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SciFinder Web使用介绍

刘衍兰

SciFinder培训专员

2014.10

提纲

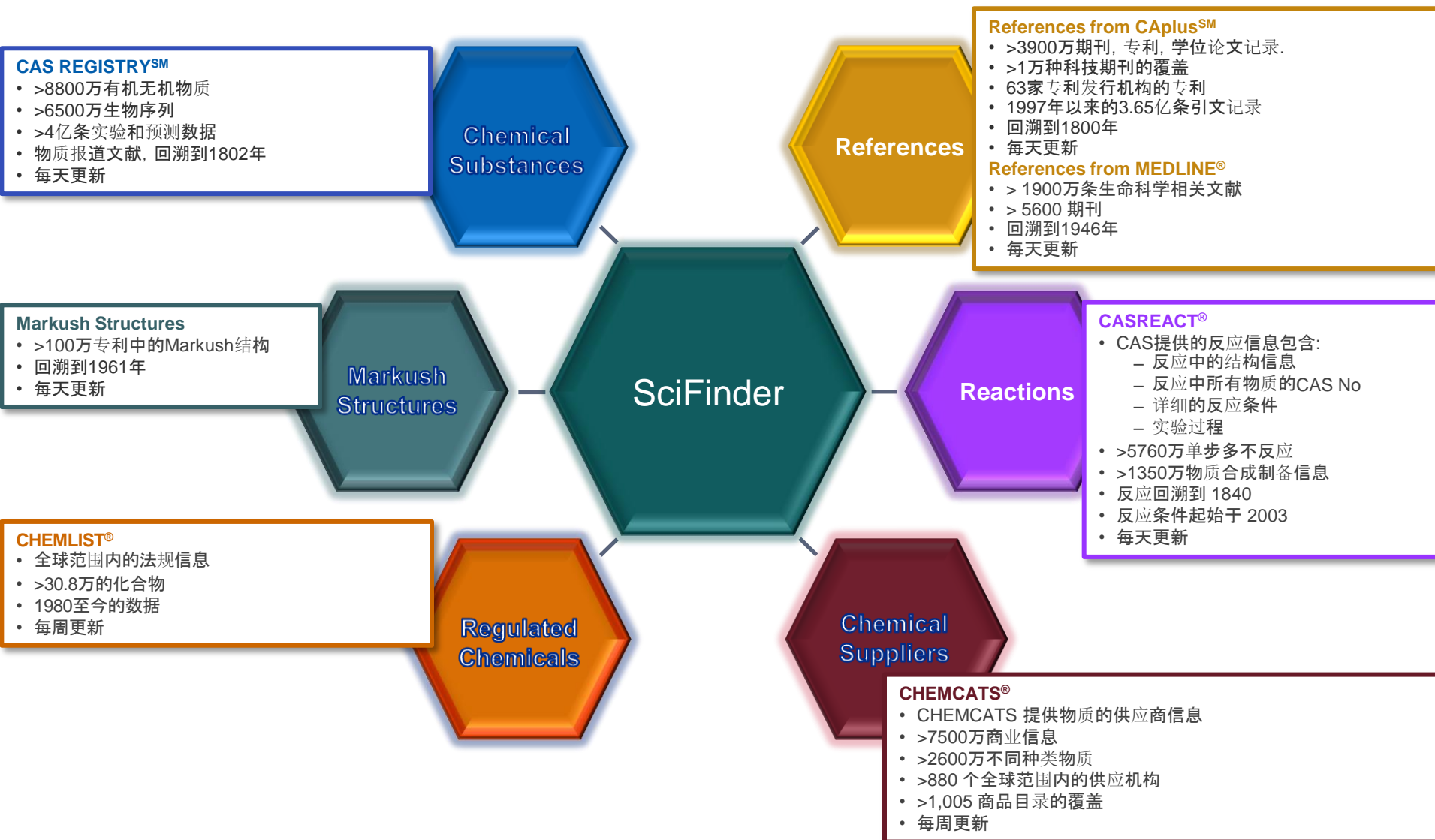
- 介绍
 - SciFinder Web中的内容
 - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索技巧
 - SciFinder Web中的反应记录及反应检索技巧
- **SciFinder Web的注册和常见问题**

美国化学文摘社—Chemical Abstract Service

- 创建于1907年
- ACS的分支机构
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- 最早创立了《化学文摘》
- 总部坐落于俄亥俄州的哥伦布市



SciFinder的覆盖内容



提纲

- 介绍
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Non-Java结构面板

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, a navigation bar contains 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar menu lists categories: REFERENCES (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (with sub-item: Reaction Structure). The 'SUBSTANCES' category is currently selected. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It features a 'Structure Editor' section with two tabs: 'Java' and 'Non-Java'. The 'Non-Java' tab is highlighted with a red rectangle. Below the tabs is a large text box that says 'Click to Edit'. To the right of the editor, there is a 'Search Type' section with three radio buttons: 'Exact Structure', 'Substructure' (which is selected), and 'Similarity'. Below this is a checkbox labeled 'Show precision analysis'. At the bottom of the main area, there is an 'Import CXF' link, a large blue 'Search' button, and a link for 'Advanced Search'.

美国专利全文PDF链接

SciFinder®

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Welcome Tony Liu

Explore Saved Searches SciPlanner

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Patent "US 20130273560 A1" > references (2)

REFERENCES

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Analyze Refine Categorize

Sort by: Accession Number

0 of 2 References Selected

Analyze by: Author Name

Cooks Robert Graham 2

Eberlin Livia Schiavinato 2

Dill Allison Lisa 1

Ferreira Christina Ramires 1

1. Analyzing a metabolite level in a sample by mass spectrometry in a nondestructive manner so that the metabolite level can be correlated to its originating source

Quick View Full Text PDF

By Cooks, Robert Graham; Kerian, Kevin Scott; Jarmusch, Alan Keith; Hamid, Ahmed Mohamed; Eberlin, Livia Schiavinato
From U.S. Pat. Appl. Publ. (2013), **US 20130273560 A1** 20131017. | Language: English, Database: CAPLUS

The invention method technique originates solvent diagnosis

(19) United States

(12) Patent Application Publication

Cooks et al.

(10) Pub. No.: US 2013/0273560 A1

(43) Pub. Date: Oct. 17, 2013

(54) ANALYZING A METABOLITE LEVEL IN A SAMPLE

(60) Provisional application No. 61/487,363, filed on May 18, 2011, provisional application No. 61/791,100, filed on Mar. 15, 2013, provisional application No. 61/778,292, filed on Mar. 12, 2013.

(71) Applicant: Purdue Research Foundation, West Lafayette, IN (US)

(72) Inventors: Robert Graham Cooks, West Lafayette, IN (US); Kevin Scott Kerian, Lafayette, IN (US); Alan Keith Jarmusch, Lafayette, IN (US); Ahmed Mohamed Hamid, West Lafayette, IN (US); Livia Schiavinato Eberlin, Lafayette, IN (US)

(21) Appl. No.: 13/909,619

(22) Filed: Jun. 4, 2013

Related U.S. Application Data

(63) Continuation-in-part of application No. 13/475,305, filed on May 18, 2012.

Publication Classification

(51) Int. Cl. G01N 27/62 (2006.01)

(52) U.S. Cl. CPC G01N 27/62 (2013.01) USPC 435/7.1; 435/40.52

(57) ABSTRACT

The invention generally relates to methods for analyzing a metabolite level in a sample. In certain embodiments, methods of the invention may involve obtaining a sample, analyzing the sample using a mass spectrometry technique to determine a level of at least one metabolite in the sample, and correlating the metabolite level with an originating source of the sample, thereby analyzing the sample.

1998-至今的美国
专利全文

CAS is a division of the American Chemical Society.

SciFinder和ChemDraw整合

The image illustrates the integration between ChemBioDraw Ultra and SciFinder. On the left, the ChemBioDraw Ultra window shows the chemical structure of Canagliflozin. A SciFinder search dialog is open, allowing for a Substance Search or Reaction Search. The SciFinder results window displays the chemical structure of Canagliflozin and its properties, including the molecular formula $C_{28}H_{35}F_{10}O_{15}S$ and the name Canagliflozin.

