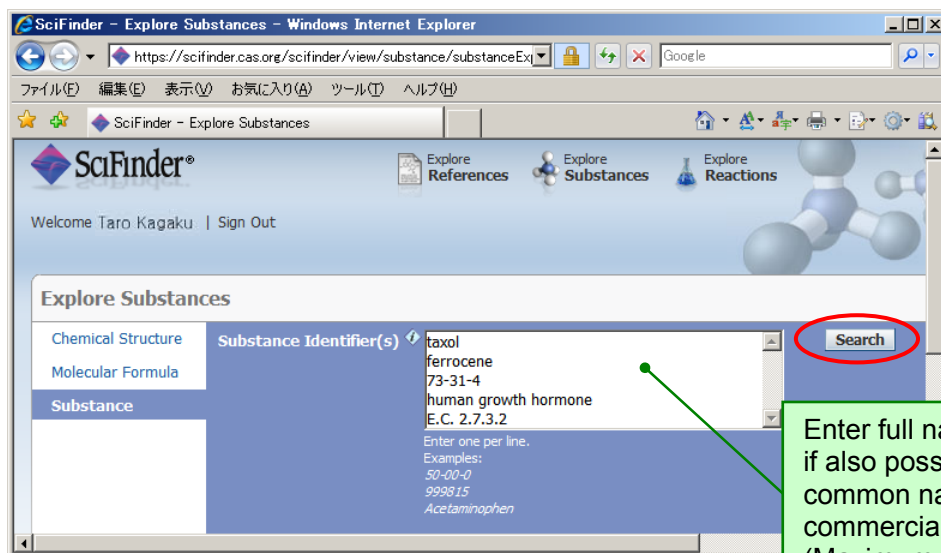


Search from Substance Information

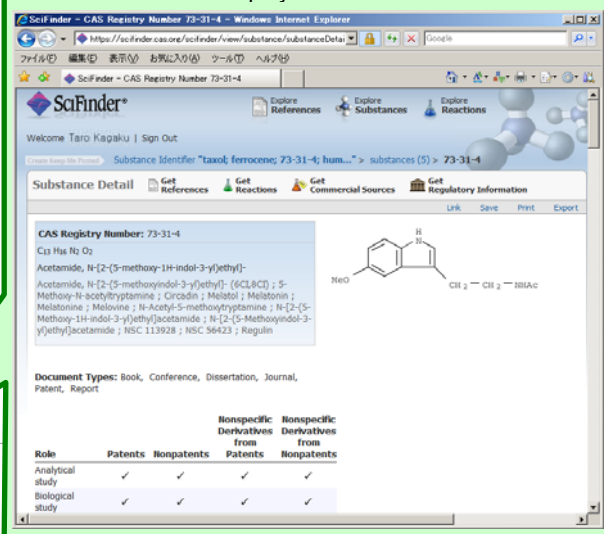
- ◆ Chemical substance search (chemical substance name, CAS Registry Number) <REGISTRY file>

534-23
trimet

- Substance can be retrieved from CAS Registry Number and name.



Click the CAS Registry Number and detailed information will be displayed.



Search from Substance Information

- ◆ Link function to chemical substance related information.

- Link to reference information

~16194 References

Get References

You can search for references by using the text button beneath each substance (for single substance), or “Get References” link button at the top of the screen (for single substance and multiple substances). In that instance, you can also restrict the references by the following 15 types of perspectives.

SciFinder - Substance Answer Set - Windows Internet Explorer

Substance Identifier "taxol; ferrocene; 73-31-4; hum..." > substances (5) > 73-31-4

Substances 5 Substances 1 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number

1. 33069-62-4
Absolute stereochemistry. Rotation (-).
C₄₇H₅₁N O₁₄
Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)-

2. 12629-01-5
Somatotropin (h)

3. 9001-15-4

Get References

Retrieve references for:
☐ All substances
☒ Selected substances

For each substance, retrieve:
☐ All references
☒ References associated with:
☐ Adverse Effect, including toxicity
☐ Analytical Study
☐ Biological Study
☐ Combinatorial Study
☐ Crystal Structure
☐ Formation, nonpreparative
☐ Miscellaneous
☐ Occurrence
☐ Prophetics in Patents
☒ Preparation
☐ Process
☐ Properties
☐ Reactant or Reagent
☐ Spectral Properties
☐ Uses

For each sequence, retrieve:
☐ Additional related references, e.g., activity studies, disease studies.

Get References Cancel

Synthetic references (since 1907)
 ★ When you selected an items other than "Preparation", the references obtained are from 1967 and later

SciFinder - Reference Answer Set - Windows Internet Explorer

Substance Identifier "taxol; ferrocene; 73-31-4; hum..." > substances (5) > get references (2851)

References 2851 References 0 Selected Keep Selected Remove Selected Remove Duplicates Save Print Export

Select All Deselect All Sort by: Accession Number

1. Enhanced production of taxanes by cell cultures of Taxus species
By Brigg, Venkatarani; Kadade, Prakash G.; Prince, Christopher L.; Roach, Braden L.
From Can. Pat. Appl. (1997), CA 2638292 A1 19971127. Language: English. Database: CAPLUS
The invention provides methods for the prodn. of taxol, baccatin III and other taxanes in very high yield using cell cultures of all known Taxus species such as T. brevifolia, T. canadensis, T. cuspidata, T. baccata, T. globosa, T. floridana, T. wallichiana, T. media and T. chinensis. Specifically, the invention provides culture media and conditions that enhance prodn. yields of various taxanes from cell cultures of all species of Taxus. Preferred cell culture enhancement agents include silver ions and their complexes, jasmonic acid and its derivs., auxin-related growth regulators and inhib...

2. Semi-synthesis of taxane intermediates and their conversion to paclitaxel and docetaxel
By Naidu, Ragina
From U.S. Pat. Appl. Publ. (2008), US 2008262250 A1 20081023. Language: English. Database: CAPLUS
A process is provided for the semi-synthesis of taxane intermediates, e.g., I [Boc = CO₂Me₃; Bz = C(O)Ph], useful in the prepn. of paclitaxel [II; R = Ac, R' = C(O)Ph] and docetaxel [II; R = H, R' = Boc], in particular, the semi-synthesis of protected taxane intermediates. The process comprises: (a) protecting the C(7)-hydroxy group

Search from Substance Information

- Link to reaction information



You can search for chemical reaction by using the conical flask icon beneath each substance (for single substance), or the “Get Reactions” link button at the top of the screen (for single substance and multiple substances).

SciFinder - Substance Answer Set - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/substance/substanceList.js

SciFinder - Substance Answer Set

Welcome Taro Kagaku | Sign Out

Create Keep Me Posted Substance Identifier "taxol; ferrocene; 73-31-4; hum..." > substances (5) > 73-31-4

Substances Get References Get Reactions Get Commercial Sources

5 Substances 1 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number

1. 33069-62-4

Absolute stereochemistry. Rotation (-).

C₄₇ H₅₁ N O₁₄

Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)-

~16194 References

Reactions Commercial Sources Regulatory Information Link

2. 12629-01-5

Somatotropin (human) (9CI)

Sequence Length: 191

Protein Sequence

~1761 References

Reactions Commercial Sources Regulatory Information Link

3. 9001-15-4

No Structure Diagram Available

Unspecified

Get Reactions

Retrieve reactions for:

☐ All substances ☒ Selected substances

Select a reaction role:

☒ Product

☐ Reactant

☐ Reagent

☐ Reactant or reagent

☐ Catalyst

☐ Solvent

☐ Any role

Choose a reaction role

Get Reactions Cancel

- ◆ Chemical substances search (Molecular formula) <REGISTRY File>

SciFinder - Explore Substances - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/substance/substanceE

SciFinder - Explore Substances

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Explore Substances

Chemical Structure Molecular Formula C₁₅ H₁₂ O₃ Search

Molecular Formula

Substance Identifier

Examples:

H₄SiO₄

H₄O₄Si

H₄SiO₄

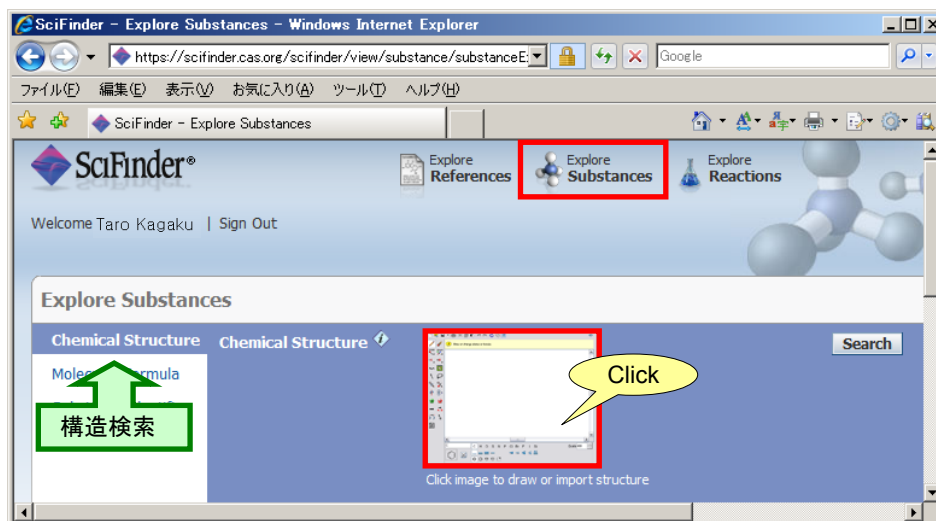
Chemical Structure Search

◆ Chemical substance search (Chemical structure formula) <REGISTRY File>

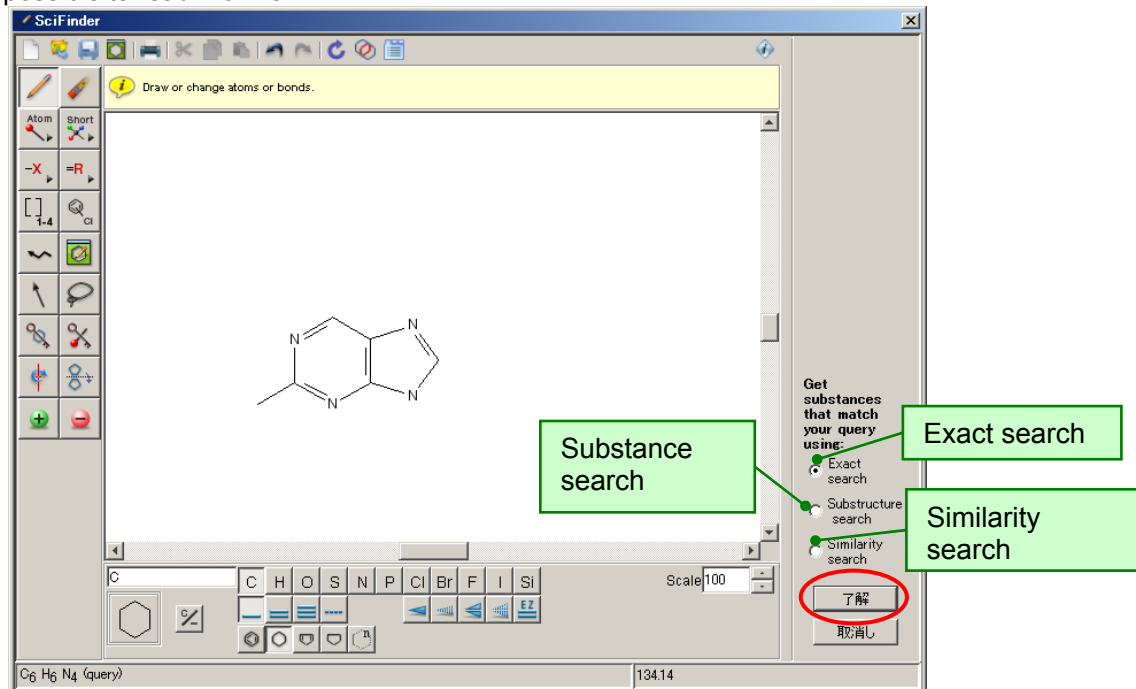


- It is possible to directly search for chemical substances from structure (including salt, compounds and copolymers).

