



SciFinder Web

新平台，新内容，新功能

上海师范大学--SciFinder Web培训

李凤梅

SciFinder培训专员

2012.6.6



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提纲

■ 介绍

- SciFinder Web中的内容
- SciFinder Web特色功能
- SciFinder Web的注册和登陆

■ SciFinder Web中的检索和后处理

- SciFinder Web中的文献检索
- SciFinder Web中的物质检索
- SciFinder Web中的Markush检索
- SciFinder Web中的反应检索

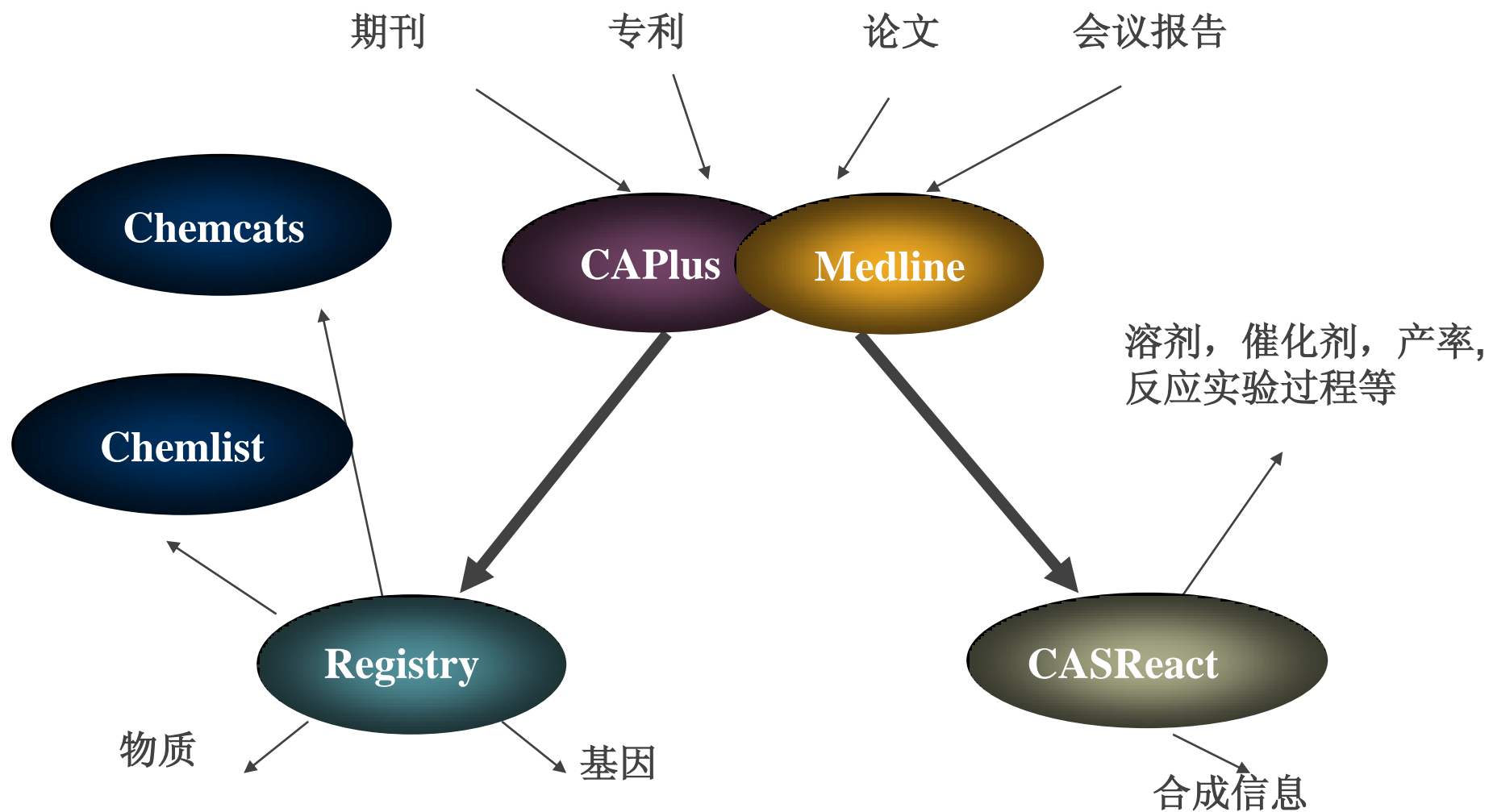
■ SciFinder Web使用常见问题和网络资源

美国化学文摘社—Chemical Abstract Service

- 创建于1907年
- ACS的分支机构
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 最早创立了《化学文摘》
- 总部坐落于俄亥俄州的哥伦布市



SciFinder Web中的内容



SciFinder Web中的内容

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>1400万物质合成制备信息

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每周更新3-5万条单步多步反应

反应回溯到1840年

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- SciFinder Web中的反应检索

■ SciFinder Web使用常见问题和网络资源

SciFinder Web特色功能—KMP定题查询

设定Email提醒，一旦有新的记录，会发邮件通知

SciFinder®

Welcome Amy | Sign Out

Add KMP Alert Research Topic "soil or clay with washing" > references (3216)

References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

3216 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4 5 6 ... 161 | Display: [icon]

☐ 1. Low-temperature cold pressing and binary continuous refining process for production of oil-tea camellia seed oil | Full Text

By Liu, Yun; Pan, Shenguo; Li, Heping; Li, Shuyuan; Xiao, Haiqing

From Faming Zhuanli Shenqing (2012), CN 102329690 A 20120125. | Language: Chinese, Database: CAPLUS

The method comprises removing impurities from oil-tea camellia seeds, sieving to remove shells, air drying, flaking and steam cooking and pressing to give crude oil and cakes, leaching the cakes with solvent No.6 to give crude oil and dregs, degumming a mixt. of hot water and crude oil, neutralizing the degreased oil with alkali soln. and then desaponifying, **washing** the se give degummed and disacidified oil, decolorizing the degummed and disa

☐ 2. Preparation method for artificial sand for sand control of oil well, and

By Wang, Yuxian; Zhu, Qianhou

From Faming Zhuanli Shenqing (2012), CN 102320857 A 20120118. | Language: Chinese

The artificial sand is prepd. by (1) pulverizing coke 100 and quartz 0.3- parts by stirring uniformly; (3) placing into rotary kiln with passing time of C to 960°C; (4) taking out, and cooling. The application process of the **washing** deposited sand in oil well; (2) arranging sand-control tubular co

Create Keep Me Posted Profile ⓘ

* Required

Title: *

soil with washing

Description:

Characters Remaining: 1024

Duration

Expires On: Jan 31, 2013 | Change

Frequency

Send updates once every Week

☐ Exclude previously retrieved references.

Create Cancel

Search:

Explore references by research topic: soil or clay with washing

Candidates Selected:

References which contain the two concepts "clay" and "washing" closely associated with one another

设置提醒文件名和失效时间

SciFinder Web特色功能—根据引文排序

SciFinder®

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Add KMP Alert Research Topic "soil or clay with washing" > references (3216)

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

3216 References 0 Selected

Select All Deselect All Sort by Citing References

Answers per Page [20] 1 2 3 4 5 6 ... 161

Display: — = ≡

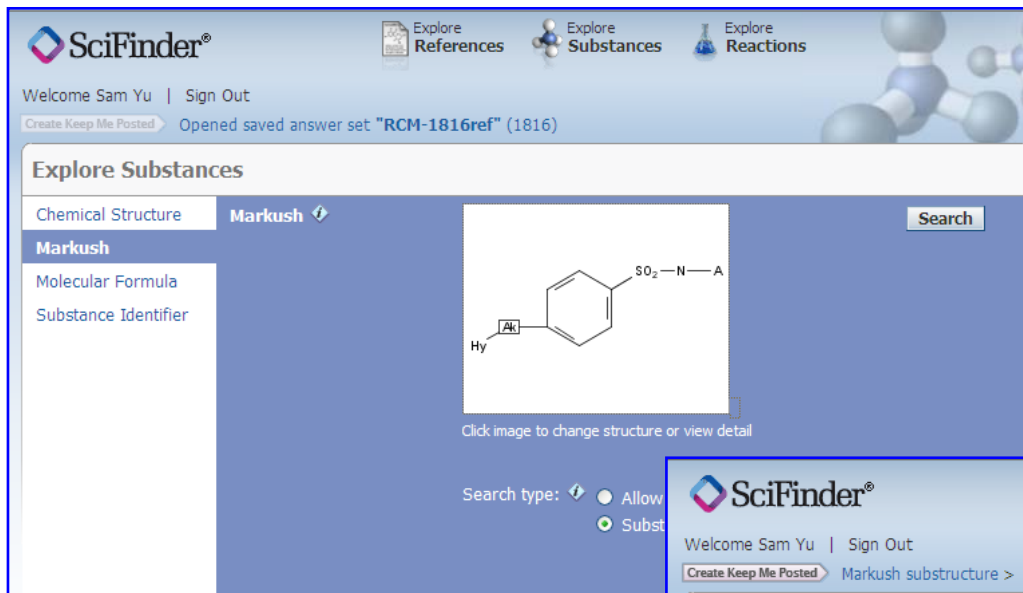
1. **Extraction of Heavy Metals by Biodegradable Chelating Agents** Full Text
 By Tandy, Susan; Bossart, Karin; ...
 From Environmental Science and Technology (2004), 38(3), 937-944. | Language: English, Database: CAPLUS
 Heavy metal soil pollution is widespread worldwide and clean-up is a difficult task. One possible remediation method is ex-situ soil **washing** using chelating agents. EDTA is a very effective chelating agent for this purpose but has a disadvantage: it is quite persistent in the environment due to its low biodegradability. This work examd. biodegradable chelating agents, [S,S]-ethylenediaminedisuccinic acid (EDDS), iminodisuccinic acid (IDSA), methylglycine diacetic acid (MGDA), and nitrilotriacetic acid (NTA) as potential alternatives and compared them to EDTA for effectiveness. Kinetic expt...

2. **Polymerization of adsorbed monolayers. I. Preparation of the clay-polymer complex** Full Text
 By Blumstein, Alexandre
 From Journal of Polymer Science, Part A: General Papers (1965), 3(7), 2653-64. | Language: English, Database: CAPLUS
 Unimol. layers of methyl methacrylate (I) adsorbed on the surface of sodium montmorillonite **clay** were polymerized with γ -irradiation or by Bz2O2 or azodiisobutyronitrile. No spontaneous polymerization was observed. The unimol. layers were prepd. by shaking the **clay** with 2.5 times its wt. of I for 30 min., centrifuging, and **washing** with heptane. The yield of adsorption was obtained by subtracting the quantity of I in the centrifugate (dett. by uv spectrophotometry) from the total wt. of I. The procedure was repeated to attain the desired yield of adsorption. **Washing** with the hydrocarbon re...

3. **Transformation of Bacillus subtilis by DNA bound on clay in non-sterile soil** Full Text
 By Gallori, E.; Bazzicalupo, M.; Dal Canto, L.; Fani, R.; Nannipieri, P.; Vettori, C.; Stotzky, G.
 From FEMS Microbiology Ecology (1994), 15(1-2), 119-26. | Language: English, Database: CAPLUS
 Chromosomal DNA from Bacillus subtilis and different forms of plasmid pHV14 (covalently closed circular (CCC), linear monomer (M), and linear multimer (LM)) were adsorbed and bound on the **clay** mineral montmorillonite. After extensive **washing** of the **clay**-DNA complexes with DNA buffer (pH 7.5), ~25% of the chromosomal DNA, and approx. 30, 90, and 5%, resp., of the CCC, M, and LM form remained bound. Chromosomal and plasmid DNA bound on **clay** were capable of transforming competent cells with different specific activities. The **clay**-DNA complexes persisted in non-sterile soil and retained transf...

~159
~98
~91

SciFinder Web特色功能—Markush检索



SciFinder®

Welcome Sam Yu | Sign Out

Create Keep Me Posted Opened saved answer set "RCM-1816ref" (1816)

Explore Substances

Chemical Structure **Markush**

Markush

Molecular Formula


Substance Identifier

Search

Click image to change structure or view detail

Search type: ☐ Allow ☒ Subst

直接检索和结构有关的专利，
用于做初步的专利评估



SciFinder®

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Create Keep Me Posted Markush substructure > references (1503)

References

1503 References 0 Selected Save Print Export




Select All Deselect All Sort by: Accession Number Answers per Page [20] **1** 3 4 5 6 ... 76

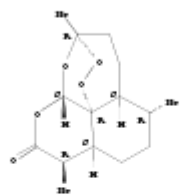
☐ **1. Preparation of pyridinylpyrrole derivatives as tyrosine kinase modulators**
By Guo, Xialing; Zhu, Zhen
From U.S. Pat. Appl. Publ. (2011), US 20110053905 A1 20110303. Language: English, Database: CAPLUS
Title compds. I [X = NR1, O, and S(O)n; n = 0-2; R1 = H, alkenyl, alkoxyalkyl, etc.; R1 = H, halo, alkyl, etc.; m = 0-3; RII = H, alkoxy, alkoxyalkoxy, etc.; n = 0-2; Y = O, NH, CO, etc.; ring A = Ph, naphthyl, 5- to 6-membered monocyclic heteroaryl, etc.; RIII = alkyl, haloalkyl, alkoxy, etc.; Z = C(O)NH, NHS(O)2, S(O)2NHCH2, etc.; ring B = Ph, naphthyl, 5- to 6-membered monocyclic heteroaryl, etc.; RIV = alkoxy, alkoxyalkyl, alkoxyalkoxy, etc.], and their pharmaceutically acceptable salts or prodrugs, are prepd. and disclosed. Thus, e.g., II was prepd. by amidation of 3-methyl-2-furoic ac...
 ~0 Citings 0 Comments 0 Tags

☐ **2. HIV integrase inhibitors**
By Wai, John S.; Su, Dai-Shi; Wiscount, Catherine M.
From PCT Int. Appl. (2011), WO 2011025683 A1 20110303. Language: English, Database: CAPLUS
4-Pyridinone and 4-pyranone compds. of Formula I (X = O or N(R3); Y = CH(R4) or CH(R4)CH(R4); R1 is substituted alkyl; R2 = H, C1-6 alkyl, etc.; R3 = H, C1-6 alkyl, etc.; R4 = H or C1-6 alkyl) are inhibitors of HIV integrase and inhibitors of HIV replication. The compds. are useful for the prophylaxis or treatment of infection by HIV and the prophylaxis, treatment, or delay in the onset or progression of AIDS. The compds. are employed against HIV infection and AIDS as compds. per se (or as hydrates or solvates thereof) or in the form of pharmaceutically acceptable salts. The compds. and the...
 ~0 Citings 0 Comments 0 Tags

