



# Web version of SciFinder®: new interface and features

Bhawat Ruangying, CAS representative

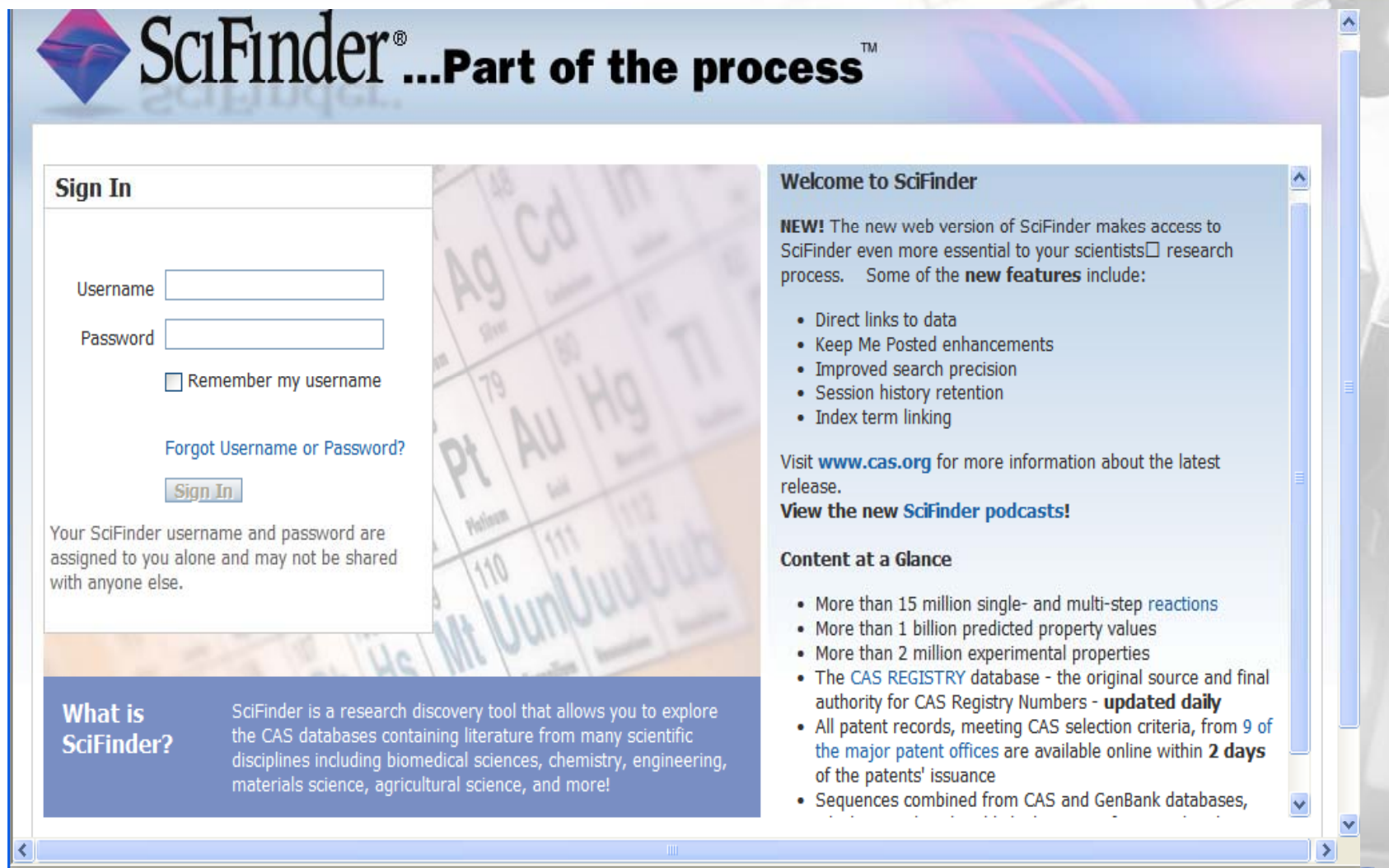
Updated at 22 Dec 2009

[www.cas.org](http://www.cas.org)



*A division of the American Chemical Society*

# SciFinder web interface



**SciFinder**® ...Part of the process™

### Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

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

### Welcome to SciFinder

**NEW!** The new web version of SciFinder makes access to SciFinder even more essential to your scientists' research process. Some of the **new features** include:

- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Visit [www.cas.org](http://www.cas.org) for more information about the latest release.

**View the new SciFinder podcasts!**

### Content at a Glance

- More than 15 million single- and multi-step reactions
- More than 1 billion predicted property values
- More than 2 million experimental properties
- The **CAS REGISTRY** database - the original source and final authority for CAS Registry Numbers - **updated daily**
- All patent records, meeting CAS selection criteria, from **9 of the major patent offices** are available online within **2 days** of the patents' issuance
- Sequences combined from CAS and GenBank databases,

### What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!



# Technical aspects of SciFinder Web

- SciFinder URL : <http://scifinder.cas.org>
  - Windows-based browsers Internet Explorer 6.x and 7.x as well as FireFox 2.x
  - Mac browser support for Firefox and Safari
  - Java applet (J2SE Runtime Environment 6.0, which installs Java 1.6 version) installed on users' computers for CASDraw to operate
- No software or sife.prf required
- Network requirement:
  - https (SSL) connection via port 443 to scifinder.cas.org
  - http connection on port 80 to chemport.cas.org
- Client based SciFinder will continue to be fully supported by CAS



# Online user registration consists of two steps

## Key Contact Setup

- Log on to myCAS to use set-up registration capabilities
- Verifies email domain(s) are correct and sufficient
- Sends CAS corrections or updates as needed
- Generates unique registration URL for distribution to users

## User Registration

- Obtains the registration URL
- Creates a new username and password online
- Enters required email address and other information
- Confirms registration via email



# User enters the information

**SciFinder**

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

**CONTACT INFORMATION**

First Name\*:   
Last Name\*:   
E-mail\*:   
Confirm E-mail\*:   
Phone Number:   
Fax number:   
Area of Research:  Select one  
Job Title:  Select one

**USERNAME AND PASSWORD**

Username\*:  [Tip](#)  
Password\*:   
Re-enter Password\*:

**SECURITY INFORMATION**

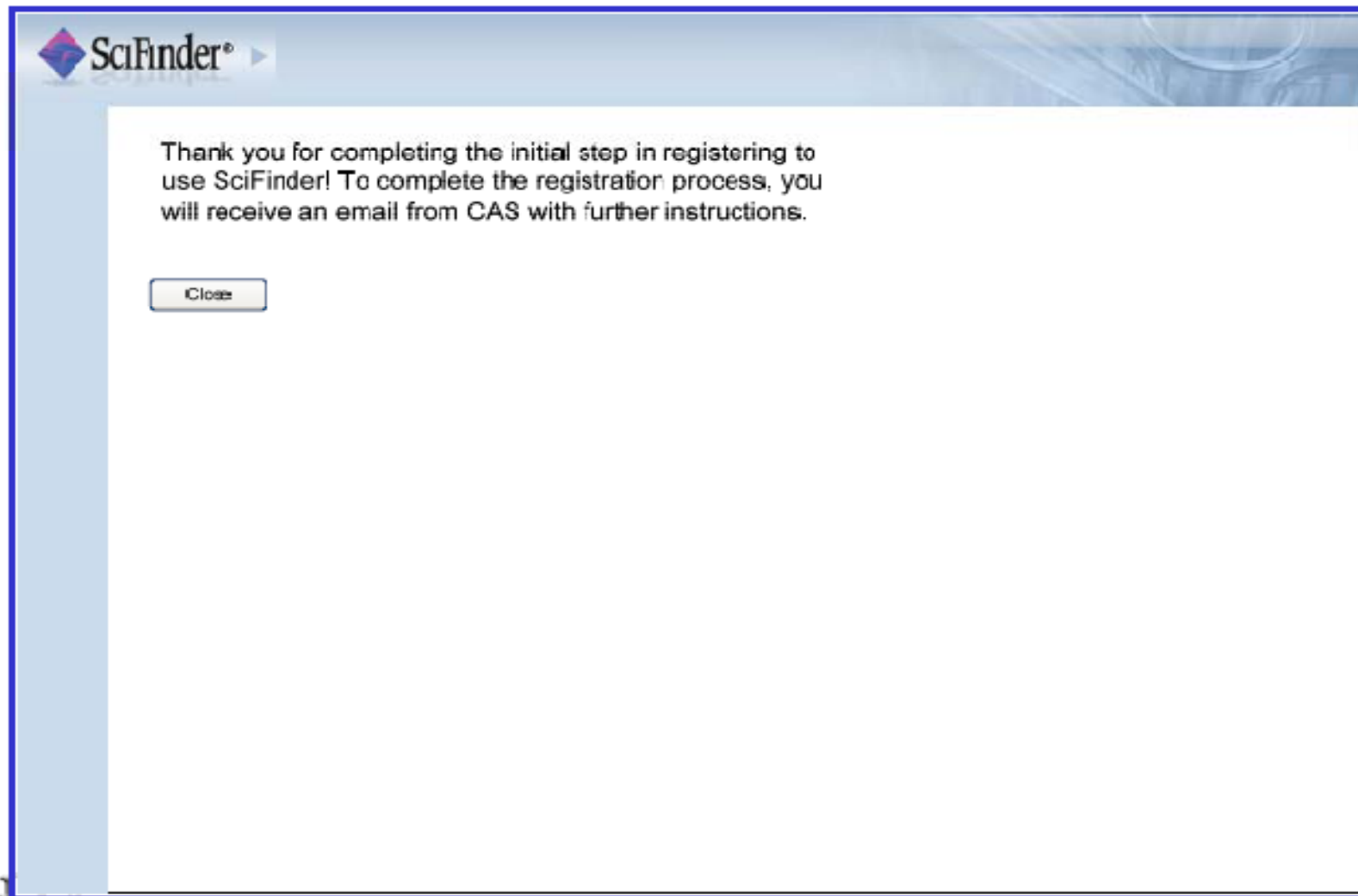
Security Question\*:  Select one [Why?](#)  
Answer\*:

**Email domain must match valid domain(s) and the entire address must be unique.**

**Username and password must meet minimum requirements and be unique.**

- What is your favorite color?
- What is the name of the city where you grew up?
- What is the name of your favorite pet?
- What is your favorite musical instrument?
- What is your ideal vacation location?

# Email validation for new IDs





# User receives email confirmation

Generic Email Message Tool

To... <End user email address>

Cc...


Subject: SciFinder Registration Completion

From: CAS

Dear <Username>,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.

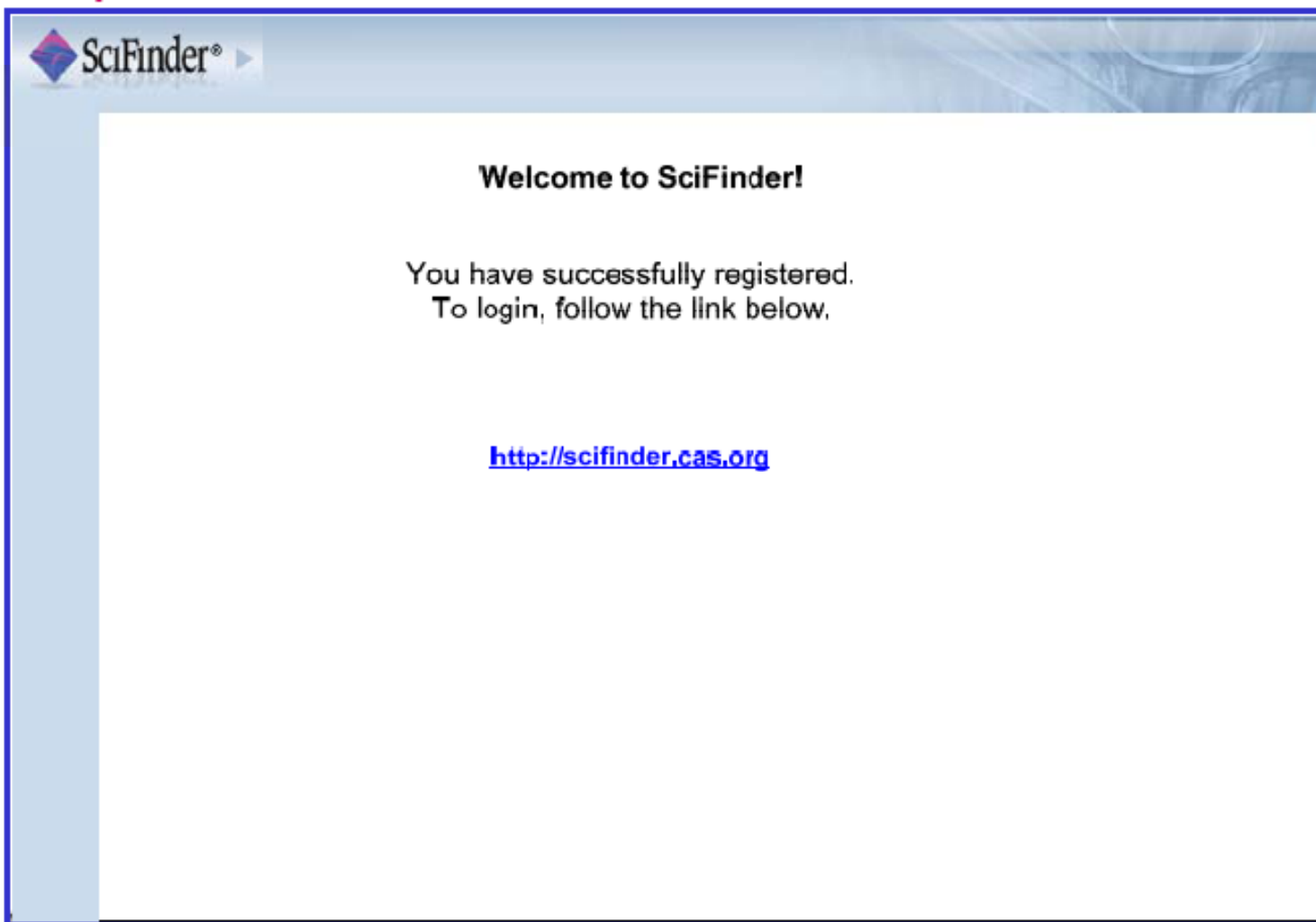
 <registration complete link>

If you need assistance at any time, consult the key contact at your organization.

