

# SciFinder Start-up Guidance

Hokkaido University  
Northern Campus Library  
October 2019



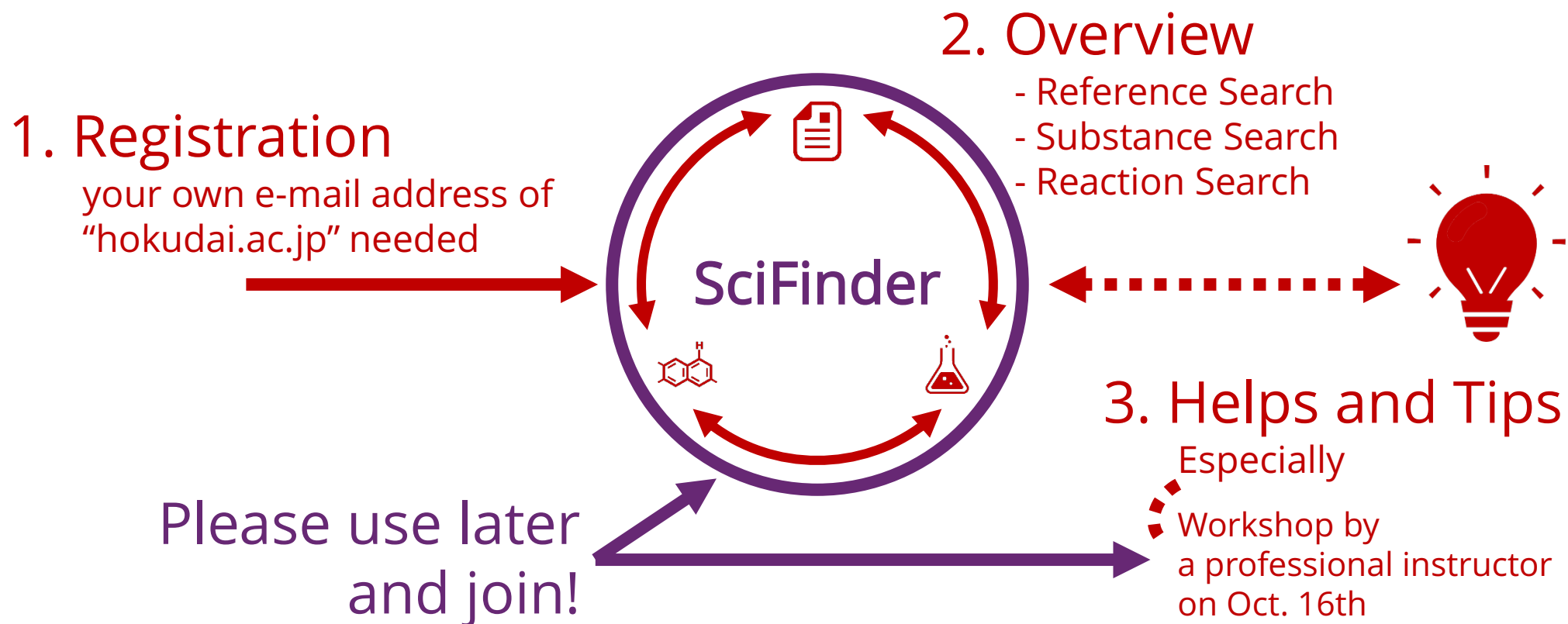
# SciFinder Start-up Guidance

## SciFinder

- an online database provided by CAS (Chemical Abstract Service), a division of ACS (American Chemical Society)
- provides information of
  - References (papers, conference papers, patents ...)
  - Substances (containing all CAS Registry Number)
  - Reactions ...
- requires one account per person

# SciFinder Start-up Guidance

From the perspective of a non-chemist



# 1. Registration










<https://www.lib.hokudai.ac.jp/en>





[Humanities / Social Sciences / Life Sciences / Medical / Science and Engineering / All / End Note Basic, Mendeley institutional version \(to research support page\)](#)





● Find Databases by Keywords (for words contained within the title or de

Search

● Popular Databases

- [\[Web of Science Core Collection\]](#)  : articles & cited references from major journals worldwide ([More Info](#))
- [\[CINII\]](#)  : article database provided by the National Institute of Informatics ([More Info](#))
- [\[SciFinder Web\]](#)  : chemistry and other scientific information from articles and patents ([More Info](#))
- [\[Reaxys\]](#)  : chemical compounds, bibliographic data and chemical reactions ([More Info](#))
- [\[Japana Centra Revuo Medicina\]](#)  : medical and nursing science articles ([More Info](#))
- [\[MEDLINE EBSCOhost\]](#) : international literature on biomedicine and health care ([More Info](#))
- [\[PubMed HOKUDAI ver.\]](#)   ⇒ It is provided by the National Medical Library ([More Info](#))
- [\[WESTLAW JAPAN\]](#)  ⇒ Westlaw Japan's legal information online service ([More Info](#))
- [\[LEX/DB Internet\]](#) : full text of cases since 1875 (Meiji 8) ([More Info](#))
- [\[Nikkei BP article search service\]](#)  : full text of articles in Nikkei BP's magazines ([More Info](#))

Site map  FAQ  Contacts  Access  Japanese

Learning/Teaching  Research Support Information  About Library  Link to Branches Libraries 

