

CAS SciFinderⁿ Search Guide

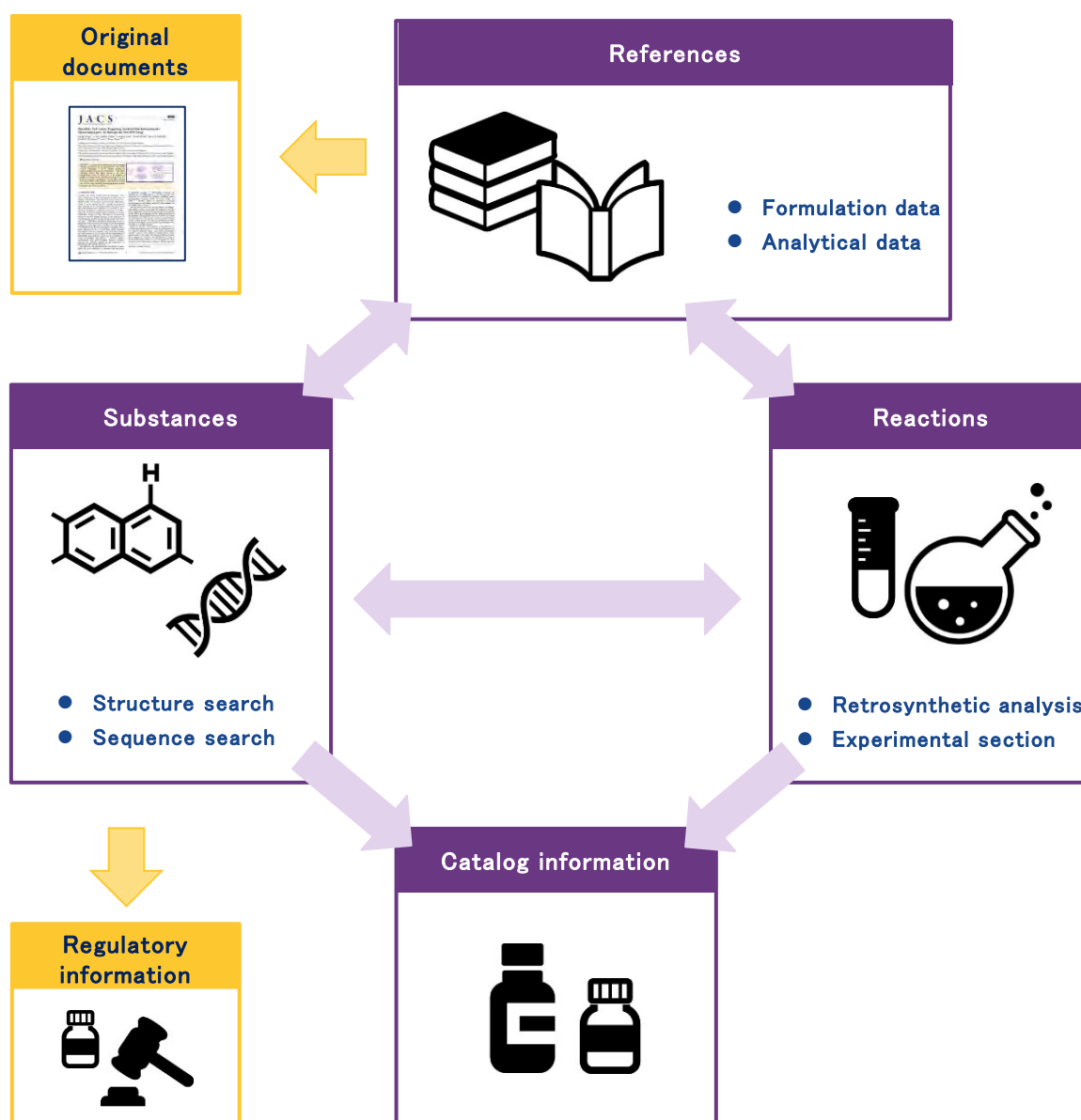
August 2021

<https://scifinder-n.cas.org/>



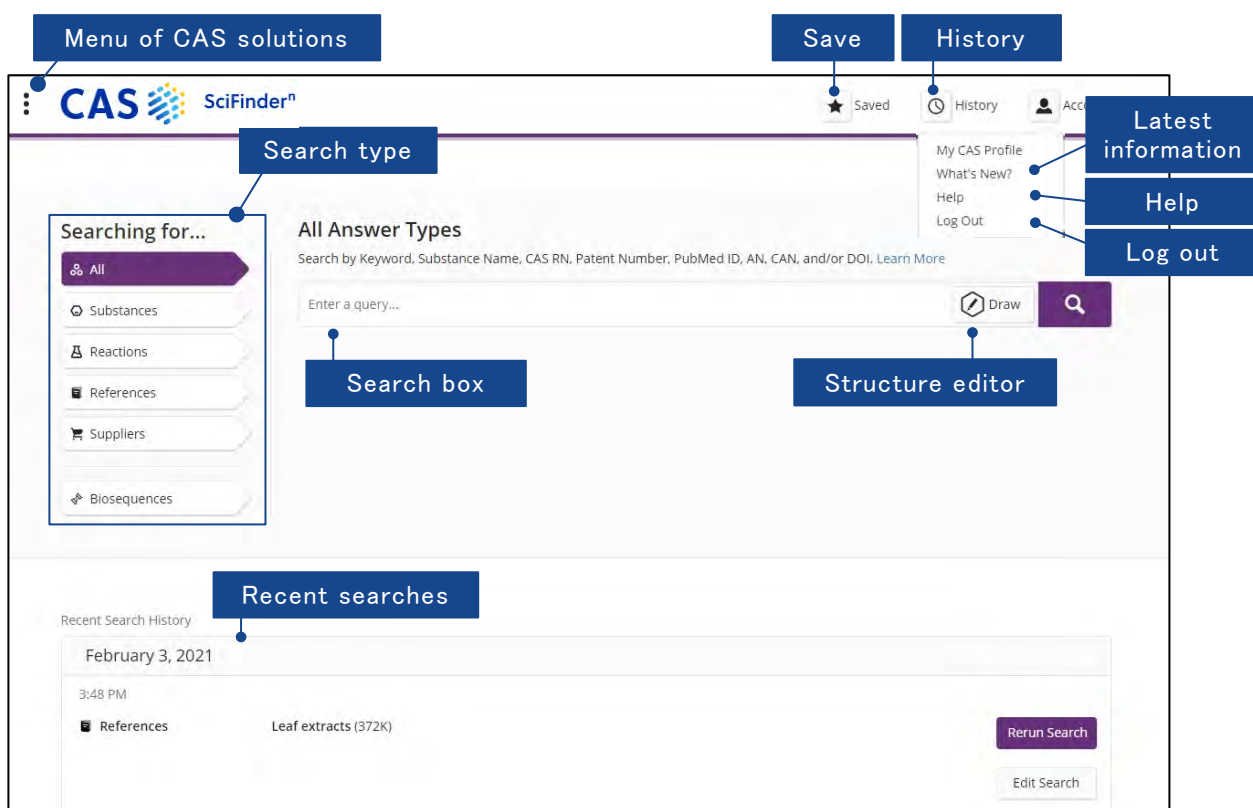
Features in CAS SciFinderⁿ

- CAS SciFinderⁿ is an online search tool for CAS databases designed for researchers.
 - Contain scientific information such as references, substances, reactions and so on
 - Access to the largest substance database containing all CAS RN[®]*
 - * CAS RN[®] is a unique and unambiguous identifier for a specific substance
 - Suitable for searching information on scientific area
 - Used globally by companies or main scientific faculties in universities (science, technology, pharmacy, agriculture, etc)
- You can search references, substances, reactions, and catalog information in CAS SciFinderⁿ
 - Each information is linked through CAS Registry Number (CAS RN[®])



Home page

■ Top of the Home page



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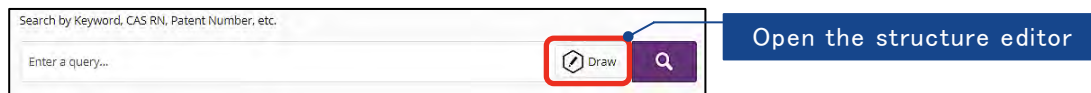
All search

- All finds substances, reactions, references, and suppliers that match your query.