提纲

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 - SciFinder Web中的内容
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- **SciFinder Web的注册和常见问题**

SciFinder中的文献记录

REFERENCE DETAIL ?	Get Substances	Get Related Citations	Get Full Text	Send to SciPlanner
Return				Previous Next
1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials By: Cavani, F.; Trifiro, F. A review, with 202 refs., on the selective oxidn. of light (C ₂₋₆) alkanes to bulk and industrial chems., with emphasis on catalyst-gas phase interactions. Attention was given mainly to: (1) the role of the redox properties of transition metal oxide-based systems, and (2) the contribution of radical-type, homogeneous and heterogeneously-initiated homogeneous reactions over nonreducible metal oxide and noble metal catalysts. Other topics included: (1) key factors in selective oxidn. of light alkanes, (2) bulk and surface properties of catalysts, (3) oxidative dehydrogenation, (4) control of oxygen supply to the catalyst, (5) non-redox-type metal oxides (e.g., alk. earth oxides, rare earth oxides, boron oxides, tin oxides, and silica). Some research examples are: (1) oxidn. of propane to acrylic acid and isobutane to methacrylic acid over Keggin-type heteropolymolybdates, (2) oxidative dehydrogenation of alkanes to alkenes over vanadium oxide-based catalysts, and (3) oxidn. of butane and pentane over vanadyl pyrophosphate.				
Indexing Fossil Fuels, Derivatives, and Related Products (Section51-0) Section cross-reference(s): 35, 45				
Concepts Redox reaction catalysts catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems. Alkaline earth oxides Rare earth oxides catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems. Catalyst use; Properties; Uses				
Substances 12026-66-3 58834-75-6 catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems. Catalyst use; Uses 1303-86-2 Boron oxide, uses 1332-29-2 Tin oxide 7631-86-9 Silica, uses				
QUICK LINKS 0 Tags, 0 Comments SOURCE <i>Catalysis Today</i> Volume51 Issue3-4 Pages561-580 Journal; General Review 1999 CODEN:CATTEA ISSN:0920-5861 DOI:10.1016/S0920-5861(99)00041-3 COMPANY/ORGANIZATION Dipartimento di Chimica Industriale e dei Materiali Bologna, Italy 40136 ACCESSION NUMBER 1999:340014 CAN131:159478 CAPLUS PUBLISHER Elsevier Science B.V.				

Citations

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 Lee, J; Catal Rev-Sci Eng 1988, 30, 249
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 Trifiro, F; Oxidative dehydrogenation and alternative dehydrogenation processes 1993
 Cavani, F; Catal Today 1995, 24, 307

一篇完整的文献界面包括:

1. 题录信息
2. 摘要信息
3. 文献中重要的概念
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质, 反应, 引文等
7. 文献中的引文信息

SciFinder中的文献检索方法

- 功能方面


- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 从物质，反应获得文献

- 检索方法推荐

- 关注某特定领域的文献——主题检索
- 关注物质有关的文献——先获得物质，再获得文献
- 关注某科研人员的文献——作者名检索

SciFinder Web中的主题检索

主题： VEGFR inhibitor with anticancer(VEGFR抑制剂在抗肿瘤方面的研究进展)



The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is visible. Below it, a navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows the search results for the topic 'VEGFR Inhibitor with anticancer', indicating 618 references. On the left, a sidebar lists various search criteria under 'REFERENCES' and 'SUBSTANCES'. The 'REFERENCES' section is currently selected, showing a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags, and Substances. The 'SUBSTANCES' section lists: Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The main search area shows the search term 'VEGFR inhibitor with anticancer' entered into a search box. Below the search box, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is prominently displayed. Below the search button, there is a link to 'Advanced Search'.

Research Topic "VEGFR Inhibitor with anticancer..." > references (618)

REFERENCES

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

SUBSTANCES

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

REFERENCES: RESEARCH TOPIC

VEGFR inhibitor with anticancer

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

Search

[Advanced Search](#)

使用介词 (of, with, in)
来连接关键词

主题检索的候选项

[Explore ▼](#)
[Saved Searches ▼](#)
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Research Topic "VEGFR inhibitor with anticanc..."

REFERENCES ?

[Select All](#)
[Deselect All](#)

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 6 references were found containing <u>"VEGFR inhibitor with anticancer" as entered.</u>	6
<input checked="" type="checkbox"/> 618 references were found containing the two concepts <u>"VEGFR inhibitor" and "anticancer" closely associated with one another.</u>	618
<input type="checkbox"/> 2888 references were found where the two concepts <u>"VEGFR inhibitor" and "anticancer" were present anywhere in the reference.</u>	2888
<input type="checkbox"/> 5255 references were found containing the concept <u>"VEGFR inhibitor".</u>	5255
<input type="checkbox"/> 1001993 references were found containing the concept "anticancer".	1001993

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- ◆ “as entered” 表示完全匹配
- ◆ “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
- ◆ “present anywhere in the reference” 表示同时出现在一段话中

SciFinder 中的文献检索结果及后处理

文献分析、
限定工具 系统分类工具

Research Topic "VEGFR inhibitor with anticanc..." > **references (618)**

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Analyze by: ?

Author Name

Ciardiello Fortunato	15
Troiani Teresa	11
Myers Jeffrey N	9
Fontanini Gabriella	8
Jiang Yuyang	8
Tan Chunyan	8
Tan Yuting	8
Tortora Giampaolo	8
Zhang Shixi	8

- Evidence for G-quadruplex in the promoter of *vegfr-2* and its targeting to inhibit tumor angiogenesis**
 Quick View Full Text
 By Salvati, Erica; Zizza, Pasquale; Rizzo, Angela; Iachettini, Sara; Cingolani, Chiara; D'Angelo, Carmen; Porru, Manuela; Randazzo, Antonio; Pagano, Bruno; Novellino, Ettore; et al
 From Nucleic Acids Research (2014), 42(5), 2945-2957. | Language: English, Database: CAPLUS

Tumor angiogenesis is mainly mediated by vascular endothelial growth factor (VEGF), a pro-angiogenic factor produced by **cancer** cells and active on the endothelium through the VEGF receptor 2 (**VEGFR-2**). Here we identify a G-rich sequence within the proximal promoter region of **vegfr-2**, able to form an antiparallel G-quadruplex (G4) structure. This G4 structure can be efficiently stabilized by small mols. with the consequent **inhibition** of **vegfr-2** expression. Functionally, the G4-mediated redn. of **VEGFR-2** protein causes a switching off of signaling components that, converging on actin cytoskele...
- Icrucumab, a fully human monoclonal antibody against the vascular endothelial growth factor receptor-1, in the treatment of patients with advanced solid malignancies: a Phase 1 study**
 Quick View Full Text
 By Lo Russo, Patricia M.; Krishnamurthi, Smitha; Youssoufian, Hagop; Hall, Nancy; Fox, Floyd; Dontabhaktuni, Aruna; Grebennik, Dmitri; Remick, Scot
 From Investigational New Drugs (2014), 32(2), 303-311. | Language: English, Database: CAPLUS

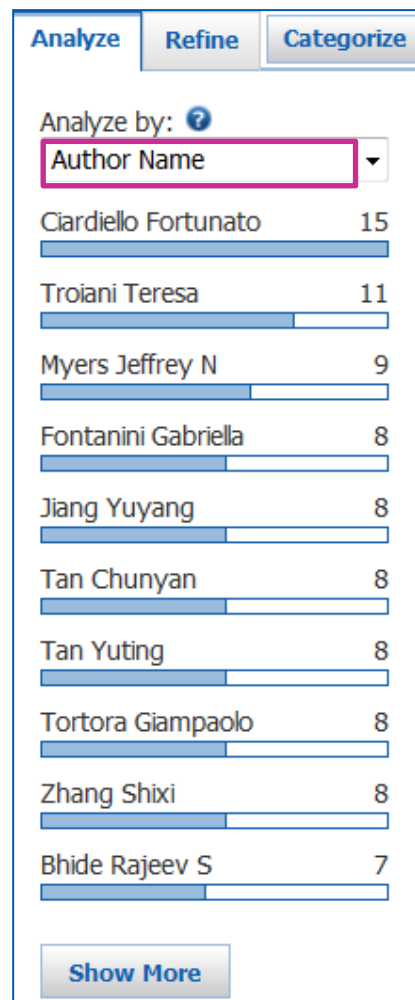
Background IMC-18F1 (icrucumab), a human monoclonal antibody against vascular endothelial growth factor receptor-1 (**VEGFR-1**), potently **inhibits** ligand-dependent phosphorylation of **VEGFR-1** and downstream signaling, making icrucumab an attractive candidate for **antitumor** activity. Objectives The primary objective was to det. the safety profile and max. tolerated dose of icrucumab in patients with advanced solid **tumors** that were previously unresponsive to std. therapy or for which no std. therapy was available. Methods In this open-label, dose-escalation, Phase 1 study, patients received icrucum...