Remote Access

Tadoku Marathon

E-Journals

E-Books

Databases

Northern studies collection

HUSCAP

The Class of made-to-order

Contribution

summer vacation (August 6, 2019 to September 26, 2019)

more

サイト内検索

Google カスタム検索

Search

# 1. Registration

HOME > English HOME > Databases > Database List

Result: 1 hit  
[TOP] [Explanation of table] [Sort: (interior/abroad) > (ABC:title)]

## SciFinder<sup>R</sup> Navi

### [Chemistry] Bibliographies/Abstracts/Index, Cited References

Limit on Number of Users: Unlimited	Chemistry
-------------------------------------	-----------

**CAS Information Use Policies - CAS Information Use Policies (Japanese, PDF)**  
Database to access chemistry and other scientific information provided by CAS (Chemical Abstracts Service).  
Information on chemical substances, in addition to **CAPLUS** files, organic chemical reactions, commercially available chemicals, regulations on chemical substances, chemical-related patents and medical documents (MEDLINE) are provided.  
**\*First you need to create your own username and password. Please register [here](#).**

- [User registration guide \(PDF\)](#)
- [SciFinder Training Materials](#)

JAICI Science Dictionary is a Japanese-English / English-Japanese bilingual dictionary and thesaurus for improving convenience in SciFinder search. It contains technical terms gathered from domestic and international papers and patent information related to chemistry, medicine and pharmaceutical science.


Remo  
Tadoku  
E-J  
E-  
Dat  
Northern st  
HU  
The Class of  
Cont

Q サイ  
Google カス  
Search

... or access →




# 1. Registration



**Welcome to User Registration for SciFinder®**

Click Next to begin registration as a new user.

**Next >>**



**License Agreement**

SciFinder® is for Educational use ONLY.  
Commercial use of your University account is strictly prohibited.


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

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

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

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

**Accept** **Decline**



**Registration Information**

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

**Contact Information**

First Name\*:

Last Name\*:

**Email\***

**Confirm Email\***

Phone Number:

Fax Number:

Area of Research\*:

Job Title\*:

**Username and Password**

**Username\***

**Password\***

Re-enter Password\*:

**Security Information**

Security Question\*:

Answer\*:

xxx@xxx.hokudai.ac.jp  
\* unavailable: @frontier.hokudai.ac.jp

5 - 15 half-width characters  
\* available: - \_ . @

7 - 15 half-width characters  
AND  
including 3 types  
of the followings:  
- Uppercase letter(s)  
- Lowercase letter(s)  
- Number(s)  
- @ # % & \* ...

# 1. Registration

After clicking the link in **the e-mail** from CAS,  
access <http://scifinder.cas.org>



## Sign In

Username

Password

☐ Keep me signed in  
(Do not use on a shared computer)

[Forgot Username or Password?](#)

By using SciFinder®, you agree to the [License Agreements and Policies](#)

**New to SciFinder?**  
[Learn more about gaining access to SciFinder.](#)

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



## News & Updates

**Welcome to SciFinder!**

SciFinder<sup>®</sup> is here!

Learn more about the power of n.

Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

**Join ACS now!**  
The American Chemical Society is committed to supporting its members with the resources they need to grow professionally, build knowledge, connect with colleagues around the world, and stay on top of all the latest developments in the chemical sciences.

**Shape the Future of SciFinder**

Help shape the future of scientific discovery and [sign up to share your insights](#) on upcoming SciFinder enhancements.



## 2. Overview

The screenshot displays the SciFinder web interface. On the left, a sidebar contains three main search categories: REFERENCES, SUBSTANCES, and REACTIONS, each with a list of sub-options. The REFERENCES category is highlighted with a red box. The main content area shows the 'REFERENCES: RESEARCH TOPIC' search interface, including a search bar, a 'Search' button, and an 'Advanced Search' link. Below the search bar, there are icons for a document, a chemical structure, and a reaction flask. A diagram in the center of the page illustrates the cross-linking of search results: a document icon at the top is connected by red arrows to a chemical structure icon at the bottom left and a reaction flask icon at the bottom right, which are also connected to each other by a red arrow, forming a circular flow.

REFERENCES: RESEARCH TOPIC

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

Search

Advanced Search

REFERENCES: RESEARCH TOPIC

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

SUBSTANCES

Chemical Structure  
Markush  
Molecular Formula  
Property  
Substance Identifier

REACTIONS

Reaction Structure

SAVED ANSWER SETS

You have no saved answer sets.

Learn how to:  
Create Saved Answer Sets

Import

KEEP ME POSTED

You have no profiles.

Learn how to:  
Create Keep Me Posted

You can move from one search category to the others.  
For example, after you find a reference,  
you can also find the substances and reactions mentioned on it.