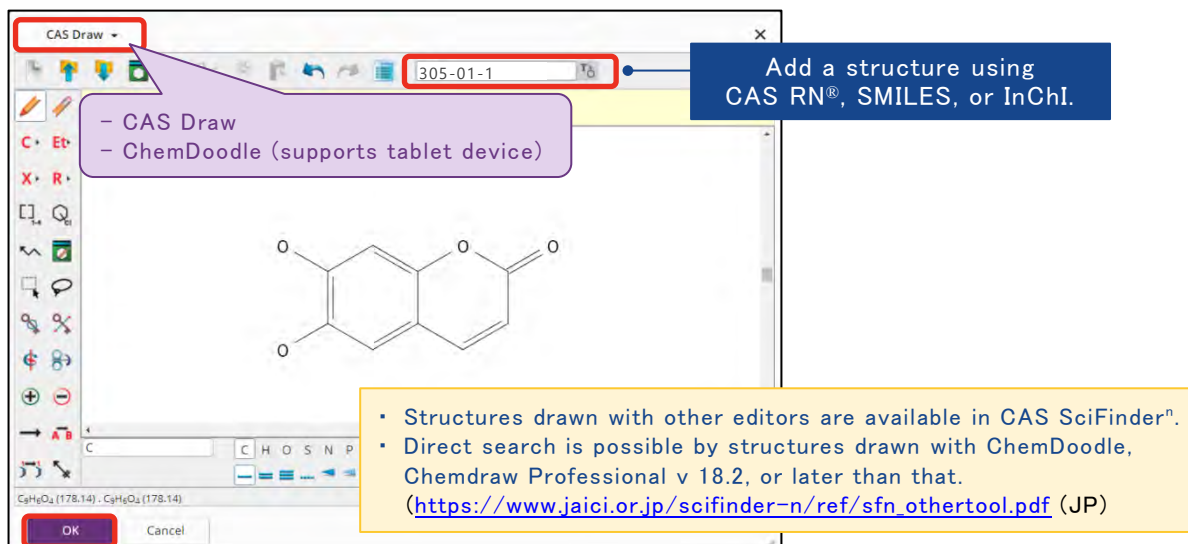
The screenshot shows the CAS SciFinder search results for 'caffeine'. The interface is divided into several sections:

- Search Bar:** Located at the top, with a search box containing 'caffeine' and a search button. A callout box says: "Enter a keyword, CAS Registry Number (CAS RN®), patent number, etc."
- Search Results Summary:** On the left, a sidebar shows the number of results for each category: Substances (26), Reactions (1,337), References (81,213), and Suppliers (151). A callout box says: "Links to each result (can be opened in a separate tab)".
- Substance Results:** The top section shows two substance results:
 - 1. 58-08-2: Caffeine (Chemical structure: CN1C=NC2=C1C(=O)N(C(=O)N2C)C). It has 63K references, 1,337 reactions, and 143 suppliers.
 - 2. 52622-68-1: Unspecified Coffeylin. It has 3 references, 0 reactions, and 0 suppliers.
- Reaction Results:** The middle section shows a reaction scheme (Scheme 1) with 3 reactions. It includes chemical structures and reagents (Na). It has 5 suppliers for the first reagent, 49 for the second, and 143 for the product.
- Reference Results:** The bottom section shows a reference titled "Caffeine and Adenosine" by Ribeiro, Joaquim A.; Sebastiao, Ana M. It has 2 substances, 0 reactions, 174 citations, and a citation map.
- Supplier Results:** The bottom section shows a table of suppliers for Caffeine, anhydrous. The first supplier is KANTO CHEMICAL Japan, with a purity of 95-98% and typically in stock.

- To search by chemical structure, click the Draw button and draw a structure.



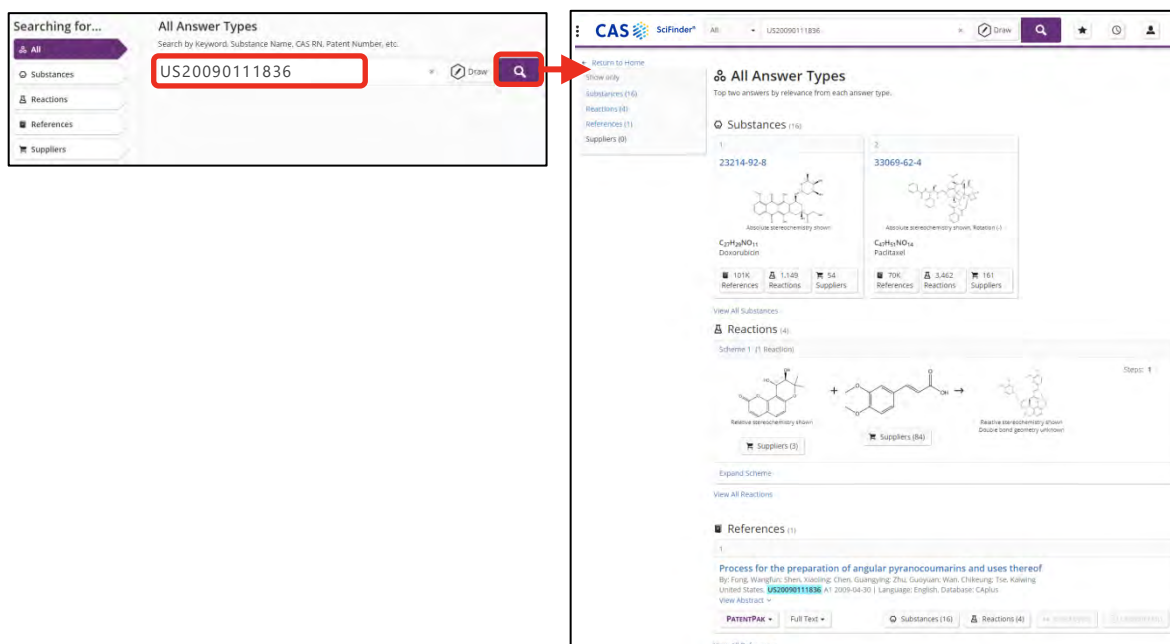
- You can select CAS Draw or ChemDoodle.



- Click the Search button.



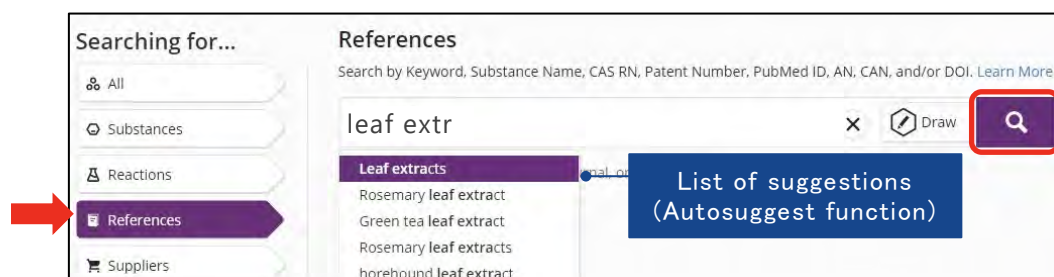
- Searching a patent number in All search retrieves substances and reactions mentioned in the patent in addition to its patent record..



Reference search

- In the Reference search, you can find references by keyword, author name, journal information (journal name, volume number, issue number, etc.), organization or document identifier.

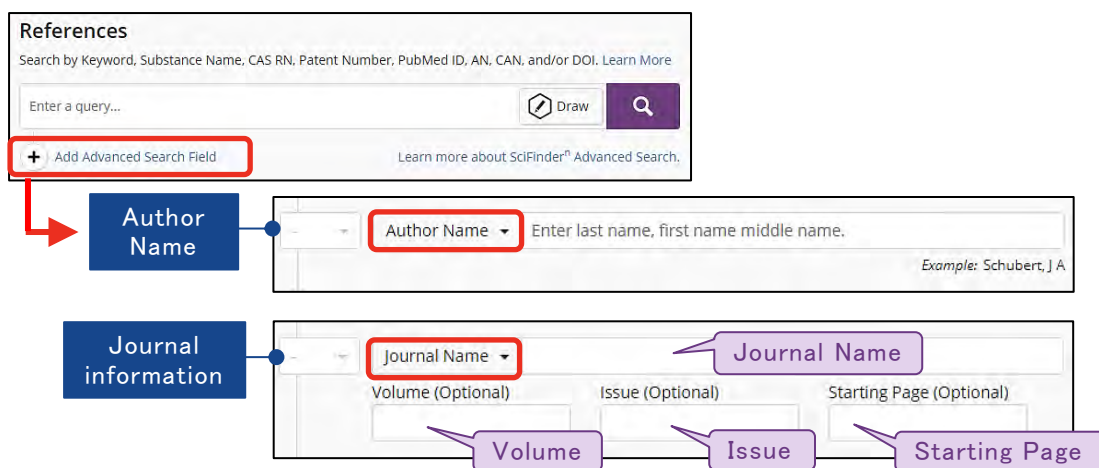
- Keyword and Document Identifier (Patent Number, DOI, Accession Number, etc.)



- Boolean search operators (AND, OR, NOT) or wildcards (*, ?) are available when combining keywords (See www.jaici.or.jp/scifinder-n/ref/sfn_boolean.pdf).
- The main search field searches title, abstract, indexing, and document identifier. If you search terms in other information or choose a field to search, please see below.

- Author name, Journal Information and Organization

- You can combine multiple author names, journal information, organization, etc.
- Click Add Advanced Search Field and choose a field to search.



- Click Add Advanced Search Field and choose OR operator when combining multiple author names, journal information and organizations.



- You can combine the main search field and Add Advanced Search Fields.

■ Answers are sorted by Relevance by default.

▪ You can select other sort orders with Sort menu.

■ Select filters to display or exclude answers that match the applied filters.

The screenshot displays the CAS SciFinder search results page for the query "cosme*". The interface includes a top navigation bar with the CAS logo, search bar, and user profile. The main content area shows a list of references, each with a title, authors, and publication details. Annotations highlight key features:

- Sort results:** A dropdown menu showing options: Relevance (selected), Times Cited, Publication Date: Newest, and Publication Date: Oldest.
- Filters:** A sidebar on the left with sections for Document Type, Language, Publication Year, and Search Within Results. The "Document Type" section is expanded, showing "Journal (4,655)" and "Patent (16K)" selected.
- Document Type:** A callout box pointing to the "Journal, Patent" selection in the filters.
- Links to related data:** A callout box pointing to the "Substances (2)" and "Cited By (752)" links for the first reference.
- Access full-text options (P.9):** A callout box pointing to the "Full Text" dropdown menu for the first reference.
- View Citation Map (Citing and Cited information):** A callout box pointing to the "Citation Map" link for the first reference.
- Keyword: cosme*:** A callout box pointing to the search bar.
- Download filter data:** A callout box pointing to the "Download filter data from this result set" button.