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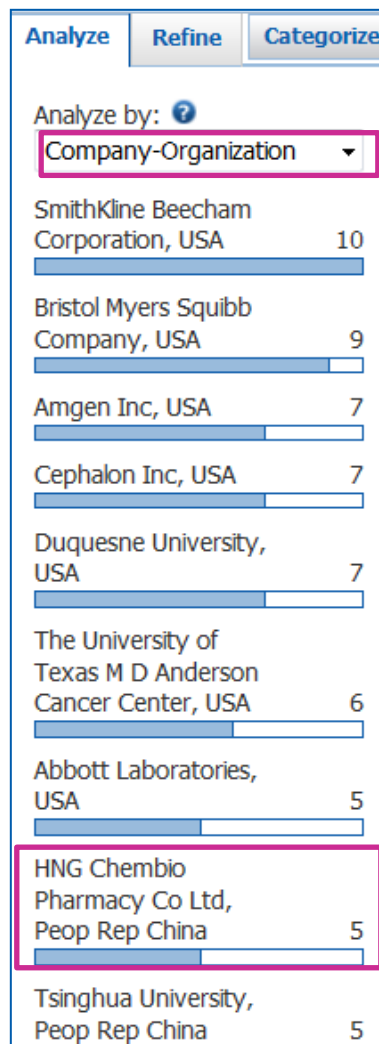
CAS is a division of the American Chemical Society.

SciFinder中的Analyze

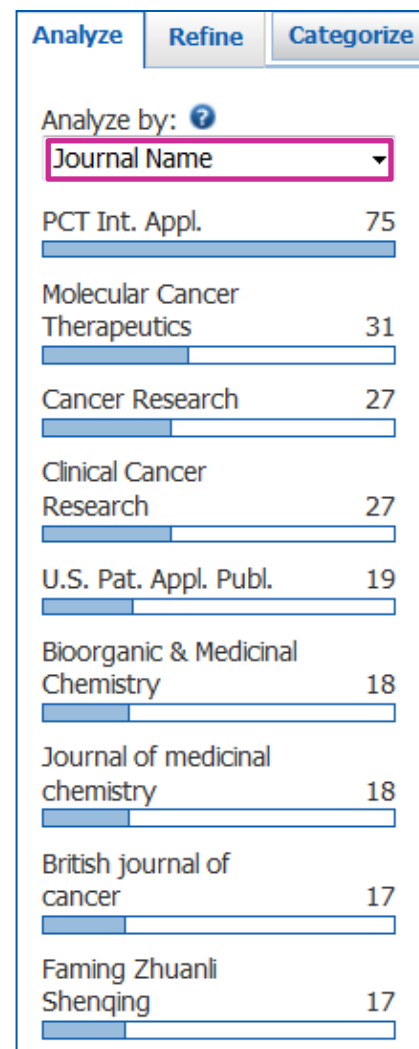
领域内主要研究人员，专家



主要研究机构，合作伙伴，竞争对手

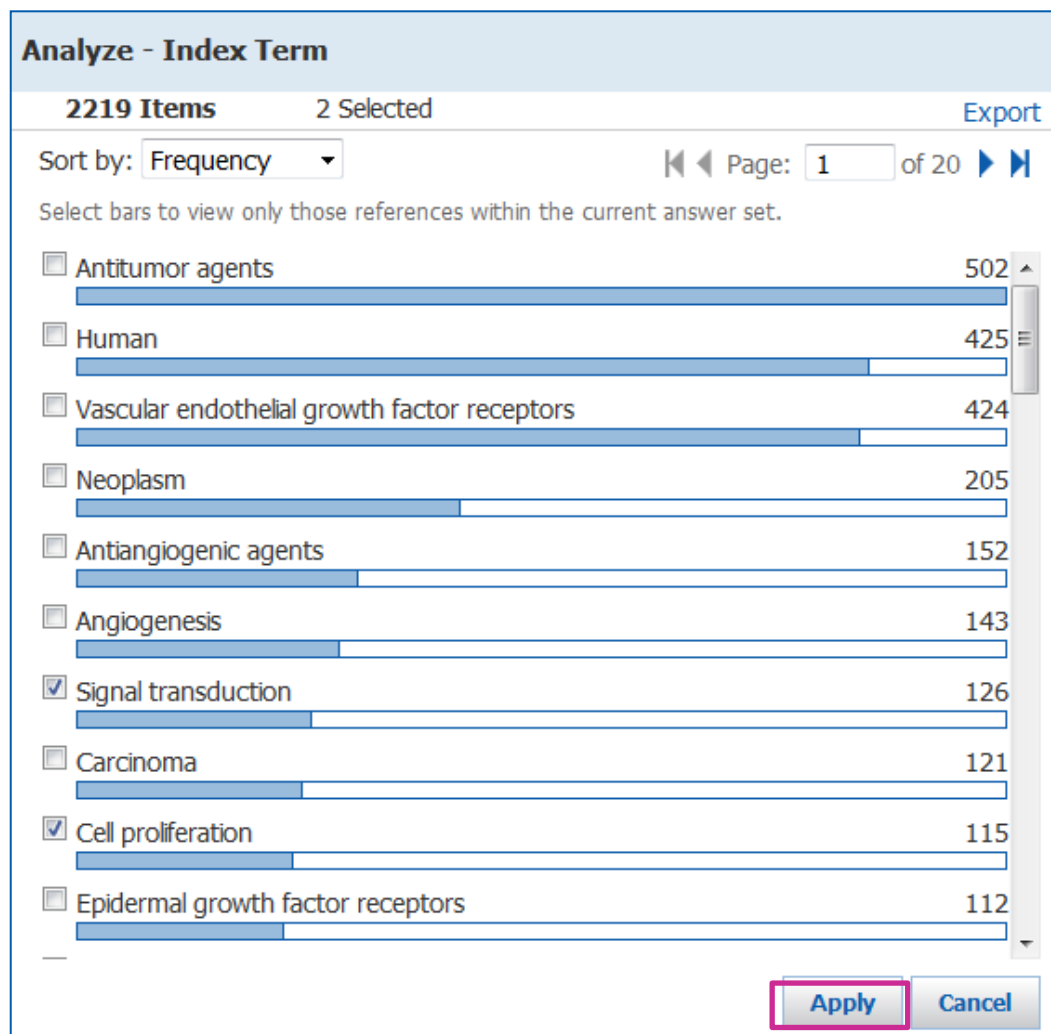
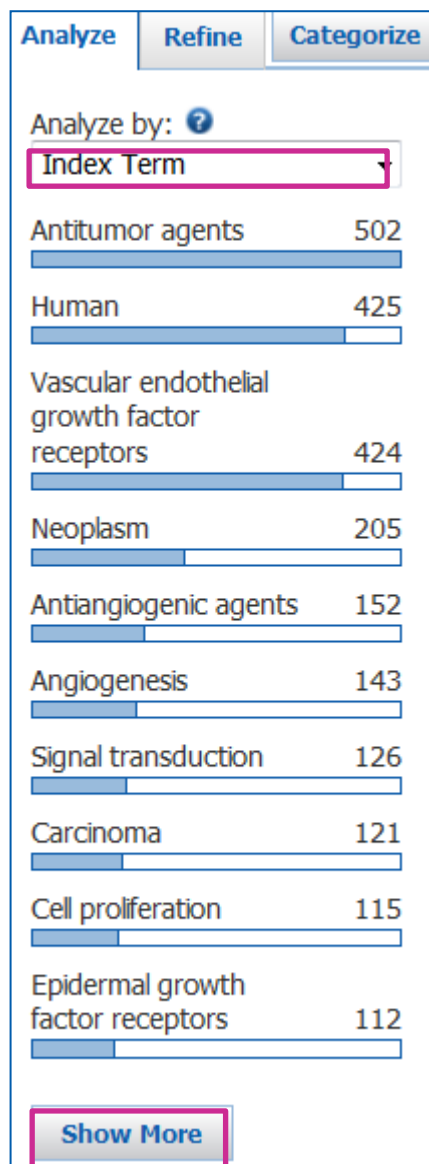


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索引词 (Index Term)：可以帮助我们大致了解文献的内容



SciFinder中的Refine

文献类型限定：获得最新综述类文献

Analyze
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Refine by: ?