Thank you!



# User is now ready to access



The screenshot shows a web browser window with the SciFinder logo in the top left corner. The main content area is white and contains the following text:

**Welcome to SciFinder!**

You have successfully registered.  
To login, follow the link below.

<http://scifinder.cas.org>



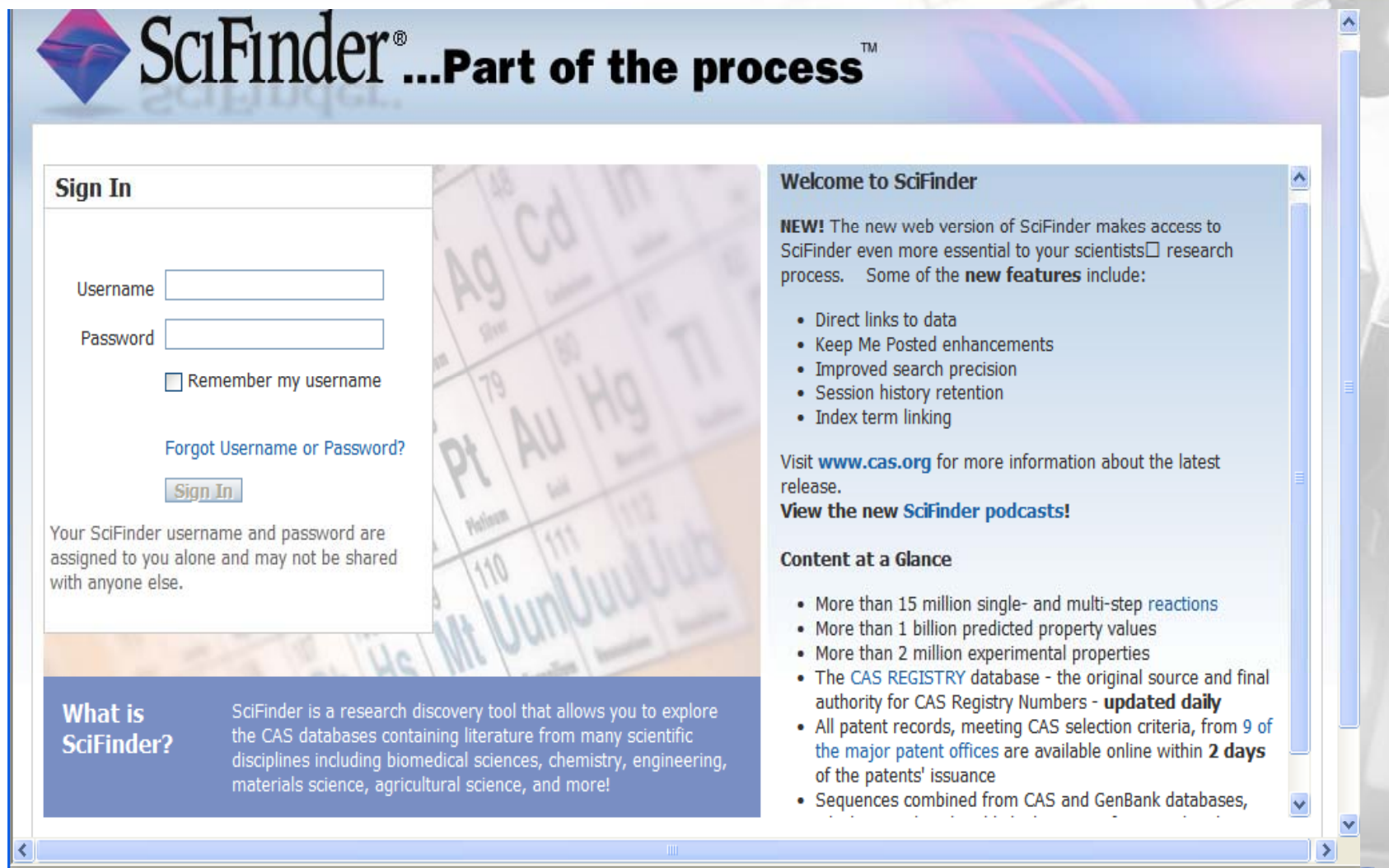




## A variety of ways to explore

- Research Topics
- Chemical names or structures
- Reaction structure drawings
- Functional group transformation

# SciFinder web interface



**SciFinder® ...Part of the process™**

### Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

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

### Welcome to SciFinder

**NEW!** The new web version of SciFinder makes access to SciFinder even more essential to your scientists' research process. Some of the **new features** include:

- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Visit [www.cas.org](http://www.cas.org) for more information about the latest release.

**View the new SciFinder podcasts!**

### Content at a Glance




- More than 15 million single- and multi-step reactions
- More than 1 billion predicted property values
- More than 2 million experimental properties
- The **CAS REGISTRY** database - the original source and final authority for CAS Registry Numbers - **updated daily**
- All patent records, meeting CAS selection criteria, from **9 of the major patent offices** are available online within **2 days** of the patents' issuance
- Sequences combined from CAS and GenBank databases,

### What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

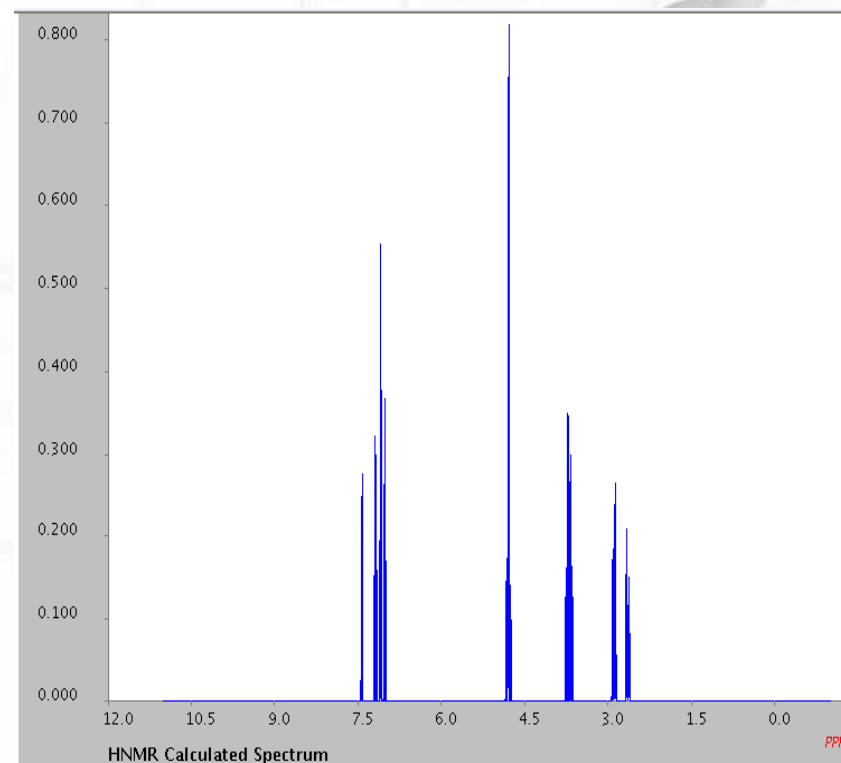


# SciFinder allows for integrated searching of these essential resources for scientists

Type of information	Content and coverage	Starting points for locating chemical synthesis information
 <b>References</b>	<ul style="list-style-type: none"> <li>• &gt;31 million references from 59 patent authorities worldwide and &gt;10,000 major scientific journals</li> <li>• &gt;18 million references from MEDLINE<sup>®</sup></li> <li>• 1907 to present, plus selected pre-1907 articles and patents</li> </ul>	<ul style="list-style-type: none"> <li>• Research topic</li> </ul>
 <b>Substances</b>	<ul style="list-style-type: none"> <li>• &gt;51 million organic and inorganic substances</li> <li>• &gt;61 million sequences</li> <li>• &gt;2.6 billion predicted and experimental properties, spectra, and data tags, plus &gt;29.6 million proton NMR spectra and 29.7 million predicted <sup>13</sup>C-NMR spectra</li> <li>• 1957 to present, plus selected substances back to the early 1900s</li> <li>• Commercial source information from &gt;1,000 suppliers for &gt;38 million substances</li> <li>• Regulatory information for &gt; 270,000 substances</li> </ul>	<ul style="list-style-type: none"> <li>• Chemical name or CAS Registry Number<sup>®</sup></li> <li>• Molecular formula</li> <li>• Chemical structure drawing</li> </ul>
 <b>Reactions</b>	<ul style="list-style-type: none"> <li>• &gt;29 million preparations, including &gt;21 million single- and multi-step reactions</li> <li>• 1840 to present</li> </ul>	<ul style="list-style-type: none"> <li>• Reaction structure drawing</li> <li>• Functional group transformation</li> </ul>

## New content added – more property data

- **1.9 billion** predicated and experimental properties, spectra and data tags
- **23.8 million** newly released predicted proton NMR spectra
- Thousands of new experimental NMR, IR, and Mass spectra as well as experimental physical properties now appear in Substance Details



# Prophetic Substance

A new role for substances indexed as prophetics. It is a specific substance located in the examples of a patent that has no supporting data (e.g property data or yields)

7758-29-4 Sodium tripolyphosphate

antimicrobial compns. and methods to eradicate and remove fungi and bacteria from indoor and outdoor structures and materials

Other use, unclassified; Technical or engineered material use; Uses; **Prophetic**

Reference Detail

Get Substances ⓘ

Retrieve substances for:

All references  Selected references

For each reference, retrieve:

All Substances

Substances associated with:

Adverse Effect, including toxicity  **Prophetics in Patents**

Analytical Study  Preparation

Biological Study  Process

Combinatorial Study  Properties

Formation, nonpreparative  Reactant or Reagent

Miscellaneous  Uses

Occurrence

Get Substances Cancel

Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical study	✓	✓		
Biological study	✓	✓	✓	✓
Formation, nonpreparative	✓	✓		
Miscellaneous		✓		
Occurrence		✓		
Preparation	✓	✓	✓	
Process	✓	✓		
Properties	✓	✓		
<b>Prophetic in patents</b>	✓			
Reactant or reagent	✓	✓		
Uses	✓	✓		

Substance Detail



## New content added – New reaction information

- More than 29 million preparations
- Thousands of evaluated reactions from several Wiley reference works:
  - Encyclopedia of Reagents for Organic Synthesis (EROS)
  - Organic Syntheses
  - Organic Reactions
- Giving access to important older reactions





# Reference Search



# Clear search interface at one page

The screenshot shows the SciFinder search interface. At the top, there are three navigation buttons: "Explore References" (highlighted with a red box), "Explore Substances", and "Explore Reactions". To the right, a user menu (highlighted with a blue box) includes "Answer Sets", "Keep Me Posted Results", "Help", "History", and "Preferences". The main search area is titled "Explore References" and features a "Research Topic" dropdown menu (highlighted with a red box) with options: "Author Name", "Company Name", "Document Identifier", "Journal", and "Patent". Next to it is a search input field with a "Search" button and example queries: "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds". Below the search area are filters for "Publication Year(s)", "Document Type(s)", and "Language(s)", each with a list of checkboxes and example values.

-Choose for references, substances and reactions search from the top

-Choose for the search way from the left

-Entry the search queries in the middle

# Informative references answer page

SciFinder®

Welcome Windy Wu | Sign Out

Explore References | Explore Substances | Explore Reactions

Answer Sets | Help | Keep Me Posted Results | History | Preferences

Create Keep Me Posted | Research Topic "anticancer drug for liver" > references (1227)

References | Get Substances | Get Reactions | Get Cited | Get Citing

1227 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | 1 2 3 4 5 6 ... 62

1. **Pharmaceutical composition containing salviannolic acid A and glycyrrhizic acid or its derivatives for preventing and/or treating cancer and cardiovascular and liver diseases**  
By Gu, Qun; Li, Zhigang; Qu, Shoufeng; Guo, Xiaopeng; Liu, Yan; Mi, Changjiang; Li, Yanbin; Lin, Zhirong; Shan, Huizhen; Jin, Zhigang  
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2008), CN 101292986 A 20081029. Language: Chinese, Database: CAPLUS  
The medical compn. contains 1-10 wt. part salviannolic acid A extd. from Salvia miltiorrhiza, and 1-20 wt. part glycyrrhizic acid or its derivs., and a suitable amt. of medical adjuvant. The content of salviannolic acid A in the medical compn. is 50-100%, and the compd. glycyrrhizic acid or its derivs is from Glycyrrhiza ext. Salviannolic acid A is obtained by extg. S. miltiorrhiza with water or ethanol, adjusting pH value, press filtering, and purifying on macroporous adsorbent resin column with 30-70% ethanol soln. as eluent, and/or refining on Sephadex LH-20 column with 50-95% ethanol soln. ...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

2. **Preparation of water soluble stilbene derivatives as anticancer drugs.**  
By Lee, Ruey-Min; Simoni, Daniele  
From PCT Int. Appl. (2008), WO 2008131320 A1 20081030. Language: English, Database: CAPLUS

Analysis | Refine

Sample Analysis

Author Name

Waxman David J

Sasaki Kenichi

Ishikawa Masaaki

Kestell Philip

Paxton James W

Waxman D J

Zhou Shufeng

-Abstract information for quick reference, with the keyword highlighted

-Get related information for particular or all references

-Analyses are performed automatically for getting more ideas of answer set

# A CPlus record (1)

SciFinder®

Welcome Windy Wu | Sign Out

Research Topic "anticancer drug for liver" > references (1227) > Pharmaceutical composition con...