SciFinder Web特色功能—物质的靶点和生物活性

1. Substance Detail
63968-64-9

~2756   



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

Spectra
Experimental Properties

在物质详细信息栏，可以查询到物质的生物活性信息和靶点标记信息

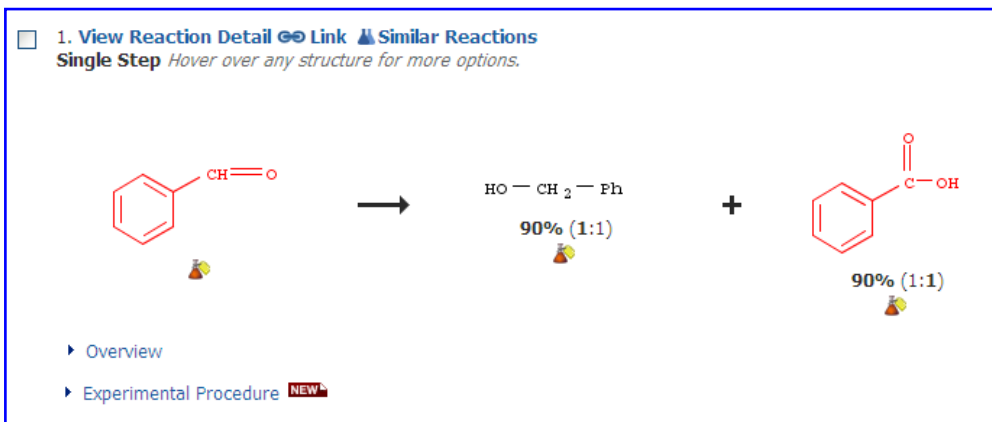
▼ Bioactivity Indicators NEW

	References
Anti-infective agents (all) >>> Antiviral agents	31
Anti-infective agents (all) >> Parasitocides	42
Anti-infective agents (all) >>> Antimalarials	755
Anti-inflammatory agents (all) > Anti-inflammatory agents	38
Antitumor agents (all) > Antitumor agents	153
Natural products MD pharmaceutical	100

▼ Target Indicators NEW

	References
Cytokines (all) >> Chemokines	13
Cytokines (all) >> Tumor necrosis factors	11
DNA-binding proteins (all) >>> Transcription factor NF-κB	21
Enzymes (all) >>>> Adenosine triphosphatase	14
Enzymes (all) >>> 26S proteasome	15
Enzymes (all) >>>>>> Src kinase	13
Glycoproteins (all) >> P-glycoproteins	13
Hemoproteins (all) >>> Cytochrome P 450	10
Hemoproteins (all) >>> Cytochrome P 450 3A4	11
Phosphoproteins (all) >> P-glycoproteins	13
Proteins	19
Receptors (all) > Toll-like receptors	13
RNA formation factors (all) >>> Transcription factor NF-κB	21
Transport proteins (all) >> P-glycoproteins	13
Transport proteins (all) >> Sarcoplasmic-endoplasmic reticulum calcium pumps	10

SciFinder Web特色功能—反应过程的获取



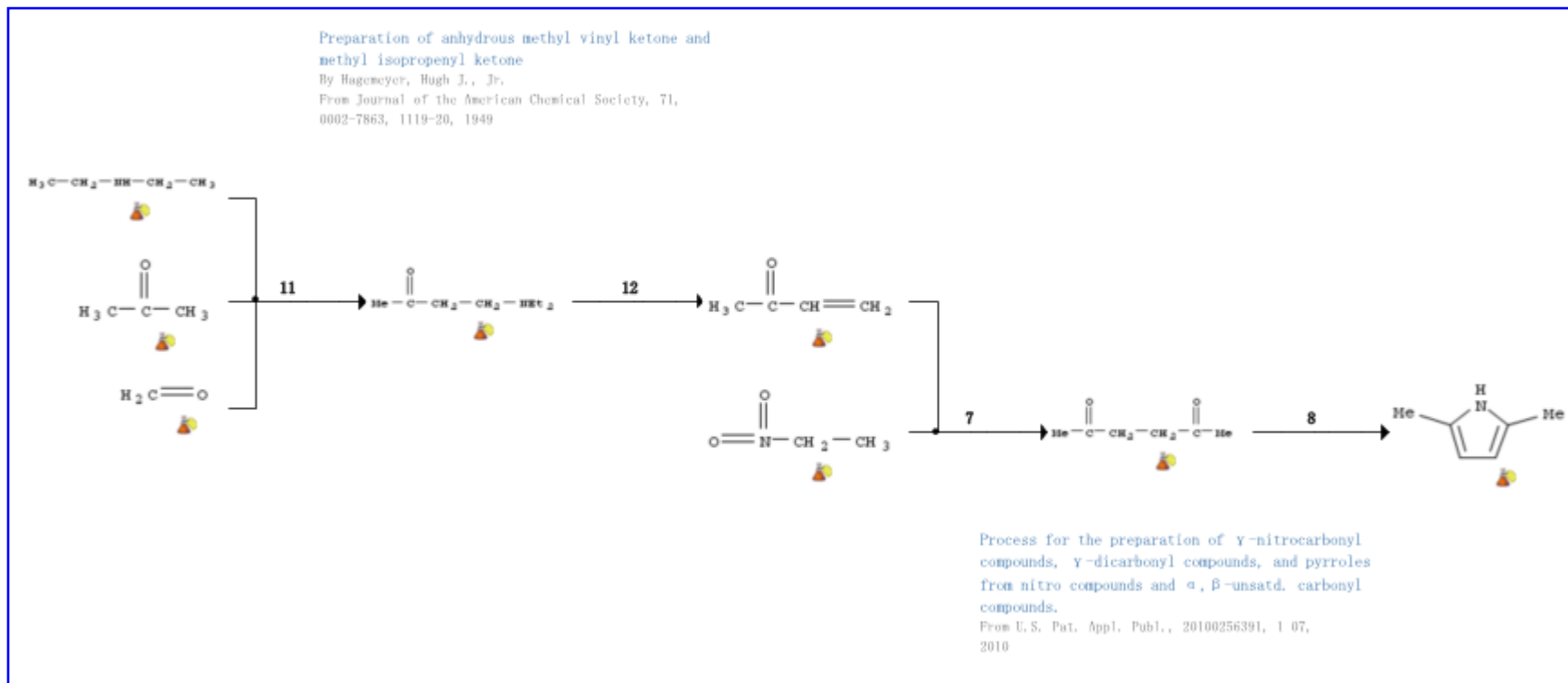
SciFinder中的部分源自期刊和专利中的反应，提供了反应过程信息，使得科研工作者不需要阅读原文，就可以获得对应的反应历程。

Experimental Procedure **NEW**

Organic LETTERS

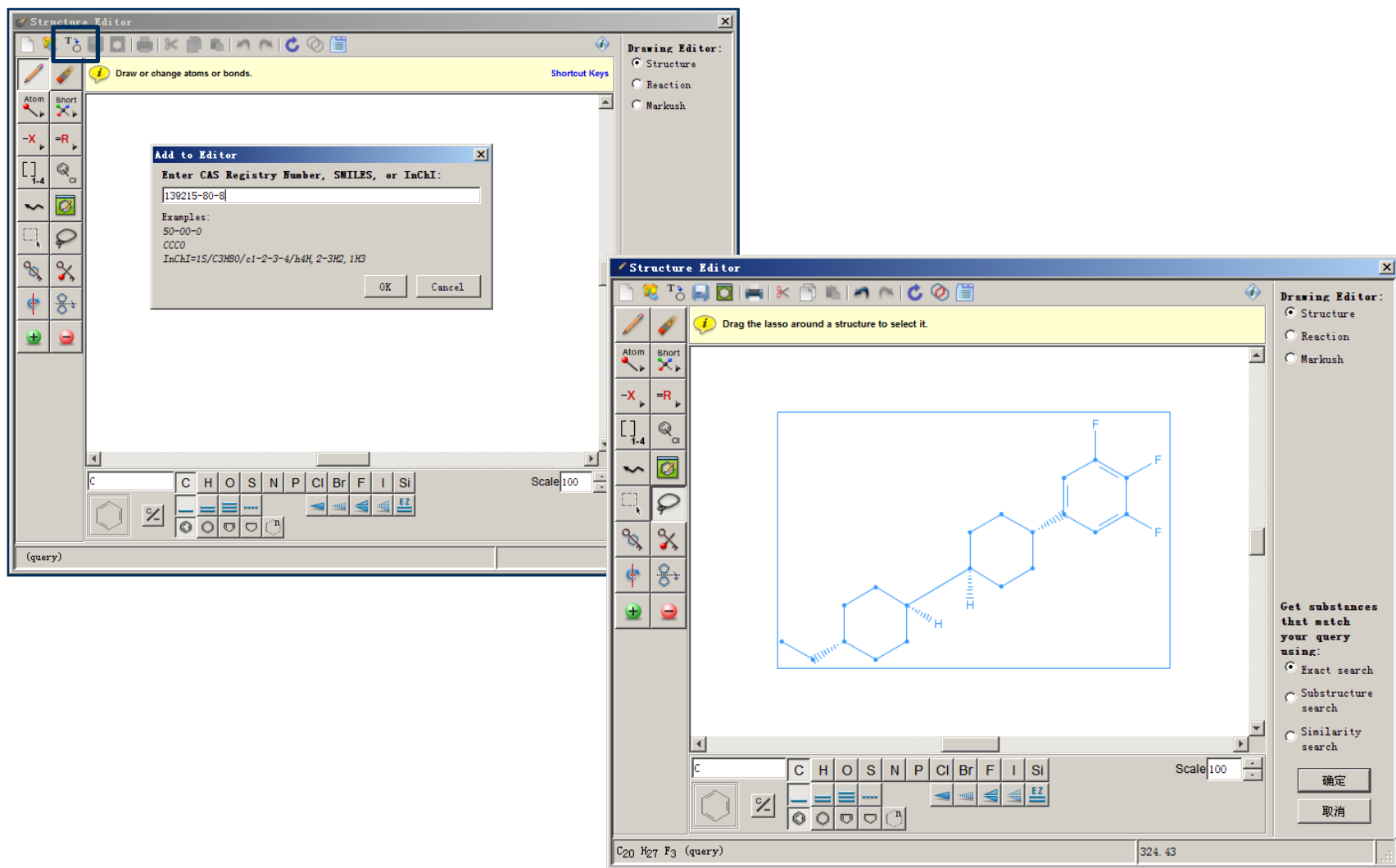
a) LiBr catalyzed Cannizzaro reactions a) LiBr catalyzed Cannizzaro reactions a) LiBr catalyzed Cannizzaro reactions A mixture of LiBr (2 mmol), the aldehyde (4 mmol), and triethylamine (6 mmol) was stirred for 2 days at room temperature under inert atmosphere until complete consumption of the aldehyde was observed. Progress of the reaction was monitored by TLC and GC analyses. Then the mixture was stirred with excess H₂O for 2 hours and subsequently was extracted by ether. The volatile portion of the organic phase was evaporated after being dried over Na₂SO₄. Analysis of the residue by ¹H NMR and GC-MS showed the formation of the corresponding alcohol and carboxylic acid in equal amounts. The alcohol portion was separated by bulb to bulb distillation or by basic separation of the acid portion.

SciFinder Web特色功能—SciPlanner



SciFinder Web新增功能—通过性质检索物质

SciFinder Web新增功能—将CAS RN转化为结构



SciFinder Web新增功能—Quick View

SciFinder®
Welcome Catherine Li | Sign Out
Add KMP Alert Chemical Structure substructure > substances (21)

Substances Get References Get Reactions Tools Send to SciPlanner

21 Substances 0 Selected Save Print Export
Select All Deselect All Sort by: Relevance (New) Answers per Page [15] 1 2 View: [Icons]

1. Substance Detail 448257-37-2
2. Substance Detail 448257-81-6

Quick View

C₂₇ H₃₃ F₃
Benzene, 1,2,3-trifluoro-5-[(*trans,trans*-4'-[(2*S*)-2-phenylpropyl][1,1'-bicyclohexyl]-4-yl]-

Absolute stereochemistry.

预览物质信息

点击CAS RN可直接查看物质详情

Quick View

CAS Registry Number: 448257-37-2
Formula: C₂₇ H₃₃ F₃
CA Index Name: Benzene, 1,2,3-trifluoro-5-[(*trans,trans*-4'-[(2*S*)-2-phenylpropyl][1,1'-bicyclohexyl]-4-yl]-

Number of References
~1

Document Types
Patent

Properties
Predicted

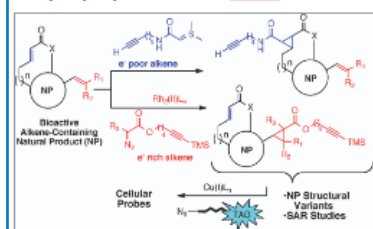
Commercial Sources
Not Available

Absolute stereochemistry.

SciFinder Web新增功能—Quick View

7. Cyclopropanations of Olefin-Containing Natural Products for Simultaneous Arming and Structure Activity Studies

Full Text



By Robles, Omar; Serna-Saldivar, Sergio O.; Gutierrez-Uribe, Janet A.; Romo, Daniel
From Organic Letters (2012), 14(6), 1394-1397. | Language: English, Database: CAPLUS

Cyclopropanations of **alkene-contg. natural products**, e.g., carvone (I), that proceed under mild conditions are reported for simultaneous arming and structure-activity relationship studies. An alkynyl diazo ester, $R_1C(:N_2)CO_2(CH_2)_4C\equiv CR_2$ [$R_1 = R_2 = H$; $R_1 = C_6H_4Br-4$, $R_2 = H$; $R_1 = CN$, $R_2 = H$, $SiMe_3$], under $Rh(II)$ catalysis is employed for cyclopropanations of electron-rich **olefins** while an alkynyl sulfonium ylide, $HC\equiv C(CH_2)_4NHC(:O)CH_2S+Me_2 Br^-$, is used for electron-poor **olefins** to give cyclopropanes, e.g., II [$R_1 = R_2 = H$, $X = O$; $R_1 = C_6H_4Br-4$, $R_2 = H$, $X = O$; $R_1 = CN$, $R_2 = H$, $SiMe_3$, $X = O$]. This approach enables simultaneous **natural product** derivatization for SAR studies and arming (i.e., via alkyne attachment) for subsequent conjugation with reporter tags (e.g., biotin, fluorophores, photoaffinity labels) for mechanism of action studies including cellular target identification and proteome profiling expts.

Quick View

Cyclopropanations of Olefin-Containing Natural Products for Simultaneous Arming and Structure Activity Studies

Full Text

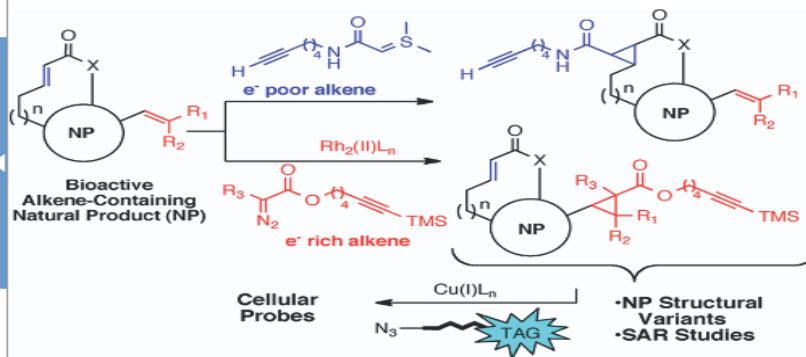
By Robles, Omar; Serna-Saldivar, Sergio O.; Gutierrez-Uribe, Janet A.; Romo, Daniel
From Organic Letters (2012), 14(6), 1394-1397. | Language: English, Database: CAPLUS

Cyclopropanations of alkene-contg. natural products, e.g., carvone (I), that proceed under mild conditions are reported for simultaneous arming and structure-activity relationship studies. An alkynyl diazo ester, $R_1C(:N_2)CO_2(CH_2)_4C\equiv CR_2$ [$R_1 = R_2 = H$; $R_1 = C_6H_4Br-4$, $R_2 = H$; $R_1 = CN$, $R_2 = H$, $SiMe_3$], under $Rh(II)$ catalysis is employed for cyclopropanations of electron-rich olefins while an alkynyl sulfonium ylide, $HC\equiv C(CH_2)_4NHC(:O)CH_2S+Me_2 Br^-$, is used for electron-poor olefins to give cyclopropanes, e.g., II [$R_1 = R_2 = H$, $X = O$; $R_1 = C_6H_4Br-4$, $R_2 = H$, $X = O$; $R_1 = CN$, $R_2 = H$, $SiMe_3$, $X = O$]. This approach enables simultaneous natural product derivatization for SAR studies and arming (i.e., via alkyne attachment) for subsequent conjugation with reporter tags (e.g., biotin, fluorophores, photoaffinity labels) for mechanism of action studies including cellular target identification and proteome profiling expts.