① Start structure search screen. You will need Java plugins in order to start it.



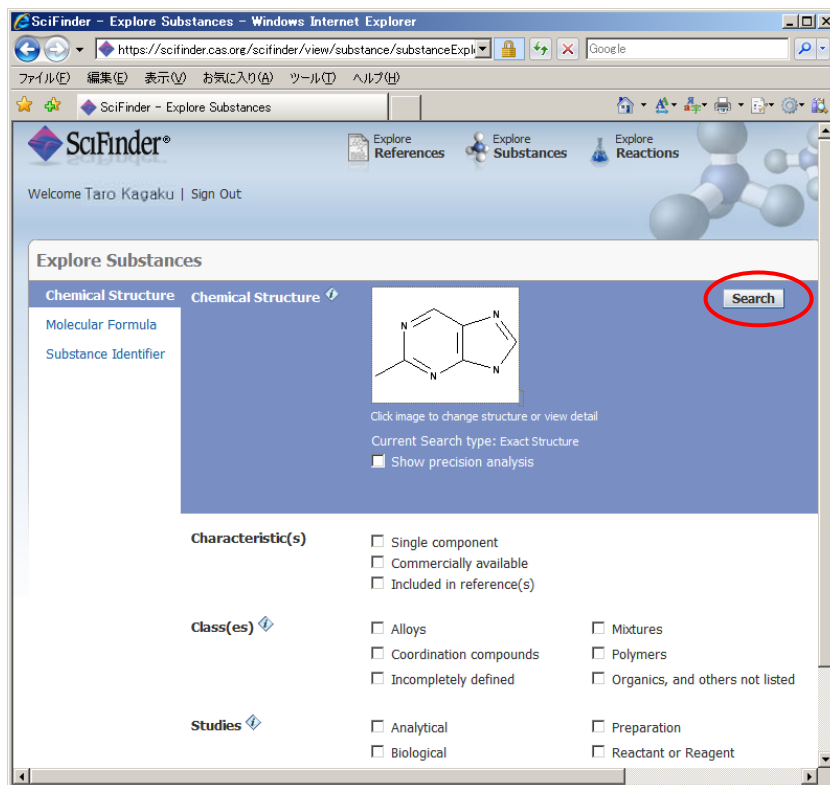
② Draw the backbone you are interested in and select search options. In addition, it is also possible to read mol file.



- Substructure search will comprehensively search every structure that contain the structure drawn, and display recent records first. You will need substructure search option agreement to use this search.
- Similar structure search will search for structures beyond the prescribed structure similarity and display the structures with high similarity on top. You will need substructure search option agreement to use this search.

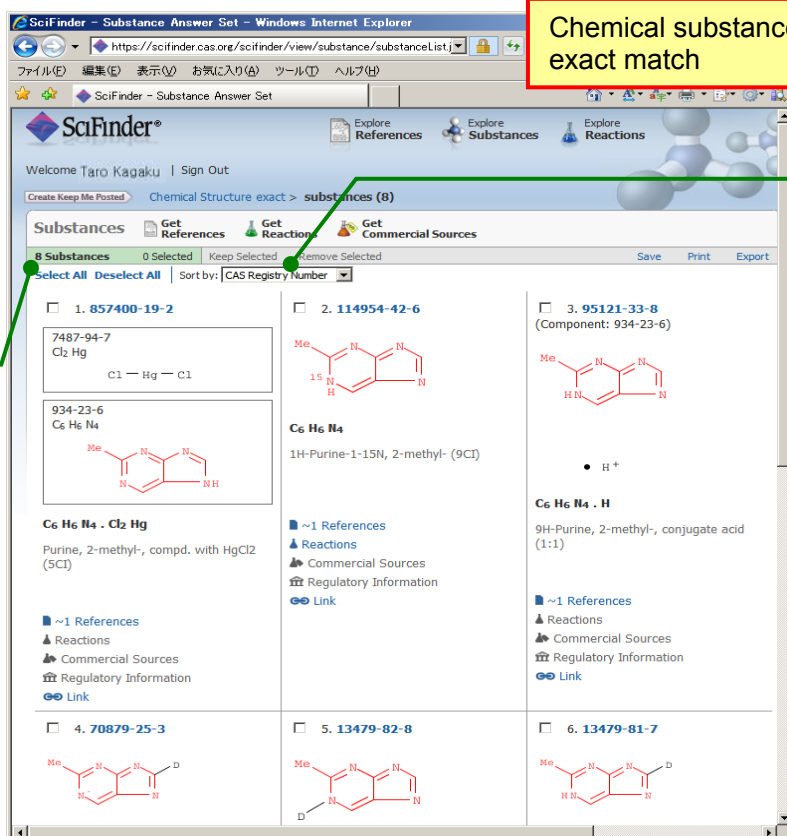
Chemical Structure Search

- ③ Execute the search after selecting the substance to search as necessary. You can also restrict the search to polymers, coordination compound and single component substances in this screen.



Restriction is possible to

- ④ Search result is displayed. You can also perform reference search after this.



Chemical substance hit in exact match

Number of hits

Click to sort
(Less than 10,000 items)

CAS Registry Number

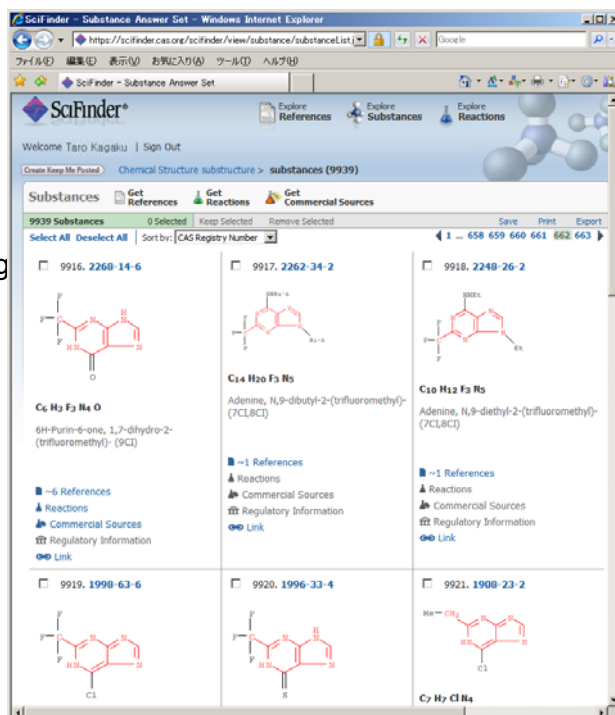
CAS Registry Number

Number of References

Chemical Structure Search

【When you executed substructure search】

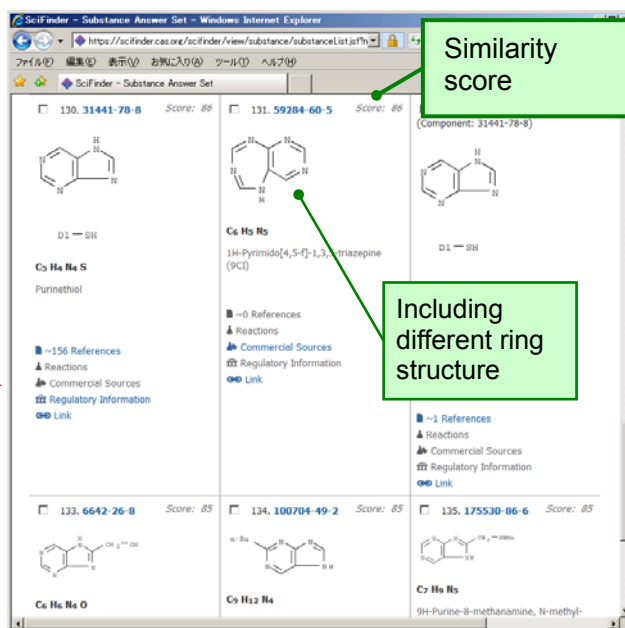
- You can use variable substituents Such as “halogen”, “alkyl group”, and “heterocyclic ring” in the structure drawing.
- You can restrict the search result using another substructure, reference availability, and substance information availability and the like.
- The number of substance uploaded by SciFinder is the largest in the world.



【When you executed similar structure search】

- The score is calculated based on Tanimoto algorithm and the number of items is displayed by the score at first.
- Because the hit included even substances with different ring size or type of elements, you will find structures that you did not expect.

Similarity Candidates		Substances
<input type="checkbox"/>	≥ 99 (most similar)	8
<input type="checkbox"/>	95-98	10
<input type="checkbox"/>	90-94	5
<input type="checkbox"/>	85-89	112
<input type="checkbox"/>	80-84	47
<input type="checkbox"/>	75-79	540
<input type="checkbox"/>	70-74	325
<input type="checkbox"/>	65-69	697
<input type="checkbox"/>	60-64 (least similar)	1432
Get Substances		



* Ambiguous structures such as variable atoms or R Groups cannot be used in similar structure search Queries.

Chemical Structure Search

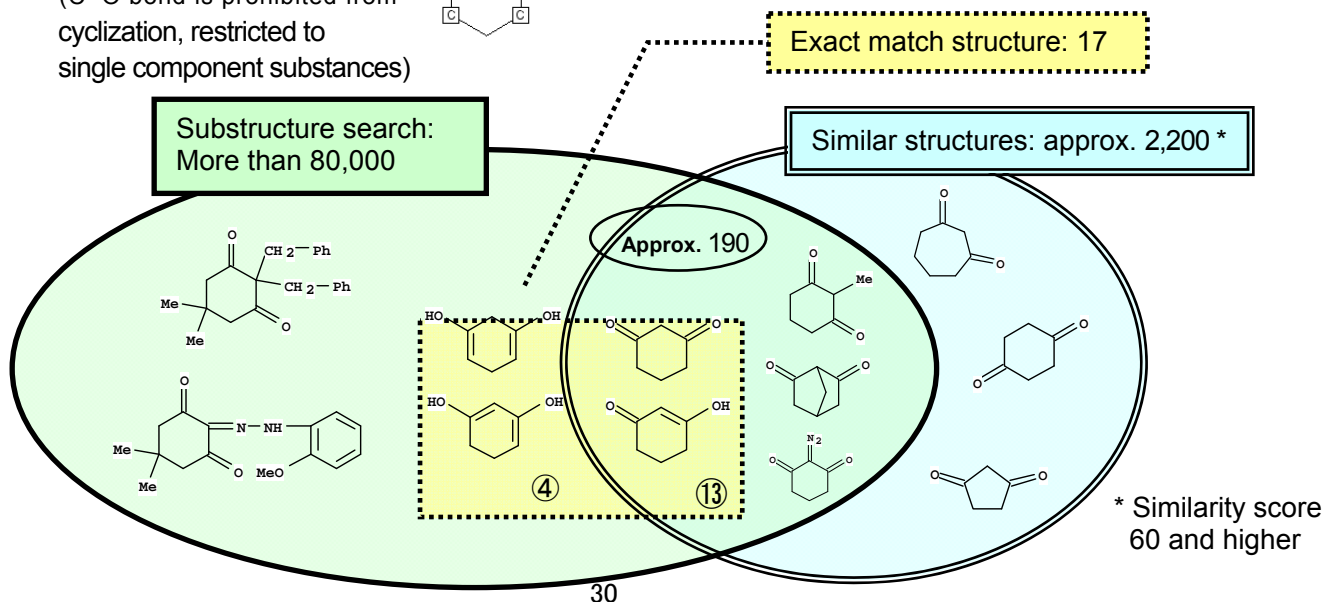
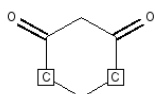
- Differences in results obtained with various search types.