## 2. Overview

CAS Solutions  
**SciFinder**  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Hiroyuki Chiba

Explore | Saved Searches | SciPlanner

**REFERENCES**

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


**SUBSTANCES**

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

**REACTIONS**

- Reaction Structure

**REFERENCES: RESEARCH TOPIC**



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

**Search**

[Advanced Search](#)

**Publication Years**

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

**Document Types**

<input type="checkbox"/> Biography	<input type="checkbox"/> Historical
<input type="checkbox"/> Book	<input type="checkbox"/> Journal
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Letter
<input type="checkbox"/> Commentary	<input type="checkbox"/> Patent
<input type="checkbox"/> Conference	<input type="checkbox"/> Preprint
<input type="checkbox"/> Dissertation	<input type="checkbox"/> Report
<input type="checkbox"/> Editorial	<input type="checkbox"/> Review

**Languages**

<input type="checkbox"/> Chinese	<input type="checkbox"/> Japanese
<input type="checkbox"/> English	<input type="checkbox"/> Polish
<input type="checkbox"/> French	<input type="checkbox"/> Russian
<input type="checkbox"/> German	<input type="checkbox"/> Spanish
<input type="checkbox"/> Italian	

**Author**

Last Name *	First	Middle
<input type="text"/>	<input type="text"/>	<input type="text"/>

**Company**

Examples:  
Minnesota Mining and Manufacturing  
DuPont

**SAVED ANSWER SETS**

You have no saved answer sets.

Learn how to:  
[Create Saved Answer Sets](#)

[Import](#)

**KEEP ME POSTED**

You have no profiles.

Learn how to:  
[Create Keep Me Posted](#)

## 2. Overview

The image shows a screenshot of the SciFinder web interface. The main search area is titled "REFERENCES: RESEARCH TOPIC" and contains a search bar with the text "suzuki coupling". Below the search bar are examples of search results: "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds". A red arrow points from the "Search" button to a detailed view of the search results.

The detailed view shows the search results for "suzuki coupling". It includes a table with two columns: "Research Topic" and "References". The table lists two results:

Research Topic	References
20525 references were found containing "suzuki coupling" as entered.	
26519 references were found containing the concept "suzuki coupling".	

A red box highlights the table content. The interface also includes a sidebar with navigation options like "REFERENCES", "SUBSTANCES", and "REACTIONS". The top navigation bar includes "Explore", "Saved Searches", and "SciPlanner". The bottom right corner shows a "Get References" button.

## 2. Overview

**Sort the results by:**

- Accession Number
- Author Name
- Citing References
- Publication Year
- Title

**Refine the results by:**

- Research Topic
- Author
- Company Name
- Publication Year
- Language
- Database

Research Topic "suzuki coupling" > references (26519)

REFERENCES ?

Analyze **Refine** Categorize

Sort by: Accession Number

0 of 26519 References Selected

Sample Analysis: ?

Author Name

Zhou Mingjie ≥ 335

Wang R

Zhang

Cao Y

Zhang

Moland

Langer

Huang

Huang

Yang Wei ≥ 73

Show More

1. **Highly Active Monoligated**

Quick View Other Sources

By Zhang, Chunming; Ogawa, Kelli; Tu, Siyu; Zu, Chengli; Ringer, Jim; Derstine, Chris; Do, Hien; Fontaine, Philip P.; Klosin, Jerzy  
From Organic Process Research & Development (2019), Ahead of Print. | Language: English, Database: CAPLUS

complexes with amide, urea, and carbamate frameworks have been developed and were found to be highly active for **Suzuki-Miyaura cross-couplings**. These palladacycle precatalysts are derived from simple, inexpensive... The most active congeners among those tested are the urea-based palladacycles, which in conjunction with a  $t\text{Bu}_3\text{P}$  ligand induce high conversions for a range of aryl halide and boronate **coupling** partners. Notably, aryl... relatively mild co...

Machine Translation].

190927. | Language: Chinese, Database: CAPLUS

tion relates to the field of intermediate synthesis, in particular to a preparation method of an RE-021 intermediate, which is characterized in that a compound shown by a formula 9 is obtained by mixing pinacol borate with... flux condition of 1, 4-dioxane, and  $\text{Pd}(\text{dppf})\text{Cl}_2$  is used as a catalyst, so that the stability is high, and the activity is strong; the method has the advantages that the catalytic efficiency is high, then the **Suzuki coupling** product... mula ...

ed melamine-formaldehyde polymer as an efficient heterogeneous catalyst for **Suzuki-Miyaura coupling reactions**

san; Mariyappan, Mathappan; Siva, Ayyanar  
Print. | Language: English, Database: CAPLUS

Abstr.: This work is described as an environmental friendly approach for  $\text{Cu}(\text{OAc})_2$  entrapped on ethylene glycol-modified melamine-formaldehyde-based polymeric material ( $\text{Cu@MCOP}$ ) which has been successfully synthesized by simple approaches using com. available starting materials via solvothermal techniques and without using any toxic reagents and chems. The structural, morphol., physicochem. characteristics and catalytic activity of the heterogeneous catalyst ( $\text{Cu@MCOP}$ ) were analyzed by various instrumental methods including powder X-ray diffraction, FT-IR, UV-DRS, XPS, SEM and elemental mapping...

4. **Bay substituted thiaza[5]helicenes: Synthesis and implications on structural and spectroscopic properties**

Quick View Other Sources

By Daniels, Mathias; de Jong, Flip; Vandermeeren, Tom; Van Meervelt, Luc; Van der Auwerera, Mark; Dehaen, Wim  
From Journal of Coordination Chemistry (2019), Ahead of Print. | Language: English, Database: CAPLUS

A series of bay substituted thiaza[5]helicenes was synthesized to investigate the effect of different substituents on the properties of these helicenes. These thiaza[5]helicenes with different substituents were prepd. in a straightforward manner through indole- and benzo[b] thiophene synthesis, palladium catalyzed **Suzuki coupling**, oxidative cyclization and functional group interconversion **reactions**. We investigated the impact of these different bay area substituents compared to the unsubstituted thiaza[5]helicene on the structural parameters and studied the steady state electronic spectroscop...