Reference Images

Substance Images

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SciFinder Web的注册和登陆

SciFinder Web的系统要求

Windows用户支持IE 8.x或者FireFox 3.6.x

Mac 用户支持 Firefox 和 Safari

Java 安装（初次使用结构时自动安装）

在图书馆相关页面上找到SciFinder Web注册用的网址



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本馆概况
上海师范大学图书馆分设徐汇和奉贤两地，馆舍总面积达35146平方米，藏书近300万册，数据库90多个。

INTO

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新闻聚合
本馆概况
应用指南
信息服务

SciFinder (CA网络版)

资源语言	外文
英文名称	SciFinder (CA网络版)
中文名称	美国化学文摘 (CA网络版)

备注

浏览器版安装使用说明：

1. 访问 SciFinder 用户注册页面：<https://origin-scifinder.cas.org/registration/index.html?corpKey=1627561DX86F35055X1B9B87B9163118FE25>

2. 注册个人信息

1) 您的用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- (破折号)
- _ (下划线)
- . (句点)

@ (表示 “at” 的符号)

2) 您的密码必须包含 7-15 个字符，并且满足下面情形中的至少三项：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

点击URL创建SciFinder Web账号



Welcome to User Registration for SciFinder®!

Would you like to:

☒ Create a new username and password?

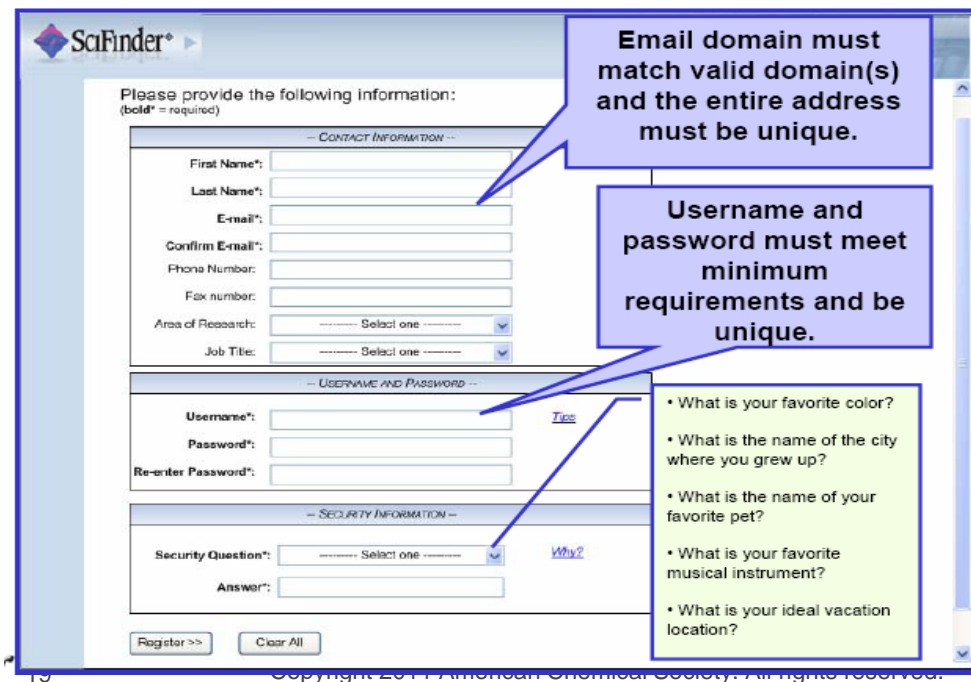
☐ Use an existing username and password? [Examples](#)

[Next >>](#)

开始创建SciFinder Web帐号

创建ID所用的IP不能是代理服务
器的IP

使用学校后缀名的邮箱
注册



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*:

Password*:

Re-enter Password*:

— SECURITY INFORMATION —

Security Question*: Select one

Answer*:

[Why?](#)

[Register >>](#) [Clear All](#)

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?

设置用户名及密码注意事项

用户名：

必须是唯一的，且包含 **5-15** 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- （破折号）
- _（下划线）
- .（句点）
- @（表示“at”的符号）

密码：

必须包含 **7-15** 个字符，并且至少包含三个以下字符：

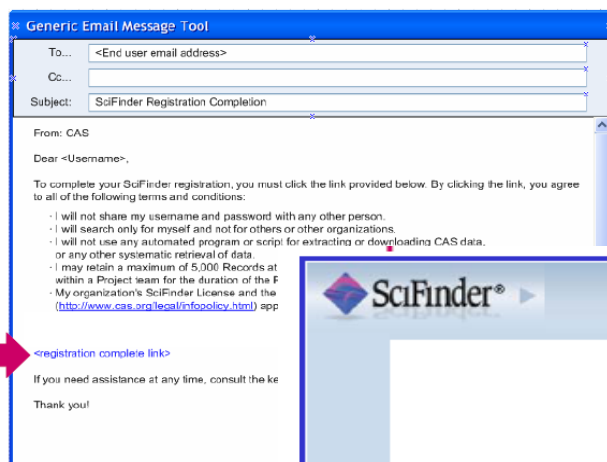
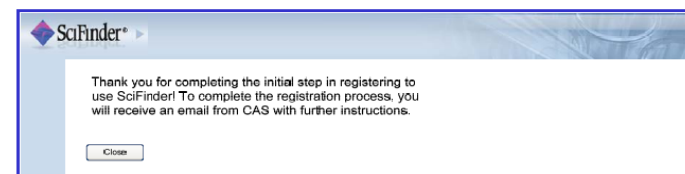
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

密码设置小技巧：

- 1：不要和账号中有重复的字符**
- 2：密码格式最好是abc@123**

对新ID的Email确认

需要点击邮件中的确认链接



上海师范大学注册SciFinder Web注意事项

浏览器版安装使用说明：

1.访问 SciFinder 用户注册页面：[https://origin-scifinder.cas.org/registration/index.html?](https://origin-scifinder.cas.org/registration/index.html?corpKey=1627561DX86F35055X1B9B87B9163118FE25)

[corpKey=1627561DX86F35055X1B9B87B9163118FE25](https://origin-scifinder.cas.org/registration/index.html?corpKey=1627561DX86F35055X1B9B87B9163118FE25)

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- (破折号)

_ (下划线)

. (句点)

@ (表示 “at” 的符号)

2) 您的密码必须包含 7-15 个字符，并且满足下面情形中的至少三项：

字母

混合的大小写字母

数字

非字母数字的字符 (例如 @、#、%、&、*)

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文献，物质，反应检索入口，
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Research Topic

Author Name

Company Name

Document Identifier

Journal

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Publication Year(s)

Document Type(s)

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Book

Clinical Trial

Commentary

Conference

Dissertation

Editorial

Historical

Journal

Letter

Patent

Preprint

Report

Review

Saved Answer Sets

pyridine Substructure-20100909

Markush-20100908

exa-markush

sss-markush

Total reaction -20100820

Demo File

End-reaction

Total Reaction--20100518

Xie ke Chang

Autosaved Reaction Set

View All

Import

Keep Me Posted Results

China -bone tissue engineering scaffold

Apr 09, 2011 (23)

Mar 05, 2011 (25)

Jan 29, 2011 (33)

View All

提纲

■ 介绍

- SciFinder Web中的内容
- SciFinder Web特色功能
- SciFinder Web的注册和登陆

■ SciFinder Web中的检索和后处理

- SciFinder Web中的文献检索
- SciFinder Web中的物质检索
- SciFinder Web中的Markush检索
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■ SciFinder Web使用常见问题和网络资源

SciFinder中的文献检索

主题检索举例：coating materials with rare earth

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this, a user is logged in as 'Catherine Li'. The main section is titled 'Explore References'. On the left, a sidebar lists search criteria: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The 'Research Topic' section is active, showing a search box with the text 'coating materials with rare earth'. A blue arrow points from the text '使用介词来连接关键词，点击Search' to the search box. To the right of the search box is a 'Search' button, which is highlighted with a blue rectangle. Below the search box, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. At the bottom, there are filters for 'Publication Year(s)', 'Document Type(s)', and 'Language(s)', each with a list of options and checkboxes.

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Research Topic Research Topic

coating materials with rare earth

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Photocyanation of aromatic compounds

Search

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Journal
Patent
Tags

Publication Year(s)

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

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<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
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Research Topic Candidates

5 Topics 1 Selected

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Research Topic Candidates	References
<input type="checkbox"/> 140 references were found containing "coating materials with rare earth" as entered.	140
<input checked="" type="checkbox"/> 1515 references were found containing the two concepts "coating materials" and "rare earth" closely associated with one another.	1515
<input type="checkbox"/> 4060 references were found where the two concepts "coating materials" and "rare earth" were present anywhere in the reference.	4060
<input type="checkbox"/> 594835 references were found containing the concept "coating materials".	594835
<input type="checkbox"/> 215432 references were found containing the concept "rare earth".	215432

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“Concept”表示做了同意词的扩展

“Closely associated with one another”

表示同时出现在一个句子中

“were present anywhere in the reference”

表示同时出现在一段话中

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1515 References 0 Selected Save Print Export

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Answers per Page [20] 1 2 3 4 5 6 ... 76

1. **Synthesis and characterization of smart functional coatings by chemical solution deposition methods** Full Text
By Torres, A. E. Mendez; Brinkman, K. S.; Weeks, G.; Krementz, D.; Verst, C.; Reppert, J.
From Annual Meeting Proceedings of the Institute of Nuclear Materials Management (2011), 52nd, a277/1-a277/7. | Language: English, Database: CAPLUS
New **coating** technol. enables the fabrication of low cost structural health monitoring (SHM) and tamper indication devices that can be and international safeguards objectives. In particular, such innovations could serve the safeguards community by improving both confidence in verification and monitoring. This work investigates the synthesis of functional surface **coatings** using chem. solns. de deposition has recently received attention in the **materials** research community due to its unique advantages such as low temp. proce products and the ability to fabricate **materials** with controlled surface properties and pore structures. The synthesis of functional o **materials** cond. and optical properties was investigated by the incorporation of transition element (e.g. Cr+3) and **rare earth** (e.g. polymer or gel matrix. The structural and morphol. investigation of the as-deposited films was carried out using UV/Vis and photolumines deposited **coating** was further investigated by SEM and energy dispersive x-ray microscopy.

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From Jpn. Kokai Tokkyo Koho (2012), JP 2012094767 A 20120517. | Language: Japanese, Database: CAPLUS
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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

Analysis Refine

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MEDLINE	2

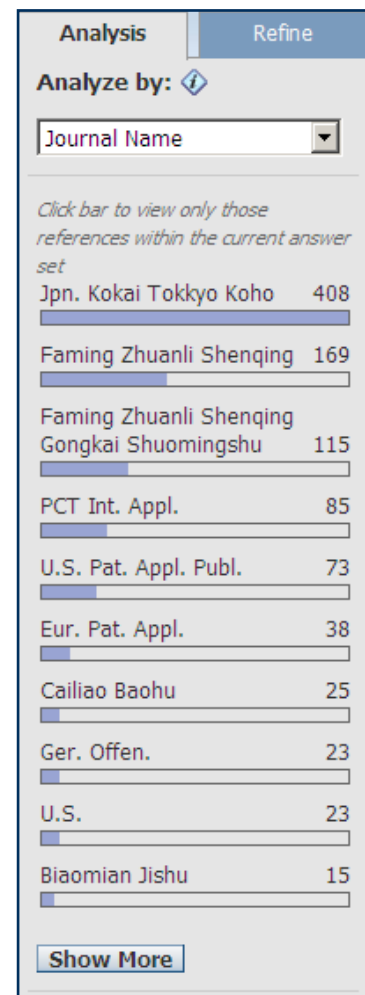
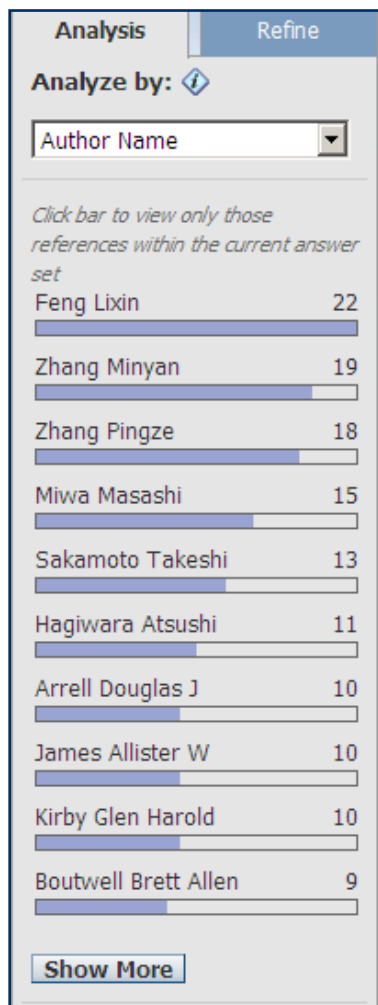
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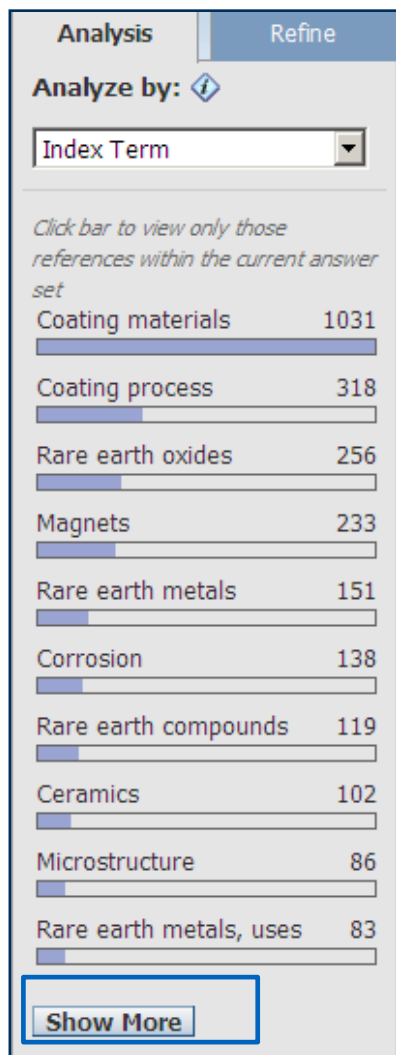
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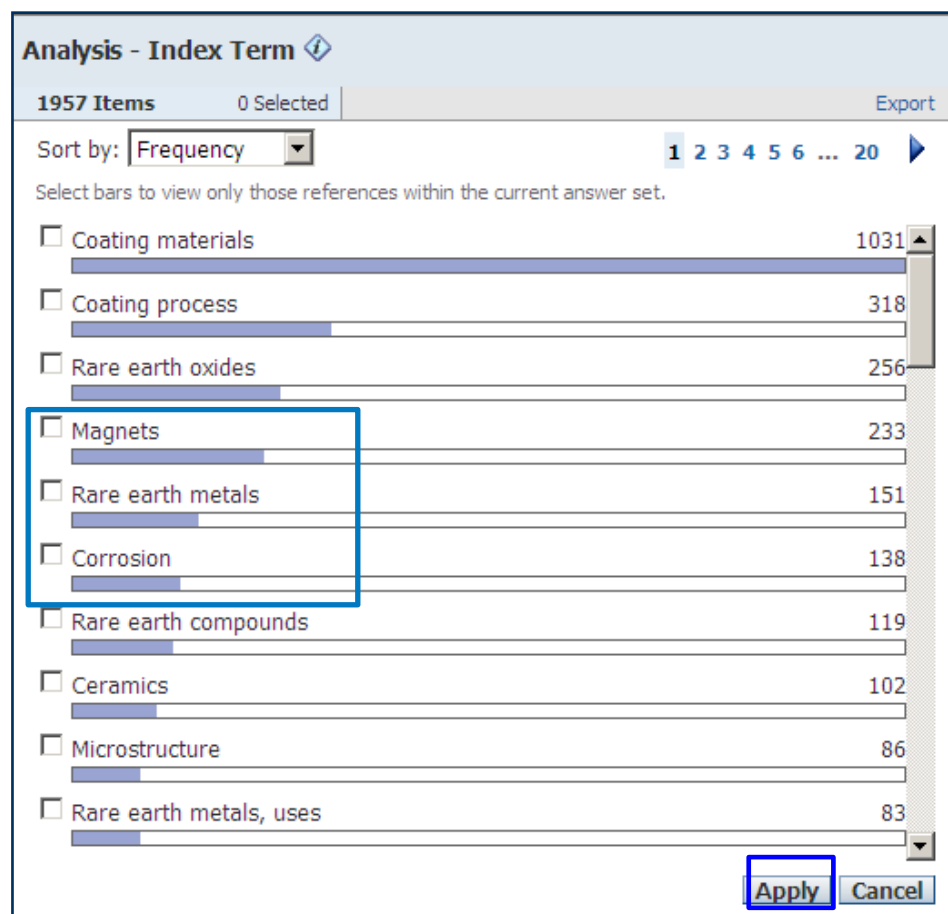
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 ☐ Company Name
 ☒ Document Type
 ☐ Publication Year
 ☐ Language
 ☐ Database