Search type	Results you will obtain	Results you will not obtain
Exact Search (Perfect match structure search)	<ul style="list-style-type: none"> Substances matching structure drawn and multi-component substances that contain the drawn structure (salts, Polymers, compounds, etc.) Tautomers 	<ul style="list-style-type: none"> Substances with substituents at the free space in the drawn structure
Substructure Search (Partial structure search)	<ul style="list-style-type: none"> Substances matching the structure drawn and multi-component substances containing the said structure (such as salts, polymers, and compounds) Tautomers Substances with substituents at the free space in the drawn structure 	<ul style="list-style-type: none"> Structures with less matching part than the structure drawn (For example, methyl groups will not be included if you draw ethyl group).
Similarity Search (Similar structure search)	<ul style="list-style-type: none"> Substances matching the structure drawn and multi-component substances containing the said structure (such as salts, polymers, and compounds) Substances having different structural elements, substituents and its position, but similar structures of the drawn structure. Substances with less parts matching the drawn structure, but having similar structure Substances with different ring structure and size to the drawn structure (You may draw 6-5 membered ring and get 6-6 membered ring) 	<ul style="list-style-type: none"> Substances with larger substituent parts than the parts drawn (because the similarity level becomes low)

- Relationship between search types

Query example:

(C=O bond is prohibited from cyclization, restricted to single component substances)



Chemical Structure Search

■ Search Result Restrict and Analyzing Function (Analyze/Refine)

- After analyzing based on 4 types of data, you can restrict it as necessary, or refine it with 7 types of perspectives for result listings of substances obtained from various search.

The screenshot displays the SoFinder Chemical Structure Search interface. The main window shows a list of search results with chemical structures. The 'Analysis' panel on the left allows for sample analysis with various filters. The 'Refine' panel on the right allows for refining the search results based on different criteria.

Analysis Panel:

- Sample Analysis:** Includes filters for Substance Role, Preparation, Biological study, Uses, Reactant or reagent, Properties, Prophetic in patents, Process, Formation, nonpreparative, Analytical study, and Combinatorial study.
- Show Full Analysis:** A button at the bottom of the Analysis panel, circled in red, with an annotation: "Click for full analysis".
- Click to select perspective:** A callout box pointing to the Substance Role dropdown menu, showing options: Substance Role, Commercial Availability, Elements, Reaction Availability, and Substance Role.

Refine Panel:

- Refine by:** A list of criteria to refine the search: Chemical Structure (selected), Isotope-Containing, Metal-Containing, Commercial Availability, Property Availability, Reference Availability, and Atom Attachment. Annotations include:
 - "Structure formula" pointing to Chemical Structure.
 - "Catalog information availability" pointing to Commercial Availability.
 - "Properties availability" pointing to Property Availability.
- Chemical Structure:** A chemical structure diagram of a purine derivative is shown. An annotation "Click to draw structure" points to the structure.
- Click image to change structure or view detail:** A callout box pointing to the chemical structure diagram.
- Current Search type:** Substructure.
- Only retrieve substances that:** A list of checkboxes: Have references, Are commercially available, Are a single component, Are in specific substance classes, and Appear in specific types of studies.
- Refine:** A button at the bottom of the Refine panel, circled in red.

System limitation information:

- Maximum data to be analyzed is 20,000 hits
- Sample analysis will not be displayed for a listing of 1,000 hits and below
- Maximum 500 items display when sorting by frequency in all items

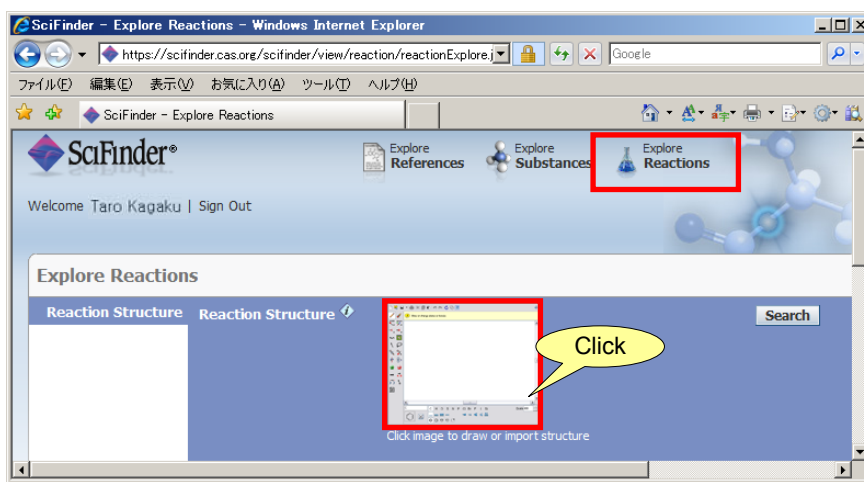
Chemical Reaction Search

◆ Chemical Reaction Search <CASREACT File>

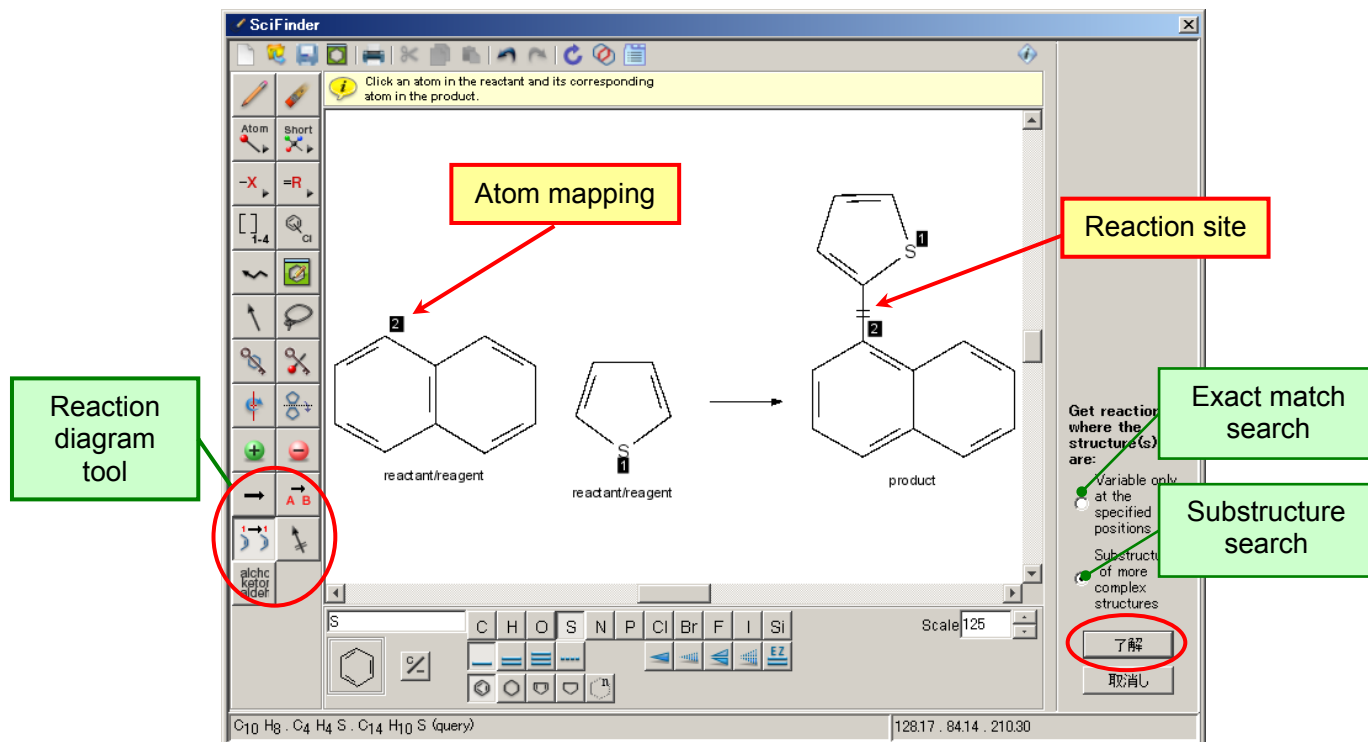


- You can designate the product and reactant/reagent and search the chemical reaction with substructure search.
- You can increase the search accuracy by indicating reaction site, and atom mapping in the reactants and products.
- You can also draw multiple structure fragments for reactants and products separately.

① Start reaction diagram screen. To start it, you will need Java plugin.



② Draw the backbone you are interested in, and select search options.



Chemical Reaction Search

- ③ Perform the search after selecting the substance to be searched as necessary. In this screen, you can also restrict the search to the source of reaction information or the number of steps in this screen.

SciFinder - Explore Reactions - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/reaction/reactionExplore.jsf

SciFinder®

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Explore Reactions

Reaction Structure

Search

Click image to change structure or view detail

Current Search type: Substructure

Classification(s)

- ☐ Biotransformation
- ☐ Catalyzed
- ☐ Chemoselective
- ☐ Combinatorial
- ☐ Electrochemical
- ☐ Gas-phase
- ☐ Non-catalyzed
- ☐ Photochemical
- ☐ Radiochemical
- ☐ Regioselective
- ☐ Stereoselective

Source(s)

- ☒ Any source
- ☐ Patents only
- ☐ Sources other than patents

Publication Year(s)

Examples: 1995, 1995 - 1999, 1995 -, 1995

Number of Steps

Examples: 1, 1 - 3, 1 -, - 3

Restriction is also possible

- ⑤ Search result is displayed. When you click the reaction scheme, you can see its detailed information.

SciFinder - Reaction Answer Set - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/reaction/reactionList.jsf?nav=00ABXQAAV

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Create Keep Me Posted

Reaction Structure substructure > reactions (262) > reaction 46 (of 262)

Reactions

Get References

262 Reactions 0 Selected Keep Selected Remove Selected

Select All Deselect All Display: All Reactions

46. Reaction Detail Link

NOTE: Reactants: 2, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 2

Palladium-Catalyzed Cross-Coupling of Five-Membered Heterocyclic Silanates

By Denmark, Scott E. et al

From Journal of Organic Chemistry, 73(4), 1440-1455; 2008

47. Reaction Detail Link

Link to references

Click and you can switch the display format (less than 10,000 items)

All Reactions

All Reactions

One Reaction Per Reference

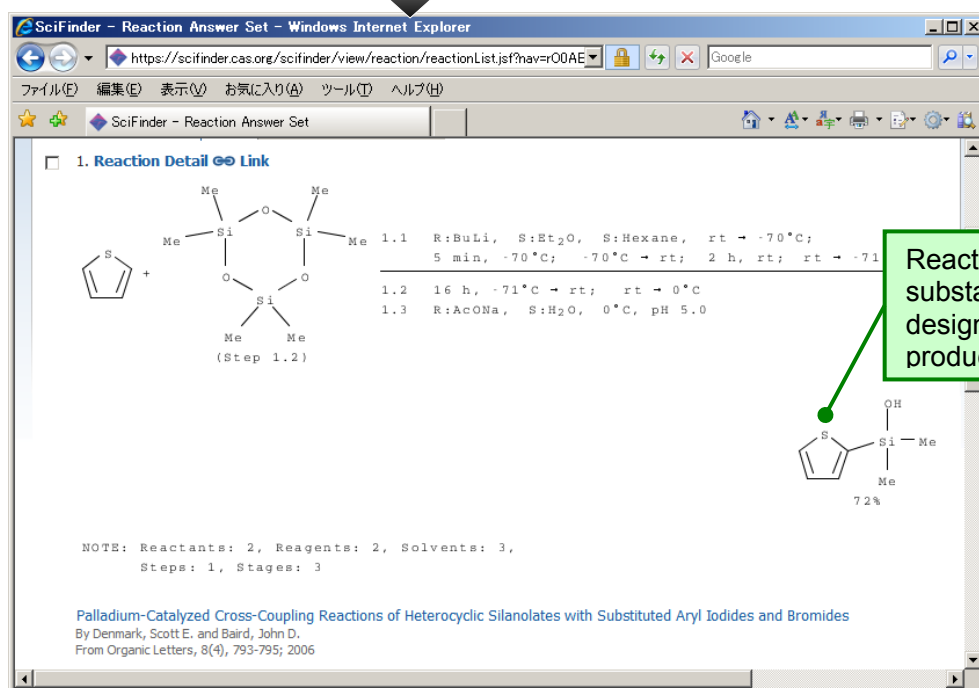
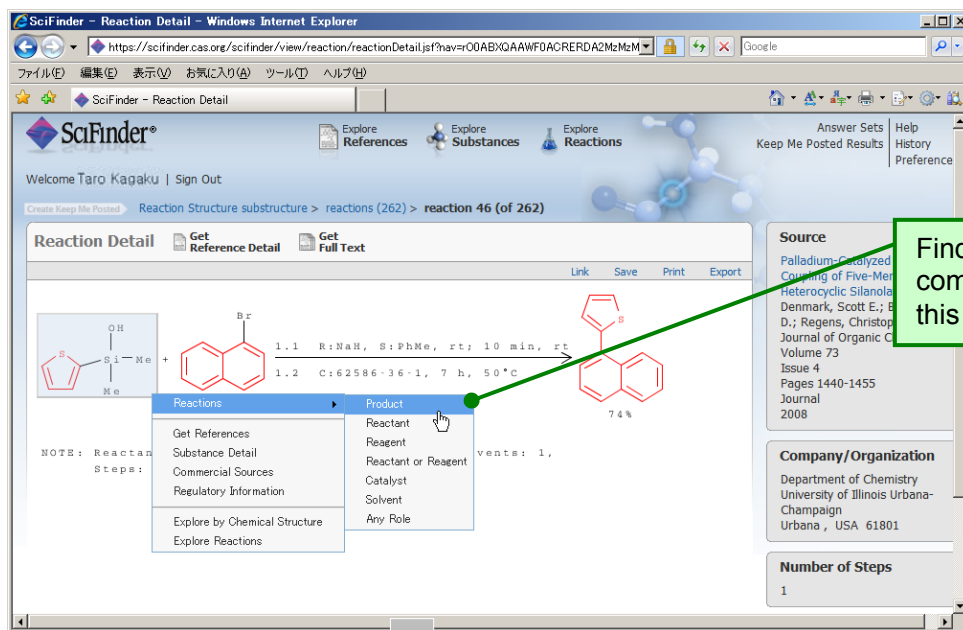
Click (see next page)