- Research Topic
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- Document Type**
- Publication Year
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Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review**

Refine

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Page: 1 of 6

- VEGF Signal System: The Application of Antiangiogenesis**
[Quick View](#) [Full Text](#)
 By Liang, Xuewu; Xu, Fuming; Li, Xiaoguang; Ma, Chunhua; Zhang, Yingjie; Xu, Wenfang
 From Current Medicinal Chemistry (2014), 21(7), 894-910. | Language: English, Database: CAPLUS

A review. Among the numerous endogenous promoters of angiogenesis, vascular endothelial growth factor (VEGF) plays a leading role in angiogenesis, which has huge impact on proliferation, survival, migration and permeability of **tumor** cells. VEGF signal system also becomes remarkable **anticancer** targets, including VEGF, vascular endothelial growth factor receptor (**VEGFR**), and VEGF downstream signal pathways. So far, there has been many clin. or approved **anticancer** drugs that directly or indirectly interfere with VEGF signal system applied in the treatment of various **tumors** and other diseases as...
- Clinical Pharmacology of Axitinib**
[Quick View](#) [Full Text](#)
 By Chen, Ying; Tortorici, Michael A.; Garrett, May; Hee, Brian; Klamers, Karen J.; Pithavala, Yazdi K.
 From Clinical Pharmacokinetics (2013), 52(9), 713-725. | Language: English, Database: CAPLUS

A review. Axitinib is a potent and selective second-generation **inhibitor** of vascular endothelial growth factor receptors 1, 2, and 3 that is approved in the US and several other countries for treatment of patients with advanced renal cell **carcinoma** after failure of one prior systemic therapy. The recommended clin. starting dose of axitinib is 5 mg twice daily, taken with or without food. Dose increase (up to a max. of 10 mg twice daily) or redn. is permitted based on individual tolerability. Axitinib pharmacokinetics are dose-proportional within 1-20 mg twice daily, which includes the clin...
- BIBF 1120/nintedanib: a new triple angiokinase inhibitor-directed therapy in patients with non-small cell lung cancer**
[Quick View](#) [Full Text](#)
 By Rolfo, Christian; Raez, Luis E.; Bronte, Giuseppe; Santos, Edgardo S.; Papadimitriou, Kostantinos; Buffoni, Lucio; van Meerbeeck, Jan P.; Russo, Antonio
 From Expert Opinion on Investigational Drugs (2013), 22(8), 1081-1088. | Language: English, Database: CAPLUS

A review. Introduction: Several new targeted agents with **anti**-angiogenic properties have been developed recently, including vandetanib, sunitinib, sorafenib, bevacizumab and others. **Tumor** development, progression, metastasis are strongly linked to angiogenesis. Targeted agents like bevacizumab, a monoclonal antibody which targets VEGF, have been fully developed in several solid **tumors**. These new agents strongly advocate that targeting angiogenesis is one of the best approaches for **cancer** therapy. Areas covered: Those agents that target addnl. pro-angiogenic intracellular signaling pathways...

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Fontanini Gabriella	8
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Tan Chunyan	8
Tan Yuting	8
Tortora Giampaolo	8
Zhang Shixi	8
Bhide Rajeev S	7

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Quick View Full Text

By Salvati, Erica; Zizza, Pasquale; Rizzo, Angela; Iachettini, Sara; Cingolani, Chiara; D'Angelo, Carmen; Porru, Manuela; Randazzo, Antonio; Pagano, Bruno; Novellino, Ettore; et al
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2. Icrucumab, a fully human monoclonal antibody against the vascular endothelial growth factor receptor-1, in the treatment of patients with advanced solid malignancies: a Phase 1 study

Quick View Full Text

By Lo Russo, Patricia M.; Krishnamurthi, Smitha; Youssoufian, Hagop; Hall, Nancy; Fox, Floyd; Dontabhaktuni, Aruna; Grebennik, Dmitri; Remick, Scot
From Investigational New Drugs (2014), 32(2), 303-311. | Language: English, Database: CAPLUS

Background IMC-18F1 (icrucumab), a human monoclonal antibody against vascular endothelial growth factor receptor-1 (**VEGFR-1**), potentially **inhibits** ligand-dependent phosphorylation of **VEGFR-1** and downstream signaling, making icrucumab an attractive candidate for **antitumor** activity. Objectives The primary objective was to det. the safety profile and max. tolerated dose of icrucumab in patients with advanced solid **tumors** that were previously unresponsive to std. therapy or for which no std. therapy was available. Methods In this open-label, dose-escalation, Phase 1 study, patients received icrucum...

3. Use of neural stem cells for treatment of malignancy using a biocompatible adhesive at the post-surgical site to **inhibit** angiogenesis

Quick View Full Text PDF

By Crawford, Susan E.

Categorize系统分类功能，基于Index Term，对文献依学科方向进行分类

SciFinder中的Categorize

一级目录

二级目录

和二级目录相关的
Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in medicine (8704)
General chemistry	Medicine (323)
Biotechnology	Substances in biological uses (1035)
Synthetic chemistry	Substances in adverse effects (165)
Genetics & protein chemistry	Toxicology & forensics (23)
Biology	Agriculture (22)
Physical chemistry	Food (6)
Polymer chemistry	
Analytical chemistry	
Technology	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	
Page: 1 of 88	
Select All Deselect All	
<input type="checkbox"/> ZD6474	54
<input checked="" type="checkbox"/> Sorafenib	46
<input type="checkbox"/> Antitumor agents	36
<input type="checkbox"/> Antibodies and Immunoglobulins	34
<input type="checkbox"/> Bevacizumab	33
<input checked="" type="checkbox"/> Paclitaxel	33
<input type="checkbox"/> Sunitinib	33
<input type="checkbox"/> Gefitinib	28
<input type="checkbox"/> Vascular endothelial growth factor receptors	27
<input type="checkbox"/> Erlotinib	22
<input type="checkbox"/> 5-Fluorouracil	21
<input type="checkbox"/> Cetuximab	21
<input type="checkbox"/> Cisplatin	21
<input type="checkbox"/> Carboplatin	20

Selected Terms

Click 'x' to remove the category from 'Selected Terms'

☒ Biotechnology > Substances in medicine (2 Terms)

索拉菲尼
紫杉醇

Biotechnology > Substances in medicine > 2 Index Term(s) Selected

OK

Cancel

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 Get Reactions
 Get Related Citations
 Get Full Text
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Sort by: Citing References
 NEW Display Options

0 of 485 References Selected
 Page: 1 of 25

1. Stability of food allergens to digestion in vitro

Quick View Full Text

By Astwood, James D.; Leach, John N.; Fuchs, Roy L.
 From Nature Biotechnology (1996), 14(10), 1269-1273. | Language: English, Database: CAPLUS

An integral part of the **safety** assessment of **genetically modified** plants is consideration of possible human health effects, esp. **food** allergy. Prospective testing for allergenicity of proteins obtained from sources with no prior history of causing allergy has been difficult because of the absence of valid methods and models. **Food** allergens may share physicochem. properties that distinguish them from nonallergens, properties that may be used as a tool to predict the inherent allergenicity of proteins newly introduced into the **food** supply by **genetic** engineering. One candidate property is stab...