5. **Bioactive NHC-derived palladium complexes: synthesis, catalytic activity for the Suzuki-Miyaura coupling of aryl chlorides and bromides and their antibacterial activities**

Quick View Other Sources

By Boubakri, Lamia; Al-Ayed, Abdullah S.; Mansour, L.; Abutaha, Nael; Harrath, Abdel Halim; Ozdemir, I.; Yasar, S.; Hamdi, Naceur  
From Journal of Coordination Chemistry (2019), Ahead of Print. | Language: English, Database: CAPLUS

$\text{Pd}(\text{II})$ -bis(NHC) complexes (where NHC = N-heterocyclic carbene) bearing asym. and sym. substituted NHC-ligand have been synthesized via deprotonation of 5,6-dimethylbenzimidazolium salts. The NHC precursors have been achieved via the two step N-alkylation of 5,6-dimethylbenzimidazole. The resultant salts were deprotonated with  $\text{PdCl}_2$  and  $\text{K}_2\text{CO}_3$  in dry THF for (). The obtained complexes were identified and characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR, FT-IR, DART-TOF mass spectrometry and elemental anal. These new  $\text{Pd}(\text{II})$ -bis(NHC) complexes were applied as catalyst precursors for **Suzuki-Miyaura cross-coupli...**

## 2. Overview

CAS Solutions

SciFinder

Preferences | SciFinder Help | Sign Out

Welcome Hiroyuki Chiba

Link Save Print Export

Research Tools

REFERENCE

Return

Get Reactions Get Related Citations Link to Other Sources

Send to SciPlanner

6. Dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring: inverse temperature dependence of subunit mobility

By: Kawai, Hidetoshi; Umehara, Takeshi; Fujiwara, Kenshu; Tsuji, Takashi; Suzuki, Takanori

Imine bridges between the axle and ring components in rotaxanes allow simple rotaxane synthesis and a novel method for motion control to be developed. The submol. mobility in this rotaxane-type assembly is regulated by the imine-bond formation/cleavage. The relative abundance of the rotaxane increases with decreasing temp. under dynamic equil. conditions.

Indexing

Physical Organic Chemistry (Section22-5)

Section cross-reference(s): 75

Concepts

Hydrolysis

acid, enthalpy-driven, of imine-bridged rotaxanes and pseudorotaxanes; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Imination catalysts

dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Imination

entropy-driven; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Silica gel

imination catalyst; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Substances

108-95-2 Phenol, reactions

Friedel-Crafts; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Reactant; Reactant or reagent

904930-18-3P

Friedel-Crafts; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Reactant; Synthetic preparation; Preparation; Reactant or reagent

904930-09-2P

Suzuki coupling, redn./hydrolysis; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

Purification or recovery; Reactant; Synthetic preparation; Preparation; Reactant or reagent

2,6-Dibromoaniline

66-74-(tert-Butyldimethylsilyloxy)phenylboronic acid

Suzuki coupling; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

References cited by this reference below

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Angewandte Chemie, International Edition

Volume45

Issue26

Pages4281-4286

Journal

2006

CODEN:ACIEF5

ISSN:1433-7851

DOI:10.1002/anie.200600750

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Hokkaido University

Sapporo, Japan 060-0810

ACCESSION NUMBER

2006:651951

CAN145:210475

CAPLUS

PUBLISHER

Wiley-VCH Verlag GmbH & Co. KGaA

LANGUAGE

English



## 2. Overview

**Citing / cited references**

**Link to the full-text of this reference**  
\* The full-text Hokkaido University does not subscribe is unavailable

**Reactions**

**Substances**

**6. Dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring; inverse temperature dependence of subunit mobility**  
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**Indexing**

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**Concepts**

Hydrolysis

acid, enthalpy-driven, of imine-bridged rotaxanes and pseudorotaxanes; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

**Imination catalysts**

dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

**Imination**

entropy-driven; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

**Silica gel**

imination catalyst; dynamic covalently bonded rotaxanes cross-linked imine bonds between the axle and ring and inverse temp. dependence of subunit mobility

**Catalyst use; Uses**

**Molecular sieves**

**References**

1. Kawai, H.; Umehara, T.; Fujiwara, K.; Tsuji, T.; Suzuki, T. *Angewandte Chemie, International Edition* 2006, 45, 4281-4286. CODEN:ACIEF5. ISSN:1433-7851. DOI:10.1002/anie.200600750.

**COMPANY/ORGANIZATION**

Division of Chemistry,  
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2006:651951  
CAN145:210475  
CAPLUS

**PUBLISHER**

Wiley-VCH Verlag GmbH & Co. KGaA

**LANGUAGE**

English

## 2. Overview

The image displays three screenshots of the SciFinder web interface, illustrating different search methods. Red boxes and arrows highlight key features and navigation paths.