Number of hits

Link to references

Chemical Reaction Search

- ⑤ You can confirm the intermediary of multi-steps reaction, or yield for each step in the reaction details screen. In addition, you can also search and display various information related to each substance such as its details, reference, catalog or reactions.



Hint

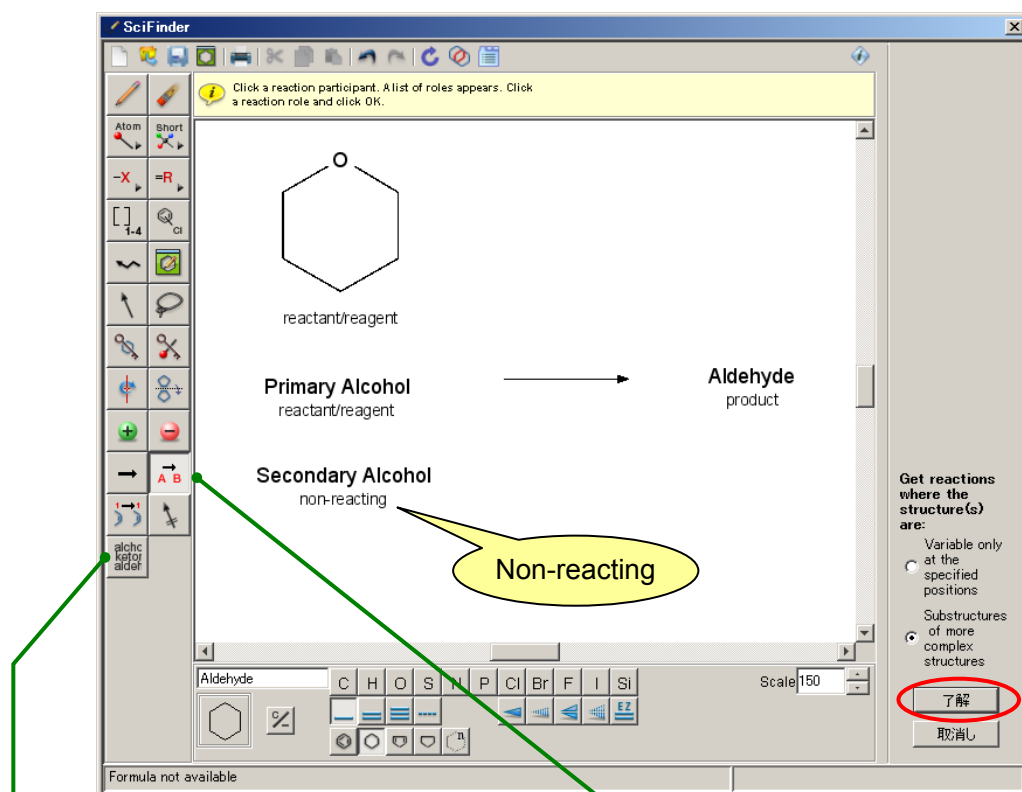
You can also perform reaction search by using "Get Reactions" from chemical substances.
(→ p.26)



Chemical Reaction Search

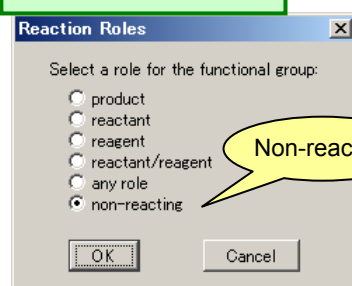
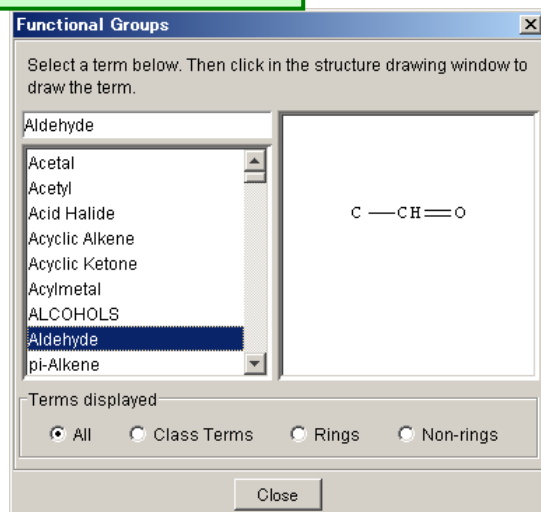
【Reference】

- You can also have a comprehensive search if you use functional group names. You can also indicate the “Non-reacting functional groups” in functional group names.



Functional group tools

Reaction role tools



Chemical Reaction Search

◆ Search result restrict and analyze function (Analyze/Refine)

- For result records obtained by reaction search, you can analyze the based on 5 types of data and refine it with 5 types of perspectives.

The image shows the SciFinder web interface. At the top, there's a navigation bar with 'Reactions' selected. Below it, a list of reactions is shown, with reaction 46 highlighted. To the right of the reaction list, there's an 'Analyze by' panel. Below the main interface, there are two detailed panels: 'Analysis' and 'Refine'.

Analysis Panel:

Analyze by: Catalyst

Click bar to view only those reactions within the current answer set

Pd(PPh ₃) ₄	91
Pd(OAc) ₂	16
PdCl ₂ (PPh ₃) ₂	13
(C ₆ H ₁₁) ₃ P	10
Ni complex	9
KBr	7
Na ₂ CO ₃	7
224311-51-7	5
AlCl ₃	4
Bu ₄ N ⁺ • Br ⁻	4

Show More

Refine Panel:

Refine by:

- ☒ Reaction Structure
- ☐ Product Yield
- ☐ Number of Steps
- ☐ Reaction Classification
- ☐ Excluding Reaction Classification

Click image to change structure or view detail

Current Search type: Substructure

Refine

System limitation information

- Maximum data to analyze is 20,000 hits
- Sample analysis will not be displayed for records with 1,000 hits and below
- In full analysis detailed display, maximum 500 items is displayed for frequency sorting

Author Name Search

◆ Author name search



- In a search related to author name (inventor for patents), the many spelling for the name (for example, Ito, itoh, ItoU) will be displayed. You can choose the appropriate spelling and search.

SciFinder - Explore References - Windows Internet Explorer

SciFinder - Explore References - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/textExplore.jsf

SciFinder - Explore References

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Explore References Explore Substances Explore Reactions

Research Topic Author Name Ito Takeshi Search

Author Name

Company Name

Document Identifier

Journal

Patent

SciFinder - Author Candidates - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/authorCandidates.jsf?n

SciFinder - Author Candidates

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Create Keep Me Posted Author Name "Ito, Takeshi"

Author Name Candidates

24 Authors 5 Selected

Select All Deselect All

Author Candidates	References
<input type="checkbox"/> ETO	1
<input type="checkbox"/> ETO T	438
<input type="checkbox"/> ETO T A	4
<input type="checkbox"/> ETO T K	3
<input type="checkbox"/> ETO TAKESHI	12
<input type="checkbox"/> ETO TAKESHI KURT	1
<input type="checkbox"/> ETTO T L	2
<input type="checkbox"/> ITO	12
<input checked="" type="checkbox"/> ITO T	4823
<input type="checkbox"/> ITO T A	3
<input type="checkbox"/> ITO T I	20
<input type="checkbox"/> ITO T I M	
<input type="checkbox"/> ITO T K	
<input type="checkbox"/> ITO T M	54
<input type="checkbox"/> ITO T TAJIMA N	1
<input type="checkbox"/> ITO T U	14
<input type="checkbox"/> ITO T Y	4
<input checked="" type="checkbox"/> ITO TAKESHI	947
<input type="checkbox"/> ITOH	3
<input checked="" type="checkbox"/> ITOH T	2617
<input type="checkbox"/> ITOH T J	20
<input checked="" type="checkbox"/> ITOH TAKESHI	202
<input type="checkbox"/> ITOU T	106
<input checked="" type="checkbox"/> ITOU TAKESHI	5

Get References

Check the possible name

Other Search

◆ Company name (University name) Search



- You can search for references by combining words that contain the name of the institution the author belongs to, or patent applications.

SciFinder - Explore References - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/textExplore.jsf

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Welcome Taro Kagaku | Sign Out

Explore References | Explore Substances | Explore Reactions

Explore References

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent

Company Name

Examples:
3M
DuPont

◆ Search from reference information



- You can search for reference from fragmentary information as author name, journal name, volume number, or number of pages.