Reference Detail

Get Substances Get Reactions Get Cited Get Citing Get Full Text

Link Save Print Export

Pharmaceutical composition containing salvianolic acid A and glycyrrhizic acid derivatives for preventing and/or treating cancer and cardiovascular diseases

Gu, Qun; Li, Zhigang; Qu, Shoufeng; Guo, Xiaopeng; Liu, Yan; Mi, Changjiang; Li, Yanbin; Lin, Zhirong; Zhigang

Assignee: Beijing Bencao Tianyuan Pharmaceutical Research Institute

The medical compn. contains 1-10 wt. part salvianolic acid A or its derivs., and a suitable amt. of medical adjuvant. The content of glycyrrhizic acid or its derivs is from Glycyrrhiza ext. S... ethanol, adjusting pH value, press filtering, and purifying on me... eluent, and/or refining on Sephadex LH-20 column with 50-95% ethanol soln. as eluent, and/or adjusting pH value, extg. with Et acetate (Pr acetate, Bu acetate, n-butanol or isopropanol), concg., and drying or freeze drying. The content of salvianolic acid A in the medical compn. is detd. by HPLC on NUCLEODUR ODS C18 column (4.6 mm x 250 mm, 5µm) at column. temp. of 35 °C, flow rate of 1.0 mL/min and wavelength for measurement of 286 nm with acetonitrile-0.2% acetic acid aq. soln. as gradient mobile phase. The medical compn. may be used to process the medical dosage forms, such as tablet, capsule, granule, soft capsule, micropill, dripping pill, oral soln., injection, infusion soln., or freeze-dried powder injection, for preventing and/or treating liver injury, liver fibrosis, neoplasm and cardiovascular and cerebrovascular diseases.

Patent Information

Patent No.	Kind	Date	Application No.	Date
CN 101292986	A	Oct 29, 2008	CN 2007-10097271	Apr 29, 2007

Permalink: Sharing the links for records

https://scifinder.cas.org/scifinder/view/link\_v1/reference.js?l=Bm...

Patent Information

Oct 29, 2008  
CN 101292986

Source

Faming Zhuanli Shengqing  
Gongkai Shuomingshu  
Volume  
Issue  
39pp.  
Patent  
2008  
CODEN: CNXXEV

Accession Number

2008:1322210  
CAN 149:519088  
CAPLUS

Language

# A CPlus record (2)

## Indexing

Pharmaceuticals (Section 63-6) ⓘ

Section cross-reference(s): 1

## Concepts ⓘ

Porous materials

adsorbents; pharmaceutical compn. contg. salvanolic acid A and glycyrrhizic acid or its derivs. for preventing and/or treating cancer and cardiovascular and liver diseases

Cardiovascular agents      Cytoprotective agents

cardioprotective agents; pharmaceutical compn. contg. salvanolic acid A and glycyrrhizic acid or its derivs. for preventing and/or treating cancer and cardiovascular and liver diseases

Liver, disease

fibrosis; pharmaceutical compn. contg. salvanolic acid A and glycyrrhizic acid or its derivs. for preventing and/or treating cancer and cardiovascular and liver diseases

Freeze-dried drug delivery systems      Pharmaceutical injections

## Substances ⓘ

471-53-4P Glycyrrhetic acid  
1405-86-3P Glycyrrhizic acid  
96574-01-5P Salvanolic acid A

pharmaceutical compn. contg. salvanolic glycyrrhizic acid or its derivs. for preventing cancer and cardiovascular and liver diseases

Analyte; Pharmacological activity; Purification; Therapeutic use; Analytical study; Biological Preparation; Uses

542-78-9 Malondialdehyde  
9000-86-6 ALT  
9000-97-9 AST

pharmaceutical compn. contg. salvanolic acid A and glycyrrhizic acid or its derivs. for preventing and/or treating cancer and cardiovascular and liver diseases

Biological study, unclassified; Biological study

64-17-5 Ethanol, uses  
67-63-0 Isopropanol, uses  
71-36-3 n-Butanol, uses

- CAS scientists index for novel concepts and substances
- Concepts heading with sub-heading for detailed information
- Index terms are linked for faster exploring
- CAS registry number is indexed for substance with specific role





# Analyze the results by different ways

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions' are in the center. On the right, there are links for 'Answer Sets', 'Help', 'Keep Me Posted Results', 'History', and 'Preferences'. Below the header, a user greeting 'Welcome Windy Wu | Sign Out' is visible. The main search area shows the query 'Research Topic "anticancer drug for liver" > references (1227) > Pharmaceutical composition con...'. A secondary navigation bar includes 'References', 'Get Substances', 'Get Reactions', 'Get Cited', and 'Get Citing'. Below this, a toolbar contains '1227 References', '0 Selected', 'Keep Selected', 'Remove Selected', 'Remove Duplicates', 'Save', 'Print', and 'Export'. A 'Sort by: Accession Number' dropdown is present, along with a pagination control showing '1 2 3 4 5 6 ... 62'. The search results list three entries, each with a checkbox, a title, author information, and a brief abstract. The first entry is '1. Pharmaceutical composition containing salvianolic acid A and glycyrrhizic acid or its derivatives for preventing and/or treating cancer and cardiovascular and liver diseases'. The second is '2. Preparation of water soluble stilbene derivatives as anticancer drugs.'. The third entry is partially visible: 'Method for extraction of ellagic acid compounds from Chinese medicine Euphorbia and application in anticancer drugs'. On the right side, a 'Analysis' sidebar is open, showing a list of analysis categories with corresponding bar charts and counts. The categories and their counts are: Neoplasm inhibitors (213), Animals (165), Carcinoma (165), Drug Delivery Systems (161), Metabolism (147), and Humans (138). The 'Index Term' category is currently selected in the dropdown menu.

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Windy Wu | Sign Out

Create Keep Me Posted | Research Topic "anticancer drug for liver" > references (1227) > Pharmaceutical composition con...

References | Get Substances | Get Reactions | Get Cited | Get Citing

1227 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | 1 2 3 4 5 6 ... 62

1. **Pharmaceutical composition containing salvianolic acid A and glycyrrhizic acid or its derivatives for preventing and/or treating cancer and cardiovascular and liver diseases**  
By Gu, Qun; Li, Zhigang; Qu, Shoufeng; Guo, Xiaopeng; Liu, Yan; Mi, Changjiang; Li, Yanbin; Lin, Zhirong; Shan, Huizhen; Jin, Zhigang  
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2008), CN 101292986 A 20081029. Language: Chinese, Database: CAPLUS  
The medical compn. contains 1-10 wt. part salvianolic acid A extd. from Salvia miltiorrhiza, and 1-20 wt. part glycyrrhizic acid or its derivs., and a suitable amt. of medical adjuvant. The content of salvianolic acid A in the medical compn. is 50-100%, and the compd. glycyrrhizic acid or its derivs is from Glycyrrhiza ext. Salvianolic acid A is obtained by extg. S. miltiorrhiza with water or ethanol, adjusting pH value, press filtering, and purifying on macroporous adsorbent resin column with 30-70% ethanol soln. as eluent, and/or refining on Sephadex LH-20 column with 50-95% ethanol soln. ...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

2. **Preparation of water soluble stilbene derivatives as anticancer drugs.**  
By Lee, Ruey-Min; Simoni, Daniele  
From PCT Int. Appl. (2008), WO 2008131320 A1 20081030. Language: English, Database: CAPLUS  
Title compds. [I; WS = H<sub>2</sub>O-sol. moiety separable from an amido linkage to a stilbene by hydrolysis; R = H, (substituted) alkyl, alkoxy], were prepd. Thus, (Z)-5-[2-(3,5-dimethoxyphenyl)viny]l-2-methoxyaniline [I; R = OMe, WS = H] in dioxane was treated with trichloromethyl chloroformate followed by heating at 60° for 2 h to give an isocyanate residue. The latter in dioxane was treated with 4-(2-hydroxyethyl)morpholine followed by heating at 60° for 12 h to give 45% (Z)-[5-[2-(3,5-dimethoxyphenyl)viny]l-2-methoxyphenyl]carbamic acid 2-morpholin-4-ylethyl ester [I; R = OMe, WS = CO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-(mor...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

**Method for extraction of ellagic acid compounds from Chinese medicine Euphorbia and application in anticancer drugs**  
By Guo, Zhenjun; Tan, Lin; Xu, Ying; Bo, Xiaodian

**Analysis** | Refine

Analyze by:

Index Term

- 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

Neoplasm inhibitors	213
Animals	165
Carcinoma	165
Drug Delivery Systems	161
Metabolism	147
Humans	138



# Keep selected records and analysis display

SciFinder®

Welcome Windy Wu | Sign Out

Research Topic "anticancer drug for liver" > references (1227) > keep analysis "Index Term" (569)

References | Get Substances | Get Reactions | Get Cited | Get Citing

569 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Save | Print | Export

569 references with Index Term **Antitumor agents** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number

1. **Pharmaceutical composition containing salvianolic acid A and glycyrrhizic acid or its derivatives for preventing and/or treating cancer and cardiovascular and liver diseases**  
By Gu, Qun; Li, Zhigang; Qu, Shoufeng; Guo, Xiaopeng; Liu, Yan; Mi, Changjiang; Li, Yanbin; Lin, Zhirong; Shan, Huizhen; Jin, Zhigang  
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2008), CN 101292986 A 20081029. Language: Chinese, Database: CAPLUS  
The medical compn. contains 1-10 wt. part salvianolic acid A extd. from Salvia miltiorrhiza, and 1-20 wt. part glycyrrhizic acid or its derivs., and a suitable amt. of medical adjuvant. The content of salvianolic acid A in the medical compn. is 50-100%, and the compd. glycyrrhizic acid or its derivs is from Glycyrrhiza ext. Salvianolic acid A is obtained by extg. S. miltiorrhiza with water or ethanol, adjusting pH value, press filtering, and purifying on

Analysis | Refine

Analyze by: Index Term

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

Antitumor agents	569
Liver, neoplasm	363
Human	283
ver	166
arcinoma	158
rug delivery systems	142
intestine, neoplasm	128
neoplasm	124
ung, neoplasm	97
lammary gla... plasm	80

- Keep/Remove selected records

-Output options

-Save (on CAS server, up to 20,000 answers per answer set)

-Print answers

-Export in different kinds of format (.akx, .pdf, .txt.)

-Keep analysis result

# Categorize helps to refine to specific index terms

method comprises the steps of: (1) pulverizing the air-dried roots and overground parts of *Euphorbia hylonoma*, extg. with ethanol, and cong., and (2) extg. with chloroform and Et acetate, applying a chromatograph column, and eluting to obtain the two ellagic acid compds. **Anticancer** pharmacol. expts. show that the two compds. have obvious **inhibiting** effects on the growth of **liver** ...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

**Categorize**  
More detailed analysis based on CAS indexing  
**Categorize**

**Categorize**

Select a heading and category. Then select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Nucleic acids	<b>Select All Deselect All</b>	<b>Genetics &amp; protein chemistry</b>
Biotechnology	Proteins & peptides	<input checked="" type="checkbox"/> Gene therapy 22	> <b>Genetics</b>
General chemistry	Genetics	<input type="checkbox"/> Molecular cloning 13	Gene therapy <a href="#">Deselect</a>
Biology	Miscellaneous substances	<input checked="" type="checkbox"/> Genetic vectors 9	Genetic vectors <a href="#">Deselect</a>
Physical chemistry	Protein & peptide topics	<input type="checkbox"/> PCR (polymerase chain reaction)	
<b>Genetics &amp; protein chemistry</b>		<input type="checkbox"/> Plasmid vectors 9	
Synthetic chemistry		<input type="checkbox"/> cDNA sequences 9	
Polymer chemistry		<input type="checkbox"/> DNA sequences 7	
Technology		<input type="checkbox"/> Mutation 6	
Analytical chemistry		<input type="checkbox"/> Nucleic acid hybridization 5	
Environmental chemistry		<input type="checkbox"/> Transcriptional regulation 5	
Catalysis		<input type="checkbox"/> Transformation, genetic 5	
		<input type="checkbox"/> Chromosome 4	
		<input type="checkbox"/> DNA formation 4	
		<input type="checkbox"/> DNA repair 4	
		<input type="checkbox"/> Northern blot hybridization 4	
		<input type="checkbox"/> DNA formation, replication 3	
		<input type="checkbox"/> Electroporation 2	

Genetics & protein chemistry > Genetics > 2 Selected

[Refine](#) [Cancel](#)

# Refine the answer sets to particular interest

**SciFinder®** Explore References Explore Substances Explore Reactions Answer Sets Help  
Keep Me Posted Results History Preference