Document Type(s)

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 ☐ Book
 ☐ Clinical Trial
 ☐ Commentary
 ☐ Conference
 ☐ Dissertation
 ☐ Editorial
 ☐ Historical
 ☐ Journal
 ☐ Letter
 ☐ Patent
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49 References 0 Selected
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☐ 1. Ceramic materials for thermal barrier coatings
 By Cao, X. Q.; Vassen, R.; Stoever, T.
 From Journal of the European Ceramic Society 24(1), 1-10. | Language: English, Database: CAPLUS
 A review. This paper summarizes the basic properties of ceramic materials for thermal barrier coatings. Ceramics, in contrast to metals, are often more resistant to oxidn., corrosion, and wear, as well as being better thermal insulators. Except yttria-stabilized zirconia, other materials such as lanthanum zirconate and rare earth oxides are also promising materials for thermal barrier coatings.

☐ 2. Borides in thin film technology
 By Mitterer, Christian
 From Journal of Solid State Chemistry 133(1), 279-291. | Language: English, Database: CAPLUS
 A review with 91 refs. The borides of transition and rare-earth metals are considered for application as wear- and corrosion-resistant, decorative or thermionic coatings. After a review of phys. vapor deposition (PVD) techniques used for the deposition of these coatings, a survey of investigations to apply these coatings is given. As a result of the strong directionality of covalent boron-boron bonds, boride coatings show an increasing tendency to amorphous film growth with increasing B/Me at. ratio and, for rare-earth hexaborides, with decreasing metallic radius of the rare-earth metal. Mech. and optical properties are strongly influenced by the crystallog. structure of the boride phase. Because of their high hardness combined with good adhesion, cryst. films based on the diborides of transition metals seem to be promising candidates for wear resistant coatings on cutting tools. Alloying of these films with nitrogen by reactive PVD processes results in the formation of extremely fine-grained multiphase hard coatings with excellent tribol. and corrosion behavior, thus offering new applications in the coating of engineering components. Because of their distinct colorations, some of the hexaborides of rare-earth elements may be used as decorative coatings on consumer products like wristwatch casings or eyeglass frames. Another promising field is the development of thermionic coatings based on rare-earth hexaborides, which may offer the possibility of the prodn. of inexpensive and simple high emission filaments.

☐ 3. Application of rare earths in thermal barrier coating materials
 By Cao, Xueqiang
 From Journal of Materials Science & Technology (Shenyang, China) 22(1), 15-35. | Language: English, Database: CAPLUS
 A review. Rare earths are a series of minerals with special properties that make them essential for applications including miniaturized electronics, computer hard disks, display panels, missile guidance, pollution controlling catalysts, H2-storage and other advanced materials. The use of thermal barrier coatings (TBCs) has the potential to extend the working time and the life of a gas turbine by providing a layer of thermal insulation between the metallic substrate and the hot gas. Y2O3 as one of the most important rare earth oxides, has already been used in the typical TBC material YSZ (yttria-stabilized zirconia). In the development of the TBC materials, esp. in the latest 10 years, rare earths were found to be more and more important. All the new candidates of TBC materials contain a large quantity of rare earths, such as R2Zr2O7 (R = La, Ce, Nd, Gd), CeO2-YSZ, RM eAl10O19 (R = La, Nd; Me = Ca, Sr) and LaPO4. The concept of double-ceramic-layer coatings based on the rare earth materials and YSZ is effective for the improvement of the thermal shock life of TBCs at high temp.

Analysis

Refine

Analyze by:

Index Term

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Coating materials	30
Rare earth metals	14
Rare earth oxides	9
Thermal barrier coatings	9
Corrosion	8
Rare earth metals, uses	7
Ceramics	6
Coating process	6
Superconductors	6
Rare earth compounds	5

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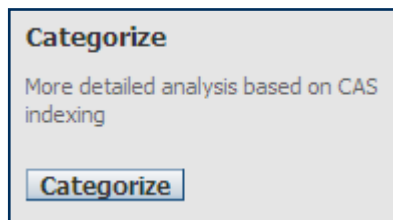
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Index Term

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1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in processes (1892)	1 2 ▶	Click 'x' to remove the category from 'Selected Terms'
Technology	Substances in property studies (1586)	Select All Deselect All	
General chemistry	Gas, liquid, & solid phenomena (184)	<input type="checkbox"/> Microstructure 86	✕ Physical chemistry > Substances in processes (1 Terms)
Physical chemistry	Mechanics (61)	<input type="checkbox"/> Surface structure 46	✕ Physical chemistry > Gas, liquid, & solid phenomena (2 Terms)
Polymer chemistry	Electric & magnetic phenomena (83)	<input type="checkbox"/> Films 37	
Synthetic chemistry	Surface phenomena (42)	<input type="checkbox"/> Glass 29	
Biotechnology	Miscellaneous substances (132)	<input type="checkbox"/> Melting 22	
Catalysis	Particle phenomena (39)	<input type="checkbox"/> Coercive force (magnetic) 21	
Environmental chemistry	Spectra & spectroscopy (63)	<input type="checkbox"/> Thermal conductivity 17	
Genetics & protein chemistry	Thermodynamics (29)	<input type="checkbox"/> Thermal expansion 15	
Biology	Subatomics (19)	<input checked="" type="checkbox"/> Crystal structure 13	
Analytical chemistry		<input type="checkbox"/> Phase composition 13	
		<input checked="" type="checkbox"/> Nanocrystals 12	
		<input type="checkbox"/> Grain size 11	
		<input type="checkbox"/> Remanence 11	
		<input type="checkbox"/> Crystallization 10	
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1. Production of nano alumina-based composite ceramic coating capable of resisting plasma gas corrosion in a high voltage environment

By Wang, Hao; Cheng, Jingqing

From Faming Zhuanli Shenqing (2012), CN 102443753 A 20120509. | Language: Chinese, Database: CAPLUS

The nano alumina-based composite ceramic coating is prepd. by thermal spraying, and its coating thickness is 50 µm-2 mm. The composite ceramic coating is prepd. from alumina 20-75, zirconia 10-40, and rare earth oxides 10-60 wt.%; the rare earth oxide is yttria, lanthanum oxide, gadolinium oxide, cerium oxide, dysprosium oxide, neodymium oxide or/and europium oxide. The composite ceramic coating is prepd. by (1) mixing alumina, zirconia and rare earth oxide, adding ethanol, wet ball milling for 10-24 h, drying, and sieving to obtain a powder material with a particle size of 20-100 µm; and (2) atm. plasma spraying or high-speed oxy fuel spraying the powder material on the substrate. The composite ceramic coating has a good nanostructure, compact structure and resistance to 24-29 kV/mm elec. breakdown and to corrosion by F-contg. plasma; it is used for surface-protective coating of parts in various plasma devices.

2. Photosensitive composition comprising hydroxyapatite or its precursor for dental use

By Sibbeth, Wilsons Brown; Christian Thomas Alcinu; Jha, Animesh; Milne, Steven John; Robinson, Colin; Duggal, Mandee Singh; Toubma, Kyriacos Jack

From PCT Int. Appl. (2012), WO 2012046082 A2 20120412. | Language: English, Database: CAPLUS

The present invention relates to a photosensitive compn. comprising synthetic nanocryst. hydroxyapatite (HAp) or a synthetic precursor thereof doped with a rare earth ion, the use of the compn. in restorative or cosmetic dentistry, a process for prepg. the compn. and a method of generating an image of an exposed dentinal surface of a tooth. For example, compns. contg. a rare-earth oxide activated nanoscale HAp are useful for the treatment of hypersensitivity, dental caries and tooth wear by forming a protective layer. Thus, a nanocryst. HAp powder was prepd. by reaction of calcium nitrate tetrahydrate and diammonium hydrogen phosphate in water at pH -6.5-7, and doped with rare earth oxide (Er2O3), CaF2 and AlPO4. Dentin was dip coated with AlPO4-CaF2-Er2O3-doped HAp and subjected to laser irrads. As a result of rapid melting and sintering, the resseted crystals grow and spread to invade the dentinal tubules. This points towards the fact that adhesion between the underlying natural enamel and the synthetic material may be occurring.

3. Method for manufacturing dense rare earth metal oxide coating film sealing porous ceramic surface

By Park, Dong Su; Lee, Byeong Guk; Han, Byeong Dong; Lee, Jeong Hwan; Byun, Eung Seon

From Repub. Korea (2012), KR 1108692 B1 20120125. | Language: Korean, Database: CAPLUS

The title method comprises the steps of: (1) forming a porous ceramic coating layer on a substrate with plasma then roughness of the porous ceramic coating layer reaches 0.4-2.3 µm, and (3) coating the porous ceramic coating layer with a dense rare earth metal oxide coating film. The method can be used for manufg. a dense rare earth metal oxide coating film sealing the porous ceramic coating film has the advantages of equiv. thickness, high voltage resistance and high corrosion resistance. The dense rare earth metal oxide coating film is used in semiconductor etching devices and various semiconductor devices.

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☒ Portable Document Format (*.pdf)

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- 尽量选择包含**Concept**和**Closed Associated with**的候选项
- 通过**SciFinder** 的**Analyze/Refine**功能来缩小检索的范围
- 尝试将不同的**Analyze/Refine**功能组合起来用，会有更多的收益
- 使用**Categorize**可以让系统来实现自动分类

更多细节化内容，请参考

www.igroup.com.cn/cas

提纲

■ 介绍

- SciFinder Web中的内容
- SciFinder Web特色功能
- SciFinder Web的注册和登陆

■ SciFinder Web中的检索和后处理

- SciFinder Web中的文献检索
- SciFinder Web中的物质检索
- SciFinder Web中的Markush检索
- SciFinder Web中的反应检索

■ SciFinder Web使用常见问题和网络资源

SciFinder中的物质标识符检索

在SciFinder 中查找三聚氰胺（Melamine）

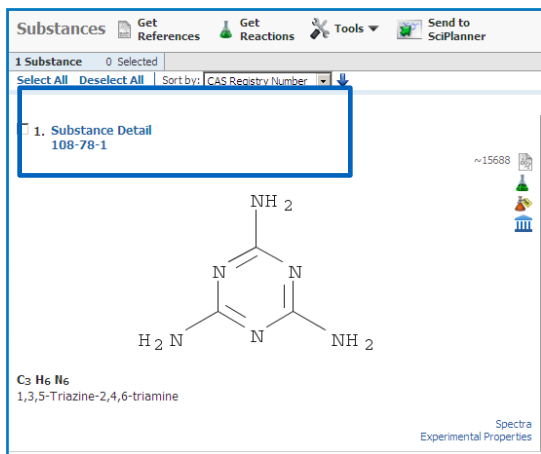
The screenshot displays the SciFinder homepage. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below these, a user is logged in as 'Catherine Li'. The main search area is titled 'Explore Substances'. On the left, there is a sidebar with options: 'Chemical Structure', 'Markush', 'Molecular Formula', 'Property' (marked with a 'NEW' tag), and 'Substance Identifier'. The 'Substance Identifier' option is selected. In the center, there is a large text input field labeled 'Substance Identifier(s)' containing the text 'Melamine'. Below this field, there is a note: 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. To the right of the input field, there is a 'Search' button. A blue arrow points to the input field with the text '在此处输入CAS RN或化学名称' (Enter CAS RN or chemical name here).