The first reference is "Rapid biological synthesis of silver nanoparticles using plant leaf extracts" by Song, Jee Yong; Kim, Beom Soo, published in "Bioprocess and Biosystems Engineering" (2009), 32(1), 79-84. The second reference is "Phytochemical analysis and gastroprotective activity of the leaves of *Phytolacca frutescens* L." by Dekanski, Dragana; Janicijevic-Hudomal, Snezana; Todric, Vanja; Markovic, Goran; Arsic, Ivana; Mitrovic, Dusan M., published in "Journal of the Serbian Chemical Society" (2009), 74(4), 367-377. The third reference is "Liquid-Liquid Extraction for the Enrichment of Edible Oils with Phenols from Olive Leaf Extracts" by Japon-Lujan, R.; Luque de Castro, M. D., published in "Journal of Agricultural and Food Chemistry" (2008), 56(7), 2505-2511. The fourth reference is "Drying and storage of olive leaf extracts. Influence on polyphenols stability" by Ahmad-Qasem, Margarita H.; Ahmad-Qasem, Begona H.; Barrajon-Catalan, Enrique; Micol, Vicente; Carcel, Juan A.; Garcia-Perez, Jose V., published in "Industrial Crops and Products" (2016), 79, 232-239. The fifth reference is "Green synthesis of silver nanoparticles using Ginkgo biloba leaf extracts" by Ren, Yan-yu; Yang, Hui; Wang, Tao; Wang, Chuang, published in "Physics Letters A" (2016), 380(45), 3773-3777.

- To open the Reference Detail page, click the title.

Stevia rebaudiana Bert. leaf extracts as a multifunctional source of natural antioxidants

By: Gawel-Reben, Katarzyna; Bujak, Tomasz; Nizioł-Lukaszewska, Zofia; Antosiewicz, Beata; Jakubczyk, Anna; Karas, Monika; Rybczynska, Kamila
Molecules (2015), 20(4), 5468-5486 | Language: English, Data Source: PubMed
| MethodsNow: Analysis
View Abstract ▾

Reference Detail (17 of 17)

Substances (8) | Cited By (33) | Citation Map

Journal
Source
Molecules
Volume: 20
Issue: 4
Pages: 5468-5486
Journal: Article; Research Support, Non-U.S. Gov't
2015
DOI: 10.3390/molecules20045468

Database Information
AN: 2015-612048
CAN: 163-270423
PubMed ID: 25826787
CAPUS and MEDLINE

Company/Organization
Department of Public Health, Dietetics & Lifestyle Disorders
The University of Information Technology and Management in

Indexed Concepts
k.gawel@wziz.rzeszow.pl
Publisher: MDPI AG
Language: English

Abstract
The aim of the presented study was to characterize the content and biol. activity of **extracts** prepared from **leaves** with potential application in the food or **cosmetic** industry. Aqueous (A), ethanolic (E) and analyzed for the content of polyphenols and proteins, showing that the highest amount of phenols (mg/g) contained GA. All **extracts** contained significant amount of protein (69.40-374.67 mg/g). Between analyzed **extracts** (HPLC) GA contained the highest amount of polyphenols, especially ferulic (5.50 mg/g) and rosmarinic (4.95 mg/g) acids derivatives. The highest antiradical activity against DPPH• and ABTS•+ was noted for GA and E (IC50 = 0.38 and 0.71 µg flavonoids/mL). The highest ability to chelate Fe2+ was observed for E (IC50 = 2.08 µg flavonoids/mL). **Stevia extracts** were also analyzed for their cytotoxicity and fibroblast irritation potential in vitro. E and GA were the most cytotoxic and irritating, probably due to the high content of biol. active phytochemicals. On the other hand, a **extract** was the most tolerable by the cells. To summarize, the presented study evaluated the potential application of A, E and GA **stevia extracts** as natural source of antioxidants in the food and **cosmetic** industry.

Keywords: Stevia, leaf extract, antioxidant activity

Access full-text options (P.9)
Full Text ▾

Indexed by CAS (Derived from CAS References)
Concepts
Cytotoxicity
Fibroblast
Role: Biological Study, Unclassified

Indexed by PubMed (Derived from MEDLINE)
MEDLINE® Medical Subject Headings
Antioxidants
Qualifier: chemistry; pharmacology
Cell Line
Plant Extracts
Qualifier: chemistry; pharmacology

Indexed Substances
Substances (8)
20283-92-5
Absolute stereochemistry shown, Rotation (+)
Double bond geometry shown
C₁₅H₁₄O₈
Rosmarinic acid
Role: Biological Study, Unclassified, Biological Study

491-70-3
C₁₅H₁₀O₆
Luteolin
Role: Biological Study, Unclassified, Biological Study

490-46-0
Absolute stereochemistry shown, Rotation (-)
C₁₅H₁₄O₆
Epicatechin
Role: Biological Study, Unclassified, Biological Study

Analytical Data
Analytical Methods
Title:
Analysis of Flavonoids in Stevia rebaudiana by Solvent extraction
Analysis of Caffeic acid in Stevia rebaudiana by Solvent extraction
Analysis of Phenols in Stevia rebaudiana by Solvent extraction
CAS Method Number:
1-124-CAS-312400
1-374-CAS-312592
690

Access detail page*

Analytical methods, materials, instrumentation, and validation data retrieved by CAS (CAS Analytical Methods) www.jaici.or.jp/cas-analytical-methods/cam.pdf

Citation Information
Citations
Citations (75)
1) Ahmad, N. J Med Plants Res. 2011, 5, 3293
2) Durak, A. Food Chem. 2013, 141, 2177
3) Ghosh, S. Int J Integr Biol. 2008, 2, 27

Retrieve references that are cited by this document*

Retrieve references that cite this document*

Bibliographic Information

Access full-text options (P.9)

Indexed Concepts

Indexed Substances

Analytical Data

Access detail page*

Analytical methods, materials, instrumentation, and validation data retrieved by CAS (CAS Analytical Methods) www.jaici.or.jp/cas-analytical-methods/cam.pdf

Citation Information

Retrieve references that are cited by this document*

Retrieve references that cite this document*

Bibliographic Information

* For the detail of citation searching with CAS SciFinder®, see www.jaici.or.jp/scifinder-n/ref/sfn_citation.pdf.

- Patent record

Reference Detail

(36 of 21,085)

Substances (22) Cited By (4) Citation Map

Patent

Patent Information

Patent Number
WO2011068812

Publication Date
2011-06-09

Application Number
WO2010-US58464

Application Date
2010-12-01

Assignee
Colgate-Palmolive Company,
United States

Source
World Intellectual Property
Organization

Database Information
AN: 2011:721251
CAN: 155:21397
CAPUS

Language
English

Oral hygiene compositions containing a combination of natural extracts and related methods for treating xerostomia

By: Trivedi, Harsh M.; Gittins, Elizabeth K.

The present invention relates to oral hygiene compositions, such as toothpastes and mouthwashes comprising a combination of extracts containing a mixture of extracts from at least three of Punica granatum, Myristica fragrans, Zingiber officinale, and Zizyphus joazeiro and a natural extract other than the extract from at least these three extracts, and an orally acceptable carrier, and methods of preparing and using the same for the treatment of xerostomia. A mouthwash containing 0.02 weight% of a mixture of extracts was exemplified.

Keywords: antibacterial plant extract dentifrice oral hygiene product xerostomia

PATENTPAK Viewer Full Text

Access CAS PatentPak (P.9)

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2011068812	English	A1	PDF PDF+ Viewer	2011-06-09	WO2010-US58464	2010-12-01
		P			US2009-G1266700P	2009-12-04
CA2780324	English	A1		2011-06-09	CA2010-2780324	2010-12-01
AU2010326134	English	A1	PDF			
JP2013512906	Japanese	T	PDF			
AU2010326134	English	B2	PDF			

Abstract and indexing are created based on a patent in the first line of Patent Family.

Indexed Concepts

Abelmoschus moschatus Modifier: extract	Myristica fragrans Modifier: extract
Abrasives	Ocimum sanctum
Carapa procera Modifier: extract	Phenols Role: Cosmetic Use; Therapeutic Use
Cinnamomum camphora	

Indexed Substances

Substances (22)

7631-86-9

O=Si=O

O₂Si
Cosme Silica BQ 60
PATENTPAK
Role: Cosmetic Use; Biological Study, Uses
Notes: Zeodine 11

601397-13-4

C1OC1

56265-03-3

C6H6O7.Na.Zn
Sodium zinc citrate
PATENTPAK
Role: Cosmetic Use; Therapeutic Use, Biological Study, Uses

Access location of indexed substances in full-text (CAS PatentPak)

Formulations Data

Oral Composition: Dentifrices or Toothpastes

View CAS Formulus® Detail

Access detail page *

Location: Claim 1, 2, 4, 5, 6, 8, 11

Purpose: Dentifrices, Toothpastes

Target: human

Component	Function	Amount Reported
Group: extract extracts	active agent	-
Group: additional ingredients	antibacterial agents	-
Group: additional ingredients		
Pharmaceutical carriers		

Formulations data retrieved by CAS (CAS Formulus)
www.jaici.or.jp/scifinder-n/ref/sfn_formulations.pdf

* Only those who make a contract for companies or government research institutions can access CAS Formulus and CAS Analytical Methods.