Welcome Windy Wu | Sign Out

Create Keep Me Posted Research Topic "anticancer drug for liver" > references (1227) > keep analysis "Index Term" (569) > refine "Hong Kong" (10)

References Get Substances Get Reactions Get Cited Get Citing

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

Select All Deselect All Sort by: Accession Number

1. **Leachianone A as a potential anti-cancer drug by induction of apoptosis in human hepatoma HepG2 cells**  
By Cheung, Crystal Sao-Fong; Chung, Karen Ka-Wing; Lui, Julian Chun-Kin; Lau, Ching-Po; Hon, Po-Ming; Chan, Judy Yuet-Wa; Fung, Kwok-Pui; Au, Shannon Wing-Ngor  
From Cancer Letters (Amsterdam, Netherlands) (2007), 253(2), 224-235. Language: English, Database: CAPLUS  
The Chinese herbal medicine Radix Sophorae is widely applied as an **anti-carcinogenic/ anti-metastatic** agent against **liver cancer**. In this study, Leachianone A, isolated from Radix Sophorae, possessed a profound cytotoxic activity against human hepatoma cell line HepG2 in vitro, with an IC50 value of 3.4 µg/mL post-48-h treatment. Its action mechanism via induction of apoptosis involved both extrinsic and intrinsic pathways. Its **anti-tumor** effect was further demonstrated in vivo by 17-54% redn. of **tumor** size in HepG2-bearing nude mice, in which no toxicity to the heart and **liver** tissues was ...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

2. **Evidence of a novel antiapoptotic factor: role of inhibitor of differentiation or DNA binding (Id-1) in anticancer drug-induced apoptosis**  
By Zhang, Xiaomeng; Ling, Ming-Tat; Wong, Yong-Chuan; Wang, Xianghong  
From Cancer Science (2007), 98(3), 308-314. Language: English, Database: CAPLUS  
Id-1 (**inhibitor** of differentiation or DNA binding), a member of the basic helix-loop-helix transcription factor family, is up-regulated in many types of human **cancer** and its expression levels are correlated with poor treatment outcome and shorter survival. In this study, we provided evidence to suggest that Id-1 is a universal survival factor that plays a key role in protection against **anticancer drug**-induced apoptosis. Using nine **anticancer drugs** and five **cancer** cell lines derived from nasopharyngeal **carcinoma** (CNE1), cervical **carcinoma** (HeLa), breast **cancer** (MCF7), hepatocarcinoma (Huh7) a...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#)

3. **Pseudolaric Acid B, a Novel Microtubule-Destabilizing Agent That Circumvents Multidrug Resistance Phenotype and Exhibits Antitumor Activity In vivo**

**Refine**

Analysis **Refine**

Refine by:

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

Company Name:

Examples:  
*3M*  
*DuPont*

**Refine**

# Combine answer sets for references, substances and reactions

SciFinder®

Explore References   Explore Substances   Explore Reactions

Welcome Windy Wu | Sign Out

Answer Sets | Help  
Keep Me Posted Results | History  
Preferences

Create Keep Me Posted   Research Topic "anticancer drug for liver" > references (1227) > keep analysis "Index Term" (569) > refine "hong kong" (10)

Saved Answer Sets   **Combine Answer Sets**

References (4)   Substances (0)   Reactions (0)

4 Answer Sets   2 Selected   Delete Selected

Answer Set Details		Date Saved
<input checked="" type="checkbox"/>	hello (19) Research reference	Nov 19, 2008
<input checked="" type="checkbox"/>	bird flu (2) Research	
<input type="checkbox"/>	warfarin research Research (1705) > " (19)	
<input type="checkbox"/>	nanotech anticance Research > referer refine "20	

### 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 hello that are not in bird flu
- Exclude - Include only answers from bird flu that are not in hello
- Remove duplicate references

**Combine Answer Sets**   **Cancel**

# Keep me posted for references

**SciFinder®** Explore References Explore Substances

Welcome Windy Wu | Sign Out

Create Keep Me Posted Research Topic "anticancer drug for liver" > references (1227) >

Candidates Selected:  
1227 references were found containing the two concepts "anticancer drug" and "liver" closely associated with one another.  
Answer set 4 created with  
961 answers from CAPLUS  
266 answers from MEDLINE

References **Get Substances** **Get Reactions** **Get Cited** **Get Citing**

1227 References 0 Selected Keep Selected Remove Selected Remove Duplicates Save Print Export

Select All Deselect All Sort by: Accession Number 1 2 3 4 5 6 ... 62 ▶

1. **Pharmaceutical composition containing salvanolic acid A and glycyrrhizic acid or its derivatives for preventing and/or treating cancer and cardiovascular and liver diseases**  
By Gu, Qun; Li, Zhigang; Qu, Shoufeng; Guo, Xiaopeng; Liu, Yan; Mi, Changjiang; Li, Yanbin; Lin, Zhirong; Shan, Huizhen; Jin, Zhigang  
From Faming Zhuanli Shenqing Gongkai Shuomingshu (2008), CN 101292986 A 20081029. Language: Chinese, Database: CAPLUS  
The medical compn. contains 1-10% glycyrrhizic acid or its derivs., and the medical compn. is 50-100%, and the resin is obtained by extg. S. miltiorrhiza macroporous adsorbent resin column with 50-95% ethanol soln. ...  
[Substances](#) [Reactions](#) [Citing](#)

2. **Preparation of water soluble salvanolic acid derivatives**  
By Lee, Ruey-Min; Simoni, Daniele  
From PCT Int. Appl. (2008), WO 2008131320  
Title compds. [I; WS = H<sub>2</sub>O-sol. (substituted) alkyl, alkoxy], were prepared in dioxane. WS = H] in dioxane was treated with isocyanate residue. The latter in dioxane for 12 h to give 45% (Z)-[5-[2-(3-ethoxy)ethyl]ester [I; R = OMe, WS = CO<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>].  
[Substances](#) [Reactions](#) [Citing](#)

3. **Method for extraction of ellagic acid from anticancer drugs**  
By Guo, Zhenjun; Tao, Lijun; Wu, Baomin

**Create Keep Me Posted Profile**

**Title:** \* anticancer

**Description:** drug for liver

**Status:**  Enabled  Disabled

Exclude previously retrieved references.

**Expiration Date:** 12 1, 2009

**Search:**  
Explore references by research topic: anticancer drug for liver  
**Candidates Selected:**  
References which contain the two concepts "anticancer drug" and "liver" closely associated with one another.

Create Cancel



# Download up to 10 previous history sessions

The screenshot displays the SciFinder web interface. At the top left is the SciFinder logo. Navigation links include 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Windy Wu'. The breadcrumb trail shows the current search path: 'Research Topic "anticancer drug for liver" > references (1227) > keep analysis "Index Term" (569) > refine "hong kong" (10)'. The main content area is titled 'History' and shows a session starting on December 1, 2008. The session details include: 'Explore references by research topic: anticancer drug for liver initiated, resulting in 5 candidates' at 5:18 AM; 'Explore complete Candidates Selected' with 1227 references found; 'Explore results' with 961 answers from CAPLUS and 266 from MEDLINE; 'Sample 'Index Term' analysis produced from Answer set 1'; 'Full 'Index Term' analysis produced from Answer set 1'; 'Kept 569 reference answers from Answer set 1 analyzed by 'Index Term'' with 569 answers from CAPLUS; and 'Refine Answer set 2 by company' to 'Hong Kong' with 10 answers from CAPLUS. The sidebar on the right, titled 'Previous Sessions', lists two files: 'SFSessionHistory-2008-12-01\_031951.rtf' and 'SFSessionHistory-2008-11-19\_025459.rtf'. A red box highlights the 'Previous Sessions' sidebar and the 'History' section header.















# Structure search

[www.cas.org](http://www.cas.org)









*A division of the American Chemical Society*






# Structure Drawing Tools

Icon	Tool	Icon	Tool
	Pencil (default selection)		Eraser
 Atom	Atom Menu	 Short	Shortcut Menu
	Chain		Template
	Selection		Lasso
	Rotation		Flip Structure
	Positive Charge		Negative Charge

**Structure searching with SSM** – If you have the SciFinder [Substructure Module \(SSM\)](#), six additional drawing tools are available.

Icon	Tools	Icon	Tools
 -X	Variables (X Menu)	 =R	R-group
 [ ] 1-4	Repeating Group		Variable Attachment Position
	Lock Rings		Lock Atoms

**Reaction searching** – If you are performing a [Reaction search](#), five additional reaction-specific tools are available.

Icon	Tools	Icon	Tools
	Reaction Arrow	 → A B	Reaction Role
	Atom Mapping		Reaction Site Marking
	Functional Group		

# Structure search java plug-in

The screenshot displays the SciFinder software interface. At the top, there are navigation buttons for "Explore References", "Explore Substances", and "Explore Reactions". A user greeting "Welcome Windy Wu" is visible. On the left, a sidebar contains "Explore Substances" and a menu with "Chemical Structure", "Molecular Formula", and "Substance Identification". The main workspace shows a chemical structure of a bicyclic system with two nitrogen atoms and an R<sub>1</sub> group. An "R-group Definitions" dialog box is open, showing a list of definitions: R1 = N, C, O, S; R2 = ; R3 = ; R4 = . Below the dialog, there are radio buttons for search types: "Exact search", "Substructure search" (selected), and "Similarity search". At the bottom of the dialog are buttons for "確定" (Confirm) and "取消" (Cancel). The main interface also includes a toolbar with drawing tools, a status bar with "Formula not available", and a bottom panel with a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si) and a "Scale 100" indicator.

# Structure search result

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Windy Wu | Sign Out

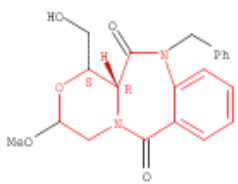
Create Keep Me Posted | Chemical Structure substructure > substances (1314) > commercial sources (240)

Substances | Get References | Get Reactions | Get Commercial Sources

1314 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | 1 2 3 4 5 6 ... 88 ▶

1. 1073249-93-0



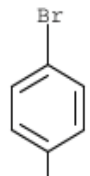
Absolute stereochemistry.

C<sub>21</sub> H<sub>22</sub> N<sub>2</sub> O<sub>5</sub>

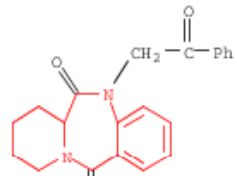
1H-[1,4]Oxazino[3,4-c][1,4]benzodiazepine-6,12(11H,12aH)-3,4-dihydro-1-(hydroxymethyl)-methoxy-11-(phenylmethyl)-, (S)

~1 References  
▲ Reactions  
👤 Commercial Sources  
🏠 Regulatory Information  
🔗 Link

2. 1050277-26-3



3. 1050276-13-5



**Analysis** | Refine

Sample Analysis

Substance Role  
Commercial Availability  
Elements  
Reaction Availability  
Substance Role

Uses

Reactant or reagent

Full Analysis

© Royal Society of Chemistry

## Automatic analysis:

- Substance roles, elements, reaction availability and commercial availability

However, the following analyses are not available yet:

- Ring skeleton, real atom attachment, variable group and R-Group

# Refine structure results by atom attachment

SciFinder®

Explore References   Explore Substances   Explore Reactions

Answer Sets   Help  
Keep Me Posted Results   History  
Preferences

Welcome Windy

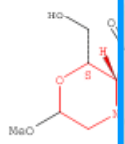
Create Keep Me Posted

Substance

1314 Substances

Select All   Description

1. 107



Absolute stereochemistry

C<sub>21</sub> H<sub>22</sub> N<sub>2</sub>

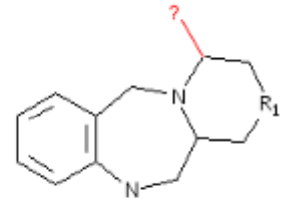
1H-[1,4]Oxazepin-2-one  
benzodiazepine  
3,4-dihydro-  
methoxy-11-

~1 Reference  
▲ Reactions  
▲ Commercial  
▲ Regulatory  
🔗 Link

### Refine by Atom Attachment

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

Substructure



Atom Attachments

Select All   Deselect All

<input type="checkbox"/> H or None	1259
<input type="checkbox"/> C	46
<input checked="" type="checkbox"/> O	9
<input type="checkbox"/> A - Any (not H)	55
<input type="checkbox"/> Q - Any (not C,H)	9

? = O

Refine   Cancel

Refine

Structure  
Containing  
Linking  
Availability  
Availability  
Availability  
Attachment

Attachments





# A substance record (1)

**SciFinder®** Explore References Explore Substances Explore Reactions Answer Sets Help  
Keep Me Posted Results History Preferences

Welcome Windy Wu | Sign Out

Create Keep Me Posted Chemical Structure substructure > substances (1314) > 41994-17-6

### Substance Detail

Get References Get Reactions Get Commercial Sources Get Regulatory Information

Link Save Print Export

**CAS Registry Number:** 41994-17-6  
C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>  
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Explore by Chemical Structure  
Explore Reactions

**Document Types:** Conference, Journal, Patent

Role	Patents	Nonpatents
Preparation	✓	✓
Properties		✓
Reactant or reagent	✓	✓

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

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	4.30	pH 1 Temp: 25 °C	(2)	
Bioconcentration Factor	4.48	pH 2 Temp: 25 °C	(2)	

# A substance record (2)

H Donors	1		(2)
H Donor/Acceptor Sum	5		(2)
logP	1.162±0.409	Temp: 25 °C	(2)
Molecular Weight	230.26		(2)