**Top Left Screenshot: SUBSTANCES: CHEMICAL STRUCTURE**

- Left Sidebar:** A red box highlights the **SUBSTANCES** section, which includes **Chemical Structure**, **Markush**, **Molecular Formula**, **Property**, and **Substance Identifier**. A red arrow points from this box to the top right screenshot.
- Main Panel:** Shows the **Structure Editor** with **Java** and **Non-Java** tabs. A chemical structure of naphthalene is shown. Search options include **Exact Structure**, **Substructure** (selected), and **Similarity**. A **ChemDraw** logo is visible.

**Top Right Screenshot: SUBSTANCES: PROPERTY**

- Left Sidebar:** A red box highlights the **SUBSTANCES** section, which includes **Chemical Structure**, **Markush**, **Molecular Formula**, **Property**, and **Substance Identifier**. A red arrow points from this box to the top left screenshot.
- Main Panel:** Shows the **Experimental** search type. A dropdown menu for **Select Property...** is open, listing various properties such as **Boiling Point (°C)**, **Density (g/cm³)**, **Electric Conductance (S)**, **Electric Resistance (ohm)**, **Electric Resistivity (ohm\*cm)**, **Glass Transition Temp. (°C)**, **Magnetic Moment (uB)**, **Median Lethal Dose (LD50) (mg/kg)**, **Melting Point (°C)**, **Optical Rotatory Power (degrees)**, **Refractive Index**, and **Tensile Strength (MPa)**. Examples are provided for some properties.

**Bottom Screenshot: SUBSTANCES: SUBSTANCE IDENTIFIER**

- Left Sidebar:** A red box highlights the **SUBSTANCES** section, which includes **Chemical Structure**, **Markush**, **Molecular Formula**, **Property**, and **Substance Identifier**. A red arrow points from this box to the top left screenshot.
- Main Panel:** Shows the **Substance Identifier** search type. A text input field is present for entering search criteria.

**Annotations:**

- A red box with the text **Search for multiple substances at once by:**
  - CAS Registry Number
  - common name
  - product name ...is located near the bottom screenshot.
- A red box with the text **Search by experimental / predicted properties** is located near the top right screenshot.

## 2. Overview

Draw a chemical structure and search by it

The image displays the SciFinder web interface, illustrating the process of drawing a chemical structure and performing a search. The interface is divided into several sections:

- Left Sidebar:** Contains navigation options under 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier) and 'REACTIONS' (Reaction Structure). A red box highlights the 'SUBSTANCES' section, with an arrow pointing to the 'Click to Edit' button in the Structure Editor.
- Structure Editor:** A central workspace for drawing chemical structures. It includes a toolbar with various drawing tools (Atom, Short, etc.) and a 'Click to Edit' button. A red box highlights the 'Click to Edit' button, with an arrow pointing to the drawing area. The structure being drawn is benzoic acid (c1ccccc1C(=O)O).
- Search Options:** A section on the right titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It includes a 'Search Type' dropdown menu with options: Exact Structure, Substructure (selected), and Similarity. A red box highlights the 'Search Type' dropdown, with an arrow pointing to the 'Substructure' option.
- Search Button:** A blue 'Search' button is located at the bottom of the search options section. A red arrow points to this button.

The bottom of the interface shows the chemical formula C7H6O2 and the molecular weight 122.12.



## 2. Overview

CAS Solutions  
**SciFINDER**  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Hiroyuki Chiba

Explore | Saved Searches | SciPlanner

Save | Print | Export

Chemical Structure substructure > substances (1804500)

**SUBSTANCES** | Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

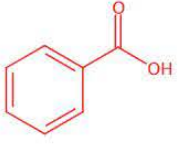
Analyze | Refine

Sort by: Relevance

0 of 1804500 Substances Selected

1. 65-85-0

~77,028 | ~200

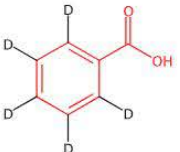


**C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>**  
Benzoic acid

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

4. 1079-02-3

~207 | ~53



**C<sub>7</sub>H<sub>5</sub>D<sub>5</sub>O<sub>2</sub>**  
Benzoic-2,3,4,5,6-d<sub>5</sub> acid

Key Physical Properties  
Regulatory Information  
Spectra  
Experimental Properties

3. 1554-28-3

8. 1554-28-3

Chemical Structure substructure > substances (1804500) > 65-85-0

**SUBSTANCE DETAIL** | Get References | Get Reactions | Get Commercial Sources

Return

1. CAS Registry Number 65-85-0

~77,028 | ~200

**C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>**  
Benzoic acid

**Molecular Weight**  
122.12

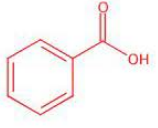
**Melting Point (Experimental)**  
Value: 122.4 °C

**Boiling Point (Experimental)**  
Value: 249.2 °C | Condition: Press: 760 Torr

**Density (Experimental)**  
Value: 1.2659 g/cm<sup>3</sup> | Condition: Temp: 15 °C

**pKa (Predicted)**  
Value: 4.20±0.10 | Condition: Most Acidic Temp: 25 °C

**Other Names**  
Benzenecarboxylic acid  
Benzeneformic acid  
Benzenemethanoic acid  
Carboxybenzene  
Dracylic acid  
View more...



EXPERIMENTAL PROPERTIES  
EXPERIMENTAL SPECTRA  
PREDICTED PROPERTIES

Detailed Data of this substance below

## 2. Overview

The image displays two screenshots of the SciFinder web interface, illustrating the process of drawing and searching chemical structures.