Access full text (CAS PatentPak, Full Text)

- To access patent PDF with locations of indexed substances, click Viewer in PatentPak menu (See https://www.jaici.or.jp/scifinder-n/ref/sfn_pat.pdf).

The screenshot shows the CAS PatentPak interface. The top section displays a patent abstract for 'Oral hygiene compositions containing a combination of natural extracts and related methods for treating xerostomia'. Below the abstract, there is a table of patent entries. The 'Full-text PDF' button is highlighted with a red box. The 'Patent PDF with locations of indexed substances' button is also highlighted with a red box. A red arrow points from the 'Patent PDF with locations of indexed substances' button to a detailed view of the patent document, which includes a chemical structure and a list of key substances.

Full-text PDF

Patent PDF with locations of indexed substances

Key Substances in Patent:

- 5. A composition according to any preceding claim, further comprising an additional antibacterial agent selected from: phenolic compounds, stannous ions, zinc ions, and mixtures thereof.
- 6. A composition according to claim 5, wherein the zinc ions are provided by one or more zinc-containing compounds selected from the group consisting of zinc acetate, zinc gluconate, zinc glycinate, zinc oxide, zinc sulfate, sodium zinc citrate, and mixtures thereof.
- 7. A composition according to any preceding claim, wherein the composition further comprises at least one additional component selected from the group consisting of humectants, abrasives, anticaries agents, anticalculus or tartar control agents, anionic carboxylate polymers, viscosity modifiers, surfactants, flavorants, pigments, and mixtures thereof.

- To view full-text options for a reference, click the Full Text button and then select one of the following options.

- Selecting View all Sources opens a page that have all options for the full text.

The screenshot shows the CAS PatentPak interface. The top section displays a patent abstract for 'Oral hygiene compositions containing a combination of natural extracts and related methods for treating xerostomia'. Below the abstract, there is a table of patent entries. The 'Full Text' button is highlighted with a red box. The 'View all Sources' button is also highlighted with a red box. A red arrow points from the 'View all Sources' button to a detailed view of the patent document, which includes a chemical structure and a list of key substances.

Journal References

Full Text

View all Sources

DOI: Link to the Web page where the full text of the journal is available
View all Sources: Link to a page that have all options for the full text

Patent References

Full Text

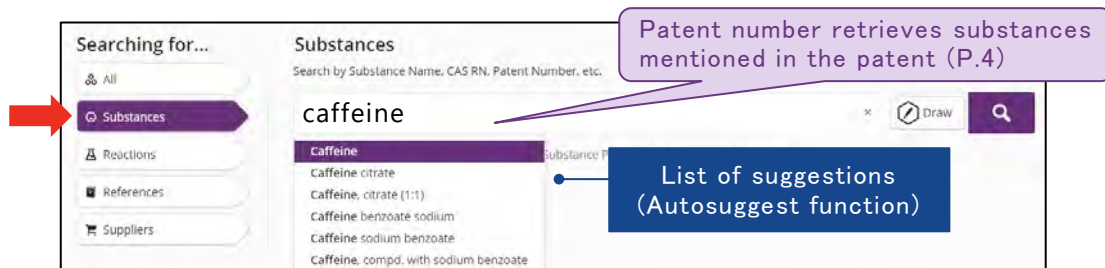
View all Sources

Espacenet: European Patent Office's Web site

Substance search

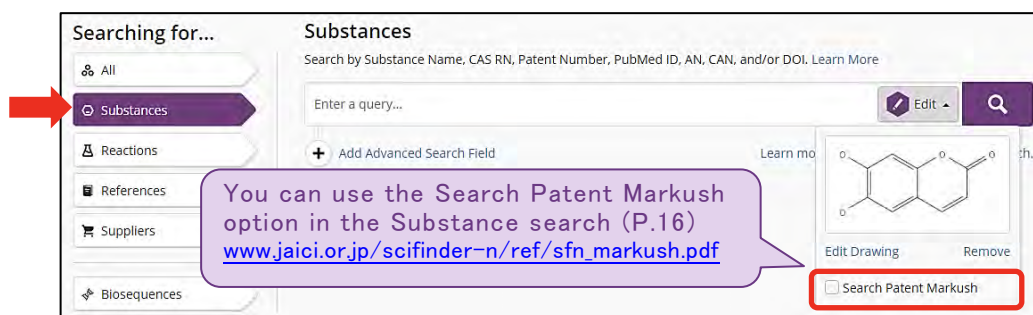
- In the Substance search, you can find substances by substance name, chemical structure, CAS Registry Number (CAS RN®), molecular formula, etc.

- Substance Name and CAS Registry Number (CAS RN®)



- When entering multiple CAS RN®s or substance names, they must be separated by a space, no commas or other punctuation.
- Substance name can search Notes in substance records with no structure information.

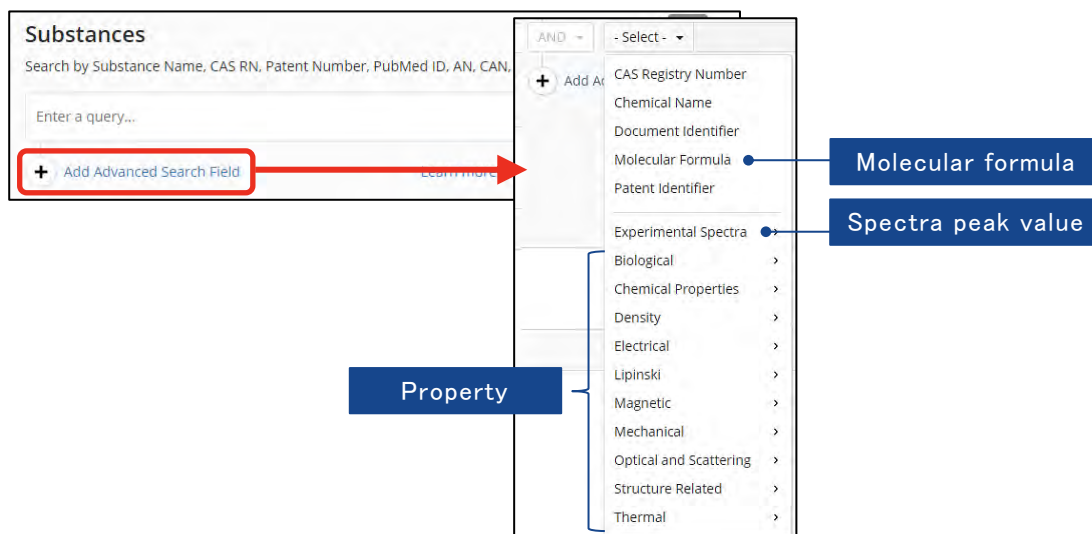
- Chemical Structure



- To find patents by Markush structure, check the box for Search Patent Markush (P.16).

- Molecular Formula, Substance Property and Experimental Spectra

- Click Add Advanced Search Field and select a field in the drop-down menu.



■ Select filters to display or exclude answers that match the applied filters.

- In chemical structure search, you can select the type of structure match.
(See P.15 for the difference of each type)

As Drawn

Substructure

Similarity

Filters

Commercial Availability

Reaction Role

Reference Role

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Data

Bioactivity Indicators (P.14)

Target Indicators (P.14)

Search within results by structure

Download filter data

Structure Match

As Drawn (21)

Substructure (7,216)

Similarity (14K)

Analyze Structure Precision

References

Reactions

Suppliers

Links to related data

Substances (1,832)

Sort: Relevance View: Partial

Filtering: Commercial Availability: Available

Clear All Filters

Available for structure search only

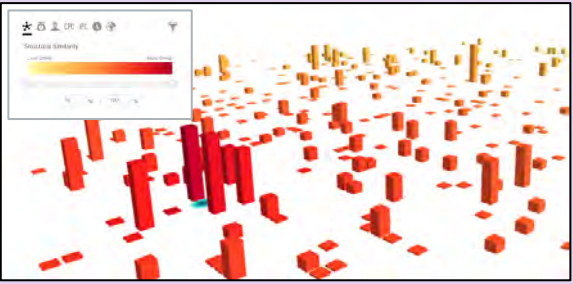
Commercially Available

Links to related data

Draw using current structure: You can modify the original query.

Visualize the similarity and patent landscape (Chemscape Analysis)

www.jaici.or.jp/scifinder-n/ref/sfn_chemscape.pdf



- To open the Substance Detail page, click the CAS RN®.

Substances (1,859) Sort: Relevance View: Partial

Filtering: Commercial Availability: Available X Clear All Filters

1 **305-01-1** 2 2088208-91-5 3 2086337-11-1

Substance Detail (1 of 1,859) Prev Next

References (2,912) Reactions (179) Suppliers (117) **Links to related data**

CAS Registry Number
305-01-1

CAS RN®

Chemical Structure

Molecular Formula
 $C_9H_6O_4$
2H-1-Benzopyran-2-one, 6,7-dihydroxy- (9CI, ACI)

Experimental Properties

Key Physical Properties	Value	Condition
Molecular Weight	178.14	-
Melting Point (Experimental)	276 °C	-
Boiling Point (Predicted)	469.7±45.0 °C	Press: 760 Torr
Density (Experimental)	1.56 g/cm ³	-
pKa (Predicted)	7.74±0.20	Most Acidic Temp: 25 °C

Experimental Properties | Spectra Expand All | Collapse All

Other Names and Identifiers **Substance Names**

Experimental Properties **Experimental Properties**

Experimental Spectra **Experimental Spectra**

Proton NMR Spectrum Detail (6 of 8)

305-01-1
Oc1cc2c(c1)oc(=O)c2
 $C_9H_6O_4$
CAS Name: Esculetin

Conditions:
Working Frequency: 400 MHz
Solvent: DMSO-d₆ (200627-1)

Spectrum Summary:
Spectrum ID: 11py10n1_38.H
Peak Data: 7.36, 6.97, 6.74, 6.16 ppm
Source: Spectral data were obtained from Advanced Chemistry Development, Inc.