Spectra Properties	Value	Conditions	Notes	Top
Proton NMR Spectrum	<a href="#">See spectrum</a>		(3)	

## Structure-related Properties

Polar Surface Area

## Thermal Properties

Boiling Point

Enthalpy of Vaporization

Flash Point

(2) Calculated using Advanced Chemistry Development, Inc. (ACD/Labs)

(3) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs)

## Experimental Properties:

### Spectra Properties

Carbon-13 NMR Spectrum

IR Absorption Spectrum

Mass Spectrum

Proton NMR Spectrum

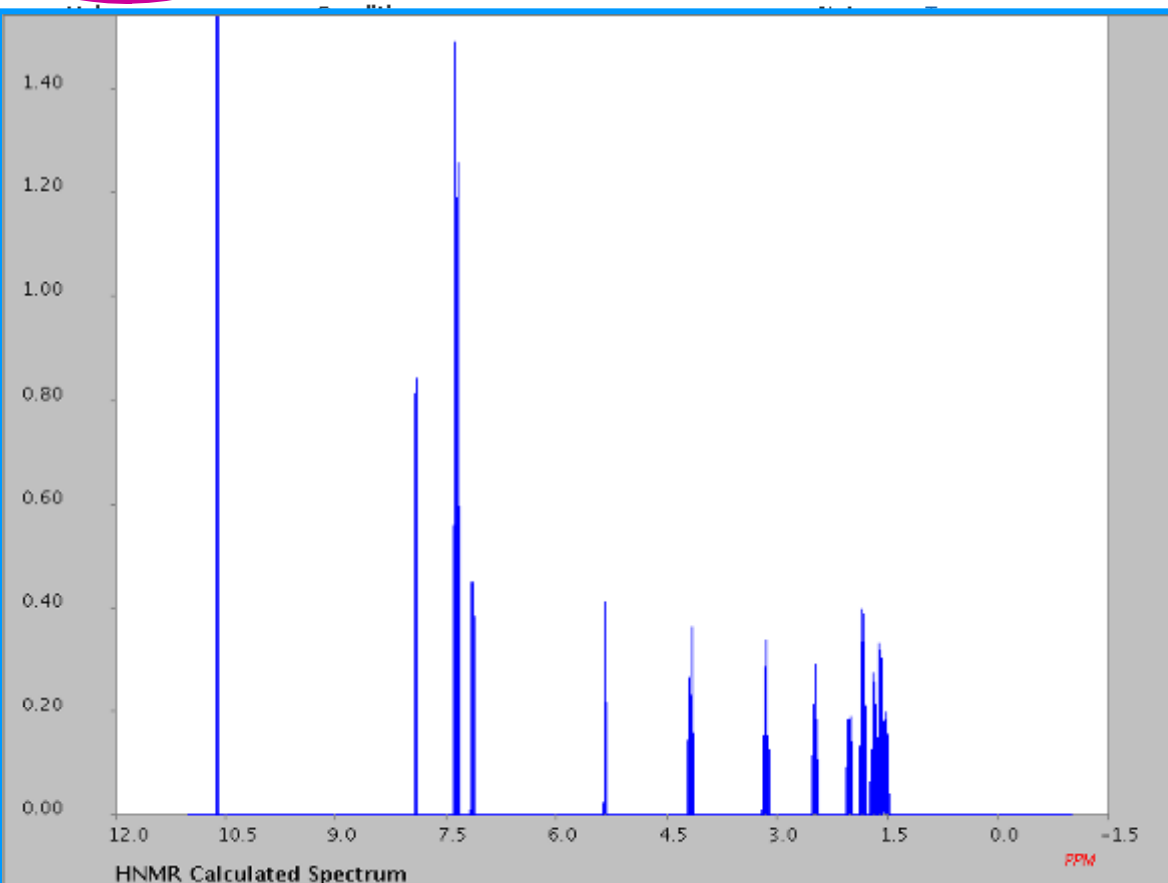
### Structure-related Properties

Crystal Structure

### Thermal Properties

Melting Point

(1) Jadidi, Khosrow; Journal of



### Nucleus

<sup>1</sup>H

### Standard

Tetramethylsilane (75-76-3)

### Temperature

25 degC

### Source

Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software v9.07 (© 2007-2008 ACD/Labs)

# Get interest references for substance

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Windy Wu'. The main content area shows the 'Substance Detail' for CAS Registry Number 41994-17-6, which is Pyrido[2,1-c][1,4]benzodiazepine. A pink box highlights the 'Get References', 'Get Reactions', 'Get Commercial Sources', and 'Get Regulatory Information' buttons. A dialog box titled 'Get References' is open, showing options to retrieve references for this substance. The 'References associated with:' section has 'Biological Study' checked. The 'For each sequence, retrieve:' section has 'Additional related references, e.g., activity studies, disease studies.' checked. The dialog box has 'Get References' and 'Cancel' buttons.

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Windy Wu | Sign Out

Create Keep Me Posted | Chemical Structure substructure > substances (1314) > 41994-17-6

Substance Detail

Get References | Get Reactions | Get Commercial Sources | Get Regulatory Information

Link Save Print Export

**Get References**

For this 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

CAS Registry Number: C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>  
Pyrido[2,1-c][1,4]benzodiazepine tetrahydro-

Document Types:

Role: Preparation, Properties, Reactant or reagent

Predicted Proper Thermal

Biological Property: Bioconcentration Factor

Bioconcentration Factor: 4.48 | pH 2 Temp: 25 °C (2)

# Get reaction information with detailed condition

Substance Detail

Get References

Get Reactions

Get Commercial Sources

Get Regulatory Information

Link Save Print Export

CAS Registry Number: 41994-17-6

C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>

Pyrido[2,1-c][1,4]  
tetrahydro-

SciFinder®

Explore References

Explore Substances

Explore Reactions

Answer Sets  
Keep Me Posted Results

Help  
History  
Preferences

Welcome Windy Wu | Sign Out

Create Keep Me Posted Chemical Structure substructure > substances (1314) > 41994-17-6 > get reactions (5)

Reactions

Get References

5 Reactions

0 Selected

Keep Selected

Remove Selected

Save

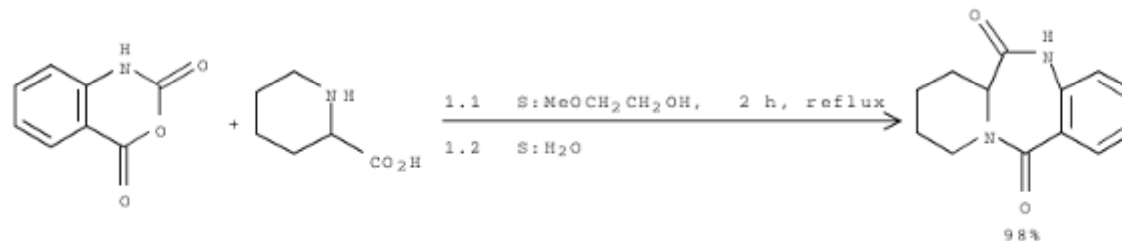
Print

Export

Select All Deselect All

Display: All Reactions

1. Reaction Detail [Link](#)



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

Simple synthesis, structure and ab initio study of 1,4-benzodiazepine-2,5-diones

By Jaddi, Khosrow et al

From Journal of Molecular Structure, 692(1-3), 37-42; 2004

2. Reaction Detail [Link](#)



Analysis

Refine

Analyze by: [?](#)

Catalyst

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

Pd(OAc)<sub>2</sub> 1

PPh<sub>3</sub> 1

Show More

# Export supplier information to excel table

SciFinder®

Explore References   Explore Substances   Explore Reactions

Welcome Windy Wu | Sign Out

Answer Sets   Help  
Keep Me Posted Results   History  
Preferences

Create Keep Me Posted   Chemical Structure substructure > substances (1314) > 41994-17-6 > commercial sources (6)

Commercial

6 Commercial Sources

Select All Deselect All

1.  **AsInEx**  
AsInEx, 10  
Order Number: 41994-17-6  
[Link](#)

2.  **Aurora**  
Aurora Fine  
Order Number: 41994-17-6  
[Link](#)

3.  **Interchim**  
Interchim,  
Order Number: 41994-17-6  
[Link](#)

4.  **Ryan Scientific**  
Ryan Scientific  
Order Number: 41994-17-6  
[Link](#)

5.  **Scientific Exchange, Inc.**  
Scientific Exchange, Inc., 4 Jun 2008

	A	B	C	D	E
1	SciFinder®				
2	CAS Registry Number: 41994-17-6				
4	Chemical Name	Catalog Name	Company Name	Street Address	City
5	Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	AsInEx Express Platinum Collection	<a href="#">AsInEx</a>	5 Gabrichevskogo St. Bldg 8	Moscow
6	Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Aurora Screening Library	<a href="#">Aurora Fine Chemicals LLC</a>	7929 Silverton Ave. Suite 609	San Diego
7	Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Aurora Screening Library	<a href="#">Aurora Fine Chemicals Ltd</a>	Reininghausstrasse 49	Graz
8	Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Interchim Intermediates	<a href="#">Interchim</a>	211 bis Av J.F. Kennedy BP 1140	Montlucon

SciFinder®

41994-17-6



# Structure search (New Enhancements)

[www.cas.org](http://www.cas.org)



*A division of the American Chemical Society*

# Structure search java plug-in

The screenshot displays the SciFinder software interface. At the top, there are navigation buttons for "Explore References", "Explore Substances", and "Explore Reactions". A user greeting "Welcome Windy Wu" and a "Sign Out" link are visible. On the left, a sidebar menu includes "Explore Substances", "Chemical Structure", "Molecular Formula", and "Substance Identification". The main workspace shows a chemical structure of a bicyclic amine with an R<sub>1</sub> group. An "R-group Definitions" dialog box is open, showing fields for R1, R2, R3, and R4. The R1 field contains the text "N, C, O, S". Below the dialog, there are radio buttons for search options: "Exact search", "Substructure search" (which is selected), and "Similarity search". Buttons for "確定" (Confirm) and "取消" (Cancel) are at the bottom right. The bottom status bar indicates "Formula not available".

SciFinder®

Explore References   Explore Substances   Explore Reactions

Welcome Windy Wu | Sign Out

Answer Sets | Help  
Keep Me Posted Results | History  
Preferences

Explore Substances

Chemical Structure  
Molecular Formula  
Substance Identification

Draw or change atoms or bonds.

Atom   Short   -X

R-group Definitions

R1 = N, C, O, S |  
R2 =  
R3 =  
R4 =

Close

Get substances that match your query using:

Exact search  
 Substructure search  
 Similarity search

確定  
取消

Formula not available

# Structure search result

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Windy Wu | Sign Out

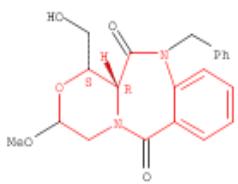
Create Keep Me Posted | Chemical Structure substructure > substances (1314) > commercial sources (240)

Substances | Get References | Get Reactions | Get Commercial Sources

1314 Substances | 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | 1 2 3 4 5 6 ... 88

1. 1073249-93-0



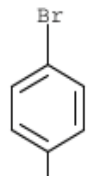
Absolute stereochemistry.

C<sub>21</sub> H<sub>22</sub> N<sub>2</sub> O<sub>5</sub>

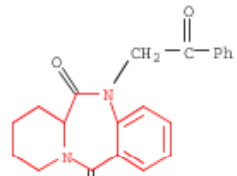
1H-[1,4]Oxazino[3,4-c][1,4]benzodiazepine-6,12(11H,12aH)-3,4-dihydro-1-(hydroxymethyl)-methoxy-11-(phenylmethyl)-, (S)

~1 References  
Reactions  
Commercial Sources  
Regulatory Information  
Link

2. 1050277-26-3



3. 1050276-13-5



**Automatic analysis:**

- Substance roles, elements, reaction availability and commercial availability

**However, the following analyses are not available yet:**

- Ring skeleton, real atom attachment, variable group and R-Group

Analysis | Refine

Sample Analysis

Substance Role

Commercial Availability

Elements

Reaction Availability

Substance Role

Uses

Reactant or reagent

Full Analysis

© 2014 Royal Society of Chemistry

# Refine structure results by atom attachment

SciFinder®

Explore References   Explore Substances   Explore Reactions

Answer Sets   Help  
Keep Me Posted Results   History  
Preferences

Welcome Windy

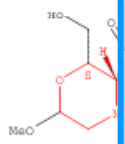
Create Keep Me Posted

Substance

1314 Substances

Select All   Description

1. 107



Absolute stereochemistry

C<sub>21</sub> H<sub>22</sub> N<sub>2</sub>

1H-[1,4]Oxazepin-2-yl  
benzodiazepine  
3,4-dihydro-2-methoxy-11H-5H-benzodiazepine

~1 Reference

▲ Reactions

▲ Commercial

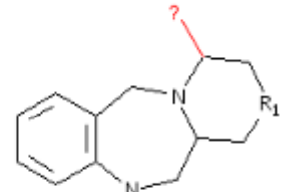
▲ Regulatory

Link

### Refine by Atom Attachment

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

Substructure



Atom Attachments

Select All   Deselect All

<input type="checkbox"/> H or None	1259
<input type="checkbox"/> C	46
<input checked="" type="checkbox"/> O	9
<input type="checkbox"/> A - Any (not H)	55
<input type="checkbox"/> Q - Any (not C,H)	9

? = O

Refine   Cancel

Refine

- Structure
- Containing
- Linking
- Availability
- Availability
- Availability
- Attachment