SciFinder - Explore References - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/text/textExplore.jsf

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Explore References | Explore Substances | Explore Reactions

Explore References

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent

Journal

Journal Name * Volume Issue Starting Page

Title Word(s)

Example: Antibiotic

Author Name

Last * First Middle

Publication Year(s)

Examples: 1995, 1995-1999, 1995-, -1995

Journal name

Volume, number, pages

Keyword (only in title)

Author name

Publication year

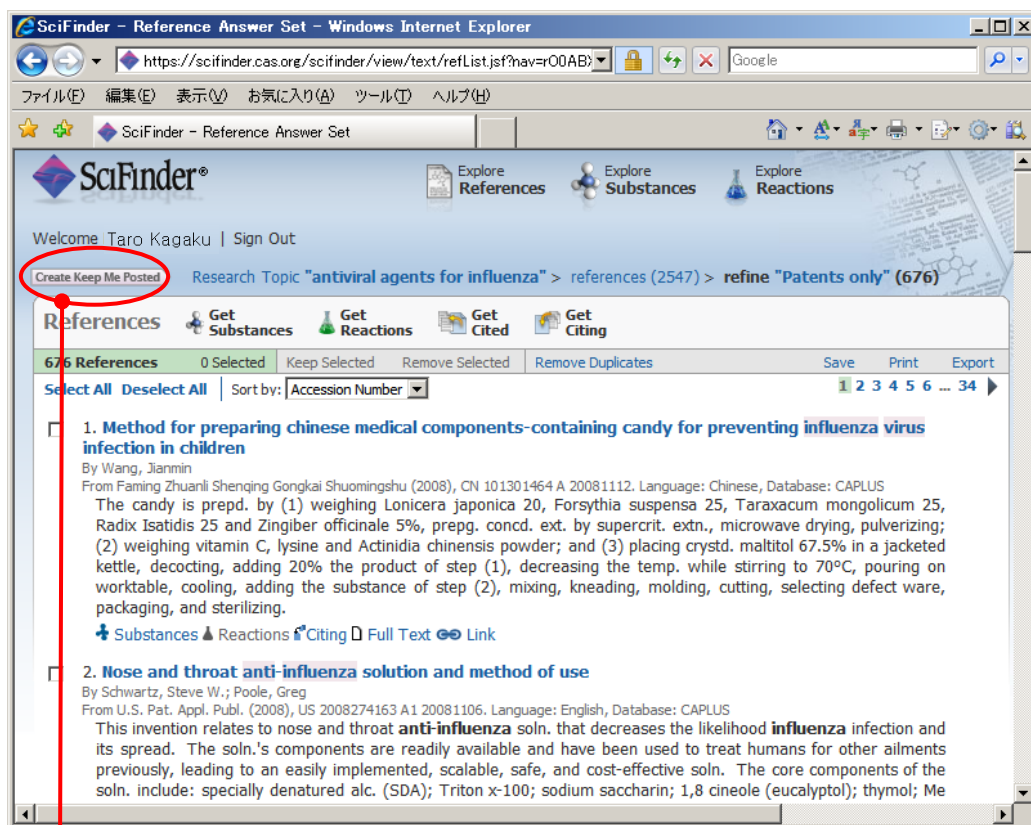
- You can use “JACS”, “J Am Chem Soc”, “Journal of the American Chemical Society” for journal name.
- Should there be any unintended references listed, you can exclude those by analyzing it by journal name..

Keep Me Posted Function

◆ Keep Me Posted Function (Alerts Search Function)



- You can get recent information by using “Keep Me Posted” (KMP) function that automatically performs a search periodically for queries registered previously.



Create Keep Me Posted Profile

* Required

Title:

Description:

Status: ☒ Enabled ☐ Disabled

☐ Exclude previously retrieved references.

Expiration Date:

Search Steps:

1. Explore references by research topic: **antiviral agents for influenza**
Candidates Selected:
 References which contain the two concepts "antiviral agents" and "influenza" closely associated with one another.
2. Reference refine by document type: **Patents only**

Create **Cancel**

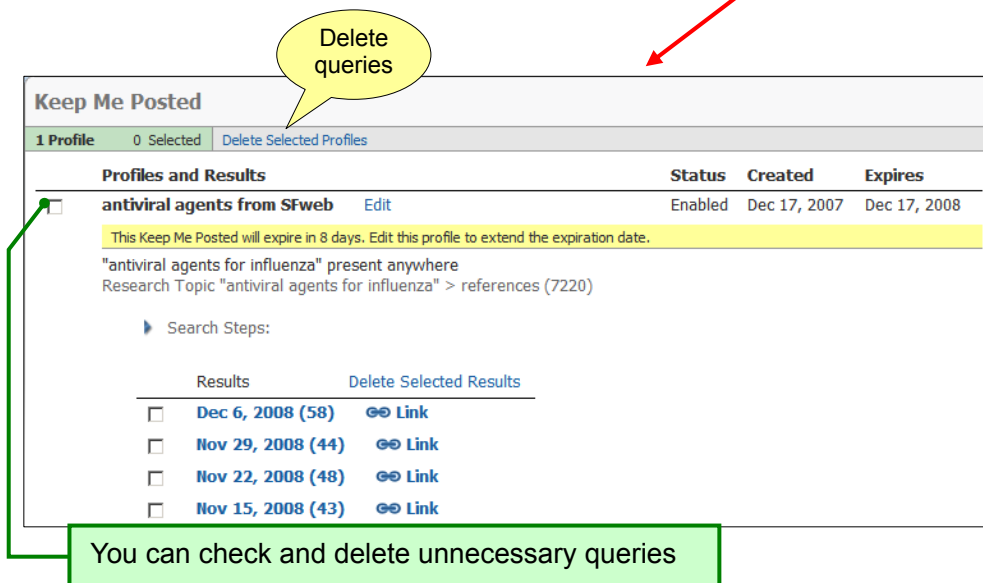
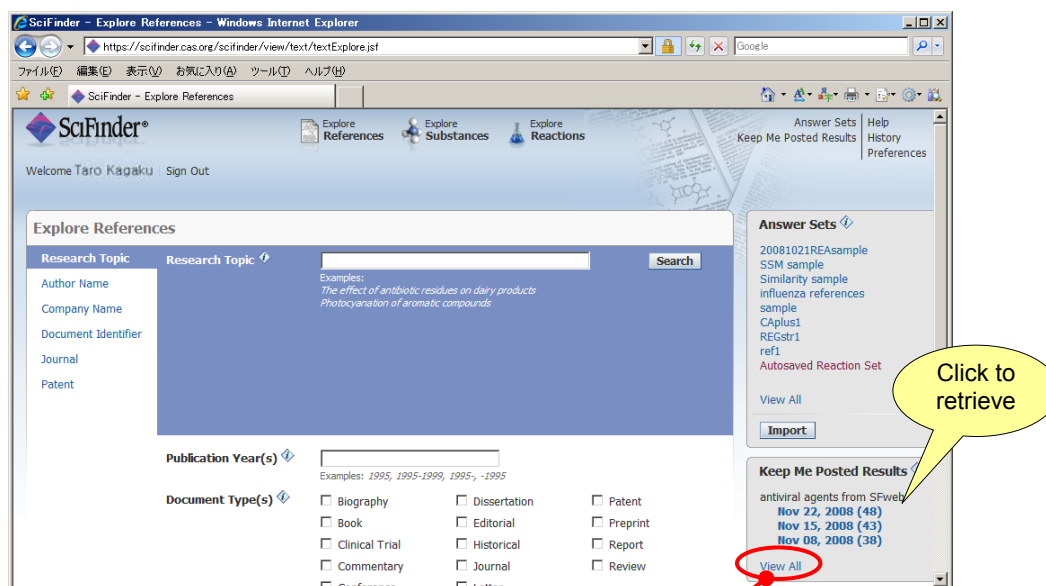
Alert expiry set to a date within 1 year.
Entry format is mm/d/y
(Example Dec 8, 2009)

If you don't check this box, you will get updated information with previously acquired results

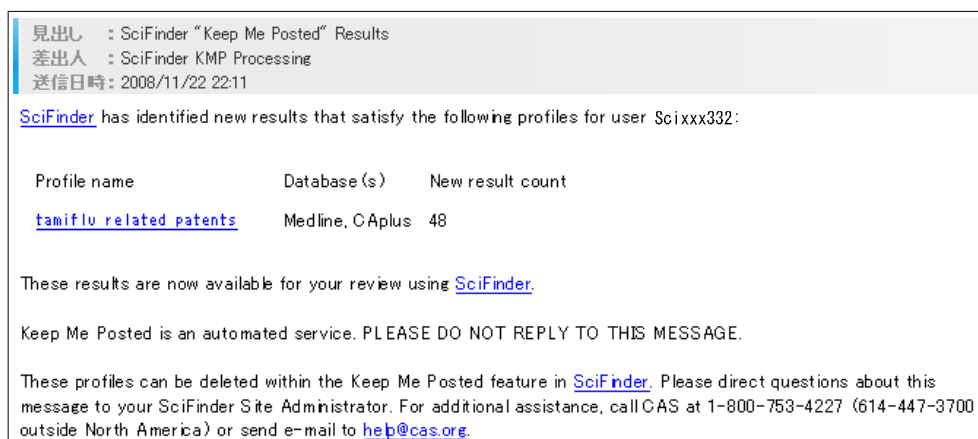
- Weekly search
- You can set it to send mail with the number of hits after the search (You can set it up in Preferences, and it will not send mail when there is no hit).
- Mail will be sent to the mail address registered with the user ID
- You cannot register the query in the result set where you cannot click the “Create Keep Me Posted” button

Keep Me Posted Function



- Retrieve result




- Submitted mail sample



Saving and Printing Results

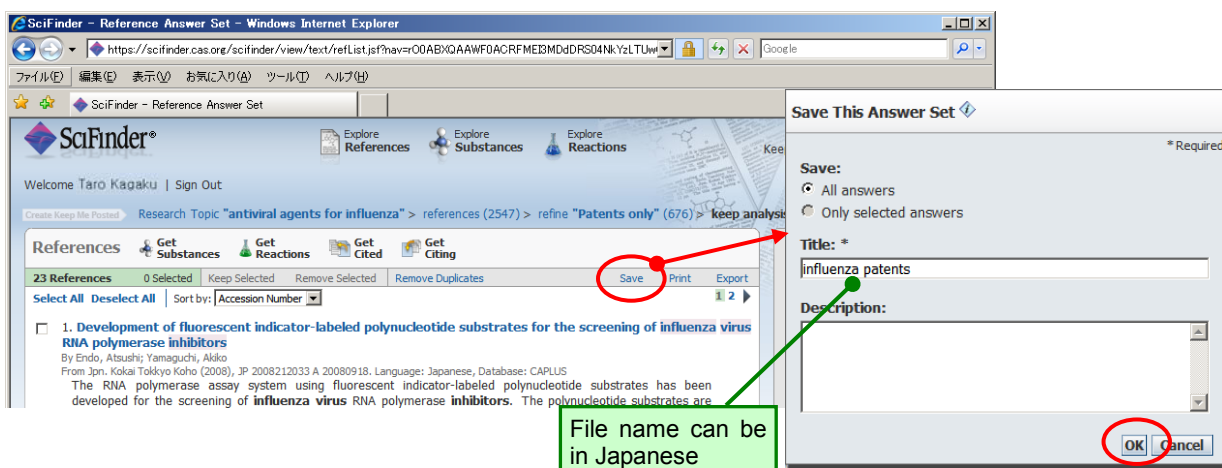
- ◆ Saving search result  

➤ There are three ways to save SciFinder results.

Save method	① Save to server 【 Recommended 】 
Description	Saving the data on the server (industries up to 100 records, universities up to 20 record)
Reproducing results with SciFinder	Possible
Maximum number of these items per save	20,000 items
Others	The structures with hits will be highlighted during reproductions, but the text hit term highlight or similarity score will not be displayed. When you are idle for 20 minutes, you will be automatically logout. The records created at that moment will be saved to the server automatically.

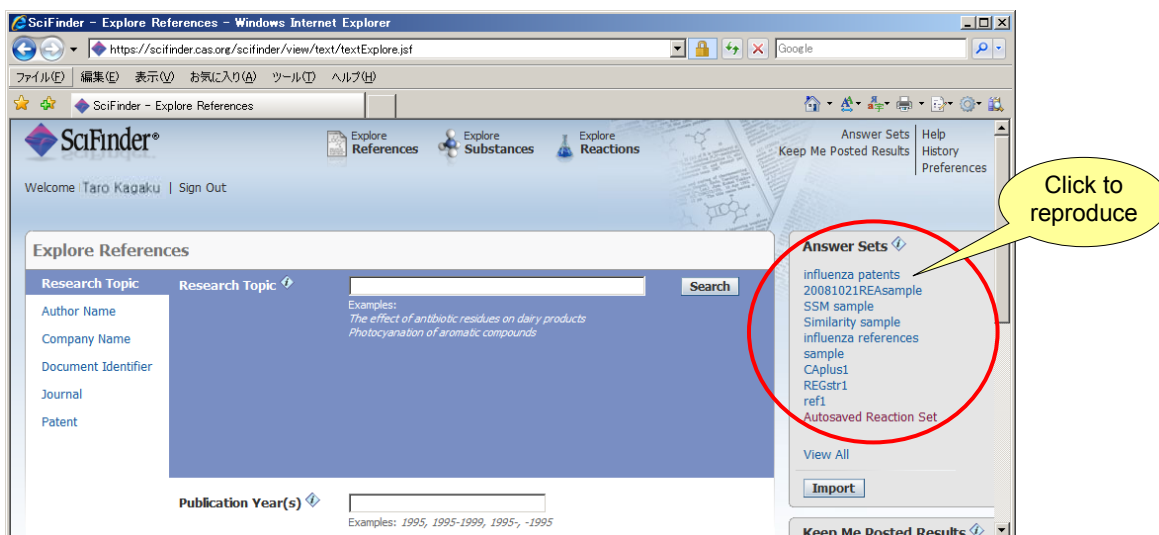
When you want to save items over the upper limit, segregate and refine your results with Refine function, and save after your items are within the allowable range.