**Left Screenshot:** The interface shows the "REACTIONS: REACTION STRUCTURE" section. The "Structure Editor" is active, displaying a benzene ring with a carboxylic acid group (COOH) labeled "reactant". A red box highlights the "REACTIONS" section in the left sidebar, and another red box highlights the "Structure Editor" toolbar. A red arrow points from the "Click to Edit" button to the "Structure Editor" area.

**Right Screenshot:** The interface shows the "Search" results page. The "Search Type" is set to "Substructure". A red box highlights the "Search Type" section. A red arrow points from the "Search" button in the left screenshot to the "Search" button in this screenshot.

**Text Box:** A red-bordered text box at the bottom left contains the text: "Draw chemical structures before / after a reaction and search by them".

## 2. Overview

Reaction Structure substructure > reactions (434533)

REACTIIONS

Group by: No Grouping Sort by: Relevance

0 of 434533 Reactions Selected

1. View Reaction Detail

Single Step Hover over any structure for more options.

~160 ~227

Overview

Steps/Stages

1.1 S:H<sub>2</sub>O, 1 h, rt → 230°C

2. View Reaction Detail

Single Step Hover over any structure for more options.

~160 ~227

Overview

Stages

1.1 S:H<sub>2</sub>O, 1 h, rt → 230°C

Notes

thermal, Na-X-type zeolite used, stainless steel autoclave used, optimization study, solvent, Reactants: 1, Solvents: 1, Steps: 1, Stages: 1

Transformation:

1. Decarboxylation of Aromatic Acids

Reaction Structure substructure > reactions (434533) > reaction 1 (of 434533)

Get Reference Detail View with PATENTPAK Get Similar Reactions Link to Other Sources

Return

1. Single Step Hover over any structure for more options.

~160 ~227

Overview

Stages

1.1 S:H<sub>2</sub>O, 1 h, rt → 230°C

Notes

thermal, Na-X-type zeolite used, stainless steel autoclave used, optimization study, solvent, Reactants: 1, Solvents: 1, Steps: 1, Stages: 1

Transformation:

1. Decarboxylation of Aromatic Acids

Sample Analysis: Reagent

HCl ≥ 9140

Et<sub>3</sub>N ≥ 7473

H<sub>2</sub> ≥ 5723

EtN(Pr-)<sub>2</sub> ≥ 5659

NaOH ≥ 5076

K<sub>2</sub>CO<sub>3</sub> ≥ 4690

NaHCO<sub>3</sub> ≥ 4408

F<sub>3</sub>CCO<sub>2</sub>H ≥ 3927

H<sub>2</sub>O ≥ 3626

EtN=C=N(CH<sub>2</sub>)<sub>3</sub>NM e<sub>2</sub> •HCl ≥ 3584

Show More

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The screenshot shows the CAS SciFinder Training page. At the top, there is a navigation bar with the CAS logo (A DIVISION OF THE AMERICAN CHEMICAL SOCIETY) and links for Support, Language, and Log In. Below this is a dark blue header with the word "Support" in yellow. On the left side, there is a vertical stack of social media icons: Facebook, Twitter, LinkedIn, and a red button with a plus sign and the number 917. The main content area has a breadcrumb trail: Home / Support / Training / SciFinder Training. The title "SciFinder Training" is prominently displayed, followed by the SciFinder logo. A paragraph states: "These on-demand SciFinder® training resources are short, targeted materials, organized by search type." Below this, there is a section titled "Overview Materials" with a bulleted list of links: "Introduction to SciFinder" (described as a tutorial for searching, analyzing results, and creating alerts), "SciFinder简介" (Chinese introduction), and "SciFinder System Requirements and Recommendations". Another section titled "Substance Searching" includes a sub-section "Substance Search Videos" with a bulleted list of links: "Input Structures Using the Drawing Editor", "Search for Chemical Compounds Using a Structure Search", and "Conduct a Substructure Search".

<https://www.cas.org/support/training/scifinder>

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The screenshot shows the JAICI SciFinder website's technical resources page. The header includes the JAICI logo, language options (Japanese/English), and a search bar. A navigation bar lists various services like STN, SciFinder, and SHIPS. The left sidebar contains a menu with categories like 'Getting Started', 'Users', and 'Related Services'. The main content area, titled 'SciFinder - 技術資料', lists various guides and resources. The link 'SciFinder Search Guide (English) (August 2018)' is highlighted with a red box. Below the main content, a URL is provided in a white box with a black border.