Attachments



# A substance record (1)

**SciFinder®** Explore References Explore Substances Explore Reactions Answer Sets Help  
Keep Me Posted Results History Preferences

Welcome Windy Wu | Sign Out

Create Keep Me Posted Chemical Structure substructure > substances (1314) > 41994-17-6

**Substance Detail** Get References Get Reactions Get Commercial Sources Get Regulatory Information

Link Save Print Export

**CAS Registry Number:** 41994-17-6  
C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>  
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Explore by Chemical Structure  
Explore Reactions

**Document Types:** Conference, Journal, Patent

Role	Patents	Nonpatents
Preparation	✓	✓
Properties		✓
Reactant or reagent	✓	✓

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

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	4.30	pH 1 Temp: 25 °C	(2)	
Bioconcentration Factor	4.48	pH 2 Temp: 25 °C	(2)	



# A substance record (2)

H Donors	1		(2)
H Donor/Acceptor Sum	5		(2)
logP	1.162±0.409	Temp: 25 °C	(2)
Molecular Weight	230.26		(2)
<b>Spectra Properties</b>			
	<b>Value</b>	<b>Conditions</b>	<b>Notes</b> <a href="#">Top</a>
Proton NMR Spectrum	<a href="#">See spectrum</a>		(3)

## Structure-related Properties

Polar Surface Area

## Thermal Properties

Boiling Point

Enthalpy of Vaporization

Flash Point

(2) Calculated using Advanced Chemistry Development, Inc. (ACD/Labs)

(3) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs)

## Experimental Properties:

## Spectra Properties

Carbon-13 NMR Spectrum

IR Absorption Spectrum

Mass Spectrum

Proton NMR Spectrum

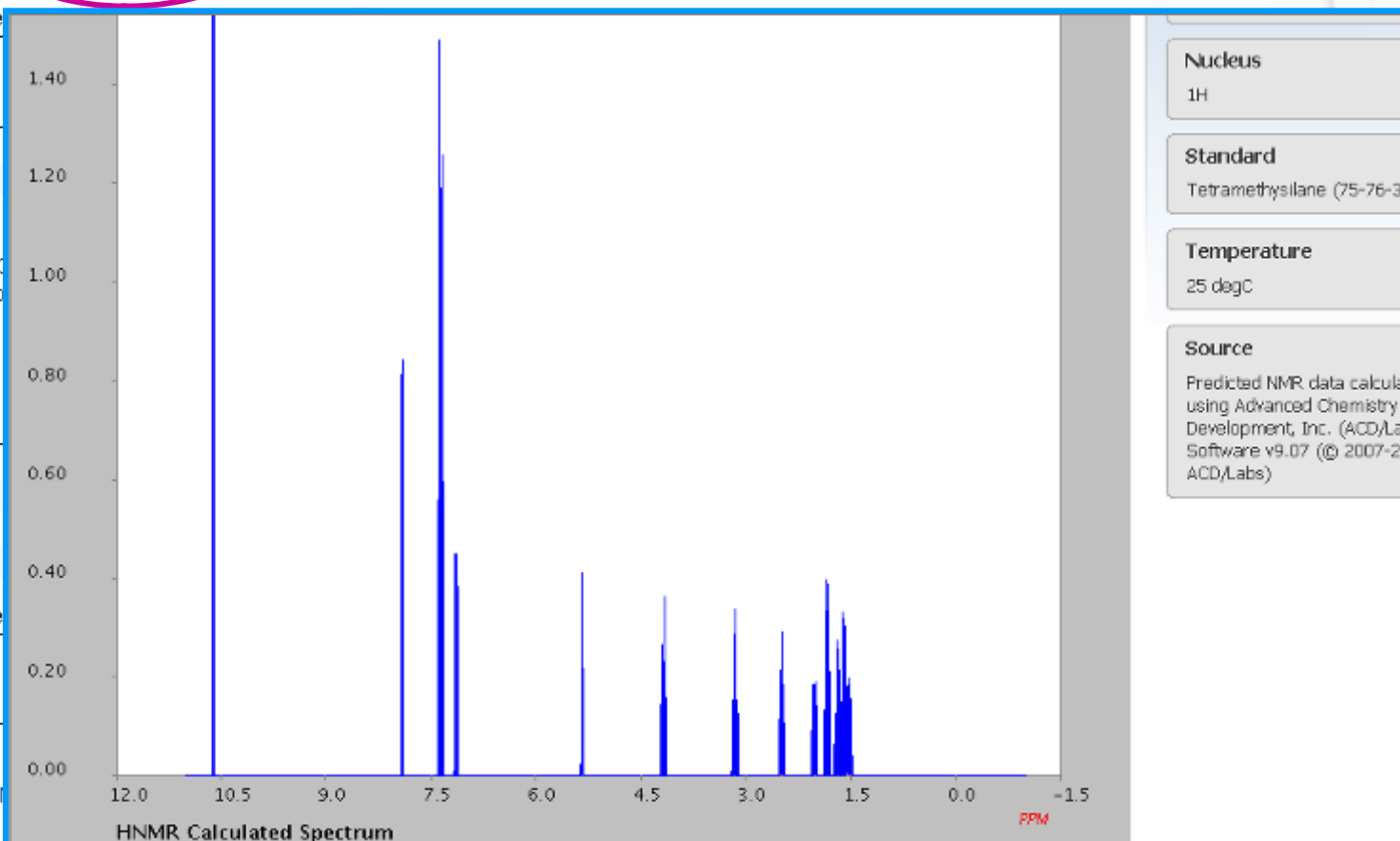
## Structure-related Properties

Crystal Structure

## Thermal Properties

Melting Point

(1) Jadidi, Khosrow; Journal of



## Nucleus

<sup>1</sup>H

## Standard

Tetramethylsilane (75-76-3)

## Temperature

25 degC

## Source

Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software v9.07 (© 2007-2008 ACD/Labs)

# Get interest references for substance

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. A user is logged in as 'Windy Wu'. The main content area shows the 'Substance Detail' for CAS Registry Number 41994-17-6, which is Pyrido[2,1-c][1,4]benzodiazepine. A pink box highlights the 'Get References' button in the top navigation bar. A dialog box titled 'Get References' is open, showing options to retrieve references for this substance. The 'References associated with:' section has 'Biological Study' checked. The 'For each sequence, retrieve:' section has 'Additional related references, e.g., activity studies, disease studies.' checked. The dialog box has 'Get References' and 'Cancel' buttons.

SciFinder®

Welcome Windy Wu | Sign Out

Explore References | Explore Substances | Explore Reactions

Answer Sets | Help  
Keep Me Posted Results | History  
Preferences

Create Keep Me Posted | Chemical Structure substructure > substances (1314) > 41994-17-6

Substance Detail

Get References | Get Reactions | Get Commercial Sources | Get Regulatory Information

Link | Save | Print | Export

**Get References**

**For this 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

CAS Registry Number: C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>  
Pyrido[2,1-c][1,4]benzodiazepine tetrahydro-

**Document Types:**

**Role**

Preparation  
Properties  
Reactant or reagent

**Predicted Properties**  
Thermal

**Biological Properties**  
Bioconcentration Factor: 4.48  
pH 2 Temp: 25 °C (2)

# Get reaction information with detailed condition

Substance Detail [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Get Regulatory Information](#)

Link Save Print Export

CAS Registry Number: 41994-17-6

C<sub>13</sub> H<sub>14</sub> N<sub>2</sub> O<sub>2</sub>  
Pyrido[2,1-c][1,4]tetrahydro-

SciFinder® [Explore References](#) [Explore Substances](#) [Explore Reactions](#)

Welcome Windy Wu | Sign Out

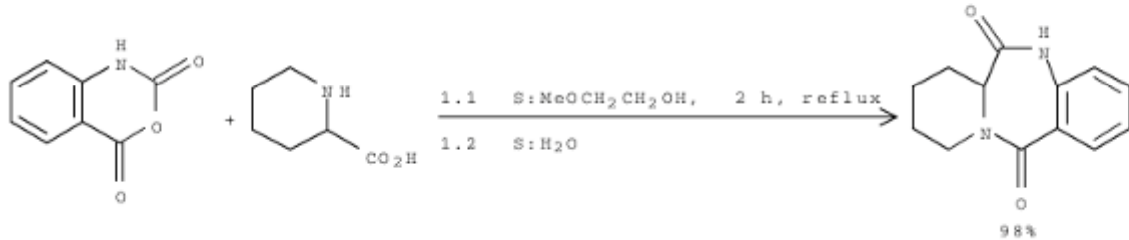
[Keep Me Posted](#) Chemical Structure substructure > substances (1314) > 41994-17-6 > **get reactions (5)**

Reactions [Get References](#)

5 Reactions 0 Selected [Keep Selected](#) [Remove Selected](#) Save Print Export

Select All Deselect All Display: All Reactions

1. Reaction Detail [Link](#)



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

Simple synthesis, structure and ab initio study of 1,4-benzodiazepine-2,5-diones  
By Jaddi, Khosrow et al  
From Journal of Molecular Structure, 692(1-3), 37-42; 2004

2. Reaction Detail [Link](#)

Analysis Refine

Analyze by: Catalyst

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

Pd(OAc) <sub>2</sub>	1
PPh <sub>3</sub>	1

Show More

# Export supplier information to excel table

SciFinder®

Explore References   Explore Substances   Explore Reactions

Welcome Windy Wu | Sign Out

Answer Sets   Help  
Keep Me Posted Results   History  
Preferences

Create Keep Me Posted   Chemical Structure substructure > substances (1314) > 41994-17-6 > commercial sources (6)

Commercial

6 Commercial Sources

Select All Deselect All

1.  **AsInEx**  
AsInEx, 10  
Order Number: 41994-17-6  
[Link](#)

2.  **Aurora**  
Aurora Fine  
Order Number: 41994-17-6  
[Link](#)

3.  **Interchim**  
Interchim,  
Order Number: 41994-17-6  
[Link](#)

4.  **Ryan Scientific**  
Ryan Scientific  
Order Number: 41994-17-6  
[Link](#)

5.  **Scientific Exchange, Inc.**  
Scientific Exchange, Inc., 4 Jun 2008

Chemical Name	Catalog Name	Company Name	Street Address	City
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	AsInEx Express Platinum Collection	<a href="#">AsInEx</a>	5 Gabrichevskogo St. Bldg 8	Moscow
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Aurora Screening Library	<a href="#">Aurora Fine Chemicals LLC</a>	7929 Silverton Ave. Suite 609	San Diego
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Aurora Screening Library	<a href="#">Aurora Fine Chemicals Ltd</a>	Reininghausstrasse 49	Graz
Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-	Interchim Intermediates	<a href="#">Interchim</a>	211 bis Av J.F. Kennedy BP 1140	Montlucon

SciFinder®

CAS Registry Number: 41994-17-6

Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Pyrido[2,1-c][1,4]benzodiazepine-6,12(5H,6aH)-dione, 7,8,9,10-tetrahydro-

Scientific Exchange, Inc., 4 Jun 2008

# Summary of Scifinder Web

- Provide quick access and user friendly interface to search for scientific information
- New features that are tailor made for the needs of researchers
- Enhanced content for properties, spectra, registration, reaction information and etc
- Personalization features (keep me posted and save as)





# Explore Reaction (Ex. Caffeine : Step 1)

Reaction Roles

Select a role for the structure fragment:

- product
- reactant
- reagent
- reactant/reagent
- any role

OK Cancel

Get reactions where the structure(s) are:

Variable only at

- the specified positions
- Substructures of more complex structures

OK Cancel

C8H10N4O2 (query) 194.19

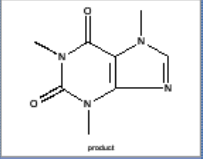
Draw a structure or Search by common name

Welcome Bhawat Ruangying | Sign Out

Create Keep Me Posted Substance Identifier "caffeine" > substances (1)

### Explore Reactions

Reaction Structure Reaction Structure



Click image to change structure or view detail

Search type:  Allow variability only as specified  Substructure

**Solvents**  Select Solvents **NEW**

Number of Steps   
Examples: 1, 1 - 3, 1 -, - 3

Classification(s)

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical

1. Draw a structure or Search by common name : Caffeine
2. Select Solvent list



# Select Solvent Limiter (Step 2)

Focus your reaction results by specifying one or more solvents.