- Saving results



File name can be in Japanese

- Retrieve results



Click to reproduce

Saving and Printing Results

Save method	② SciFinder Web Format Export	③ Download Export
Description	Save the result to hard disk in a format that can be reproduced with SciFinder later	Download the data to hard disk or other medias
File format	akx (Answers Key eXchange) format	PDF format and text format (comma delimited format or tab-delimited format)
Result reproduction with SciFinder	Possible	Impossible
Maximum per save	20,000 items	500 items (industry) 100 items (university)*
Usage Reminders	There are limitations on the saved result usage	There are limitations on the number of the downloaded data to save. *
Others	Queries are not saved, but highlights will be the same as saving to the server	Take longer to save, and file size will be larger compared to SciFinder Web format

* Limitations on the number of downloaded data to save.

③ In downloading, saving the results exceeding a total of 5,000 items is prohibited by the agreement. Make sure that you do not exceed 5,000 items by deleting unnecessary data.

● Saving results

File name using half-width English characters (Japanese not allowed)

Click to select format

Export

● Retrieve results

Click to choose a file

Import

Saving and Printing Results

◆ Printing search result [Print](#)

- Click Print link button (print up to 500 items in summary format, 100 items in detail format)

Print sample
(Reference)

The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'SciFinder - Reference Answer Set - Windows Internet Explorer'. Below it, the address bar shows the URL: 'https://scifinder.cas.org/scifinder/view/text/ref.list.jsf?nav=00ABX0AAWF0ACRFME3MD6DFSD4NkYsLTUw'. The main content area displays search results for 'Research Topic "antiviral agents for influenza" > references (2547) > refine "Patents only" (676) > keep analysis "Company/Organization" (23)'. The 'References' section is active, showing 23 references. A red circle highlights the 'Print' button in the top right of the results area, with a red arrow pointing to it from the bottom left. The first reference is titled '1. Development of fluorescent indicator-labeled polynucleotide substrates for the screening of influenza virus RNA polymerase inhibitors' by Endo, Atsushi; Yamaguchi, Akiko. The abstract mentions the use of fluorescent indicator-labeled polynucleotide substrates for screening influenza virus RNA polymerase inhibitors.

Search history will
also be printed

Print sample
(Substances)

Print sample
(Reactions)

SciFinder

1/8 ページ

Task History

Explore substances by substructure structure initiated

November 27, 2008 10:42 PM

Query

Explore complete

Explore results

Answer set 8 created with 9940 answers from REGISTRY

Refine Answer set 8 by commercial availability

includes commercially available

Answer set 10 created with 1041 answers from REGISTRY

Refine Answer set 10 by reference availability

includes 1 or more references

Answer set 12 created with 82 answers from REGISTRY

Keep 1/2 substance answers from Answer set 12 analyzed by "Substance Rule"

Answer set 13 created with 41 answers from REGISTRY

1. 932497-46-4

Cis H3x H6 O2

781 Thione-6-Carboxamide, 9-ethylthio-6-allylthio-2-[3-(hydroxyethylthio)-5-oxo-2-phenylthio]-4,5-dihydro-1,2,4-triazole-3-carboxamide (1-oxide) (1)

■ = 1 Reference

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1. 932359-20-0

C2x H2x H6 O2

784 Thione-6-Carboxamide, 5,8-dialkylthio-6-oxo-5-phenylthio-4,5-dihydro-1,2,4-triazole-3-carboxamide (1-oxide) (2)

■ = 1 Reference

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3. 863609-91-2

C2x H2x H6 O2

781 Thione-6-Carboxamide, 5,8-dialkylthio-6-oxo-5-phenylthio-4,5-dihydro-1,2,4-triazole-3-carboxamide (1-oxide) (2)

■ = 1 Reference

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4. 863609-41-0

5. 863502-35-6

6. 863502-06-1

C2x H2x H6 O2

See also

Task History

Explore reactions by substructure structures initiated

November 27, 2008 10:49 PM

Query

Explore complete
Explore results

Answer set 14 created with 91 answers from CASREACT

Refine Answer set 14 by product yield
(0)

Include answers that have no product yield

Answer set 15 created with 47 answers from CASREACT

Refine Answer set 15 by number of steps
(1)

Answer set 16 created with 27 answers from CASREACT

Keep 9 reaction answers from Answer set 16; analyze
Answer set 17 created with 9 answers from CASREACT

Scilinker

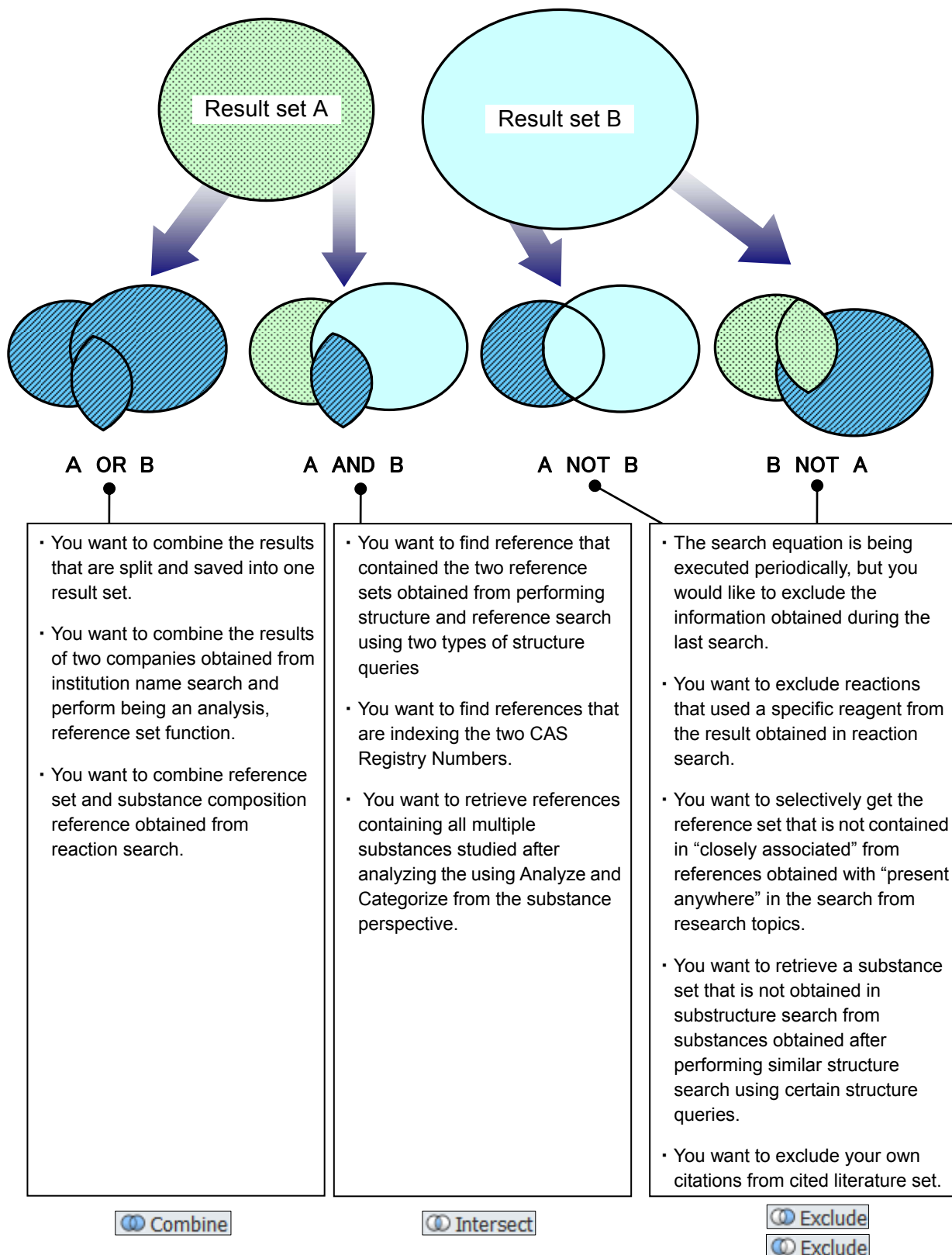
1, 2: R1R2C1=CC=CC=C1C2, 3: R1R2C1=CC=CC=C1C2, 4: R1R2C1=CC=CC=C1C2, 5: R1R2C1=CC=CC=C1C2, 6: R1R2C1=CC=CC=C1C2, 7: R1R2C1=CC=CC=C1C2, 8: R1R2C1=CC=CC=C1C2, 9: R1R2C1=CC=CC=C1C2, 10: R1R2C1=CC=CC=C1C2, 11: R1R2C1=CC=CC=C1C2, 12: R1R2C1=CC=CC=C1C2, 13: R1R2C1=CC=CC=C1C2, 14: R1R2C1=CC=CC=C1C2, 15: R1R2C1=CC=CC=C1C2, 16: R1R2C1=CC=CC=C1C2, 17: R1R2C1=CC=CC=C1C2, 18: R1R2C1=CC=CC=C1C2, 19: R1R2C1=CC=CC=C1C2, 20: R1R2C1=CC=CC=C1C2, 21: R1R2C1=CC=CC=C1C2, 22: R1R2C1=CC=CC=C1C2, 23: R1R2C1=CC=CC=C1C2, 24: R1R2C1=CC=CC=C1C2, 25: R1R2C1=CC=CC=C1C2, 26: R1R2C1=CC=CC=C1C2, 27: R1R2C1=CC=CC=C1C2, 28: R1R2C1=CC=CC=C1C2, 29: R1R2C1=CC=CC=C1C2, 30: R1R2C1=CC=CC=C1C2, 31: R1R2C1=CC=CC=C1C2, 32: R1R2C1=CC=CC=C1C2, 33: R1R2C1=CC=CC=C1C2, 34: R1R2C1=CC=CC=C1C2, 35: R1R2C1=CC=CC=C1C2, 36: R1R2C1=CC=CC=C1C2, 37: R1R2C1=CC=CC=C1C2, 38: R1R2C1=CC=CC=C1C2, 39: R1R2C1=CC=CC=C1C2, 40: R1R2C1=CC=CC=C1C2, 41: R1R2C1=CC=CC=C1C2, 42: R1R2C1=CC=CC=C1C2, 43: R1R2C1=CC=CC=C1C2, 44: R1R2C1=CC=CC=C1C2, 45: R1R2C1=CC=CC=C1C2, 46: R1R2C1=CC=CC=C1C2, 47: R1R2C1=CC=CC=C1C2, 48: R1R2C1=CC=CC=C1C2, 49: R1R2C1=CC=CC=C1C2, 50: R1R2C1=CC=CC=C1C2, 51: R1R2C1=CC=CC=C1C2, 52: R1R2C1=CC=CC=C1C2, 53: R1R2C1=CC=CC=C1C2, 54: R1R2C1=CC=CC=C1C2, 55: R1R2C1=CC=CC=C1C2, 56: R1R2C1=CC=CC=C1C2, 57: R1R2C1=CC=CC=C1C2, 58: R1R2C1=CC=CC=C1C2, 59: R1R2C1=CC=CC=C1C2, 60: R1R2C1=CC=CC=C1C2, 61: R1R2C1=CC=CC=C1C2, 62: R1R2C1=CC=CC=C1C2, 63: R1R2C1=CC=CC=C1C2, 64: R1R2C1=CC=CC=C1C2, 65: R1R2C1=CC=CC=C1C2, 66: R1R2C1=CC=CC=C1C2, 67: R1R2C1=CC=CC=C1C2, 68: R1R2C1=CC=CC=C1C2, 69: R1R2C1=CC=CC=C1C2, 70: R1R2C1=CC=CC=C1C2, 71: R1R2C1=CC=CC=C1C2, 72: R1R2C1=CC=CC=C1C2, 73: R1R2C1=CC=CC=C1C2, 74: R1R2C1=CC=CC=C1C2, 75: R1R2C1=CC=CC=C1C2, 76: R1R2C1=CC=CC=C1C2, 77: R1R2C1=CC=CC=C1C2, 78: R1R2C1=CC=CC=C1C2, 79: R1R2C1=CC=CC=C1C2, 80: R1R2C1=CC=CC=C1C2, 81: R1R2C1=CC=CC=C1C2, 82: R1R2C1=CC=CC=C1C2, 83: R1R2C1=CC=CC=C1C2, 84: R1R2C1=CC=CC=C1C2, 85: R1R2C1=CC=CC=C1C2, 86: R1R2C1=CC=CC=C1C2, 87: R1R2C1=CC=CC=C1C2, 88: R1R2C1=CC=CC=C1C2, 89: R1R2C1=CC=CC=C1C2, 90: R1R2C1=CC=CC=C1C2, 91: R1R2C1=CC=CC=C1C2, 92: R1R2C1=CC=CC=C1C2, 93: R1R2C1=CC=CC=C1C2, 94: R1R2C1=CC=CC=C1C2, 95: R1R2C1=CC=CC=C1C2, 96: R1R2C1=CC=CC=C1C2, 97: R1R2C1=CC=CC=C1C2, 98: R1R2C1=CC=CC=C1C2, 99: R1R2C1=CC=CC=C1C2, 100: R1R2C1=CC=CC=C1C2, 101: R1R2C1=CC=CC=C1C2, 102: R1R2C1=CC=CC=C1C2, 103: R1R2C1=CC=CC=C1C2, 104: R1R2C1=CC=CC=C1C2, 105: R1R2C1=CC=CC=C1C2, 106: R1R2C1=CC=CC=C1C2, 107: R1R2C1=CC=CC=C1C2, 108: R1R2C1=CC=CC=C1C2, 109: R1R2C1=CC=CC=C1C2, 110: R1R2C1=CC=CC=C1C2, 111: R1R2C1=CC=CC=C1C2, 112: R1R2C1=CC=CC=C1C2, 113: R1R2C1=CC=CC=C1C2, 114: R1R2C1=CC=CC=C1C2, 115: R1R2C1=CC=CC=C1C2, 116: R1R2C1=CC=CC=C1C2, 117: R1R2C1=CC=CC=C1C2, 118: R1R2C1=CC=CC=C1C2, 119: R1R2C1=CC=CC=C1C2, 120: R1R2C1=CC=CC=C1C2, 121: R1R2C1=CC=CC=C1C2, 122: R1R2C1=CC=CC=C1C2, 123: R1R2C1=CC=CC=C1C2, 124: R1R2C1=CC=CC=C1C2, 125: R1R2C1=CC=CC=C1C2, 126: R1R2C1=CC=CC=C1C2, 127: R1R2C1=CC=CC=C1C2, 128: R1R2C1=CC=CC=C1C2, 129: R1R2C1=CC=CC=C1C2, 130: R1R2C1=CC=CC=C1C2, 131: R1R2C1=CC=CC=C1C2, 132: R1R2C1=CC=CC=C1C2, 133: R1R2C1=CC=CC=C1C2, 134: R1R2C1=CC=CC=C1C2, 135: R1R2C1=CC=CC=C1C2, 136: R1R2C1=CC=CC=C1C2, 137: R1R2C1=CC=CC=C1C2, 138: R1R2C1=CC=CC=C1C2, 139: R1R2C1=CC=CC=C1C2, 140: R1R2C1=CC=CC=C1C2, 141: R1R2C1=CC=CC=C1C2, 142: R1R2C1=CC=CC=C1C2, 143: R1R2C1=CC=CC=C1C2, 144: R1R2C1=CC=CC=C1C2, 145: R1R2C1=CC=CC=C1C2, 146: R1R2C1=CC=CC=C1C2, 147: R1R2C1=CC=CC=C1C2, 148: R1R2C1=CC=CC=C1C2, 149: R1R2C1=CC=CC=C1C2, 150: R1R2C1=CC=CC=C1C2, 151: R1R2C1=CC=CC=C1C2, 152: R1R2C1=CC=CC=C1C2, 153: R1R2C1=CC=CC=C1C2, 154: R1R2C1=CC=CC=C1C2, 155: R1R2C1=CC=CC=C1C2, 156: R1R2C1=CC=CC=C1C2, 157: R1R2C1=CC=CC=C1C2, 158: R1R2C1=CC=CC=C1C2, 159: R1