JAICI 化学情報協会

日本語 English

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HOME > SciFinder > 技術資料

ログイン

はじめての方

- 契約プラン
- 収録内容
- PatentPak
- MethodsNow
- ChemZent
- 利用環境

ユーザーの方

- 技術資料
- e-ラーニング
- イベント
- ニュースレター
- サービス時間
- よくあるご質問
- データ利用制限
- ヘルプデスク support@jaici.or.jp (0120-003-462)

関連サービス

### SciFinder - 技術資料

- SciFinder のサポートに！専門用語の英日/日英辞書ツール [JAICI Science Dictionary](#) をお使いください。

#### 検索ガイド

- [SciFinder 検索ガイド \(2018 年 8 月\)](#)
- [SciFinder の構造作成 \(2016 年 4 月\)](#)
- [SciFinder Search Guide \(English\) \(August 2018\)](#)

#### コンテンツ & 利用規約

- [収録内容](#)
- [データ利用制限](#)
- [レコード例](#)

#### ログイン & 設定

- [SciFinder へのアクセス](#)
- [Preference \(設定・パスワード変更\)](#)
- [登録情報 \(メールアドレス、パスワード、秘密の質問\) の変更方法](#)
- [ユーザー名・パスワードを忘れた場合](#)
- [スマートフォンからのアクセス](#)

#### 文献検索 (雑誌論文、特許など)

- [キーワード検索](#)
- [引用文献の検索](#)
- [著者名検索](#)
- [文献回答の絞り込み・解析 \(Analyze/Refine\)](#)
- [会社名、大学名からの検索](#)
- [文献回答からの関連情報の抽出](#)
- [文献の書誌情報からの検索](#)
- [Categorize 機能](#)

#### 化学物質検索

- [化学物質名称、CAS 登録番号 \(CAS RN<sup>®</sup>\) 検索](#)
- [物質回答の絞り込み・解析 \(Analyze/Refine\)](#)
- [化学構造検索、構造検索タイプ](#)
- [無機化合物の検索](#)
- [他ツールの構造を使った構造検索](#)
- [ポリマー検索の概要](#)
- [マルクシェ構造検索](#)
- [化学物質関連情報へのリンク機能](#)
- [物性検索](#)

[https://www.jaici.or.jp/SCIFINDER/sci\\_tecdata.html](https://www.jaici.or.jp/SCIFINDER/sci_tecdata.html)

協会案内 このサイトについて プライバシーポリシー サイトマップ 採用情報 アクセス

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HOMEヘルプデスク

STN

SciFinder<sup>®</sup>

SciFinder

MethodsNow

NCI Global

FIZ AutoDoc

CAS Full Text Options

## ヘルプデスク

ヘルプデスクでは、検索方法に関するご質問をお受けしております。お気軽にご利用ください。

■ 技術的 なご質問の例

- こんな検索できますか？
- このファイルでどのように検索できますか？
- このファイルについてよい資料はありますか？
- このエラーは何ですか？ どのように対処したらよいですか？

■ その他 のご質問の例

- 請求書について聞きたい。
- 講習会やセミナーの申込み方法について聞きたい。
- STN の担当者を変更するにはどうしたらよいですか？

よくあるご質問

STN

FIZ AutoDoc

CAS Full Text Options

NCI Global

SciFinder<sup>®</sup>

SciFinder

MethodsNow

### STN, SciFinder<sup>®</sup>/SciFinder, NCI Global, 原報複写サービス (FIZ AutoDoc) をお使いのお客様

	TEL	e メール	FAX
技術的 なご質問	0120-003-462 (テクニカルグループ)	e メール	03-5978-4090
その他 のご質問	0120-151-462 (カスタマーグループ)	e メール	

依頼用 FAX 用紙はこちらです (PDF 形式・Microsoft Word 形式)。必ずお名前とご連絡先 (電話番号、FAX 番号、メールアドレス) を付記ください。

\* 北米及びアジア諸国の方は CAS, ヨーロッパの方は FIZ Karlsruhe が上記サービスの窓口となっております。直接お問い合わせください。

[このページのトップへ](#)

協会案内このサイトについてプライバシーポリシーサイトマップ採用情報アクセス

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<https://www.jaici.or.jp/helpdesk/index.htm>

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## JAICI Science Dictionary

専門用語豊富なシソーラス付き辞書！

あなたの用語を登録しませんか？  
★ノベルティ進呈★ 2019 用語登録キャンペーン

### どんな辞書？

JAICI Science Dictionary は…

- SciFinder<sup>®</sup> / STN ご利用のための、日英/英日の対訳辞書とシソーラスです。
- 化学や医学・薬学を中心とした科学技術関係の国内外の論文及び特許情報から集めた専門用語を収録しています。

インターネットに接続された環境と、Web ブラウザが必要です。Windows 7 以降の PC での利用を推奨しています。

### どんな言葉が調べられるの？

収録用語（約 84 万語）のうち、約 80 %は以下の分野の専門用語です。

- 生化学・ライフサイエンス（医学用語・病名を含む）
- 高分子化学（プラスチック・ゴム・繊維・界面活性剤を含む）
- 有機化学（化合物の慣用名を含む）
- 応用化学（電池・セラミックス・合金・環境・薬剤・化粧品・鉱物など）
- 物理化学・無機化学（半導体・液晶・電気化学・工学・原子力など）
- 情報工学・計算機科学（コンピュータ）

学名が充実しています。二命名法に沿った表記や、階級名に沿った生物分類が多く収録されています。シソーラス（後述）と紐付いており、階層情報を参照できます。

### 分野別の用語数内訳

■ 生化学・ライフサイエンス  
■ 高分子化学  
■ 有機化学  
■ 応用化学  
■ 物理化学・無機化学  
■ 情報工学・計算機科学  
■ その他

掲載から採択されたものについては、製造・販売会社名を参照できます。

<https://www.jaici.or.jp/jsd>

協会案内 このサイトについて プライバシーポリシー サイトマップ 採用情報 アクセス

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<https://www.lib.hokudai.ac.jp/en>

Site map FAQ Contacts Access Japanese

HOME English HOME Remote Access

Research Support Information About Library Link to Branches Libraries

Remote Access

**Remote Access Service**

\*Select the type of ID from the following\*

- ☐ Faculty and staff
- ☐ Students
- ☐ Professor emeriti
- ☐ The Other staff etc.