物质标示符包括CAS RN. 和化学名称。其中化学名称可以是通用名称、商品名、俗名

提示：

1. 一次检索最多可输入25个物质。
2. 每行一个物质标示符。

SciFinder中的物质记录



Substance Detail
获得和物质有关
的所有信息

CAS Registry Number: 108-78-1

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Export as molfile

Send to SciPlanner

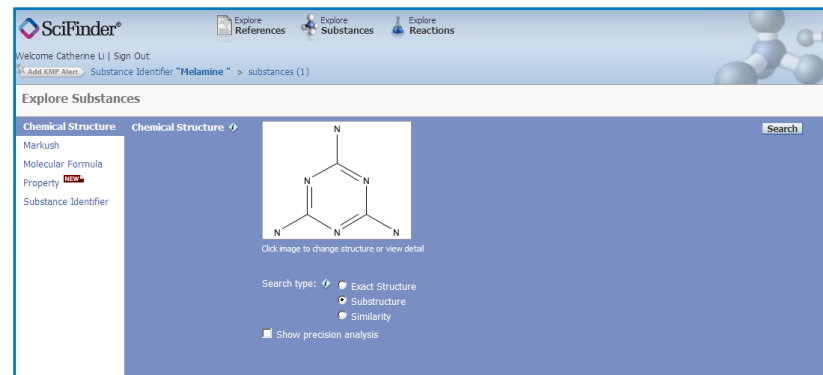
Chemical Structure

Markush Patents by Structure

Reactions

在SciFinder中，
鼠标滑过物质，
可以打开物质的
标准菜单，通过
标准菜单，可以
获得和物质有关
的所有内容

或者发起一
个结构检索
或反应检索



Substance Detail—物质详情

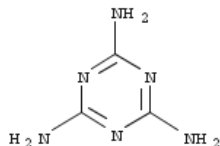
CAS Registry Number: 108-78-1

$C_3H_6N_6$


1,3,5-Triazine-2,4,6-triamine

Melamine (8CI); s-Triazine, 4,6-diamino-1,2-dihydro-2-imino- (6CI); 1,3,5-Triazine-2,4,6-(1H,3H,5H)-triimine; 2,4,6-Triamino-1,2,3-triazine; 2,4,6-Triamino-1,3,5-triazine; 2,4,6-Triamino-s-triazine; 2,4,6-Triaminotriazine; ADK Stab ZS 27; Cyanuramide; Cyanurotriamide; Cyanurotriamine; DG 002; DG 002 (amine); Flammex MEL; Isomelamine; Mark ZS 27; Mel F 40; Melafine; Melamine 2020A; Mitsui 2020A; NSC 2130; PC 1; Pluragard; Pluragard C 133; Spinflam ML 94M; Teoharn; Theoharn; Triamino-s-triazine; Triaminotriazine; Virset 656-4; Yukamelamine; ZS 27; s-Triazinetriamine

Deleted CAS Registry Numbers: 504-18-7, 65544-34-5, 67757-43-1, 68379-55-5, 70371-19-6, 94977-27-2, 130392-03-9, 169314-62-9



CAS号、分子式、
结构式、化学名、别名

按照CAS Role分类的专利、非专利文献列表。对某类文献感兴趣，仅需点击交叉处的  即可方便快捷地获取。

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

预测数据与实验数据

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

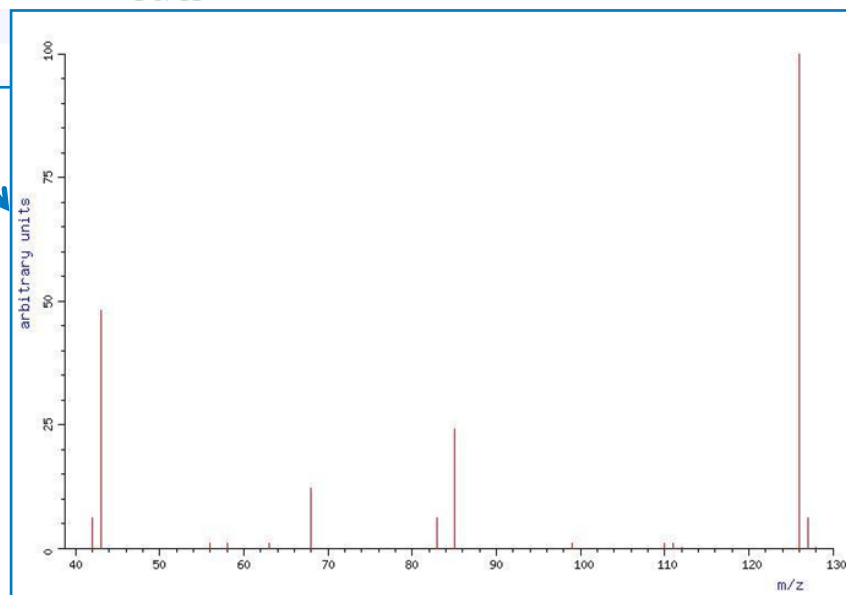
Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(39)	
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(39)	
Chemical Properties	Value	Condition	Note	Top
Koc	1.0	pH 1 Temp: 25 °C	(39)	
Koc	1.0	pH 2 Temp: 25 °C	(39)	

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

Biological Properties	Value	Condition	Note	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(2)CAS	
Half-Life (Biological)	See full text		(2)CAS	
LD50	See full text		(19)CAS	
Median Lethal Dose(LD50)	6000 mg/kg	Organism: rat Route: intragastric	(20)CAS	
Median Lethal Dose(LD50)	4300 mg/kg	Organism: mouse Route: intragastric	(20)CAS	
Median Lethal Dose(LD50)	3296 mg/kg	Organism: mouse Route: oral	(21)CAS	
Median Lethal Dose(LD50)	3161 mg/kg	Organism: rat Route: oral	(22)CAS	
Median Lethal Dose(LD50)	3161 mg/kg	Organism: rat Route: oral	(23)CAS	
Median Lethal Dose(LD50)	3161 mg/kg	Organism: rat Route: oral	(21)CAS	
Median Lethal Dose(LD50)	1000 mg/kg	Organism: rabbit Route: intradermal	(21)CAS	
Chemical Properties	Value	Condition	Note	Top
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(1)CAS	

实验谱图

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum	1 of 2	(3)AIST
Carbon-13 NMR Spectrum	See spectrum		(4)WSS
Carbon-13 NMR Spectrum	See full text		(5)CAS
IR Absorption Spectrum	See spectrum		(4)WSS
IR Absorption Spectrum	See spectrum		(4)WSS
IR Absorption Spectrum	See spectrum		(3)AIST
IR Absorption Spectrum	See spectrum		(3)AIST
IR Absorption Spectrum	See spectrum		(17)BIORAD
IR Absorption Spectrum	See spectrum		(17)BIORAD
IR Absorption Spectrum	See spectrum		(17)BIORAD
IR Absorption Spectrum	See spectrum		(17)BIORAD
IR Absorption Spectrum	See full text	1 of 11	(18)CAS
Mass Spectrum	See spectrum		(4)WSS
Mass Spectrum	See spectrum		(4)WSS



SciFinder中的结构检索

The screenshot shows the SciFinder web interface. At the top, there's a header with the SciFinder logo and navigation links: 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below the header, a welcome message 'Welcome Catherine Li | Sign Out' is visible. A green bar contains an 'Add KMP Alert' button. The main section is titled 'Explore Substances'. On the left, a sidebar lists search methods: 'Chemical Structure' (highlighted), 'Markush', 'Molecular Formula', and 'Substance Identifier'. The main content area features a large blue rectangle with a 'Search' button in the top right corner. In the center of this area, a smaller window is open, displaying 'Click to Edit' and a chemical structure editor toolbar.

点击画图版来进行结构输入，初次使用时需要安装**Java**插件

SciFinder结构绘制工具

The image shows the SciFinder Structure Editor interface with various tools labeled in Chinese. The labels are as follows:

- 铅笔 (Pencil)
- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 元素周期表 (Periodic Table)
- 常用基团 (Common Groups)
- R基团定义工具 (R-group Definition Tool)
- 可变基团 (Variable Groups)
- 可变位置连接工具 (Variable Position Connection Tool)
- 重复基团工具 (Repeating Group Tool)
- 模版工具 (Template Tool)
- 碳链工具 (Carbon Chain Tool)
- 索套选择工具 (Lasso Selection Tool)
- 选择工具 (Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 环锁定工具 (Ring Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 旋转工具 (Rotation Tool)
- C原子和单键恢复工具 (C-atom and Single Bond Restoration Tool)
- 正电子 (Positron)
- 负电子 (Electron)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 结构检索选择 (Structure Search Selection)
- Get substances that match your query using:
 - ☐ Exact search
 - ☒ Substructure search
 - ☐ Similarity search
- 确定 (OK)
- 取消 (Cancel)
- 常见环, 多元环工具 (Common Rings, Polycyclic Tools)

精确结构检索

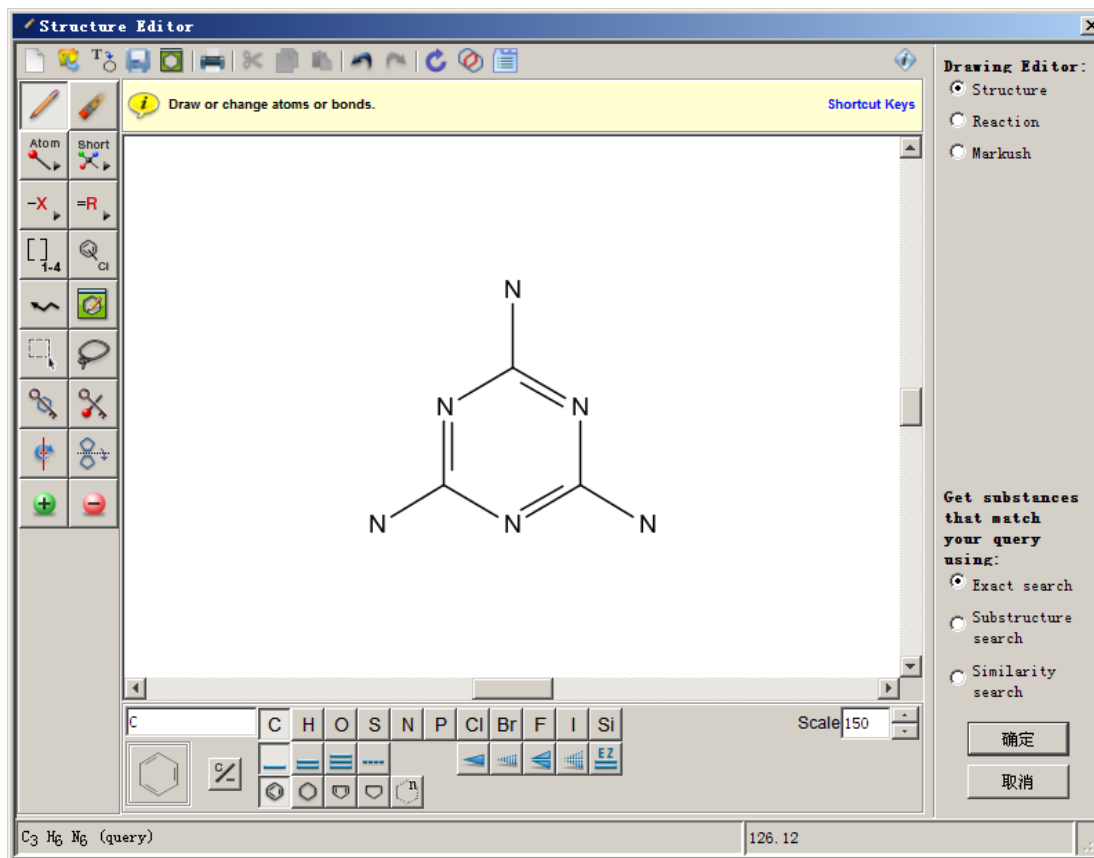
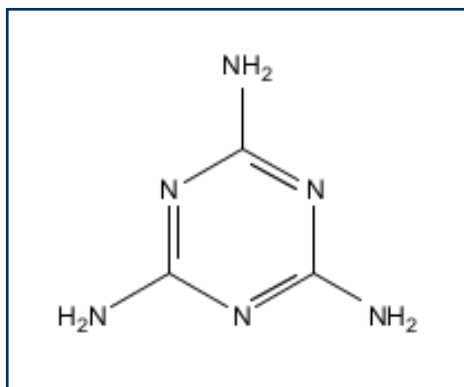
精确结构检索结果包括：

- 与已绘画结构完全相同的结构
- 互变异构体(包括酮-烯醇互变异构)
- 配位化合物
- 两性离子
- 离子化合物
- 自由基和自由基离子
- 同位素
- 所检索结构为单体的聚合物

化合物族（例如，聚合物、混合物、盐等）被自动检索包括在检索结果中。

精确结构检索

在SciFinder Web 中通过精确结构检索以下结构



检索页面

SciFinder®

Welcome Catherine Li | Sign Out

Explore References Explore Substances Explore Reactions

Add KMP Alert Substance Identifier "Melamine" > substances (1) > 108-78-1 > Mass Spectrum (ID_WID-DLO-080659-7)

Explore Substances

Chemical Structure Chemical Structure

Markush
Molecular Formula
Property **NEW**
Substance Identifier

Click image to change structure or view detail

Search type: ☒ Exact Structure
☐ Substructure
☐ Similarity

☒ Show precision analysis

Search

精确结构检索

Characteristic(s)

- ☐ Single component
- ☐ Commercially available
- ☐ Included in reference(s)

Class(es)

- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☐ Polymers
- ☐ Organics, and others not listed

Studies

- ☐ Analytical
- ☐ Biological
- ☐ Preparation
- ☐ Reactant or reagent

Saved Answer Sets

11
139215-80-8Markush
交集1
叔壳氨酸
xu jay4
Thomas Nygil
reaction
123
substructure
sheet resistance
Autosaved Substance Set

View All

Import

Keep Me Posted Results

ullmann reaction
No results

View All

可根据物质的属性、种类和被研究方向进行检索限定

精确检索结果

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Catherine Li | Sign Out

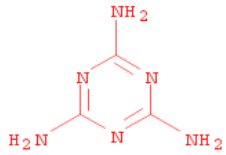
Add KMP Alert Chemical Structure exact > substances (10856)

Substances Get References Get Reactions Tools Send to SciPlanner

10856 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) Answers per Page [15] 1 2 3 4 5 6 ... 724 View: [Icons]

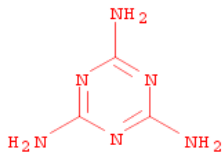
1. Substance Detail 108-78-1 ~15688



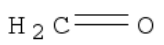
C3 H6 N6
1,3,5-Triazine-2,4,6-triamine

Spectra Experimental Properties

2. Substance Detail 9003-08-1 ~24811



108-78-1
C3 H6 N6

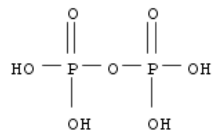


50-00-0
C H2 O

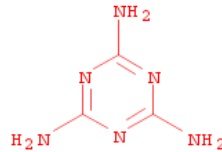
(C3 H6 N6 . C H2 O)x
1,3,5-Triazine-2,4,6-triamine, polymer with formaldehyde

Spectra Experimental Properties

3. Substance Detail 15541-60-3 ~450



2466-09-3
H4 O7 P2



108-78-1
C3 H6 N6

C3 H6 N6 . x H4 O7 P2
Diphosphoric acid, condensed with 1,3,5-triazine-2,4,6-triamine (1:?)