Search history will
also be printed

Combine Function機能

◆ Combine function Combine Answer Sets

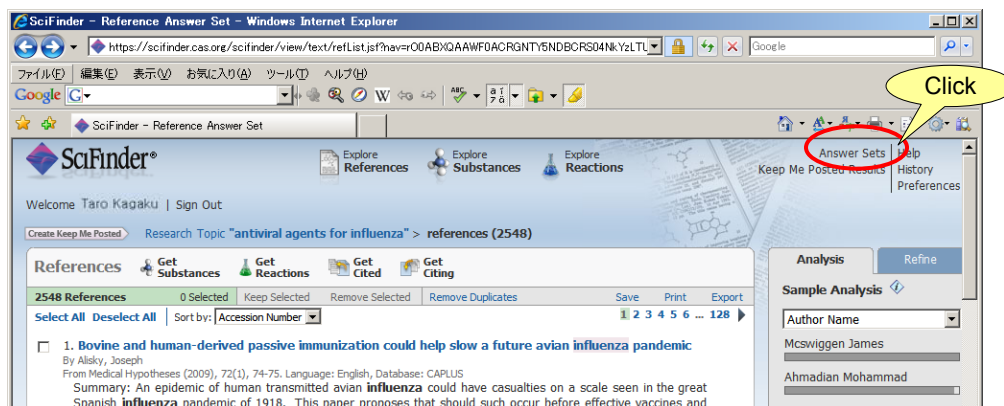
- You can assign operators among result sets obtained with SciFinder. By using this function, you will be able to combine the results split into a number of sets and saved, exclude the results obtained previously, and look at only the information recently obtained.



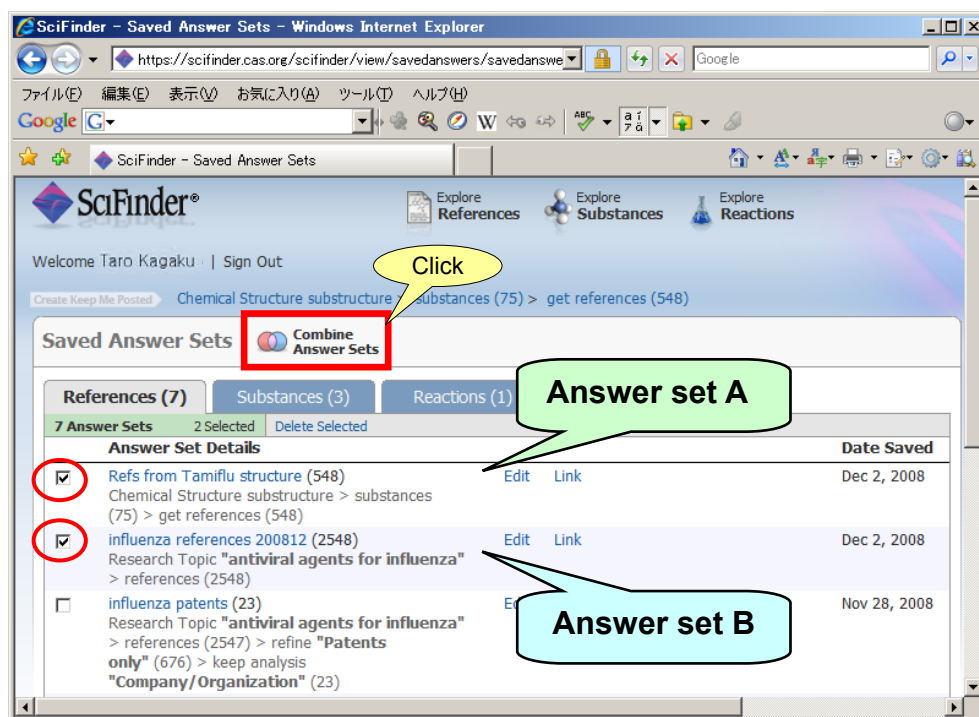
Note: Results that can be assigned operators are limited to substance record sets, reference record sets and reaction record sets.

Combine Function

- ① Save to the server all the answer sets you want to combine (→ p41).
- ② Click the “Answer Sets” at the screen top right, and list screen of answer sets will be displayed.



- ③ Check all the sets you want to combine, and click “Combine Answer Sets”. You can select more than three sets.



Combine Function

- ④ Select the operators you want to execute. In a combination of 3 sets and more, Exclude (NOT operator) option is not displayed (→ p47).

Combine Answer Sets

Select an option for combining the two selected saved answer sets:

☐ ☒ Combine - Include all references from both sets

☐ ☒ Intersect - Include only references that appear in both sets

☐ ☒ Exclude - Include only answers from Refs from Tamiflu structure that are not in influenza references 200812

☐ ☒ Exclude - Include only answers from influenza references 200812 that are not in Refs from Tamiflu structure

☐ Remove duplicate references

Combine Answer Sets **Cancel**

OR Operator (Combine sets)

AND Operator (Intersect sets)

NOT Operator: Difference of sets (A) – (B)

NOT Operator: Difference of sets (B) – (A)

- ⑤ Operation results are displayed. You can perform restriction or analysis later.

The screenshot shows the SciFinder web interface. The main content area displays a list of references under the heading 'Combine Reference Answer Sets "influenza references 200812 AN..."'. The first reference is '1. Design of Multi-Binding-Site Inhibitors, Ligand Efficiency, and Consensus Screening of Avian Influenza H5N1 Wild-Type Neuraminidase and of the Oseltamivir-Resistant H274Y Variant' by Garcia-Sosa, Alfonso T.; Sild, Sulev; Maran, Uko. The second reference is '2. Limited inhibitory effects of oseltamivir and zanamivir on human sialidases' by Hata, Keiko; Koseki, Koichi; Yamaguchi, Kazunori; Moriya, Setsuko; Suzuki, Yasuo; Yingsakmongkon, Sangchai; Hirai, Go; Sodeoka, Mikiko; von Itzstein, Mark; Miyagi, Taeko. The right sidebar shows an 'Analysis' section with a bar chart of author frequencies, listing authors like Hayden Frederick G (15), Kashiwagi Seizaburo (10), Sugaya Norio (10), Ward Penelope (10), Sidwell Robert W (9), Kim Choung U (8), Webster Robert G (8), and Gubareva Larisa V (7).

♣ System limitation information

- Highlights during search will not be reflected.
- Keep Me Posted registration cannot be done for sets after operation.
- The similar structure search score will not be displayed.

Combine Function

* As mentioned in □ previous page, when you select 3 or more sets, operator selection screen will be as shown below.

Combine Answer Sets

Select an option for combining the selected saved answer sets:

☒ Combine - Include all references from all selected answers

☐ Intersect - Include only references that appear in all selected sets

☐ Remove duplicate references

OR Operator (Combine sets)

AND Operator (Intersect sets)

Combine Answer Sets

Cancel

◆ Reference Information: SciFinder user case example

Japan Association for International Chemical Information is introducing SciFinder user case examples at the SciFinder site. Please make sure to refer to it. For those who are interested in data collection, please contact our information division.