2. The feeding value of soybeans fed to rats, chickens, catfish and dairy cattle is not altered by genetic incorporation of glyphosate tolerance

Quick View Full Text

By Hammond, Bruce G.; Vicini, John L.; Hartnell, Gary F.; Naylor, Mark W.; Knight, Christopher D.; Robinson, Edwin H.; Fuchs, Roy L.; Padgett, Stephen R.
 From Journal of Nutrition (1996), 126(3), 717-27. | Language: English, Database: CAPLUS

Animal **feeding** studies were conducted with rats, broiler chickens, catfish, and dairy cattle to determine the **feeding** value of **genetically modified** to tolerate in-season application of glyphosate. The **feeding** value of glyphosate-tolerant soybeans (GTS) to the **feeding** value of the parent soybeans was compared. The **feeding** value of GTS was not significantly different from the diets at the same concns. as used com.; dairy cows were fed 10 g/

Create Keep Me Posted Profile

Title: * 题目

Description:

Characters Remaining: 1024

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Expires On: Mar 07, 2015 Change

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Search:

Explore references by research topic: Genetically Modified Food with safety

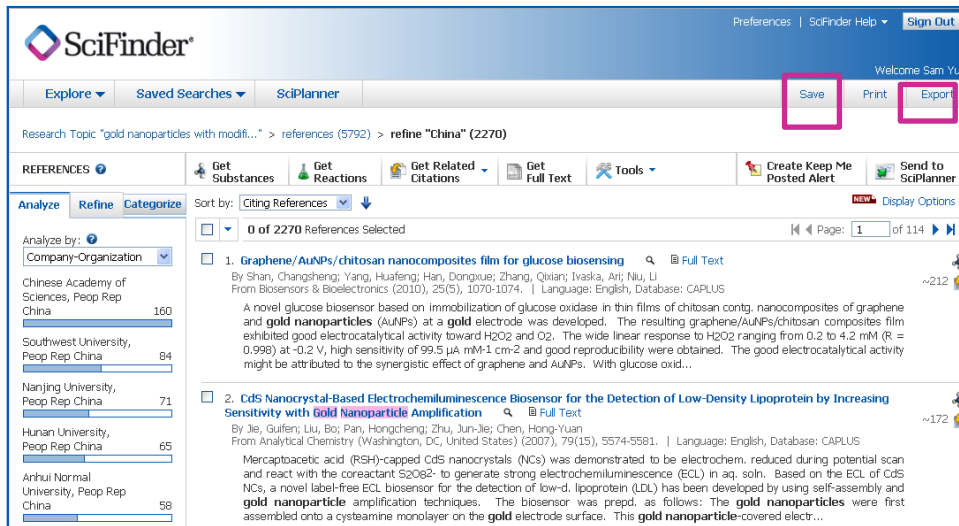
Candidates Selected:

References which contain the two concepts "Genetically Modified Food" and "safety" closely associated with one another

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Research Topic "gold nanoparticles with modifi..." > references (5792) > refine "China" (2270)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Citing References

0 of 2270 References Selected

1. Graphene/AuNPs/chitosan nanocomposites film for glucose biosensing
 By Shan, Changsheng; Yang, Huiqiong; Han, Dongxue; Zhang, Qian; Ivaska, Art; Niu, Li
 From Biosensors & Bioelectronics (2010), 25(5), 1070-1074. | Language: English, Database: CAPLUS
 ~212

2. CdS Nanocrystal-Based Electrochemiluminescence Biosensor for the Detection of Low-Density Lipoprotein by Increasing Sensitivity with Gold Nanoparticle Amplification
 By Jie, Guifeng; Liu, Bo; Pan, Hongcheng; Zhu, Jun-Jie; Chen, Hong-Yuan
 From Analytical Chemistry (Washington, DC, United States) (2007), 79(15), 5574-5581. | Language: English, Database: CAPLUS
 ~172

Export:

Citation manager: 保存成RIS格式，用于导入EndNote等文献管理工具

Offline Review: 保存过成PDF，RTF格式，用于脱机浏览

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☐ Only selected answers

Title: *

Description:

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* Required

Export:

☒ All

☐ Selected

☐ Range

Example: 2-20

For:

Citation Manager

☒ Citation export format (*.ris)

☐ Quoted Format (*.bt)

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Offline review

☐ Portable Document Format (*.pdf)

☐ Rich Text Format (*.rtf)

☐ Answer Keys (*.bt)

Saving locally

☐ Answer Key eXchange (*.alox)

Details:

File Name: *

Reference_06_26_2012_150931

Export Cancel

SciFinder主题检索小结

- ◆ 关键词的选择以及关键词用介词连接
- ◆ 候选项选择含有**concept**和**closed associated with** 的选项
- ◆ 使用**citing reference**排序可以获得被引用次数最多的文献
- ◆ 使用**KMP**功能跟踪科研进展
- ◆ 使用**Analyze, Refine**和**categorize**进行后处理
- ◆ 结果集的保存

提纲

- 介绍
 - SciFinder Web中的内容
 - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索技巧
 - SciFinder Web中的反应记录及反应检索技巧
- **SciFinder Web的注册和常见问题**

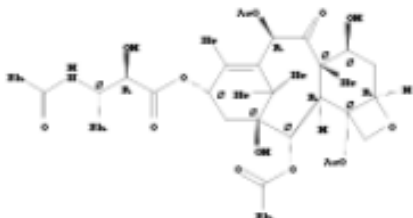
SciFinder中的物质结果界面

1.

33069-62-4

~29338

~189



Absolute stereochemistry., Rotation (-).

C47 H51 N O14

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

[Regulatory Information](#)

[Spectra](#)

[Experimental Properties](#)

紫杉醇的物质检索结果

一个完整的物质结果界面包含：

- 物质详情连接
- 文献连接
- 反应连接
- 商品信息连接
- 管制品信息连接
- 谱图连接
- 实验性质连接

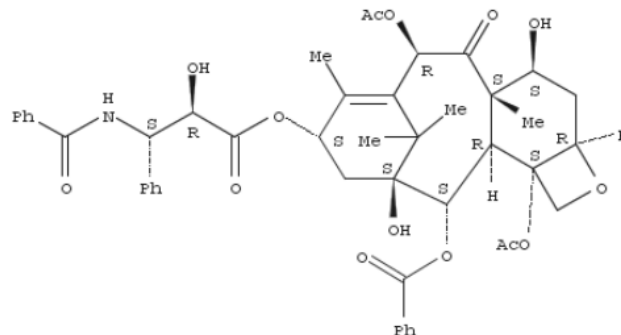
Substance Detail—查看物质详细信息

CAS Registry Number: 33069-62-4

C47 H51 N O14

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

Benzenepropanoic acid, β -(benzoylamino)- α -hydroxy-, 6,12-bis(acetyloxy)-12-(benzoyloxy)-2*a*,3,4,4*a*,5,6,9,10,11,12,12*a*,12*b*-dodecahydro-4,11-dihydroxy-4*a*,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, [2*a*,[2*a*,4*\beta*,4*a*, β ,6*\beta*,9*a*(*a*,*R**, β ,*S**),11*a*,12*a*,12*a*,12*b**a*]]-; Tax-11-en-9-one, 5*\beta*,20-epoxy-1,2*a*,4,7*\beta*,10*\beta*,13*a*-hexahydroxy-, 4,10-diacetate 2-benzoate 13-ester with (2*R*,3*S*)-*N*-benzoyl-3-phenylisoserine (8*CI*); 7,11-Methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxete, benzenepropanoic acid deriv.; (-)-Paclitaxel; 5*\beta*,20-



物质的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	✓	✓	✓	✓

生物活性和靶点信息

▼ Bioactivity Indicators	
	References
Antidiabetic agents	143
Antifibrotic agents	67
Anti-infective agents (all) >>> Antibacterial agents	155
Anti-infective agents (all) >> Antibiotics	862
Anti-infective agents (all) >>> Anti-HIV agents	94
Anti-infective agents (all) > Anti-infective agents	94
Anti-infective agents (all) >> Antimicrobial agents	122
Anti-infective agents (all) >>> Antiviral agents	367
Anti-infective agents (all) >> Fungicides	193
Anti-inflammatory agents (all) > Antiarthritics	148
Anti-inflammatory agents (all) > Anti-inflammatory agents	830
Anti-inflammatory agents (all) > Antirheumatic agents	200
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory drugs	133
Antiproliferative agents (all) > Antimitotic agents	164
Antiproliferative agents (all) > Antiproliferative agents	501
Antitumor agents (all) > Alkylating agents, biological	644
Antitumor agents (all) > Antiangiogenic agents	1027
Antitumor agents (all) > Antitumor agents	15182