Spectra

Analysis Refine

Analyze by: Substance Role

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

Uses	8400
Preparation	6820
Properties	3035
Process	539
Reactant or Reagent	243
Biological Study	139
Formation, Nonpreparative	26
Analytical Study	20
Prophetic in Patents	20
Occurrence	16

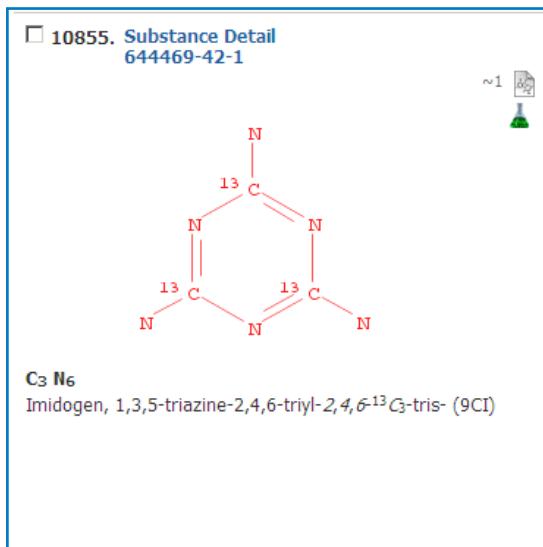
Show More

结构本身

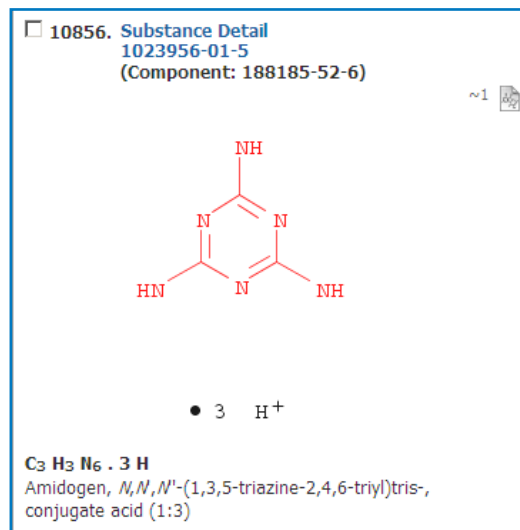
聚合物

磷酸盐

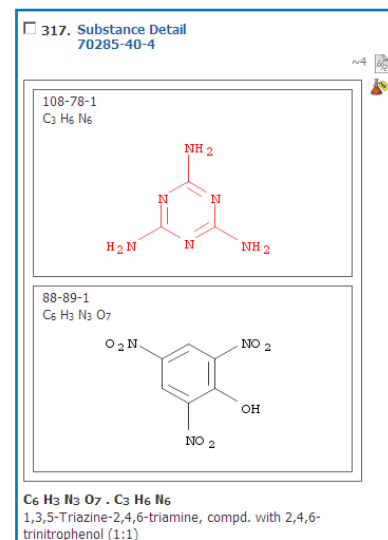
精确检索结果



同位素标记物



氢化物



混合物

物质检索结果集的限定

Analysis Refine

Refine by:

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

Select One:

- ☐ Include only isotope-containing substances
- ☒ Exclude isotope-containing substances

Refine

使用限定工具去除包含同位素的物质

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Catherine Li | Sign Out

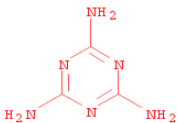
Add KMP Alert Chemical Structure exact > substances (10856) > refine "exclude isotope-containing" (10839)

Substances Get References Get Reactions Tools Send to SciPlanner

10839 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) Answers per Page [15] 1 2 3 4 5 6 ... 723 View: [] [] []

☐ 1. Substance Detail 108-78-1 ~15688

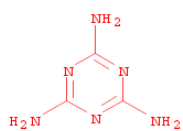


C₃ H₆ N₆
1,3,5-Triazine-2,4,6-triamine

Spectra Experimental Properties

☐ 2. Substance Detail 9003-08-1 ~24811

108-78-1
C₃ H₆ N₆



50-00-0
C₂ H₂ O

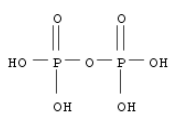
H₂C=O

(C₃ H₆ N₆ · C₂ H₂ O)_x
1,3,5-Triazine-2,4,6-triamine, polymer with formaldehyde

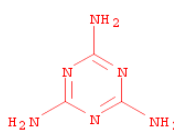
Spectra Experimental Properties

☐ 3. Substance Detail 15541-60-3 ~450

2466-09-3
H₄ O₇ P₂



108-78-1
C₃ H₆ N₆



C₃ H₆ N₆ · x H₄ O₇ P₂
Diphosphoric acid, compd. with 1,3,5-triazine-2,4,6-triamine (1:?)

Spectra

亚结构检索

亚结构检索帮助了解所输入结构的修饰信息，以及获得具有一定结构特征的物质

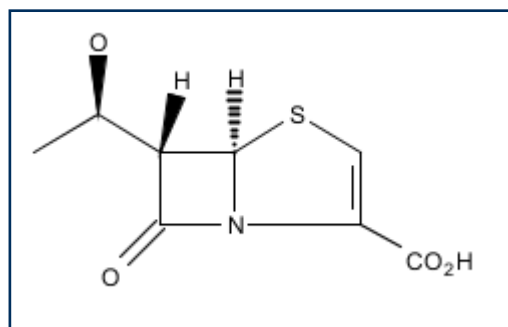
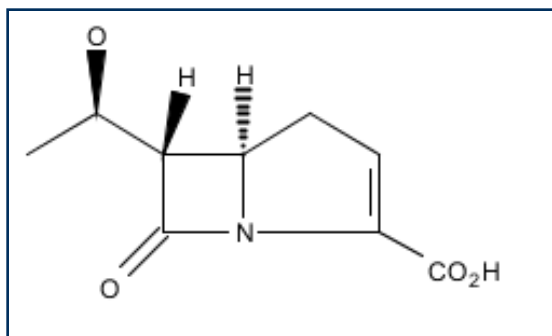
亚结构检索的结果包括：

- 亚结构检索的答案包括精确结构检索的答案，加上附加取代的答案。
- 所有的节点被假定为“开放的”，并且环体系被假定为“未锁定的”。
- 所以要 通过控制取代、控制环的形成和定义相关基团来缩小范围

相关策略参考网页<http://www.cas.org/support/scifi/strategies/windex.html>

亚结构检索

举例，检索以下母核结构的修饰物

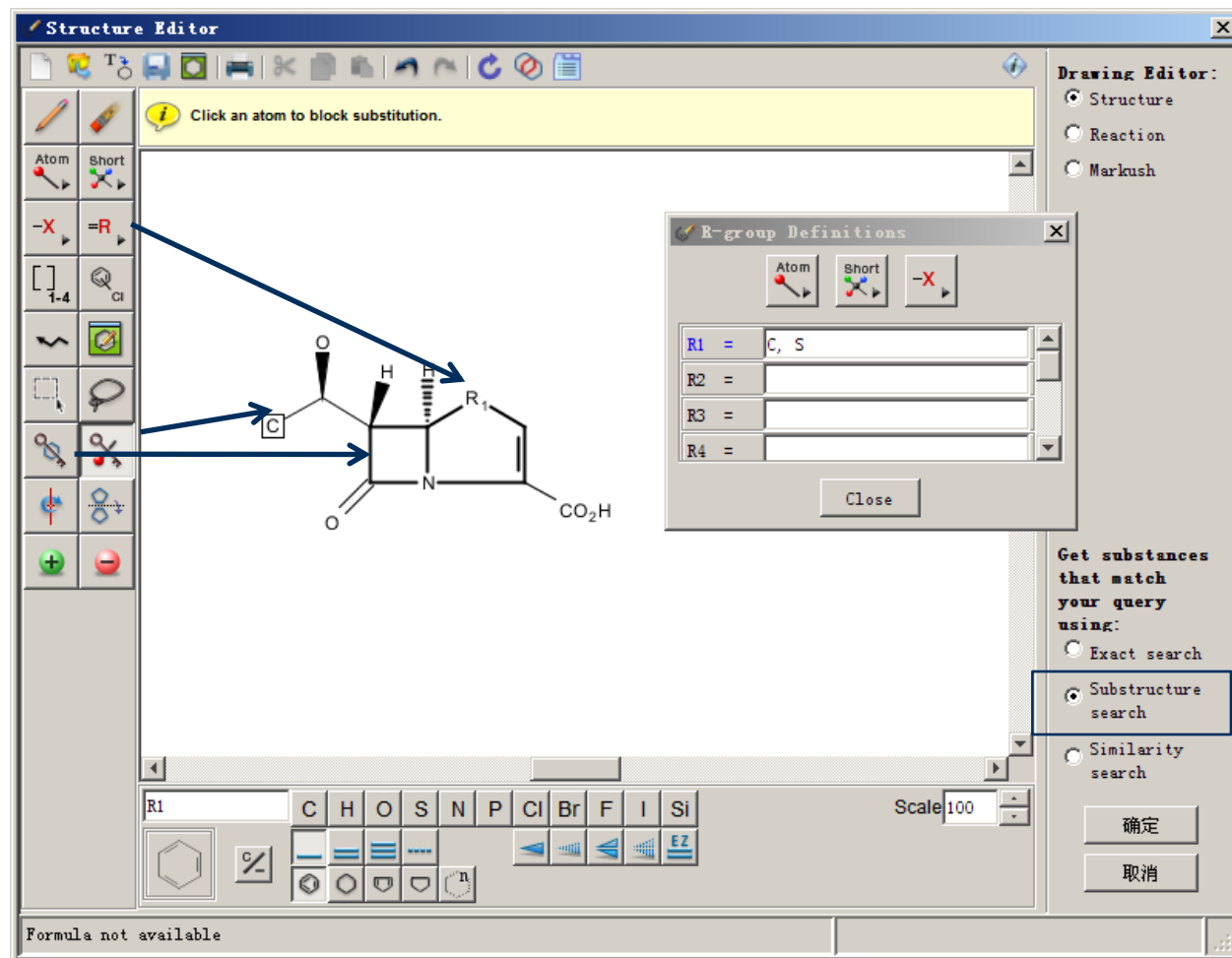


结构绘制和定义

R-基团，增加可
变性

环锁定工具控制
环的形成

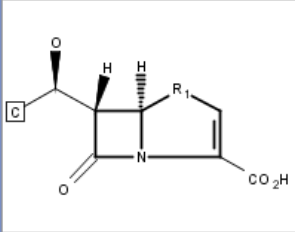
原子锁定工具
禁止发生取代



亚结构检索页面

Explore Substances

Chemical Structure
Markush
Molecular Formula
Substance Identifier

Chemical Structure


Click image to change structure or view detail

Search type: ☒ Exact Structure
☒ Substructure
☐ Similarity

☐ Show precision analysis

Search

Characteristic(s)

☒ Single component
☐ Commercially available
☐ Included in reference(s)

Class(es)

☐ Alloys
☐ Coordination compounds
☐ Incompletely defined
☐ Mixtures
☐ Polymers
☐ Organics, and others not listed

亚结构检索

单组分

立体候选项

Stereo Candidates	
5 Candidates	2 Selected
Select All Deselect All	
Stereo Candidates	Substances
<input checked="" type="checkbox"/> Absolute stereo match	13147
<input type="checkbox"/> Absolute stereo mirror image	19
<input type="checkbox"/> Relative stereo match	84
<input type="checkbox"/> Stereo that doesn't match query	1098
<input checked="" type="checkbox"/> No stereo in answer structure	3004
Get Substances	

亚结构检索结果集

物质分析工具

Substances

16151 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number

Answers per Page [15] 1 2 3 4 5 6 ... 1077 View:

☐ 1. Substance Detail
1356992-95-4

Absolute stereochemistry.

C₂₂ H₂₁ D₄ N₃ O₇ S
INDEX NAME NOT YET ASSIGNED

☐ 2. Substance Detail
1354685-52-1

Absolute stereochemistry.

C₂₀ H₂₁ N O₆
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-[(1*R*)-1-(acetyloxy)ethyl]-3-(4-acetylphenyl)-4-methyl-7-oxo-, (4*S*,5*R*,6*S*)-

☐ 3. Substance Detail
1354685-51-0

☐ 4. Substance Detail
1354685-50-9

Analysis Refine

Analyze by:

- Substance Role
- Bioactivity Indicators (New)
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Target Indicators (New)

Biological Study	9459
Uses	2972
Properties	399
Prophetic in Patents	333
Reactant or Reagent	301
Process	118
Analytical Study	45
Formation, Nonpreparative	16
Occurrence	13

[Show More](#)

物质结果集的分析

Analysis Refine

Analyze by:

Substance Role

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

Preparation	10224
Biological Study	9459
Uses	2972
Properties	399
Prophetic in Patents	333
Reactant or Reagent	301
Process	118
Analytical Study	45
Formation, Nonpreparative	16
Occurrence	13

[Show More](#)

Substance Role分析，帮助获得具有特定研究报道的物质
点击**Keep Analysis**来获取当前的结果集。

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Catherine Li | Sign Out

[Add KMP Alert](#) [Chemical Structure substructure with limiters](#) > substances (16151)

Substances Get References Get Reactions Tools Send to SciPlanner

16151 Substances 0 Selected Save Print Export

9,459 substances with the Substance Roles **Biological Study** are displayed Keep Analysis Clear Analysis

Select All Deselect All | Sort by: CAS Registry Number

Answers per Page [15] 1 2 3 4 5 6 ... 631 View:

☐ 6. Substance Detail
1353544-80-5

C₃₈ H₆₈ N₄ O₈ S₂
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-(7,7-dimethyl-3,3-dioxido-5-oxo-6-oxa-3-thia-2,4-diazahexacos-1-yl)-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-

☐ 7. Substance Detail
1353539-36-2

C₃₆ H₆₄ N₄ O₈ S₂
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-(7,7-dimethyl-3,3-dioxido-5-oxo-6-oxa-3-thia-2,4-diazatetracos-1-yl)-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-

☐ 8. Substance Detail
1353536-98-7

C₃₈ H₆₈ N₄ O₈ S₂
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-(7,7-dimethyl-3,3-dioxido-5-oxo-6-oxa-3-thia-2,4-diazahexacos-1-yl)-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-

☐ 9. Substance Detail
1353533-66-0

C₃₆ H₆₄ N₄ O₈ S₂
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-(7,7-dimethyl-3,3-dioxido-5-oxo-6-oxa-3-thia-2,4-diazatetracos-1-yl)-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-

物质结果集的排序

Chemical Structure substructure with limiters > substances (16151) > keep analysis "Substance Role" (9459)

Substances Get References Get Reactions Tools Send to SciPlanner

9459 Substances 0 Selected

Select All Deselect All Sort by: **Number of References** (dropdown menu showing: Number of References, CAS Registry Number, Molecular Weight, Molecular Formula)

Answers per Page [15] 1 2 3 4 5 6 ... 631

View: [icon] [icon] [icon]

☐ 1. Substance Detail
64221-86-9

~10718

Absolute stereochemistry.

C₁₂ H₁₇ N₃ O₄ S
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-[(1*R*)-1-hydroxyethyl]-3-[[2-[(iminomethyl)amino]ethyl]thio]-7-oxo-, (5*R*,6*S*)-

Experimental Properties

☐ 2. Substance Detail
96036-03-2

~5203

Absolute stereochemistry.

C₁₇ H₂₅ N₃ O₅ S
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[[(3*S*,5*S*)-5-[(dimethylamino)carbonyl]-3-pyrrolidinyl]thio]-6-[(1*R*)-1-hydroxyethyl]-4-methyl-7-oxo-, (4*R*,5*S*,6*S*)-

Experimental Properties

☐ 3. Substance Detail
153832-46-3

~804

Absolute stereochemistry.

C₂₂ H₂₅ N₃ O₇ S

☐ 4. Substance Detail
87726-17-8

~438

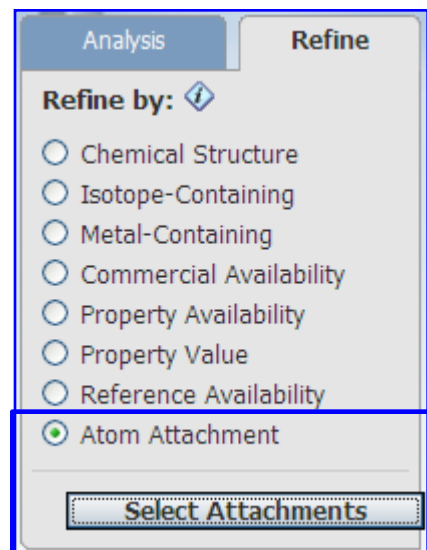
Absolute stereochemistry.