User ID

Password

Log In

**E-journals, E-books**

E-journals and E-books can be searched through the following system

[E-Journals • E-Books Portal](#)

**Databases**

Databases can be accessed through the following web page.

[Database web page](#)

- Some databases can not use via remote access. Please confirm the icon at the results page. A

**Popular Databases**

- [Web of Science Core Collection] : articles & cited references from major journals (More Info)
- [CINII] : article database provided by the National Institute of Informatics (More Info)
- [SciFinder Web] : chemistry and other scientific information from articles and patents (More Info)
- [Reaxys] : chemical compounds, bibliographic data and chemical reactions (More Info)
- [Japana Centra Revuo Medicina] : medical and nursing science articles (More Info)
- [MEDLINE EBSCOhost] : international literature on biomedicine and health care (More Info)
- [PubMed HOKUDAI ver.] : It is provided by the National Medical Library (More Info)
- [WESTLAW JAPAN] ⇒ Westlaw Japan's legal information online service (More Info)
- [LEX/DB Internet] : full text of cases since 1875 (Meiji 8) (More Info)
- [Nikkei BP article search service] : full text of articles in Nikkei BP's magazines (More Info)

**Tips : Easy way to access frequently used E-journals, E-books, Databases**

Almost all of the contents and databases can access easily by the following steps. If you use same this tip.

1. Log in the remote access service.
2. Pursue the Hokkaido University Library catalog or Database page, then access the webpage of your target.
3. Confirm the URL including the strings "ezoris.lib.hokudai".
4. Save the URL for the internet browser.
5. Afterword, in the case of not accessed on the remote access service, access the saved URL, then login page. After the login, you can use the contents or databases directly.

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- PatentPak
- MethodsNow
- ChemZent
- 利用環境

ユーザーの方

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- e-ラーニング
- イベント
- ニュース
- サービス
- よくある質問
- データ利用
- ヘルプデスク  
support@jaici.or.jp  
(0120-003333)

SciFinder Mobile

移動中、実験中、出張中、学会参加中など、これまで SciFinder をお使いいただけなかった環境下でも SciFinder Mobile を使えば、重要な情報に手軽にアクセスできます。



SciFinder Mobile では下記の機能が利用できます。

- キーワード検索
- 物質名称, CAS 登録番号 (CAS RN<sup>®</sup>) による物質検索
- 著者名検索
- 会社名 (大学名) 検索

Although the functions of this version are limited, you can use it on your smartphone just by entering your SciFinder account

<https://scifinder.cas.org/mobile>

<https://www.jaici.or.jp/SCIFINDER/sfmobile>

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Workshop

For accelerating Chemical Research!  
Workshop Series on Chemical Information Databases  
**Workshop on**  
**SciFinder**  
containing all the chemical substances registered by CAS

SciFinder is an essential tool for the chemists, with which they can comprehensively search chemicals and reaction information in addition to papers and patents!  
A professional instructor will lecture on how to use it.

**How to participate:**  
Students, faculty, and staff of Hokkaido University can join any venue.  
- Basic Course: for first-time users  
\* the own e-mail address of [hokudai.ac.jp](mailto:hokudai.ac.jp) is needed  
- Advanced Course: for those already using  
\* the own SciFinder account is needed

Please apply in advance when you join the venue marked with [Application Needed] —  
<https://www.lib.hokudai.ac.jp/?p=68938>

Date	Time	Course	Language	Venue
Wed. Oct. 16 <sup>th</sup>	13:30-14:30	Advanced	Japanese	Northern Campus [Seating Capacity: 15] Northern Campus BLDG. No. 5 (RIES) 1F Northern Campus Library
	14:45-15:45	Advanced	English	* There are <b>NO</b> computers for training at this venue. Please prepare a device that can connect to the wireless LAN, and your own ID/PW of ELMS, SSO, or iIC.
Thu. Oct. 17 <sup>th</sup>	16:30-18:00	Basic & Advanced	Japanese	Faculty of Science [Seating Capacity: 15] [Application Needed] School of Science BLDG. No. 8 1F Media Education Center Computer Room (1-04)
	14:45-16:15	Basic	Japanese	Faculty of Pharmaceutical Sciences [Seating Capacity: 30]
	16:30-17:30	Advanced	Japanese	School of Pharmaceutical Sciences BLDG. 1F Computer Room (S103)
				Faculty of Agriculture

Hokkaido University holds the workshops twice a year, usually in spring and fall

[kitacam@lib.hokudai.ac.jp](mailto:kitacam@lib.hokudai.ac.jp)   [sci@lib.hokudai.ac.jp](mailto:sci@lib.hokudai.ac.jp)   [ph@lib.hokudai.ac.jp](mailto:ph@lib.hokudai.ac.jp)   [agr@lib.hokudai.ac.jp](mailto:agr@lib.hokudai.ac.jp)

USE  
SciFinder  
AND  
JOIN  
the Workshop  
on Oct. 16th