▼ Target Indicators	
	References
Agglutinins and Lectins (all) > Galectins	10
Albuminoids (all) > Fibrins	36
Apoptosis-regulating proteins (all) > Apoptosis-inducing factors	13
Apoptosis-regulating proteins (all) > Apoptosis-regulating proteins	52
Apoptosis-regulating proteins (all) > Bad proteins	41
Apoptosis-regulating proteins (all) > Bak proteins	27
Apoptosis-regulating proteins (all) > Bax proteins	280
Apoptosis-regulating proteins (all) > Bcl-2 proteins	548
Apoptosis-regulating proteins (all) > Bcl-x proteins	180
Apoptosis-regulating proteins (all) >> Inhibitor of apoptosis proteins	108
Basigins	12
Bid proteins	35
Bim proteins	28
Blood-coagulation factors (all) > Blood-coagulation factor III	12
Blood-coagulation factors (all) > Fibrinogens	21

Substance Detail—查看物质详细信息

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

[Top](#)

Biological Properties	Value	Condition	Note
Bioconcentration Factor	591	pH 1 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 2 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 3 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 4 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 5 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 6 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 7 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 8 Temp: 25 °C	(34)
Bioconcentration Factor	590	pH 9 Temp: 25 °C	(34)
Bioconcentration Factor	582	pH 10 Temp: 25 °C	(34)

[Top](#)

Chemical Properties	Value	Condition	Note
Koc	3350	pH 1 Temp: 25 °C	(34)
Koc	3350	pH 2 Temp: 25 °C	(34)
Koc	3350	pH 3 Temp: 25 °C	(34)
Koc	3350	pH 4 Temp: 25 °C	(34)

Density Properties	Value	Condition	Note
Density	1.39±0.1 g/cm ³	Temp: 20 °C Press: 760 Torr	(34)
Molar Volume	610.5±5.0 cm ³ /mol	Temp: 20 °C Press: 760 Torr	(34)

Lipinski and Related Properties	Value	Condition	Note
Freely Rotatable Bonds	17		(34)
H Acceptors	15		(34)
H Donors	4		(34)
H Donor/Acceptor Sum	19		(34)
logP	3.950±0.808	Temp: 25 °C	(34)
Molecular Weight	853.91		(34)

Substance Detail—查看物质详细信息

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

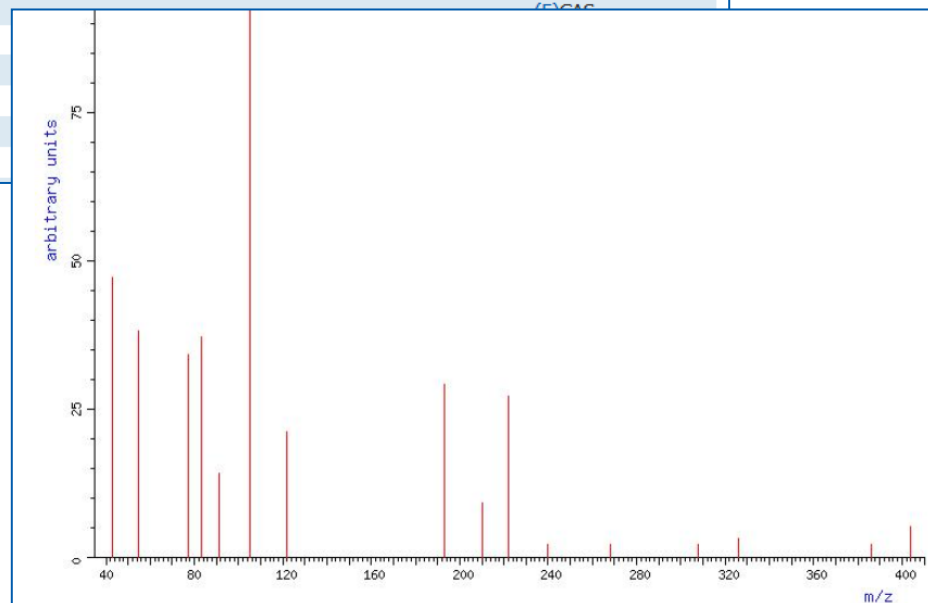
Biological Properties	Value	Condition	Note	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 72	(1)CAS	
Half-Life (Biological)	See full text	1 of 37	(7)CAS	
LC50	See full text	1 of 2	(8)CAS	
LD50	See full text		(9)CAS	
Median Lethal Dose(LD50)	8.3 mg/kg	Organism: rat Route: intravenous	(14)CAS	

Chemical Properties	Value	Condition	Note	Top
logD	See full text		(10)CAS	
logP	See full text	1 of 3	(11)CAS	
Potential of Electrode Reaction	See full text		(28)CAS	
Solubility	See full text	1 of 18	(30)CAS	

Lipinski and Related Properties	Value	Condition	Note	Top
logP	See full text	1 of 3	(11)CAS	

Optical and Scattering Properties	Value	Condition	Note	Top
Optical Rotatory Power	-48.4 °	Conc: 0.5 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm	(26)CAS	
Optical Rotatory Power	-49 °	Solv: methanol (67-56-1); Wavlen: 589.3 nm; Temp: 20 °C	(20)APC	
Optical Rotatory Power	-49 °	Solv: methanol (67-56-1); Wavlen: 589.3 nm; Temp: 20 °C	(21)NLM	
Optical Rotatory Power	-50 °	Conc: 1.0 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3	(23)CAS	

Spectra Properties				Top
Carbon-13 NMR Spectrum	See full text	1 of 5	(3)CAS	
IR Absorption Spectrum	See full text	1 of 6	(3)CAS	
Mass Spectrum	See spectrum		(12)WSS	
Mass Spectrum	See full text	1 of 20	(13)CAS	
Phosphorus-31 NMR Spectrum	See full text		(27)CAS	
Proton NMR Spectrum	See full text	1 of 12	(17)CAS	
Raman Spectrum	See full text	1 of 2	(29)CAS	
Two-Dimensional NMR Spectrum	See full text		(31)CAS	
UV and Visible Absorption Spectrum	See full text	1 of 3	(32)CAS	
Structure-related Properties				Top
Bond Length	See full text		(2)CAS	
X-Ray Diffraction Pattern	See full text	1 of 4	(33)CAS	
Thermal Properties				Top
Enthalpy	See full text		(4)CAS	
Entropy	See full text		(4)CAS	
Gibbs Free Energy	See full text	1 of 2	(5)CAS	
Glass Transition Temperature	151 °C			
Melting Point	228.6 °C			
Melting Point	223 °C			
Melting Point	216 °C			
Melting Point	213-217 °C			



物质有关的文献信息

☐ 1. **33069-62-4** 🔍

~29338

~189

Absolute stereochemistry., Rotation (-).

C47 H51 N O14
Benzenepropanoic acid, β -(benzoylamino)- α -hydroxy-, (2a*R*,4*S*,4a*S*,6*R*,9*S*,11*S*,12*S*,12a*R*,12b*S*)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, (α *R*, β *S*)-
[Regulatory Information](#)
[Spectra](#)
[Experimental Properties](#)

一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容，不勾选，默认获得全部

Get References

Limit results to:

- | | |
|---|--|
| <input type="checkbox"/> Adverse Effect, including toxicity | <input type="checkbox"/> Prophetics in Patents |
| <input type="checkbox"/> Analytical Study | <input type="checkbox"/> Preparation |
| <input type="checkbox"/> Biological Study | <input type="checkbox"/> Process |
| <input type="checkbox"/> Combinatorial Study | <input type="checkbox"/> Properties |
| <input type="checkbox"/> Crystal Structure | <input type="checkbox"/> Reactant or Reagent |
| <input type="checkbox"/> Formation, nonpreparative | <input type="checkbox"/> Spectral Properties |
| <input type="checkbox"/> Miscellaneous | <input type="checkbox"/> Uses |
| <input type="checkbox"/> Occurrence | |

For each sequence, retrieve:



- ☐ Additional related references, e.g., activity studies, disease studies.