C₁₅ H₂₁ N₃ O₄ S
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-[(1*R*)-1-hydroxyethyl]-3-[[[(3*S*)-1-(1-

按文献数量排序帮助优先浏览研究较多的热门物质

亚胺培南
美罗培南
厄他培南
帕尼培南
等

Refine-Atom Attachment获得结构中特定修饰情况



Refine下的**Atom Attachment**工具，帮助科研工作者了解结构中各个位点的修饰性

Refine by Atom Attachment

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

Substructure

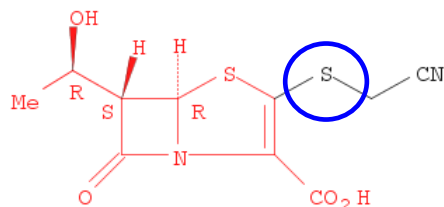
Atom Attachments

Select All Deselect All

<input type="checkbox"/> H or None	6
<input checked="" type="checkbox"/> S	6031
<input type="checkbox"/> C	3367
<input type="checkbox"/> O	22
<input type="checkbox"/> N	19
<input type="checkbox"/> Other	14
<input type="checkbox"/> A - Any (not H)	9439
<input type="checkbox"/> Q - Any (not C,H)	6072
<input type="checkbox"/> Ak - Alkyl chain	1201
<input type="checkbox"/> Cb - Carbocycle	1098
<input type="checkbox"/> Hy - Heterocycle	1080

获得特定定位点上为S的衍生物

1. Substance Detail 121470-68-6

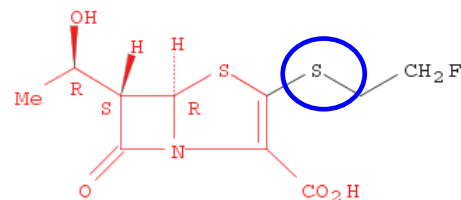


Absolute stereochemistry.

C₁₀ H₁₀ N₂ O₄ S₂

4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(cyanomethyl)thio]-6-(1-hydroxyethyl)-7-oxo-, [5*R*]-[5*a*,6*a*(*R*^{*})]- (9CI)

2. Substance Detail 85905-06-2

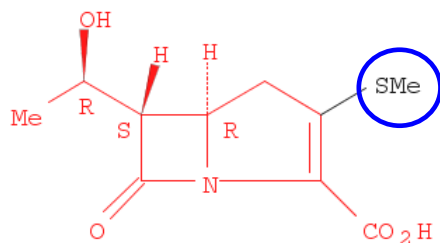


Absolute stereochemistry.

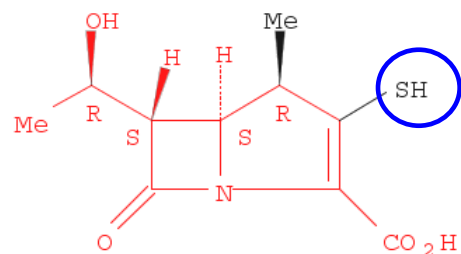
C₁₀ H₁₂ F N O₄ S₂

4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(2-fluoroethyl)thio]-6-(1-hydroxyethyl)-7-oxo-, [5*R*]-[5*a*,6*a*(*R*^{*})]- (9CI)

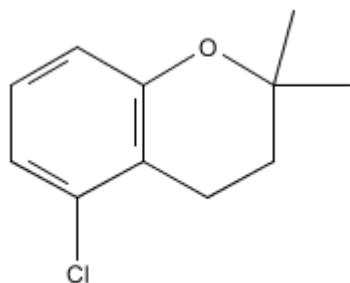
3. Substance Detail 118243-53-1



4. Substance Detail 111596-54-4



相似检索



SciFinder中的相似结构检索，帮助获得在结构上存在相似的物质。

Explore Substances

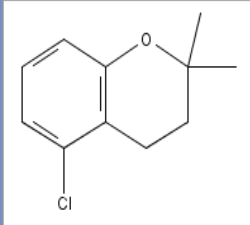
Chemical Structure

Markush

Molecular Formula

Substance Identifier

Chemical Structure



Click image to change structure or view detail

Search type:

☒ Exact Structure

☐ Substructure

☐ Similarity

☐ Show precision analysis

Characteristic(s)

☒ Single component

☐ Commercially available

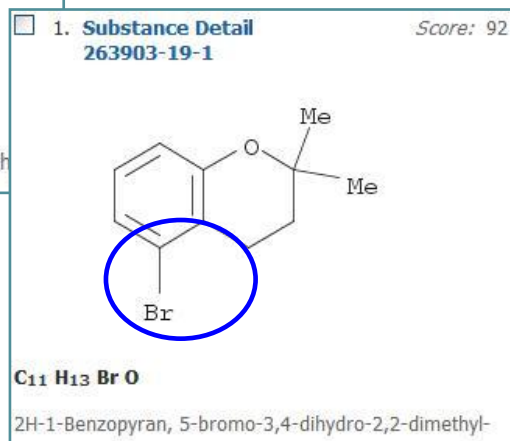
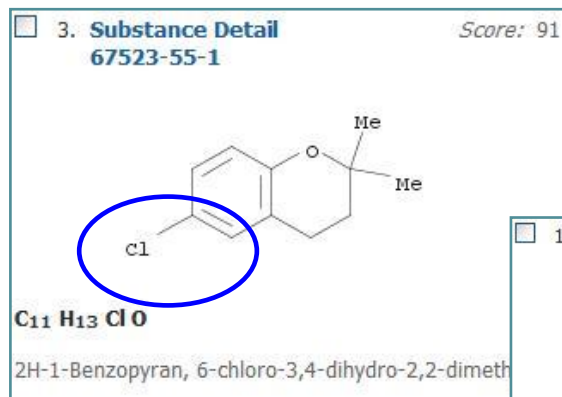
☐ Included in reference(s)

Search

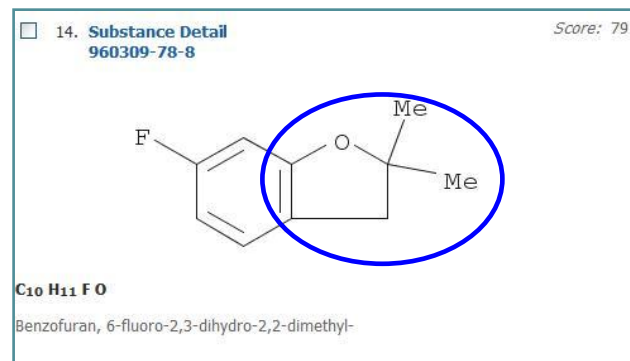
相似结构检索

Similarity Candidates	
7 Candidates	4 Selected
Select All Deselect All	
Similarity Candidates	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input checked="" type="checkbox"/> 90-94	3
<input checked="" type="checkbox"/> 85-89	7
<input checked="" type="checkbox"/> 80-84	34
<input checked="" type="checkbox"/> 75-79	114
<input type="checkbox"/> 70-74	324
<input type="checkbox"/> 65-69	1158
<input type="checkbox"/> 0-64 (least similar)	3403
Get Substances	

根据相似分值控制相似度



与原结构存在以下的区别：
取代基位置变化
取代基变化
母体结构变化



结构检索小结

- 精确结构检索：
获得物质的盐，聚合物，混合物，配合物等，母体结构不能修改，不能修饰
- 亚结构检索：
所画的结构必须存在，母体结构不能修改，但可以被修饰
- 相似结构检索：
获得相似度在**60**分以上的结构，母体结构可以修改，也可以被修饰，用相似度来控制获得的结果

提纲

■ 介绍

- SciFinder Web中的内容
- SciFinder Web特色功能
- SciFinder Web的注册和登陆

■ SciFinder Web中的检索和后处理

- SciFinder Web中的文献检索
- SciFinder Web中的物质检索
- SciFinder Web中的Markush检索
- SciFinder Web中的反应检索

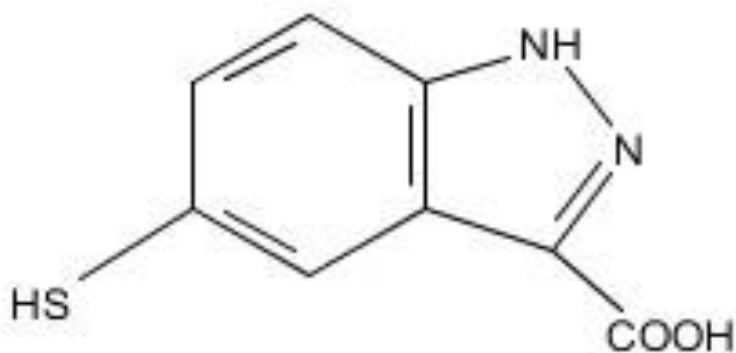
■ SciFinder Web使用常见问题和网络资源

Markush检索—帮助获取和结构有关的专利

- Markush检索能帮助我们做初步的专利评估

- 举例:

获取和该结构有关的专利



检索中的问题:

精确结构没有检索到相应结果，可以确定该物质是新物质，但是能否保证其没有被专利保护？

Markush检索直接返回保护了该结构的专利

SciFinder®

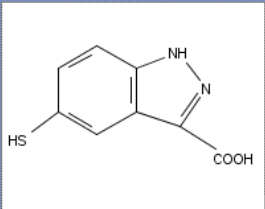
Welcome Sam Yu | Sign Out

Explore References Explore Substances Explore Reactions

Explore Substances

Chemical Structure Markush Molecular Formula Substance Identifier

Search



Click image to change structure or view detail

Search type: ☒ Allow variability only as specified ☐ Substructure

Markush检索出来的是保护了该结构的专利

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

23 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number

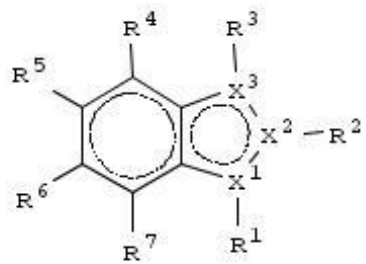
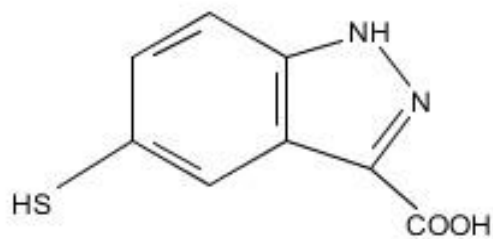
Answers per Page [20] 1 2

Display: 

☐ 1. **Bicyclic heteroaryl compounds for the treatment of cancer**
By Sun, Chung-Ming; Kuo, Min-Liang
From U.S. Pat. Appl. Publ. (2011), US 20110082143 A1 20110407. Language: English, Database: CAPLUS
The invention discloses bicyclic heteroaryl compds. I, (X1, X2, X3= C, N, where at least 2 of X1, X2, X3= N; R1, R3= H, alkyl, alkenyl, alkynyl, etc.; R2= heterocycloalkenyl, aryl, heteroaryl; R4, R5, R6, R7= H, alkyl, alkenyl, alkynyl, cycloalkyl, etc), eg. Me 2-(3,3-diphenyl-propyl)-2H-indazole-6-carboxylate. Also disclosed are the prepn. of compds. of the invention and the treatment of cancer with these compds.
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

☐ 2. **Method for manufacturing a boronic acid ester compound**
By Miki, Takashi; Shimasaki, Yasuharu; Babu, Srinivasan; Cheng, Zhigang; Reynolds, Mark E.; Tian, Qingping
From PCT Int. Appl. (2010), WO 2010110782 A1 20100930. Language: English, Database: CAPLUS
The present invention relates to a method for manufg. a boronic acid ester compd. I (Ar = substituted arom. hydrocarbon group, substituted arom. heterocyclic group; R = divalent org. group), characterized by reacting an aryl halide compd. and a diboron ester compd. in the presence of a nitrogen-contg. org. base, a nickel catalyst, a phosphine compd. and a solvent. According to the manufg. method of the present invention, even if a nickel catalyst is used as the catalyst, a desired boronic acid ester compd. can be obtained in a sufficiently high yield. Furthermore, even if anhydride or anhydride is used as a catalyst, a desired boronic acid ester compd. can be obtained in a sufficiently high yield.
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

一篇专利原文中的Claim



1. What is claimed is: 1. A compound of formula (I):

wherein

each of X1, X2, and X3, independently, is C or N, and at least two of X1, X2, and X3 are each N;
each of R1 and R3, independently, is deleted, H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocycloalkyl, heterocycloalkenyl, aryl, heteroaryl, halo, CN, NO₂, ORa, COORa, OC(O)Ra, C(O)Ra, C(O)NRaRb, C(O)N(Ra)N(Rb)C(O)Rc, NRaRb, N(Rc)SO₂NRaRb, SO₂NRaRb, or SRa, in which each of Ra, Rb, and Rc, independently, is H, alkyl, cycloalkyl, heterocycloalkyl, aryl, or heteroaryl, or Ra and Rb together with the nitrogen atom to which they are attached form heterocycloalkyl or heteroaryl;
R2 is heterocycloalkenyl, aryl, or heteroaryl;

each of R4, R5, R6, and R7, independently, is H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocycloalkyl, heterocycloalkenyl, aryl, heteroaryl, halo, CN, NO₂, ORd, COORd, OC(O)Rd, C(O)Rd, C(O)NRdRe, C(O)N(Rd)N(Re)C(O)Rf, NRdRe, N(Rf)SO₂NRdRe, SO₂NRdRe, or SRd, in which each of Rd, Re, and Rf, independently, is H, alkyl, cycloalkyl, heterocycloalkyl, aryl, or heteroaryl, or Rd and Re together with the nitrogen atom to which they are attached form heterocycloalkyl or heteroaryl.

X1, X2, X3为C、N原子，至少有两个是N原子
R1包括COOH基团，R6包括SH基团
保护了我们设计的目标化合物

提纲

■ 介绍

- SciFinder Web中的内容
- SciFinder Web特色功能
- SciFinder Web的注册和登陆

■ SciFinder Web中的检索和后处理

- SciFinder Web中的文献检索
- SciFinder Web中的物质检索
- SciFinder Web中的Markush检索
- SciFinder Web中的反应检索

■ SciFinder Web使用常见问题和网络资源

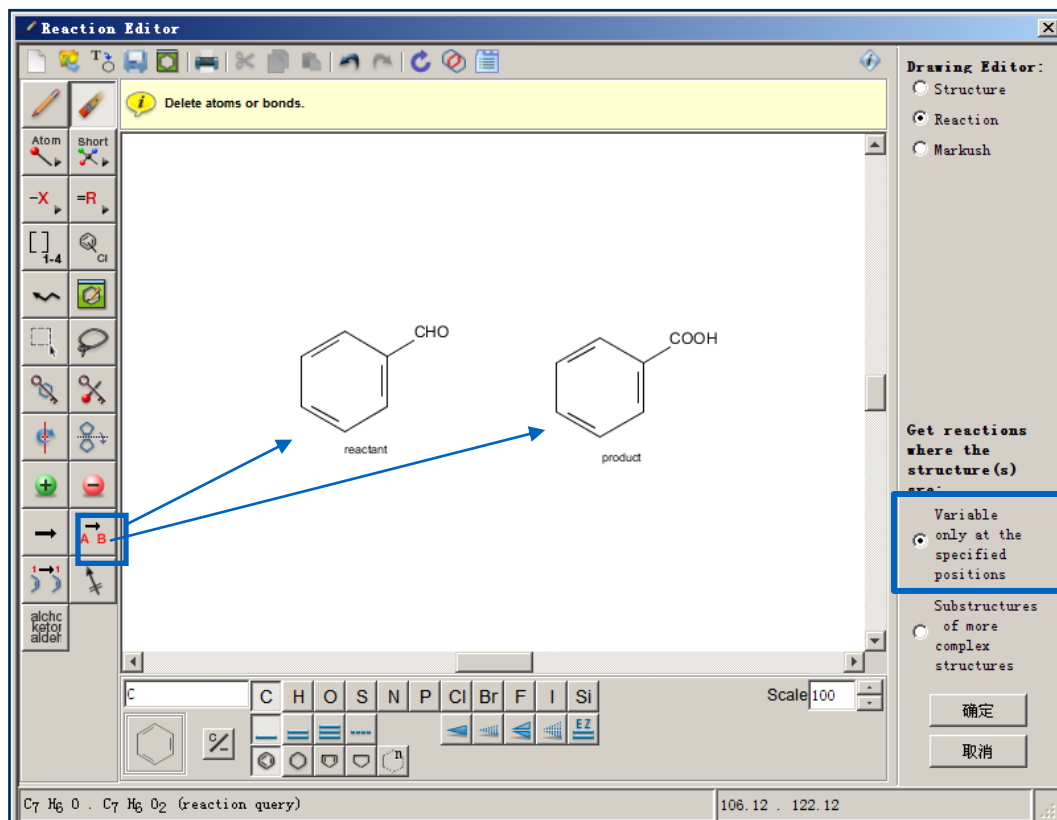
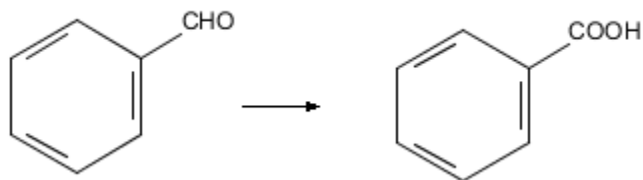
SciFinder中的反应定义工具

The screenshot shows the 'Reaction Editor' window in SciFinder. The interface includes a toolbar on the left with various chemical drawing tools, a central workspace for drawing, and a right-hand panel with 'Drawing Editor' options and search filters. Red boxes and lines highlight specific tools with Chinese labels:

- 反应箭头** (Reaction Arrow): Points to the arrow tool in the toolbar.
- 反应原子标记工具** (Reaction Atom Labeling Tool): Points to the tool that adds atom labels (A, B) to a reaction.
- 反应官能团列表** (Reaction Functional Group List): Points to the list of functional groups (aldehyde, ketone, aldol) at the bottom of the toolbar.
- 反应角色工具** (Reaction Role Tool): Points to the tool that assigns roles (e.g., reagent, catalyst) to reaction components.
- 反应位置标记工具** (Reaction Position Labeling Tool): Points to the tool that adds position labels to a reaction.