Source of Spectra

(1) Copyright Bio-Rad Laboratories. All Rights Reserved.

(4) Spectral data were obtained from Advanced Chemistry Development, Inc.

(5) Razdan, T. K.; Phytochemistry, (1987), 26(7), 2063-9, CAplus

(6) Shi, Shuyun; Journal of Chromatography A, (2008), 1209(1-2), 145-152, CAplus

(7) Liu, Renmin; Journal of Chromatography A, (2005), 1072(2), 195-199, CAplus

Predicted Properties **Predicted Properties**

Predicted Spectra **Predicted Spectra**

Bioactivity Indicators **Bioactivity Indicators (P.14)**

Target Indicators **Target Indicators (P.14)**

Regulatory Information **Regulatory Information***

Additional Details

* For the detail of regulatory information in CAS SciFinder®, see www.jaici.or.jp/scifinder-n/ref/sfn_regulatory.pdf.

- You may retrieve data related to all or specific Substance page results.
 - To retrieve data about all substance results, click the All Results button.
 - To retrieve data about specific substance results, check the box for each substance, and then click the Selected Results button.

The interface shows a list of substances with columns for 'References', 'Reactions', and 'Suppliers'. A red box highlights the 'References' column, with an arrow pointing to a detailed view of references for a specific substance. Another red box highlights the 'Selected Results' button, with an arrow pointing to a detailed view of references for selected substances. A third red box highlights the 'Reactions' column, with an arrow pointing to a detailed view of reactions for a specific substance. A fourth red box highlights the 'Suppliers' column, with an arrow pointing to a detailed view of suppliers for a specific substance.

Related references

Related reactions

Related suppliers

Substances (1,859)

Sort: Relevance View: Partial

3 Selected References Reactions Suppliers

Filtering: Get References for Substances

All Results Selected Results

For all substances For selected substances

Related data about each substance

Check the button to select a specific substance.

Filter Behavior

Filter by Exclude

Document Type

- Journal (6,322)
- Patent (690)
- Review (78)
- Clinical Trial (8)
- Commentary (1)

View All

Substance Role

- Biological Study (4,970)
- Uses (1,746)
- Preparation (1,141)
- Analytical Study (1,038)
- Properties (686)

View All

Language

References (7,065)

Substances Reactions Cited By

Accumulation of Hydroxycoumarins During Post-harvest Deterioration of Tuberous Cassava (*Manihot esculenta* Crantz)

By: Buschmann, Holger; Rodriguez, Maria X.; Tohme, Joe; Beeching, John R. Annals of Botany (London) (2000), 86(6), 1153-1160 | Language: English; Database: C.Aplus

View Abstract

Full Text

Substances (5) Cited By (5)

Substances (1,859)

3 Selected References Reactions Suppliers

Reactions (531)

References

Scheme 1 (2 Reactions)

Suppliers (122) Suppliers (117)

Reaction Summary

Steps: 1 Yield: 100% Enzymatic ortho-hydroxylation of 4-hydroxyphenylacetate 3-monooxygenase

1.1 Catalysts: 4-hydroxyphenylacetate 3-monooxygenase Solvents: Water: 12 h 37 °C

By: Van, Yajun; et al United States, US2014

View Reaction Detail

Reaction Summary

Steps: 1 Yield: 10% The persulfate oxidation of phenols and arylamines (the Elbs and the Boyland-Sims oxidations)

By: Behrman, E. J.

Suppliers (231)

Supplier Substance Purity Purchasing Details Availability

1 Wako 305-01-1 Esculetin <90% Product information 5g, JPY 19000 Bulk

2 Wako 305-01-1 Esculetin <90% Product information 1g, JPY 6100 Bulk

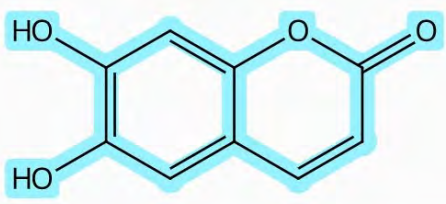
Tips: Bioactivity Indicators and Target Indicators

- Some substance records have Bioactivity Indicator and/or Target Indicators.
 - Bioactivity Indicators shows types of biological activity that substances in the result set may have.
Example: Antitumor agents, Anti Platelet agents, etc.
 - Target Indicators shows types of receptors or enzymes that substances are expected to interact with.
Example: α -amylase, dopamine receptor, etc.
 - You can retrieve the references studying bioactivities, receptors, or enzymes related to the substance by clicking a link of each indicator name.

Bioactivity Indicators

Target Indicators

CAS Registry Number
305-01-1



Predicted Spectra
 Bioactivity Indicators
 Anti-inflammatory agents (86)
 Antitumor agents (130)

Target Indicators
 Apoptosis-regulating proteins
 Bax proteins (27)
 Bcl-2 proteins (26)
 Cell cycle regulatory proteins
 Cyclin D1 (10)
 Chromoproteins
 Cytochrome c (18)
 Enzymes
 Alanine aminotransferase (16)
 Aldehyde reductase (11)
 Arachidonate 5-lipoxygenase (16)
 Arachidonate lipoxygenase (11)
 Caspase-3 (38)
 Caspase-8 (10)
 Caspase-9 (20)
 Catalase (12)
 Cyclooxygenase (18)
 Cyclooxygenase 1 (13)
 Cyclooxygenase 2 (18)
 Gelatinase B (10)
 Glutathione peroxidase (12)
 L-Lactate dehydrogenase (11)
 Lipoxygenase, general (15)
 Mitogen-activated protein kinase (11)
 Mitogen-activated protein kinase 1 (15)
 Mitogen-activated protein kinase 3 (15)
 Mitogen-activated protein kinase p38 (11)
 Monophenol monooxygenase (11)
 Nitric oxide synthase, iNOS (10)
 Poly(ADP-ribose) polymerase (13)
 Protein kinase Akt (14)
 Tumor suppressor proteins
 p53 (protein) (11)

Regulatory Information

References where 305-01-1 may be mentioned as anti-inflammatory agent

1. New secoiridoids and bioactive components extracted from *Fraxinus chinensis* and its preparation method
By: Chen, Jih Jung; Shieh, Po Chuen; Chen, Chin Yen; Hwang, Tsong Long Taiwan, TW568443 B 2017-02-01 | Language: Chinese, Database: Cplus
View Abstract

2. Chinese medicinal pellet containing *Corydalis* and *Scutellaria* and others for treating upper respiratory system infection
By: Long, Chaofeng; Xie, Chenshi; Chen, Muzhou; Zhao, Xiping China, CN101904948 A 2010-12-08 | Language: Chinese, Database: Cplus
View Abstract

3. Effects of PD and its ingredients on LPS-induced endothelial cell to secrete TNF- α , TXB₂ and 6-keto-PGF_{1 α}
By: Hu, Yiyi; Mu, Xiang; Hu, Yuanliang

References where 305-01-4 may interact with cytochrome c

1. Esculetin, a natural coumarin compound, evokes Ca²⁺ movement and activation of Ca²⁺-associated mitochondrial apoptotic pathways that involved cell cycle arrest in ZR-75-1 human breast cancer cells
By: Chang, Hong-Tai; Chou, Chiang-Ting; Lin, You-Sheng; Shieh, Pochuen; Kuo, Dai-Huang; Jan, Chung-Ren; Liang, Wei-Zhe Tumor Biology (2016), 37(4), 4665-4678 | Language: English, Database: Cplus
View Abstract

2. Esculetin induces mitochondria-mediated apoptosis in 3T3-L1 adipocytes
By: Yang, Jeong-Yeh; Della-Fera, Mary Anne; Baile, Clifton A. Apoptosis (2006), 11(8), 1371-1378 | Language: English, Database: Cplus
View Abstract

3. Esculetin induces apoptosis of SMMC-7721 cells through IGF-1/PI3K/Akt-mediated

Tips: Chemical structure search type

- Substances that match following three types will be retrieved automatically if you use a structure query.