## Sort by Solvent Hierarchy

Solvents

Close NEW

**Solvent Hierarchy**  
[View solvent list]

0 Selected | Select All | Deselect All

- Ionic liquids
  - Imidazolium derivatives
  - Nonimidazolium derivatives
- Nonpolar solvents
  - Aliphatic compounds
  - Aromatic compounds
  - Silanes
- Polar solvents
  - Polar solvents, aprotic
  - Polar solvents, protic
- Supercritical fluids

Find:  Next

## Sort by Solvent List

Close NEW

**Solvent List**  
[View solvent hierarchy]

1 Selected | Select All | Deselect All

- Valeronitrile
- Vinyl acetate
- Vinyl butyrate
- Vinyl propionate
- Water
- Water-170
- Water-180
- Water-d
- Water-d2
- Water-d2-180
- Water-t
- Water-t2
- Xylene
- Xylene-d10
- cis-1-Ethoxypropene

Find:  Next Previous

1. Draw a structure or Search by common name : Caffeine
2. Select Solvent by Solvent Hierarchy : Go to SCF category then select "Water"

# Reaction Answer Set Sort/ Solvent Exploring (Step 3)

Reactions Get References

30 Reactions 0 Selected | Keep Selected Remove Selected Save Print Export

Select All Deselect All | Sort by: Accession Number

Answers per Page [15] 1 2

Display:

1. Reaction Detail

Reactions	Product
References	Reactant
Substance Detail	Reagent
Commercial Sources	Reactant or Reagent
Regulatory Information	Catalyst
Explore by Chemical Structure	Solvent
Explore Reactions	Any role

# Analyze by Solvent (Step 4)

Reactions

Get References

30 Reactions

0 Selected

Keep Selected

Remove Selected

Save

Print

Export

Select All Deselect All

Sort by:

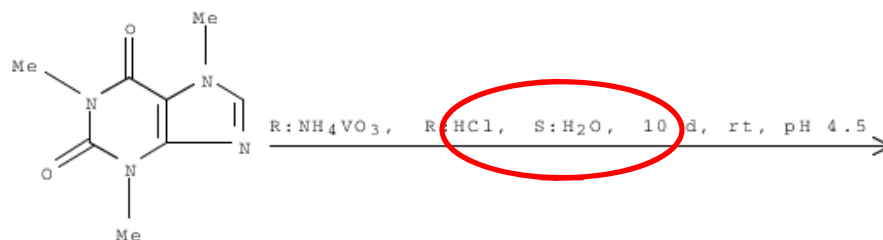
Accession Number

Answers per Page [15]

1 2


Display:  

1. Reaction Detail [Link](#)



Analysis

Refine

Analyze by: 

Solvent

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

H<sub>2</sub>O 30

DMF 11

Ac<sub>2</sub>O 9

HCO<sub>2</sub>H 7

Me<sub>2</sub>CO 7

EtOH 6

H<sub>2</sub>SO<sub>4</sub> 3


MeOH 3

POCl<sub>3</sub> 2

Show More

Analysis

Refine

Analyze by: 

Catalyst

Author Name

Catalyst

Company-Organization

Document Type

Journal Name

Language

Number of Steps

Product Yield

Publication Year

Solvent



A division of the American Chemical Society

# Export Feature (Step 5)

Welcome Bhawat Ruangying | Sign Out

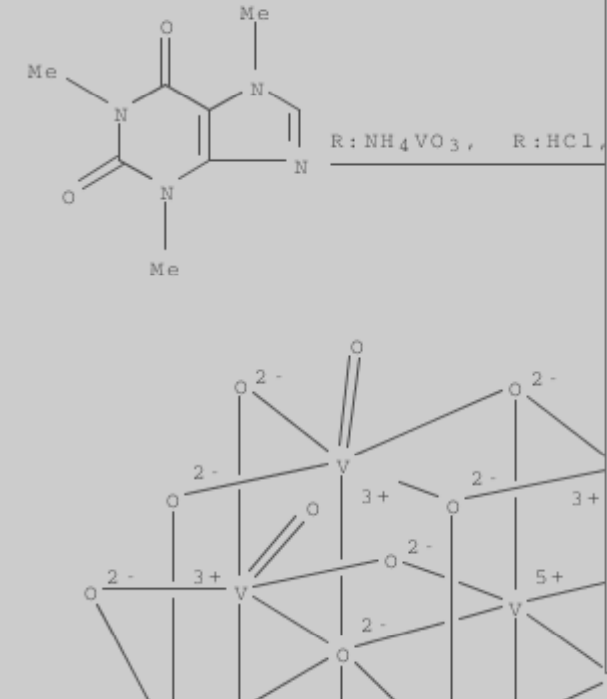
Reaction Structure structure variable only at one with limiters > reactions (30)


Reactions **Get References**

30 Reactions 0 Selected Keep Selected Remove

Select All Deselect All | Sort by: Accession Number

1. Reaction Detail [Link](#)



Export 

\* Required


**Export:**

All answers

Only selected answers

**File Name: \***

**File Type:**


Answer Key eXchange (\*.akx) 

Answer Key eXchange (\*.akx)

Portable Document Format (\*.pdf)

Rich Text Format (\*.rtf)


**History:**

product 

Limiters

1 solvent

- Water

Any source 

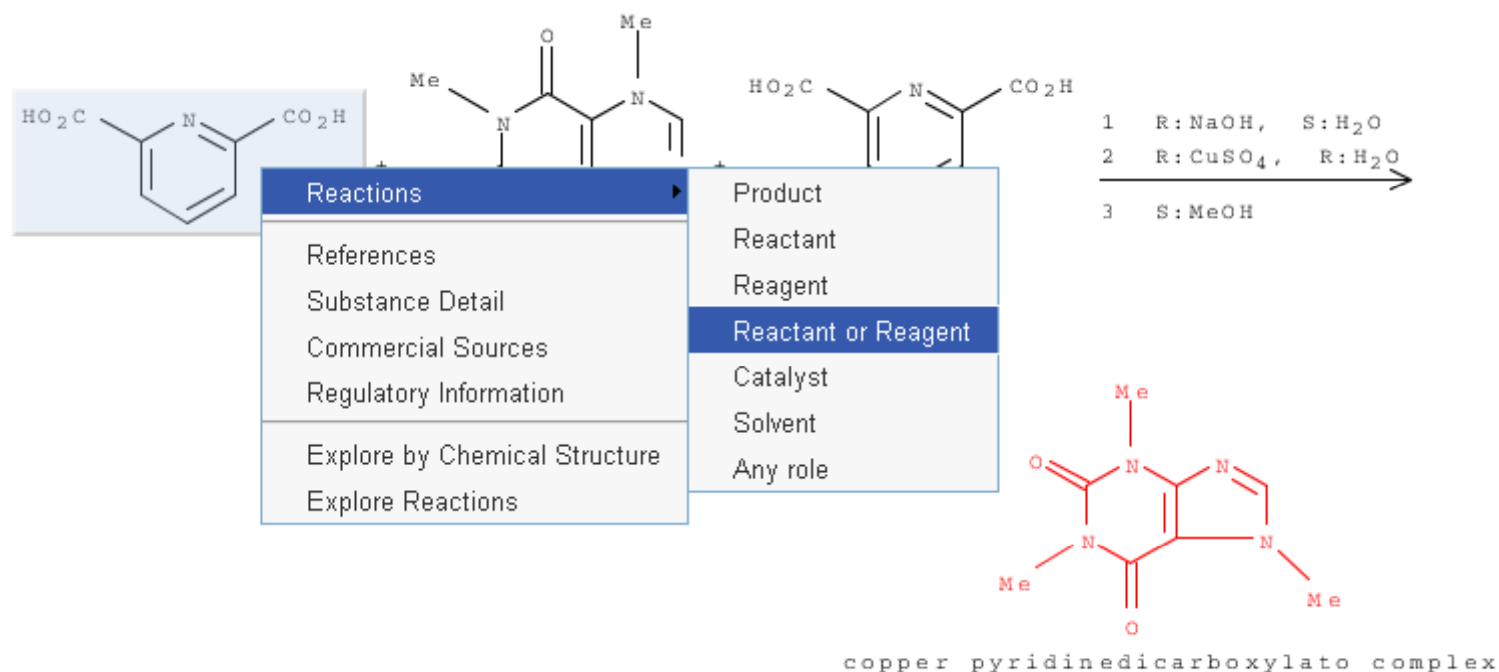
**Export** **Cancel**





# Quick Search from reaction result set (Step 6)

## 3. Reaction Detail [Link](#)



NOTE: Reactants: 2, Reagents: 4, Solvents: 2,  
Steps: 3, Stages: 3

Copper(II) pyridine-2,6-dicarboxylates. Coordination and distortion isomers of [Cu(pydca)(H<sub>2</sub>O)<sub>2</sub>]

By Koman, M. et al

From Polish Journal of Chemistry, 75(7), 957-964; 2001



A division of the American Chemical Society

# Get Similar Reactions (Step 7.1)

Find reactions that undergo similar transformations for all single step reactions

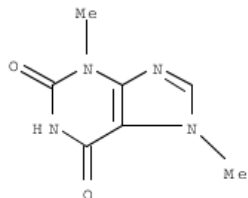
Reactions [Get References](#)

30 Reactions 1 Selected [Keep Selected](#) [Remove Selected](#) [Save](#) [Print](#) [Export](#)

12 reactions with Number of Steps 1 are displayed [Keep Analysis](#) [Clear Analysis](#)

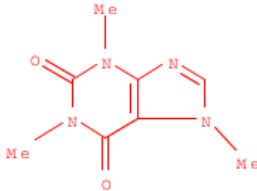
[Select All](#) [Deselect All](#) | Sort by: [Accession Number](#) [Answers per Page \[15\]](#) Display:

7. Reaction Detail [Link](#) [Similar Reactions](#) **NEW**

CN1C=NC2=C1C(=O)N(C)C2=O

1.1 R: MgCl<sub>2</sub>, C: 155215-94-4, S: H<sub>2</sub>O, 30 min, 28 °C

1.2 R: HCl, S: H<sub>2</sub>O, 28 °C

CN1C=NC2=C1C(=O)N(C)C2=O

NOTE: enzymic, biotransformation, kinetic study, purified S-adenosyl-L-methionine:theobromine 1-N-methyltransferase from developing endosperm of Coffea arabica used, alternate reaction with purified enzyme from leaves of Coffea arabica shown, S-adenosyl-L-methionine used as methyl donor,  
Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1,  
Steps: 1, Stages: 2

S-Adenosyl-L-methionine:theobromine 1-N-methyltransferase, an enzyme catalyzing the synthesis of caffeine in coffee  
By Mazzafera, Paulo et al  
From Phytochemistry, 37(6), 1577-84; 1994

**Analysis** [Refine](#)

Analyze by: [Number of Steps](#)

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

1	12
2	3
3	2
4	2
5	2
6	2
7	2
8	1
9	1
10	1

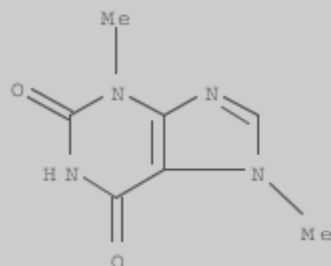
# Get Similar Reactions (Step 7.2)

Thiocyanatochromium(III) complexes with urotropine

By Ganescu, I. et al

From Analele Stiintifice ale Universitatii "Al. I. Cuza Iaasi" Matematica-Chimie, 46(1), 1992

7. Reaction Detail [Link](#) [Sim](#)



NOTE: enzymic, biotransformation of S-adenosyl-L-methionine in the endosperm of Coffea arabica from leaves of Coffea arabica donor, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1

S-Adenosyl-L-methionine:theobromine 1-N-methyltransferase, an enzyme catalyzing the synthesis of caffeine in coffee

By Mazzafera, Paulo et al

From Phytochemistry, 37(6), 1577-84; 1994

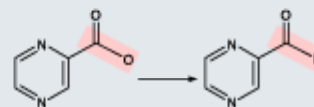
## Get Similar Reactions ⓘ

Retrieve similar reactions from:

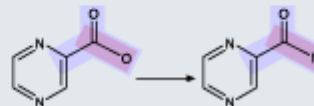
- All reactions
- Current answer set

Include this level of similarity:

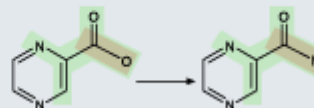
- Broad - Reaction centers only (18793)



- Medium - Reaction centers plus adjacent atoms and bonds (1595)



- Narrow - Reaction centers plus extended atoms and bonds (76)




Get Reactions

Cancel







A division of the American Chemical Society



# Similarity Matches

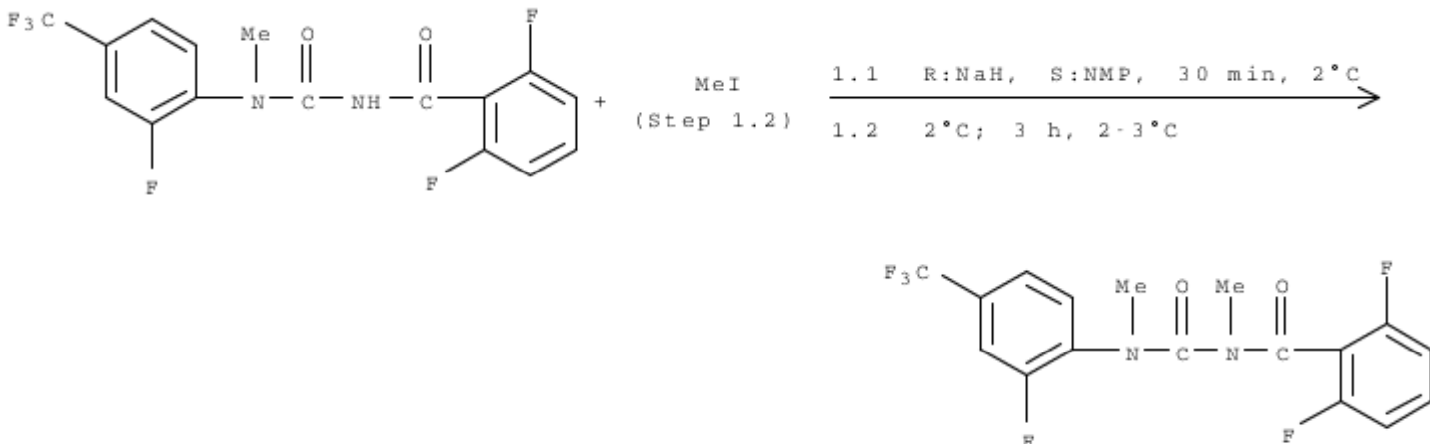
Reactions  Get References

1595 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All | Sort by: Similarity  Answers per Page [15] 1 2 3 4 5 6 ... 107 

Display:  

1. Reaction Detail  Link  Similar Reactions **NEW**



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

Novel use of (n<sup>1</sup>-methyl)benzoylurea compound for preventing a plant from damage by insect pest after germination

By Sakamoto, Norihisa and Konobe, Masato

From U.S. Pat. Appl. Publ., 2008274884, 06 Nov 2008



A division of the American Chemical Society

# Explore Substance (Ex. Aspirin, Step 1)

Welcome Bhawat Ruangying | Sign Out  
Create Keep Me Posted | Chemical Structure exact > substances (708)

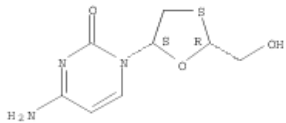
Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

708 Substances 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

Select All Deselect All | Sort by: CAS Registry Number | Answers per Page [15] 1 2 3 4 5 6 ... 48

1. Substance Detail  
1192061-68-9

134678-17-4  
C<sub>8</sub> H<sub>11</sub> N<sub>3</sub> O<sub>3</sub> S

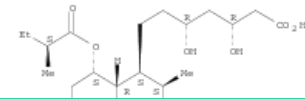


Absolute stereochemistry.  
Rotation (-).