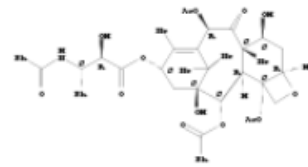
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物质有关的反应

1. **33069-62-4** 🔍

~29338  ~189 



Absolute stereochemistry., Rotation (-).

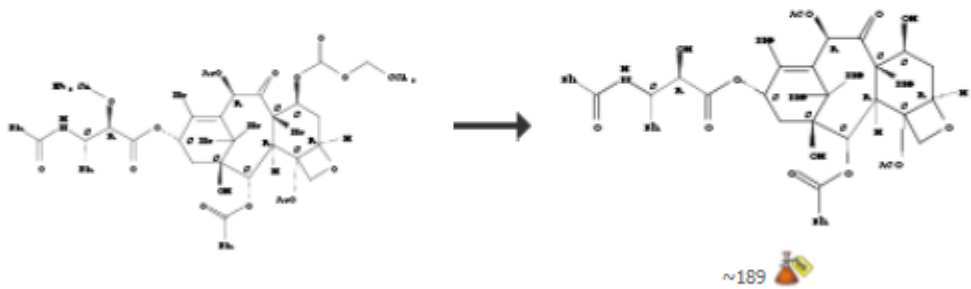
C47 H51 N O14
Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12-bis(acetyloxy)-12-(benzyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (αR,βS)-


Regulatory Information
Spectra
Experimental Properties

0 of 1990 Reactions Selected

1. **View Reaction Detail** 🔗 **Link**

2 Steps *Hover over any structure for more options.*



~189 

Overview

Get Reactions

Limit results by reaction role:

☒ **Product**

☐ Reactant

☐ Reagent

☐ Reactant or reagent

☐ Catalyst

☐ Solvent

☐ Any role

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物质有关的商品信息

1. **33069-62-4** 🔍

~29338 **~189**

Absolute stereochemistry., Rotation (-).

C47 H51 N O14
Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2a*R*,4*S*,4a*S*,6*R*,9*S*,11*S*,12*S*,12a*R*,12b*S*)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methanobenz[1,2-*b*]oxet-9-yl ester, (α*R*,β*S*

[Regulatory Information](#)
[Spectra](#)
[Experimental Properties](#)

可以直接Export到Excel中，又或者使用分析工具，对商业信息进行处理

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Substance Identifier "33069-62-4" > substances (1) > commercial sources (189)

COMMERCIAL SOURCES ⓘ

Analyze Sort by: Commercial Source ↑ Display Options

0 of 189 Commercial Sources Selected

Analyze by: ⓘ
Commercial Source

Ryan Scientific Intermediate and Building Block Compounds 7

CarboMer Catalog 5

Wako Pure Chemicals Product List 5

1. **3B Scientific Corporation Product List** Set Preference ▼
Chemical Name: Taxol
Order Number: 3B2-0277
CAS Registry Number: 33069-62-4 🔍
Quantity: 0.5g, 1g

2. **A Chemtek Product List** Set Preference ▼
Chemical Name: Taxol
Order Number: 001-10105
CAS Registry Number: 33069-62-4 🔍
Quantity: N/A

SciFinder中的物质检索方法

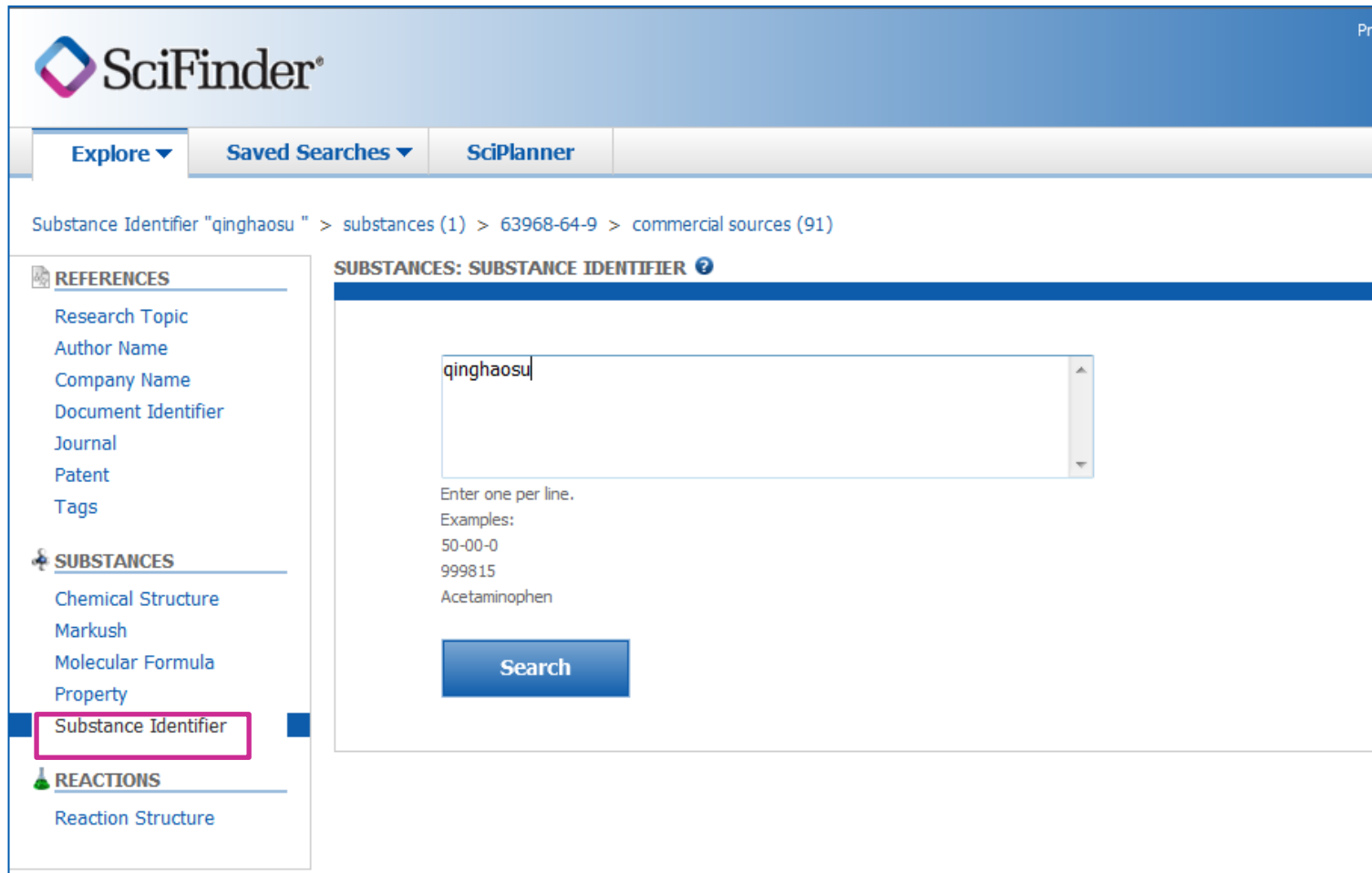
- 功能方面

- 物质名称, CAS No
- 分子式
- 结构式
- 理化性质

- 推荐的物质检索功能

- 有机物, 天然产物及衍生物 ---结构比较方便
- 无机物 ---分子式比较方便
- 高分子化合物 ---首先分子式, 其次结构

物质名称检索



Substance Identifier "qinghaosu" > substances (1) > 63968-64-9 > commercial sources (91)

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER


qinghaosu

Enter one per line.
 Examples:
 50-00-0
 999815
 Acetaminophen

Search

直接输入物质的名称，CAS No，俗名，都能检索，一次最多检索25个物质，用换行换开

理化性质检索


Pre

Explore ▾

Saved Searches ▾

SciPlanner

Substance Identifier "qinghaosu " > substances (1) > 63968-64-9 > commercial sources (91)

 REFERENCES

Research Topic

Author Name


Company Name

Document Identifier

Journal

Patent

Tags

 SUBSTANCES


Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

 REACTIONS

Reaction Structure

SUBSTANCES: PROPERTY ?

Select the category and enter an appropriate value or range.