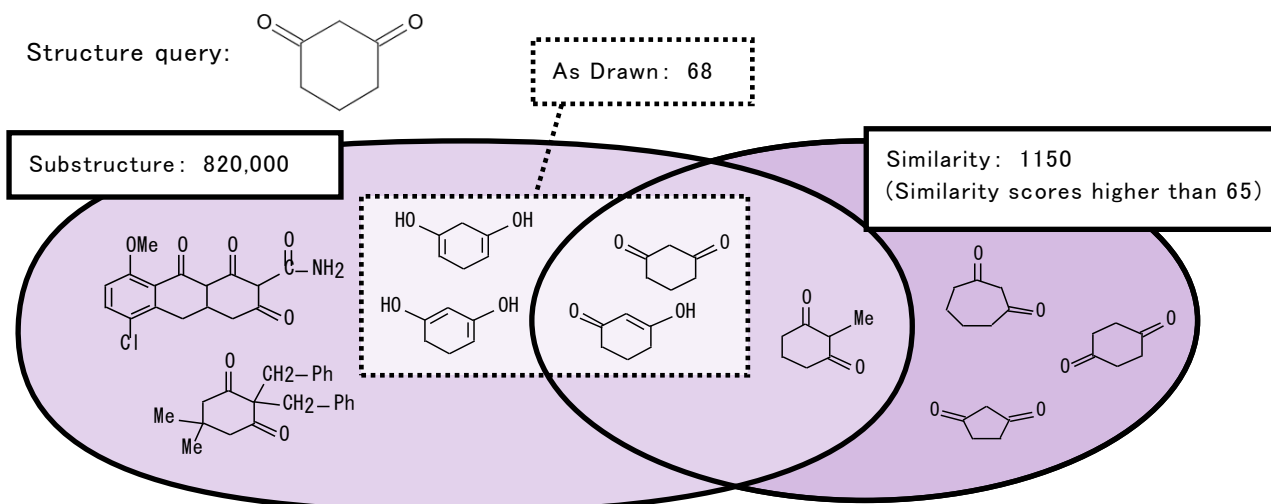
- Select the type you wish to view from Structure Match.

- Difference in each search type

Search Type	Retrieved substances
As Drawn (Exact Search)	<ul style="list-style-type: none"> Substances that match the structure exactly as drawn (including stereoisomers or isotopes) and multicomponent substances in which the queried structure appears Tautomers
Substructure (Substructure Search)	<ul style="list-style-type: none"> In addition to the substances in a As drawn match, any substituent is allowed at any open atom position.
Similarity * (Similarity Search)	<ul style="list-style-type: none"> Substances that are similar to the queried structure in addition to the substances retrieved by Exact Search <ul style="list-style-type: none"> Substances containing different elements or element's positions than the queried structure Substances that do not match the queried structure exactly (e.g.: For ethyl group, methyl group can be retrieved) Substances containing different cyclic structure than the queried structure (e.g.: For 6-5 membered ring, 6-6 membered ring can be retrieved)

* Similarity score is calculated based on a Tanimoto metric.

- Relation between three search types

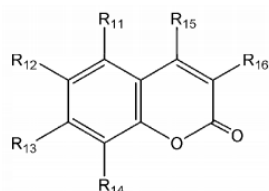


For the details, see www.jaici.or.jp/scifinder-n/ref/sfn_strtype.pdf.

Tips: Markush structure search (MARPAT)

- Use a Patent Markush search to find patents that have generic formula (Markush structure) described in the claims matching your query.

e.g.: WO2014204104



(Formula 2)

in Formula 2, R11, R12, R13, R14, R15, and R16 are each independently -H, -OH, -OR19, or -R20, and wherein R19 and R20 are each independently C1-C20 alkyl, C2-C20 alkenyl, or C2-C20 alkynyl and at least one of R11, R12, R13, R14, R15, and R16 is hydroxyl group.

- To find patents by a Patent Markush search, check the box for Search Patent Markush.

- If multiple Markush structures in the patent match your query, all those structures are retrieved.

Exact Search

Substructure Search

Patent Markush Match

- As Drawn (139)
- Substructure (423)

Filter by

- Patent Office
 - World Intellectual Property Organization (70)
 - Japan (32)
 - United States (15)
 - China (7)
 - European Patent Organization (7)
- View All

Patent Markush (139)

Sort: Relevance

View patent detail

Location of the patent

View patent full-text

Patent detail

Reference Detail

Definition of Ak (alkyl chain having 1 to 6 carbon atoms)

Tips: Biosequence search

■ In the Biosequence search, there are following three search types.

- BLAST: Search for proteins as well as nucleotides using a set of local alignment algorithms.
- CDR: Search for antibody and t-cell receptors.
- Motif: Search for short patterns in DNA, RNA, or proteins

The screenshot shows the Biosequence search interface. On the left, a sidebar lists search categories: All, Substances, Reactions, References, Suppliers, and Biosequences (highlighted with a red arrow). The main area is titled 'Biosequences' and contains a search bar with the text 'gcggtttgctctctctctcttgcg'. Below the search bar are tabs for 'BLAST', 'CDR', and 'Motif'. A red box highlights the 'Advanced Biosequence Search' dropdown. To the right, a 'Sequence Type' dropdown is set to 'Nucleotide', and a 'Search Within' section has radio buttons for 'Nucleotides' (selected) and 'Proteins'. A 'Limit Total Sequence Results to:' dropdown is set to '20000'. A red box highlights the 'Start Biosequence Search' button. Annotations include: 'Select the Search Type' pointing to the BLAST/CDR/Motif tabs, 'Select the Sequence Type' pointing to the Nucleotide/Protein dropdown, and 'Adjust Parameters' pointing to the Advanced Biosequence Search dropdown.

The screenshot shows the Biosequence search results page. On the left, a 'Search Details' panel displays search parameters: Sequence Type: Nucleotide, Search Within: Nucleotides, BLAST Algorithm: BLASTn, Alignment Identity: 80%, Query Coverage: 90%, E-Value: 10, Match with Gaps?: No, Gap Costs: Existence 5 Extension 2, Word Size: 11. Below this is a 'Bioscape Analysis' section with a 'Create Bioscape Analysis' button. A 'Filters' panel on the left allows filtering by E-Value, Query Coverage %, Subject Coverage %, and Alignment Identity %. The main results area is titled 'Biosequences (198)' and shows a table with columns for Alignment, Subject, and References. A red box highlights the 'References' column. A 'Sort results' dropdown is set to 'Alignment Identity'. A 'View More' link is present. Below the table, an 'Alignment Visualization' section shows a sequence alignment between a Query and a Subject. A 'Detail of the Sequence' section displays the alignment data, including the BLAST Score (42) and E-Value (0.0385525). A 'Detail of Source References' section shows the source of the sequence. A 'Link to related references' button is present. A 'Visualize the similarity and patent landscape (Bioscape Analysis)' section shows a heatmap of sequence similarity. Annotations include: 'Search Details' pointing to the search parameters panel, 'Filters' pointing to the filter panel, 'Sort results' pointing to the sort dropdown, 'Alignment Visualization' pointing to the sequence alignment, 'Detail of the Sequence' pointing to the alignment data, 'Detail of Source References' pointing to the source information, 'Link to related references' pointing to the related references button, and 'Visualize the similarity and patent landscape (Bioscape Analysis)' pointing to the heatmap.

For the details of Biosequences Search, Bioscape Analysis or search for nucleic acid or protein/peptide, see www.jaici.or.jp/scifinder-n/ref/sfn_bioseq.pdf.

Reaction search

- In the Reaction search, you can find reactions by substance name, chemical structure, CAS Registry Number (CAS RN®), etc.

Searching for...

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

Reactions
Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, C...

Enter a query...

Substance names or patent numbers can be entered.

Open structure editor

Retrosynthesis Planner (P.21)
Retrosynthesis Planner is a feature to generate synthetic routes including predicted steps by retrosynthesis analysis.
<https://www.jaici.or.jp/scifinder-n/retrosynthesis>

- Select the type you wish to view from Structure Match. To focus the result set, select filters from Filter by or Exclude on the left side of the page.

Exact Search
Substructure Search
Similarity Search

Filters

Yield

- 90-100% (84)
- 80-89% (120)
- 70-79% (107)
- 50-69% (156)
- 30-49% (56)

Number of Steps

- Non-Participating Functional Groups
- Reaction Mapping
- Experimental Protocols
- Synthetic Methods (84)
- Experimental Procedures

Reaction Type

- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search within Results by reaction structure

【Source Reference】

- Document Type
- Language
- Publication Year
- Publication Name

Download filter data

Structure Match

- As Drawn (0)
- Substructure (1,692)**
- Similarity (15K)

Filter Behavior

- Filter by
- Exclude

Yield: 90-100%

Synthetic Methods is available

Draw using current structure: You can modify the original query.

View reference information

Links to supplier information

- Results are grouped by scheme (default)
 - Each scheme contains reactions that have the same reactants and products.

Group: By Scheme (Default)

View: Expanded

View/Hide Reaction Summary

Reaction Summary

View Reaction Detail

Experimental Protocols (P.20)

Reference information

- By Document groups reactions by the document in which they are referenced.

Group: By Reference

View: Expanded

View reference information

View All Related Reactions

View Reaction Detail

Experimental Protocols (P.20)

Each result displays one example reaction and reaction summary per document.

- To view a reaction detail, click Experimental Protocols.