The right-hand panel includes the 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'. Below this is a section for 'Get reactions where the structure(s) are:' with options for 'Variable' (only at the specified positions) and 'Substructures' (of more complex structures). At the bottom right are '确定' (OK) and '取消' (Cancel) buttons.

反应检索—特定物质之间的反应






精确反应检索帮助获得特定物质之间的反应，点击确定

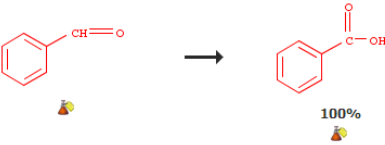
反应检索结果

Reactions [Get References](#) [Tools](#) [Send to SciPlanner](#)

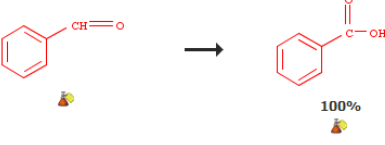
336 Reactions 0 Selected [Save](#) [Print](#) [Export](#)

Select All Deselect All Sort by: Relevance [Answers per Page \[15\]](#) 1 2 3 4 5 6 ... 23 [Display:](#)   

☐ 1. View Reaction Detail [Link](#) [Similar Reactions](#)
Single Step Hover over any structure for more options.


100% [Overview](#)




☐ 2. View Reaction Detail [Link](#) [Similar Reactions](#)
Single Step Hover over any structure for more options.


100% [Overview](#)

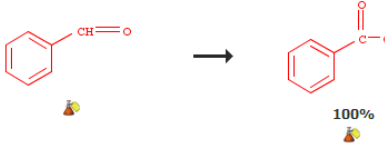
让一篇文献出现一条反应

Reactions [Get References](#) [Tools](#) [Send to SciPlanner](#)

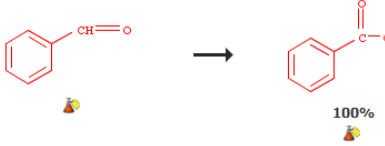
336 Reactions 0 Selected [Save](#) [Print](#) [Export](#)

Select All Deselect All Sort by: Relevance [Answers per Page \[15\]](#) 1 2 3 4 5 6 ... 17 [Display:](#)   (250 Reactions) 

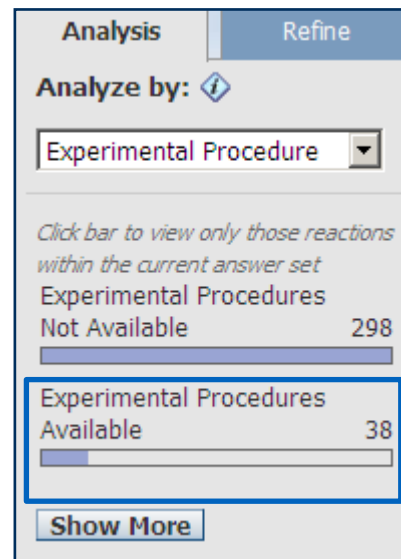
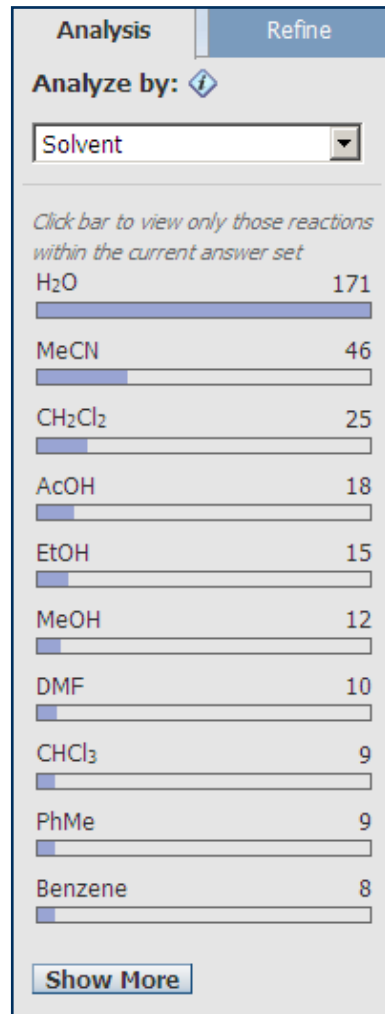
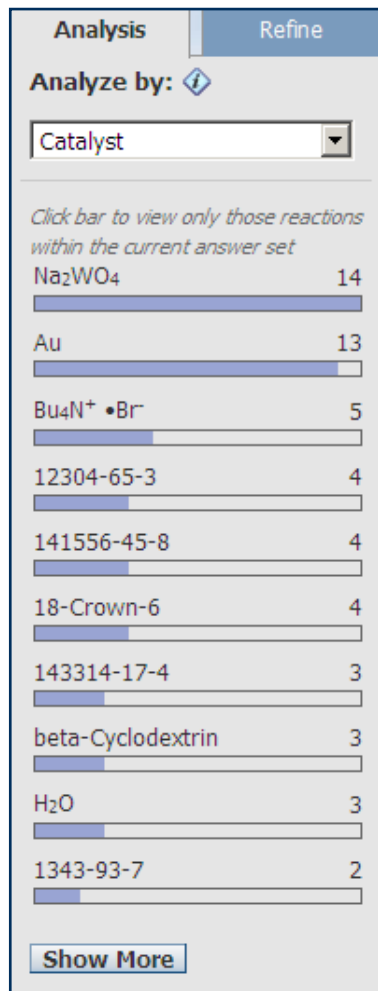
☐ 1. 1 Hits in this Reference [Similar Reactions](#)
Single Step Hover over any structure for more options.


100% [Overview](#)

☐ 2. 4 Hits in this Reference [Similar Reactions](#)
Single Step Hover over any structure for more options.


100% [Overview](#)

反应结果分析



SciFinder中可以使用
Analysis/Refine工具对反应进行
处理，这些工具的使用能让我们
更好的了解反应的信息。

获得有实验过程的反应

SciFinder®

Welcome Catherine Li | Sign Out

Reaction Structure structure variable only at spe... > reactions (336)

Reactions Get References Tools Send to SciPlanner

336 Reactions 0 Selected Save Print Export

38 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed Keep Analysis Clear Analysis

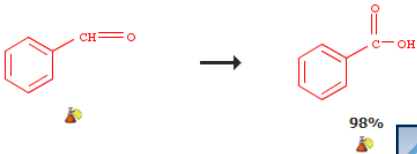
Select All Deselect All Sort by: Relevance

Answers per Page [15] 1 2 3

Display: [Icons]

☐ 5. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



► Overview

► Experimental Procedure

分析后的结果是一个预览结果，需要点击**Keep Analysis**来获得最后的结果。

SciFinder®

Welcome Catherine Li | Sign Out

Reaction Structure structure variable only at spe... > reactions (336) > keep analysis "Experimental Procedure" (38)

Reactions Get References Tools Send to SciPlanner

38 Reactions 0 Selected Save Print Export

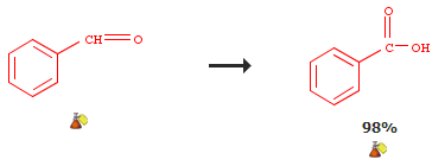
Select All Deselect All Sort by: Relevance

Answers per Page [15] 1 2 3

Display: [Icons]

☐ 1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



► Overview

► Experimental Procedure

反应信息和反应过程

Reactions Get References Tools Send to SciPlanner

38 Reactions 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3 Display:

☐ 1. View Reaction Detail Link Similar Reactions
Single Step *Hover over any structure for more options.*

► Overview

► Experimental Procedure

反应的整体概述，
每一步的溶剂，温
度，反应条件

▼ Overview

Steps/Stages	Notes
1.1 R:H ₂ O ₂ , C:1036033-11-0, S:H ₂ O, S:MeCN, 1.5 h, rt	Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1
	References Novel Michael Addition Products of Bis(amino acidato)metal(II) Complexes: Synthesis, Characterization, Dye Degradation, and Oxidation Properties Full Text By Rajalakshmi, V. et al From Inorganic Chemistry (Washington, DC, United States), 47(13), 5821-5830; 2008

反应信息和反应过程

Reactions

38 Reactions 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3

Display:

☐ 1. View Reaction Detail Link Similar Reactions

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

► Overview

► Experimental Procedure

反应实验历程
的获取

Experimental Procedure

Inorganic Chemistry

General/Typical Procedure: Catalytic Activities. Degradation of Phenol Red Dye. Complexes 1a, 2a, 3a, and 4a were used as catalysts for the degradation of PR dye in the presence of hydrogen peroxide (H_2O_2). The degradation experiments were carried out at fixed concentrations of H_2O_2 (0.01 M), complexes (0.001 M), and dye (6.0×10^{-5} M). In each degradation experiment, to a solution of 0.0034, 0.0044, 0.0037, or 0.0050 g of the catalysts 1a, 2a, 3a, or 4a, respectively, in 9.3 mL of double-distilled water was added 0.6 mL of 0.001 M dye and 0.1 mL of 0.01 M H_2O_2 , and zero-time was noted. The reaction mixture was stirred continuously, and at regular time intervals, an aliquot was withdrawn and the absorbance at 430 nm recorded. The absorbance of the dye/ H_2O_2 mixture remains constant for several hours in the absence of the catalyst. Compound No. 1a. Time 1.5 (h). product $\text{C}_6\text{H}_5\text{COOH}$. Yield 98 (%). cryst color, blue. crystal Data: space group P1. $a = 5.415(5)$ Å, $b = 7.186(5)$ Å, $c = 8.806(5)$ Å, α deg = $97.129(5)$, β deg = $100.281(5)$, γ deg = $97.274(5)$. $Z = 1$. elemental analyses (%), found C 35.72, H 4.71, N 16.62. IR (cm^{-1}) OH 3547, NH 3180, CN 2250, COO^- (asym) 1631, COO^- (sym) 1362.

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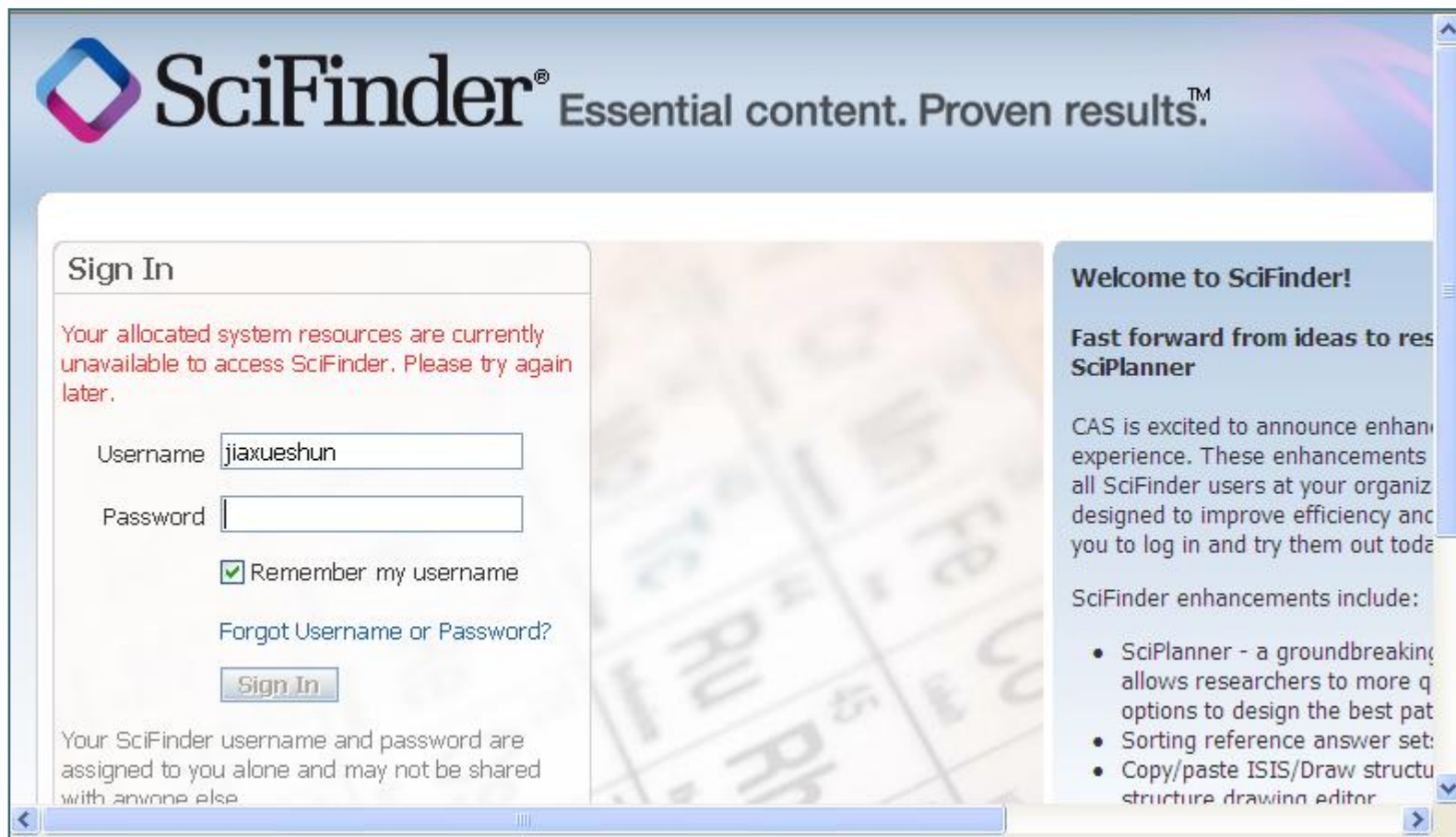
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