<http://www.jaici.or.jp/sci/SCIFINDER/user.html>

社会法人化学情報協会 JAICI | 製品とサービス | SciFinder | ユーザー事例 | - Windows Internet Explorer

http://www.jaici.jp/sci/SCIFINDER/user.html

Google

ファイル(E) 編集(E) 表示(V) お気に入り(A) ツール(T) ヘルプ(H)

Google G

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English

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SciFinder

科学関連情報が必要とする企業や政府機関等の研究者向けオンライン検索サービスです。

SciFinder のトップへ

SciFinder

Part of the process.™

お申込方法
サービス時間
必要なシステム環境
ユーザー事例
技術資料
検索例
よくあるご質問
ヘルプデスク
データ利用制限
myCAS

原稿提供サービス
CAS 原稿提供サービス
ChemPort

ユーザー事例

SciFinder をご利用いただいているユーザー事例が雑誌に掲載されました。下記に記事を PDF 形式でご用意いたしましたのでご参照ください。

エーザイ(株)	日経サイエンス 2008 年 8 月号掲載
金沢大学	金沢大学附属図書館報「こだま」2008 年 4 月号掲載
リンク・ジェノミクス(株)	日経サイエンス 2008 年 4 月号掲載
独立行政法人理化学研究所	ユーザー事例 (実験医学 2008 年 2 月号掲載) シリーズ記事2 (実験医学 2008 年 1 月号掲載) シリーズ記事1 (実験医学 2007 年 12 月号掲載)
三井農林(株)	日経サイエンス 2008 年 2 月号掲載
新日本理化(株)	日経サイエンス 2007 年 8 月号掲載
(株)ニチロ	日経サイエンス 2007 年 2 月号掲載
セントラル硝子(株)	日経サイエンス 2006 年 8 月号掲載
長瀬産業(株)	日経サイエンス 2006 年 2 月号掲載
石原産業(株)	日経サイエンス 2005 年 8 月号掲載
日本化薬(株)	日経サイエンス 2005 年 2 月号掲載
(株)ナード研究所	日経サイエンス 2004 年 8 月号掲載

APPENDIX

◆ Reference information containing Chemical Abstracts

SciFinder has been selectively compiling reference information related to substances from approximately 10,000 scientific journals and patents. A wide spectrum of references related to research that used substances, not only chemistry, but from physics to biology are being compiled. Among these journals, SciFinder has been compiling all articles since 1994 from 1,900 major journals.

○ Examples

◆ Physics

- Journal of Applied Physics
- Physical Review (A, B, C, D, E)
- Physical Review Letters
- European Physical Journal (A, B, C, D, E)
- Physics Letters (A, B)
- Journal of Experimental and Theoretical Physics
- Journal of Chemical Physics
- Japanese Journal of Applied Physics (Part 1, 2)

◆ Chemistry

- Journal of the American Chemical Society
- Journal of Physical Chemistry (A, B)
- Macromolecules
- Journal of Organic Chemistry
- Tetrahedron Letters
- Chemistry of Materials
- Journal of the Electrochemical Society
- Solid State Ionics

◆ Environmental Sciences

- Chemosphere
- Environmental Pollution (Amsterdam, Netherlands)
- Journal of Environmental Quality
- Environmental Science and Technology
- Environmental Toxicology and Pharmacology
- Journal of Environmental Science & Engineering
- Water Environment Research
- Water Research

◆ Biology

- Cell
- Molecular Biology of the Cell
- Molecular Biology and Evolution
- Journal of Biochemistry
- Plant Physiology
- Journal of Cell Biology
- Brain Research
- Nucleic Acids Research

◆ Pharmaceutical

- Bioorganic & Medicinal Chemistry
- Bioorganic & Medicinal Chemistry Letters
- Basic & Clinical Pharmacology & Toxicology
- Chemical & Pharmaceutical Bulletin
- European Journal of Pharmaceutical Sciences
- British Journal of Pharmacology
- Journal of Pharmaceutical Sciences
- Pharmaceutical Development and Technology

◆ Medicine

- Annual Review of Medicine
- Birth Defects Research, Part A, B
- New England Journal of Medicine
- Clinical and Diagnostic Laboratory Immunology
- Nature Medicine (New York, NY, United States)
- Experimental and Clinical Endocrinology & Diabetes
- Experimental and Molecular Medicine
- Journal of Clinical Investigation

◆ Agriculture & Nutrition

- Experimental Animals
- Journal of Insect Physiology
- Journal of Animal Science (Savoy, IL, U. S.)
- Journal of Agricultural and Food Chemistry
- Journal of Oleo Science
- Journal of Nutritional Science and Vitaminology
- Journal of the Science of Food and Agriculture
- Fisheries Science (Carlton, Australia)

◆ Material Science & Engineering

- Materials Science & Engineering (A, B, C)
- Biomacromolecules
- Journal of Biomedical Materials Research (A, B)
- Journal of Material Science
- International Journal of Hydrogen Energy
- Journal of the American Ceramic Society
- Materials Transactions
- Particulates and Powder Metallurgy

◆ Electrical and Electronic Engineering

- Applied Surface Science
- Ferroelectrics
- IEEE Journal of Quantum Electronics
- Journal of Electronic Materials
- Journal of Vacuum Science & Technology, B
- Quantum Electronics
- Microelectronic Engineering
- Superconductor Science and Technology

◆ Mechanical Engineering

- Corrosion Science
- Materials Science and Technology
- Journal of Thermophysics and Heat Transfer
- Combustion Science and Technology
- Archivum Combustionis
- ISIJ International
- Wear
- Journal of Japan Institute of Metals

You can view a list of published major journals at the following site

<http://www.cas.org/expertise/cascontent/caplus/corejournals.html>

APPENDIX

◆ Chemical Abstracts Compiling Division (CA section list)

- Compiled divisions are entered in reference record one by one (see page 4).
- Compiled divisions can also be used in refining references (see page 19).

Biochemistry

1. Pharmacology
2. Mammalian Hormones
3. Biochemical Genetics
4. Toxicology
5. Agrochemical Bioregulators
6. General Biochemistry
7. Enzymes
8. Radiation Biochemistry
9. Biochemical Methods
10. Microbial, Algal, and Fungal Biochemistry
11. Plant Biochemistry
12. Nonmammalian Biochemistry
13. Mammalian Biochemistry
14. Mammalian Pathological Biochemistry
15. Immunochemistry
16. Fermentation and Bioindustrial Biochemistry
17. Food and Feed Chemistry
18. Animal Nutrition
19. Fertilizers, Soils, and Plant Nutrition
20. History, Education, and Documentation

Organic Chemistry

21. General Organic Chemistry
22. Physical Organic Chemistry
23. Aliphatic Compounds
24. Alicyclic Compounds
25. Benzene, Its Derivatives, and Condensed Benzenoid Compounds
26. Biomolecules and Their Synthetic Analogs
27. Heterocyclic Compounds (One Hetero Atom)
28. Heterocyclic Compounds (More Than One Hetero Atom)
29. Organometallic and Organometalloidal Compounds
30. Terpenes and Terpenoids
31. Alkaloids
32. Steroids
33. Carbohydrates
34. Amino Acids, Peptides, and Proteins

High Polymers Chemistry

35. Chemistry of Synthetic High Polymers
36. Physical Properties of Synthetic High Polymers
37. Plastics Manufacture and Processing
38. Plastics Fabrication and Uses
39. Synthetic Elastomers and Natural Rubber
40. Textiles and Fibers
41. Dyes, Organic Pigments, Fluorescent
42. Coatings, Inks, and Related Products
43. Cellulose, Lignin, Paper, and Other Wood Products
44. Industrial Carbohydrates
45. Industrial Organic Chemicals, Leather, Fats, and Waxes
46. Surface-Active Agents and Detergents

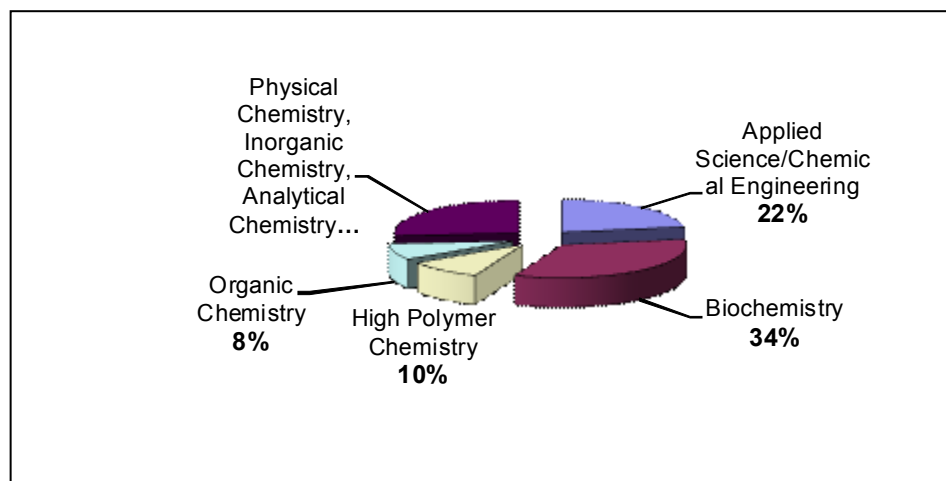
APPENDIX

Applied Chemistry and Chemical Engineering

47. Apparatus and Plant Equipment
48. Unit Operations and Processes
49. Industrial Inorganic Chemicals
50. Propellants and Explosives
51. Fossil Fuels, Derivatives, and Related Products
52. Electrochemical, Radiational, and Thermal Energy Technology
53. Mineralogical and Geological Chemistry
54. Extractive Metallurgy
55. Ferrous Metals and Alloys
56. Nonferrous Metals and Alloys
57. Ceramics
58. Cement, concrete, and Related Building Materials
59. Air Pollution and Industrial Hygiene
60. Waste Treatment and Disposal
61. Water
62. Essential Oils and Cosmetics
63. Pharmaceuticals
64. Pharmaceutical Analysis

Physical Chemistry, Inorganic Chemistry and Analytical Chemistry

65. General Physical Chemistry
66. Surface Chemistry and Colloids
67. Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms
68. Phase Equilibria, Chemical Equilibria, and Solutions
69. Thermodynamics, Thermochemistry, and Thermal Properties
70. Nuclear Phenomena
71. Nuclear Technology
72. Electrochemistry
73. Optical, Electron, and Mass Spectroscopy and Other Related Properties
74. Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes
75. Crystallography and Liquid Crystals
76. Electric Phenomena
77. Magnetic Phenomena
78. Inorganic Chemicals and Reactions
79. Inorganic Analytical Chemistry
80. Organic Analytical Chemistry



SciFinder Environment

◆ Requirements to use SciFinder (Web version)

Refer to following URL for current information about the Recommended OS and browser.
<http://www.cas.org/support/scifi/sysreqs.html>

- Recommended OS and browser (Tested OS and browser) (As of June 2010)

Recommended OS	Recommended browser
Windows XP Professional * (SP1 or later)	Internet Explorer 7.0 • 8.0 Firefox 3.0 • 3.5
Windows Vista * (Business, Enterprise, Ultimate)	Internet Explorer 7.0 • 8.0 Firefox 3.0 • 3.5
Mac OS X 10.4.11	Firefox 3.0 • 3.5 Safari 3.x • 4.0
Mac OS X 10.5 and 10.6	Firefox 3.0 • 3.5 Safari 3.x • 4.0

*Windows 64bit OS is not supported.

- Java and Java Script enabled
 (Java plugin (Java Runtime Environment (JRE) 5 or later) Installation is required)
<http://www.cas.org/misc/downloads/jreplugin.html> (English)
- Cookies enabled
- ActiveX enabled (For Internet Explorer)

ActiveX control and plugin	Internet Explorer 7 • 8
ActiveX control and plugin execution	Enabled
ActiveX display dialog for ActiveX control	Disabled
Scriptlets permission	Disabled
Run ActiveX that is not marked safe even after running the script	Disabled
Run ActiveX that is marked safe even after running the script	Enabled
Binary behavior and script behavior	Enabled
Display Web page video or animation that is not using external media player	Disabled
Download signed ActiveX control	Display dialog
Allow ActiveX control not used previously to run without warning.	Disabled
Download unsigned ActiveX control	Disabled

◆ Support (Help Desk)

Please do not hesitate to contact our help desk should you have any questions regarding SciFinder (Web Version). You can phone, fax or e-mail your questions (see cover page for our contact number).