Reactions (84) Group: By Scheme View: Expanded

Filtering: Yield: 90-100% Experimental Protocols: Synthetic Methods Clear All Filters

Scheme 1 (2 Reactions) Steps: 1 Yield: 92-99%

Suppliers (115) Suppliers (90) Suppliers (5)

Reaction Summary Steps: 1 Yield: 99% An Amphiphilic Resin-Supported Palladium Catalyst for High-Throughput Cross-Coupling in Water

1.1 Reagents: Potassium carbonate Catalysts: Palladium(1+), [1-(diphenylphosphino-κP)-N-((diphenylphosphino-κP)methyl)methan... (ArgoGel bound) Solvents: Water By: Uozumi, Yasuhiro; et al Organic Letters (2002), 4(17), 2997-3000

View Reaction Detail Experimental Protocols

Reaction Summary

Synthetic Methods

Experimental Protocols

Synthetic Methods Experimental Procedure

Products: 2-(1-Naphthalenyl)thiophene, Yield: 99%

Reactants: 2-Iodothiophene, 1-Naphthylboronic acid

Reagents: Potassium carbonate

Catalysts: Palladium(1+), [1-(diphenylphosphino-κP)-N-((diphenylphosphino-κP)methyl)methan... (ArgoGel bound)

Solvents: Water

Procedure: 1. Add aryl halide (0.5 mmol), boronic acid (0.6 mmol), K₂CO₃ (2.5 mmol), water (1.65 mL) and amphiphilic resin-supported palladium complex (33 mg, 10 μmol Pd) into a baker disposable filtration column. 2. Shake the mixture on a Libralis at 50 °C for 12 hours. 3. Filter the reaction mixture. 4. Rinse the reaction mixture with water. 5. Separate the organic layer. 6. Dry the organic layer over Na₂SO₄. 7. Concentrate the organic layer under reduced pressure. 8. Filter the residue through silica gel.

Transformation: Coupling of Aryl Compounds with A

Step-by-step procedure

Detailed reaction information by item (Synthetic Methods)

Experimental Procedure

Experimental Protocols

Synthetic Methods Experimental Procedure

General/Typical Procedure: Palladium-catalyzed Cross-Coupling in water. General Procedure for Table 2: A Baker Disposable Filtration Column was charged with 5 (0.5 mmol), 6 (0.6 mmol), K₂CO₃ (2.5 mmol), water (1.65 mL) and Pd(PPh₃)₄-adsorbed complex (33 mg, 10 μmol Pd), and the mixture was shaken on a Libralis at 50 °C for 12 h. The reaction mixture was filtered, rinsed with water (4 mL x 5) and diethyl ether (5 mL x 5). The organic layer was separated, dried over Na₂SO₄ and concentrated under reduced pressure. The residue was filtered through silica gel pad (eluent, hexanes/ethyl acetate, 7:3 v/v).

Experimental Section in the original document (Experimental Procedure)

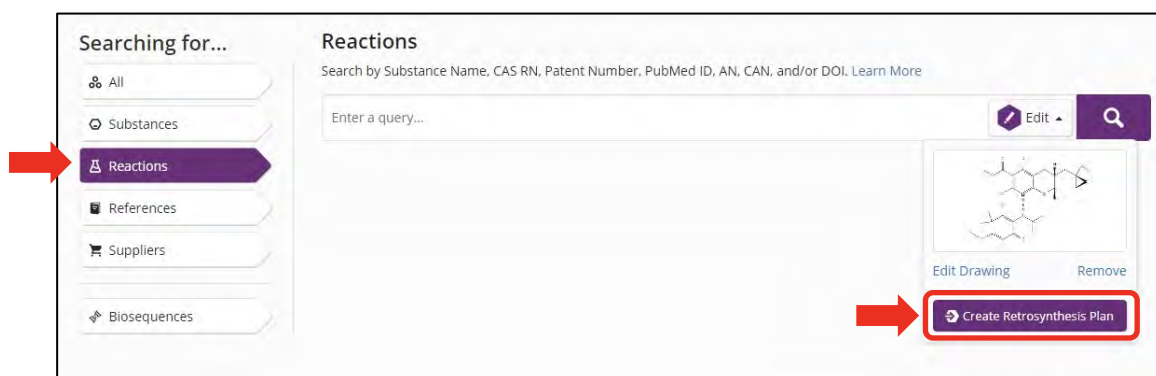
Contents of Experimental Protocols

Synthetic Methods	
Journals	2000–
ACS	: Journal of Medicinal Chemistry, Journal of the American Chemical Society
Springer	: Catalysis Letters
Taylor & Francis	: Journal of Coordination Chemistry
Elsevier	: Tetrahedron
RSC	: Chemical Science
Wiley	: Angewandte Chemie etc, (about 180 journals)
WIPO patents (English)	2010–
Experimental Procedure	
Journals	Mainly 1998–
ACS	: All journals
Taylor & Francis	: Synthetic Communications, Journal of Coordination Chemistry, etc
Springer	: 165 journals in Chemistry (1985–)
Shanghai institute of Organic Chemistry	: Youji Huaxue, Huaxue Xuebao
Thieme	: SYNLETT (1989–2013), SYNTHESIS (1980–2013)
SORD	: Selected Organic Reactions Database (dissertations, 1961–2011)
Patents	2000–
English	: US (America), EP (Europe), WIPO (World Intellectual Property Organization), CA (Canada), GB (Great Britain)
Japanese	: JP (Japan), WIPO (World Intellectual Property Organization)
German	: DE (Germany), EP (Europe), WIPO (World Intellectual Property Organization)

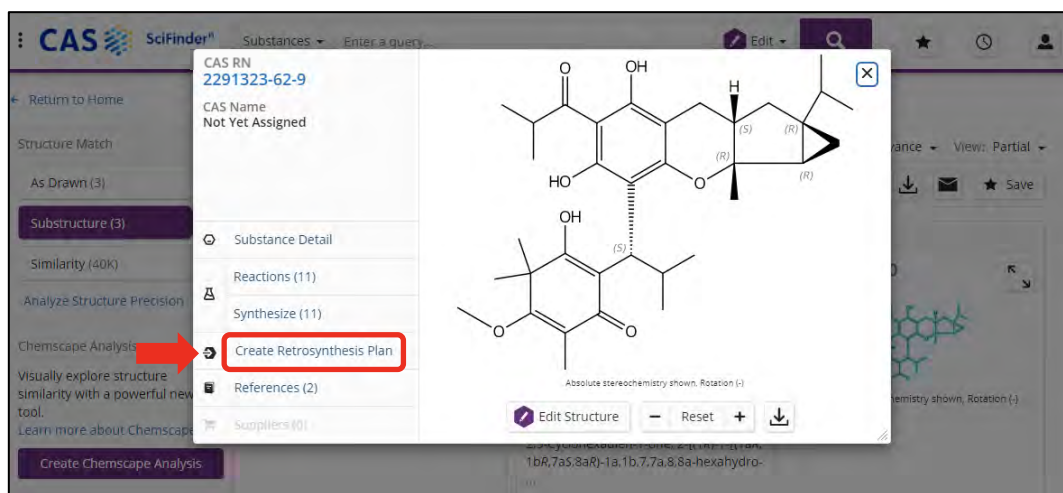
Tips: Retrosynthesis Planner

- Retrosynthesis Planner creates viable synthetic steps to the target substance based on known reactions in CASREACT (For more detail, see www.jaici.or.jp/scifinder-n/ref/sfn_retrosynthesis.pdf).

- From the Reactions Search page
 - Draw a structure on the Reactions page, and then click the Create Retrosynthesis Plan button displayed under the structure image.



- From a substance window
 - After opening the substance window by clicking a substance structure image, Click the Create Retrosynthesis Planner button on the left side of the substance window.



- You can continue to work within CAS SciFinderⁿ while waiting for your Retrosynthesis plan to complete.

Open created Retrosynthesis Plan

You can open created Retrosynthesis plan from the ★ (Save) button or the ⌚ (History) button. Saved retrosynthesis plans expire 90 days after the date they are first generated.

- Plan Options page appears after clicking the Create Retrosynthesis Plan button.

Plan Options Powered by ChemPlanner®

Select Synthetic Depth
Synthetic depth restricts the number of steps generated in the plan. [Learn More.](#)

Set Rules Supporting Predicted Reactions
Common rules are supported by many literature examples. Uncommon and Rare rules are supported by fewer examples, but may expose novel approaches. [Learn More.](#)

Break and Protect Bonds **Bond-breaking restrictions**
You may select one bond to break in the first step of the plan. Any bonds you protect will not break, though their order may change. [Learn More.](#)

☐ 1 ☐ 2 ☒ 3 ☐ 4

☒ Common ☐ Uncommon (includes Common) ☐ Rare (includes Common)

☒ Email me when my Retrosynthesis Plan is Complete

- To apply your edits to the options and generate your plan, click the Create Retrosynthesis Plan button.

- Overview and Steps tabs are displayed in Retrosynthesis Plan page. Red lines are experimental steps and green ones are predicted steps.

Retrosynthesis Powered by ChemPlanner®

Overview **Steps** **Predicted Results** ☒ 予測反応の表示

Plan Information
Estimated Yield: 20%
Overall Price: \$8,648.11 (USD per 100 grams)
Commercially Available: C, D, E

Plan Options
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
[Edit Plan Options](#)

Scoring Profiles
Complexity Reduction
Convergence
Evidence

Retrosynthesis Step Key
Hover on the options below to highlight experimental and predicted steps within this plan. [View Steps Menu.](#)

☒ Experimental Steps **Experimental steps**

☐ Predicted Steps **Predicted steps**

View/Select alternative steps

Experimental steps **Predicted steps** **Stereoselective reaction**

- The Overview tab has estimated yield, overall cost, and commercially available substances in the current retrosynthesis plan.
In the Scoring Profiles, you can set scoring profiles that determine what is displayed in the plan/alternative steps.
- The Steps tab provides the summary of all steps in the current retrosynthesis plan.
 - Evidence : View reactions and references supporting the plan step.
 - Alternative Steps : View and select alternatives for a plan step.

Supplier search

- In the Supplier search, you can find suppliers by substance name, chemical structure, etc.