2. Substance Detail  
1189571-88-7

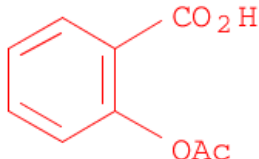
9012-76-4  
Unspecified  
No Structure Diagram Available

50-81-7  
C<sub>6</sub> H<sub>8</sub> O<sub>6</sub>

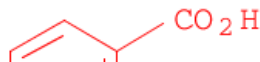


Absolute stereochemistry.

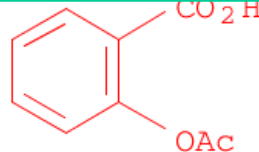
50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



Select the number of answers to show per page.  
15 | 20 | 25 | 50  
Displaying more answers per page may increase page-loading time.

**Variable number of substance answers per page**

**Analysis** [Refine](#)

Analyze by:

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

Biological Study	401
Preparation	289
Uses	251
Properties	82

Reactant or Reagent	31
Formation, Nonpreparative	15
Miscellaneous	4

# Refine by Property Value (Step 2.1)

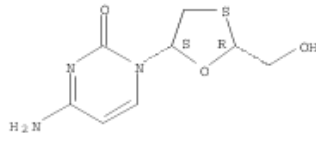
Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

708 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] 1 2 3 4 5 6 ... 48 View: [Icons]

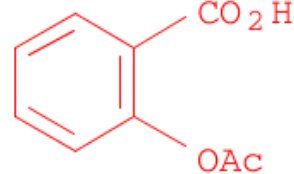
1. Substance Detail  
1192061-68-9

134678-17-4  
C<sub>8</sub> H<sub>11</sub> N<sub>3</sub> O<sub>3</sub> S



Absolute stereochemistry.  
Rotation (-).

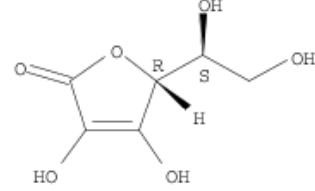
50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



2. Substance Detail  
1189571-88-7


9012-76-4  
Unspecified  
No Structure Diagram Available

50-81-7  
C<sub>6</sub> H<sub>8</sub> O<sub>6</sub>



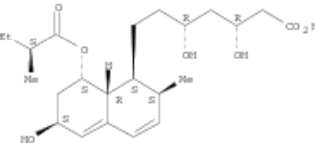
Absolute stereochemistry.

50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



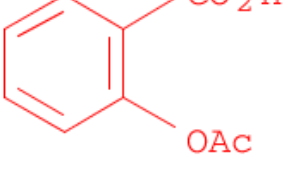
3. Substance Detail  
1188913-22-5

81093-37-0  
C<sub>23</sub> H<sub>36</sub> O<sub>7</sub>




Absolute stereochemistry.

50-78-2  
C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>



Analysis Refine

Refine by: 

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

**Select Properties**



# Refine by Property Value (Step 2.2)

## Refine by Property Value

1. Select one or more properties. Click each property to display value options.

Properties - 1 selected

**Experimental**

- Boiling Point
- Melting Point

**Predicted**

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Acceptor/Donor Sum
- Koc
- logD
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility

2. Specify values and limits.

Values - Experimental Boiling Point

Specify range (degrees C):

to

Min: -273.0      Max:

Pressure (Torr):

to

Min: 0.0      Max:

Include substances with no value for the specified properties

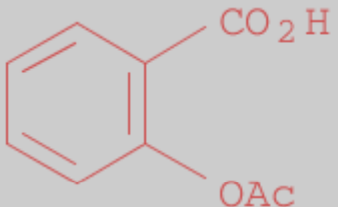


# Export Substance Property Data (Step 3.1)

1 Substance 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] View: [Icons]

1. Substance Detail  
50-78-2



CC(=O)OC1=CC=C(C=C1)C(=O)O

**C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>**  
Benzoic acid, 2-(acetyloxy)-

~25,272 References  
Reactions  
Commercial Sources  
Regulatory Information  
Link

### Export

\* Required

**Export:**  
 All answers  
 Only selected answers

**File Name: \***

**File Type:**  
Microsoft Excel Worksheet (\*.xls)

**Properties to Export:**  
 All property values  
 Only experimental property values  
 Only predicted property values  
 Select property values...

Continue Cancel

# Export Substance Property Data (Step 3.2)

## Export Selected Property Values

### Properties to Export:

Select: **All** **All Experimental** **All Predicted**

**Deselect All**

#### Experimental

- Boiling Point
- Density
- Electric Conductance
- Electric Conductivity
- Electric Resistance
- Electric Resistivity
- Glass Transition Temperature
- Magnetic Moment
- Median Lethal Dose
- Melting Point
- Optical Rotatory Power
- Refractive Index
- Tensile Strength

#### Predicted

- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- Freely Rotatable Bonds
- H Acceptor/Donor Sum
- H Acceptors
- H Donors
- Koc
- LogD
- LogP
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility
- Molar Volume
- Molecular Weight
- pKa
- Polar Surface Area
- Vapor Pressure

**Export**

**Cancel**

SciFinder®		
CAS Registry Number	CAS Index Name	Type
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental
50-78-2	Benzoic acid, 2-(acetyloxy)-	experimental

Density	Density	1.4 g/cm3
Density	Density	1.396 g/cm3
Biological	Median Lethal Dose(LD50)	1216 mg/kg
Biological	Median Lethal Dose(LD50)	1100 mg/kg
Biological	Median Lethal Dose(LD50)	880 mg/kg



# Carbon-13 NMR Spectrum (new)

Molar Volume	139.5±3.0 cm <sup>3</sup> /mol	Temp: 20 °C Press: 760 Torr	(80)
<b>Lipinski and Related Properties</b>			
Value	Conditions	Notes	Top
Freely Rotatable Bonds	3	(80)	
H Acceptors	4	(80)	
H Donors	1	(80)	
H Donor/Acceptor Sum	5	(80)	
logP	1.190±0.226	Temp: 25 °C	(80)
Molecular Weight	180.16		(80)
<b>Spectra Properties</b>			
Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum <b>NEW</b>	<a href="#">See spectrum</a>	(81)	
Proton NMR Spectrum	<a href="#">See spectrum</a>	(81)	
<b>Structure-related Properties</b>			
Value	Conditions	Notes	Top
Polar Surface Area	63.6 Å <sup>2</sup>	(80)	
<b>Thermal Properties</b>			
Value	Conditions	Notes	Top
Boiling Point	321.4±25.0 °C	Press: 760 Torr	(80)
Enthalpy of Vaporization	59.45±3.0 kJ/mol	Press: 760 Torr	(80)
Flash Point	131.1±16.7 °C		(80)

(80) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 for Solaris (© 1994-2009 ACD/Labs)

(81) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V9.07 (© 1994-2009 ACD/Labs)



A division of the American Chemical Society

# C-13 NMR and other spectra



Explore References

Explore Substances

Explore Reactions

Saved Answer Sets  
Keep Me Posted Results  
**NEW** My Connections

Help  
History  
Preferences

Welcome Bhawat Ruangying | Sign Out

Create Keep Me Posted > Chemical Structure exact > substances (708) > refine "property value" (1) > 50-78-2 > Carbon-13 NMR Spectrum (50782-CNMR)

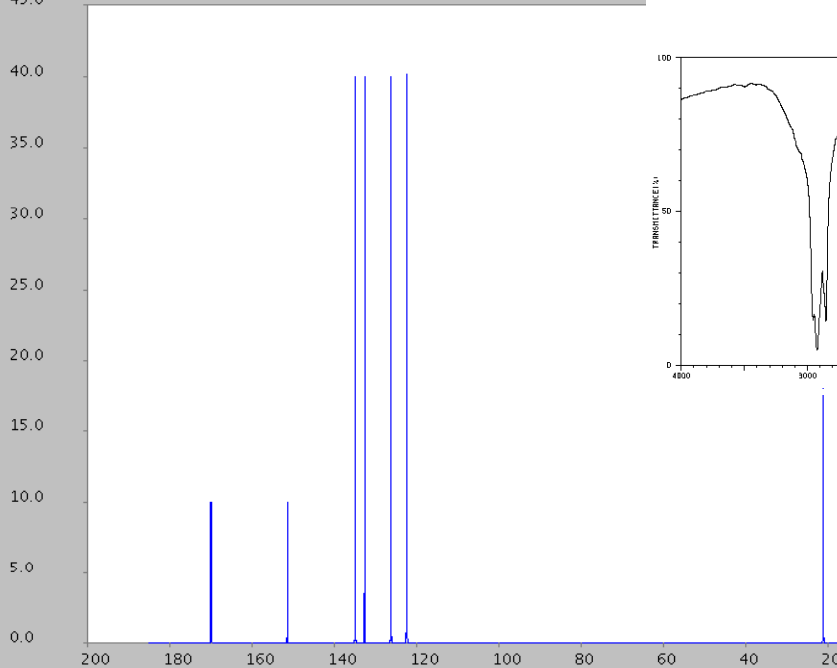
Carbon-13 NMR Spectrum

IR Absorption Spectrum

Spectrum ID

IR

ARBITRARY UNITS  
45.0

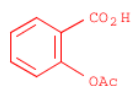


CNMR Predicted Spectrum

CAS Registry Number: 50-78-2

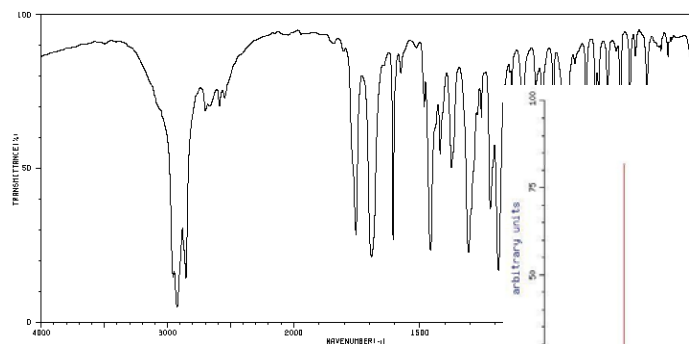
C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>

Benzoic acid, 2-(acetyloxy)-

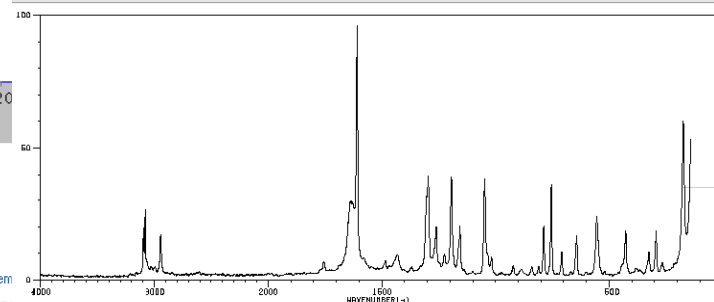


Contact Us | Copyrights and Tradem

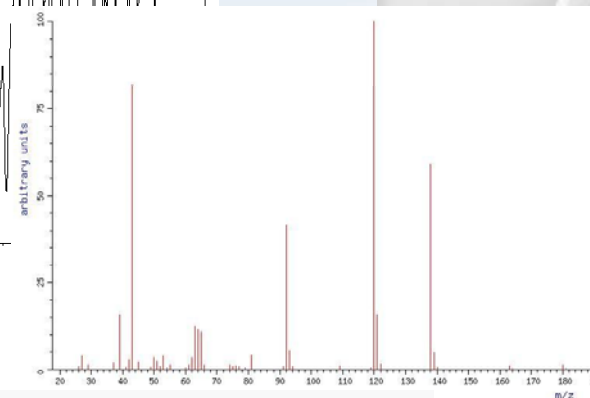
Copyright © 2009 American Chemical Society. All RI



Raman Spectrum



Isilane (75-76-3)



CO<sub>2</sub>H  
OAc



A division of the American Chemical Society

# Summary of Scifinder Web

- Provide quick access and user friendly interface to search for scientific information
- New features that are tailor made for the needs of researchers
- Enhanced content for properties, spectra, registration, reaction information and etc
- Personalization features (keep me posted and save as)







**Thank you**

**Email: [pootorn@book.co.th](mailto:pootorn@book.co.th)  
OR : [bhawatr@gmail.com](mailto:bhawatr@gmail.com)**

[www.cas.org](http://www.cas.org)



*A division of the American Chemical Society*