- Answers are sorted by Relevance by default.

- Click to specify a supplier as Preferred. Preferred suppliers will appear at the top of the list.
- Select filters to display or exclude answers that match the applied filters.
- To view its supplier detail page, click the supplier name.

Saving, Alerts, and Sharing

■ Selected results and the search can be saved or shared with other users.

- Click the Email icon to share results with a colleague via email.
 - You can share your results including keywords and/or structures with filter items you used.
 - You can share your results within the same organization.
- Click the Save button to save text/structure query including applied filter items.
 - To save individual answers, select check boxes of individual results you wish to save, and then click the Save button.
 - To set an alert, click the Save button then select a frequency from As Available (new content added), Weekly, or Monthly.

Share results

Save results

Open user's default email application

Send with CAS SciFinderⁿ

Name

Alert frequency (Manage Alert)

Save

- To access the saved searches and results, click ★ button on the top menu bar.

Filter by search type

Limit items with/without alerts

Combine saved items (See www.jaici.or.jp/scifinder-n/ref/sfn_combine.pdf)

Rerun search

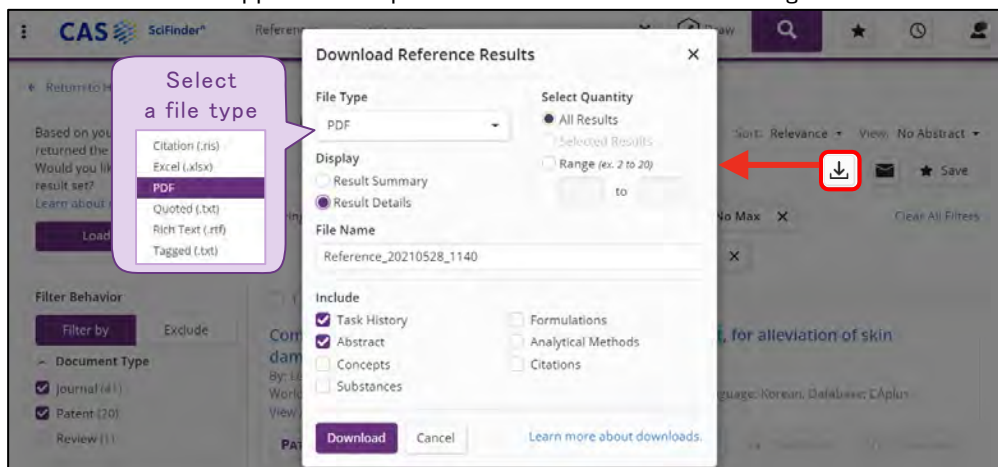
View saved answers

Open a list of alert results

View individual alert results

Download results

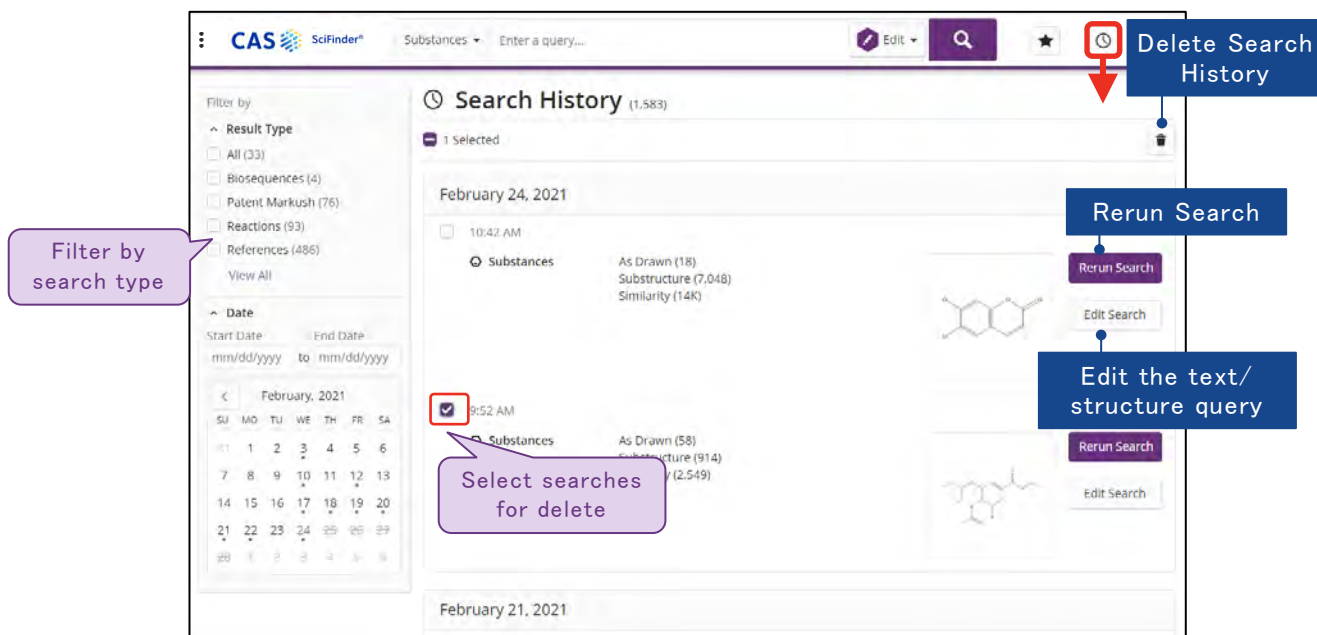
- CAS SciFinder[®] supports multiple data formats for downloading results.




- You can share your downloaded answers within the same research group.
- Up to 500 or 100 answers can be downloaded at one time
- Users are not allowed to keep more than 5,000 downloaded answers at any given time under the license agreement. Answers exceeding 5,000 shall be deleted.

Search history

- To access the search history page, click the clock icon at the top of any page.



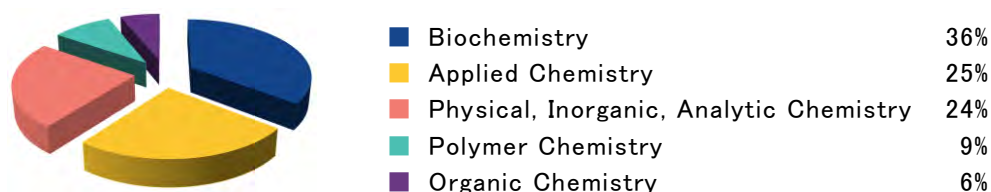
- Text/structure queries you used before clicking the  icon are recorded on the Search History page. Filters used after the search are not included.

Tips: Contents of CAS SciFinderⁿ

■ Main contents of CAS SciFinderⁿ

- References published in more 50 languages that are searchable in English
- Journal
 - Journals in science and technology fields (several thousands)*
 - * Bibliographic information of major 1,500 journals is added within 1 week of journal receipt in CAS
 - Journals in biology and medical fields (several thousands)
- Patents
 - Patents in Chemical and surrounding area around the world (several thousands)*
 - * Bibliographic information of patents from major countries is added within 2 days of the patent's issuance and fully indexed by CAS scientists in less than 27 days from the date of issue.

■ Area of contents (CAS References)



■ Substance Type

- Organic Compounds
- Nucleic acids, Proteins
- Polymers
- Inorganic Compounds
- Coordination Compounds
- Alloys

■ Searchable information in CAS SciFinderⁿ

(As of July 2021)

Category	Contents	Amount of information	Year
Reference	Chemistry and surrounding area 【CAS References】	> 54 million references	1808–
	Biology and medical area 【MEDLINE】	> 32 million References	1946–
	Patents with Markush structure 【CAS Markush】	> 54 thousand References (patent) > 1.9 million Markush structures	1961–
	Chemistry area in old era (option)【CAS ChemZent】	> 3 million References	1830 – 1969
Substance	Chemical name, CAS Registry Number (CAS RN®), molecular formula, chemical structure, sequence, physical property, etc. 【CAS REGISTRY】	> 2.47 million Substances	Early 1800–
Reaction	Organic chemical reactions 【CAS Reactions】	> 1.18 million Reactions > 1.9 million References	1840–
Catalog	Catalog information 【Commercial Sources】	Hundreds of Catalog information provided by chemical vendors around the world	As available
Regulatory	Inventory and regulatory information around the world	> 400 thousand Substances	1979–

Training materials

- JAICI offers Japanese training materials on <https://www.jaici.or.jp/scifinder-n/doc.html>. We also offer links to English training materials created by CAS.

The screenshot shows the JAICI website's technical resources page for CAS SciFinder. The header includes the JAICI logo, navigation links for various services, and a search bar. The main content area is titled 'CAS SciFinder[®] - 技術資料' and lists various resources such as search guides, literature search, and chemical reaction search. A sidebar on the left provides navigation options like 'ログイン' (Login) and 'はじめての方' (For first-time users).

- You can use another English training and on-demand materials on CAS Web site. (<https://www.cas.org/support/training/scifinder-n>)

The screenshot shows the CAS SciFinder Training page. The header includes the CAS logo and navigation links. The main content area is titled 'SciFinder[®] Training' and features a section for on-demand training resources, stating: 'These on-demand SciFinder[®] training resources are short, targeted materials, organized by search type.'

Helpdesk (9 a.m. – 5 p.m. weekdays, Japan standard time)

Users in Japan can contact us if you have questions or need information about CAS SciFinder[®].

e-mail support@jaici.or.jp

* For users outside of Japan, please contact help@cas.org for support.