☒ Experimental

Value or Range

Select Property... ▾

Examples: Individual value as 44,
range as 25-35, or open ended range
as >125 or <125

☐ Predicted

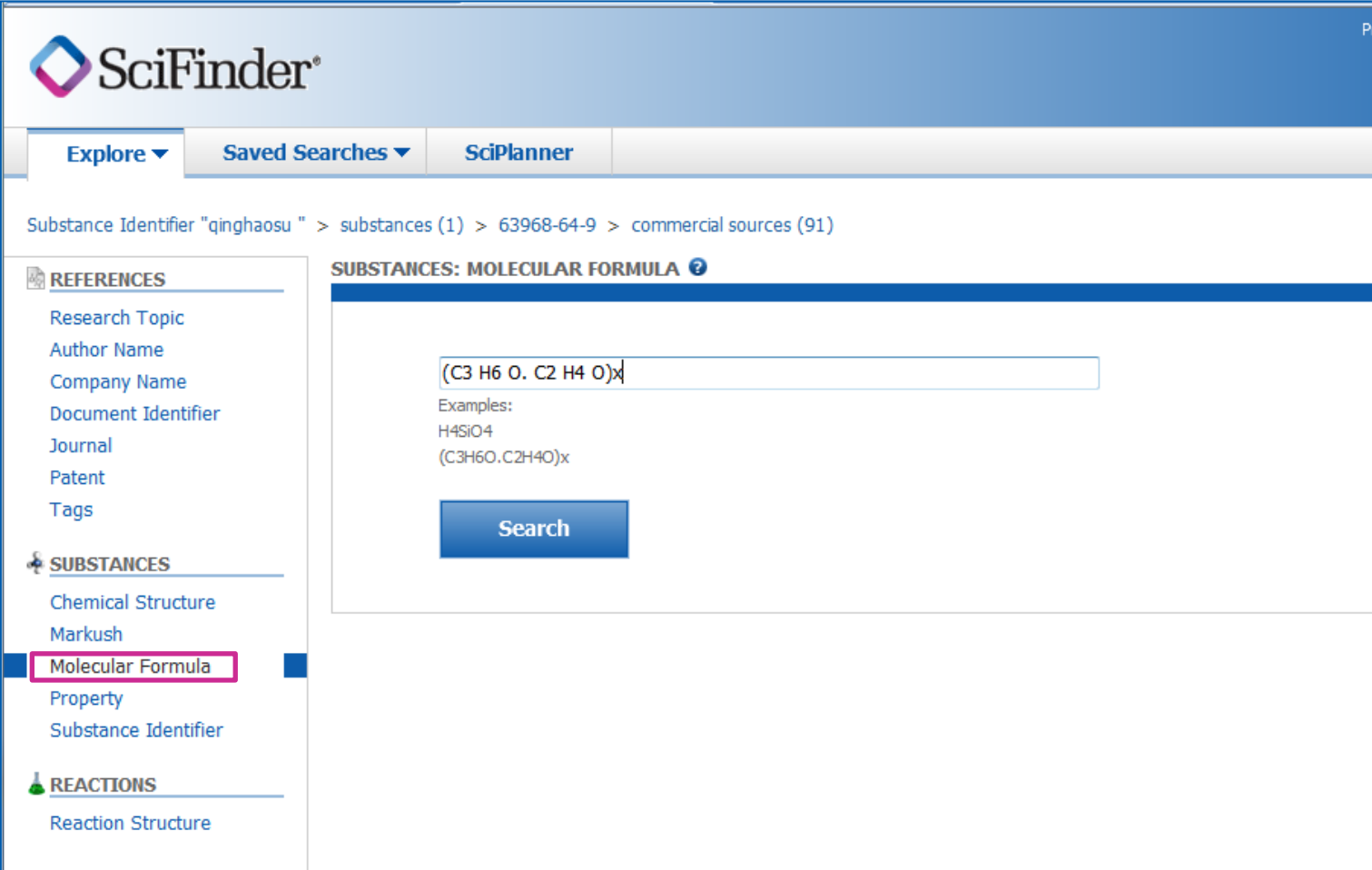
Value or Range

Select Property... ▾

Examples: Individual value as 44,
range as 25-35, or open ended range
as >125 or <125

Search

分子式检索




The screenshot shows the SciFinder homepage with the following elements:

- Navigation Bar:** Includes the SciFinder logo, a "Pre" label, and tabs for "Explore", "Saved Searches", and "SciPlanner".
- Breadcrumbs:** "Substance Identifier 'qinghaosu' > substances (1) > 63968-64-9 > commercial sources (91)".
- Left Sidebar:**
 - REFERENCES:** Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags.
 - SUBSTANCES:** Chemical Structure, Markush, **Molecular Formula** (highlighted with a red box), Property, Substance Identifier.
 - REACTIONS:** Reaction Structure.
- Main Content Area:**
 - Section: "SUBSTANCES: MOLECULAR FORMULA ?"
 - Input field: Contains the text "(C3 H6 O. C2 H4 O)x".
 - Examples: "H4SiO4" and "(C3H6O.C2H4O)x".
 - Search button: A blue button labeled "Search".

SciFinder中的分子式的检索，需要按照HILL排序方式输入，简单来说，CH写前面，其他的按照字母顺序写

结构式检索



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REFERENCES

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

SUBSTANCES

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

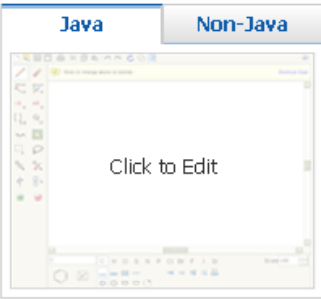
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

[Java](#) | [Non-Java](#)



Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

Import CXF

Search

[Advanced Search](#)

SAVED ANSWER SETS

- 4 step ref
- 3 step-ref
- 4 Step
- 3130
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- RCM-1816ref
- 646Ref
- Luminescent substances with organic refined
- Total reaction
- Autosaved Substance Set
- View All | Import

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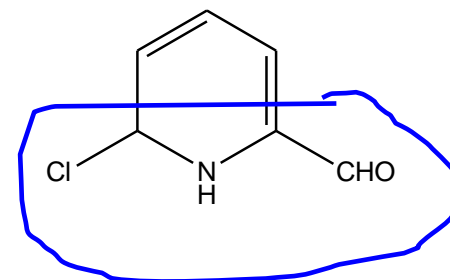
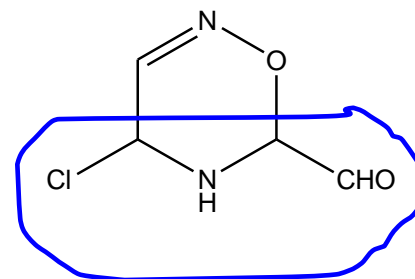
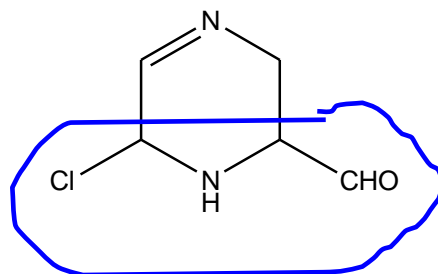
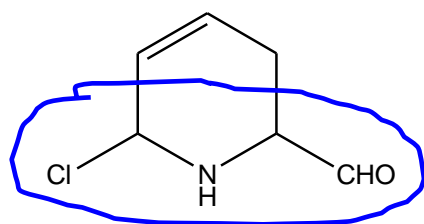
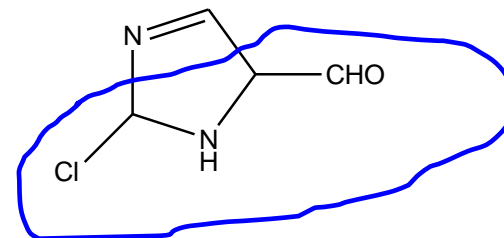
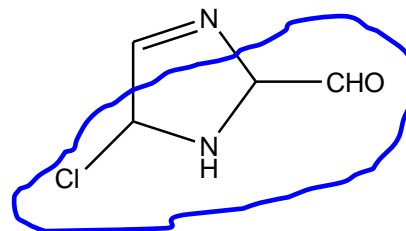
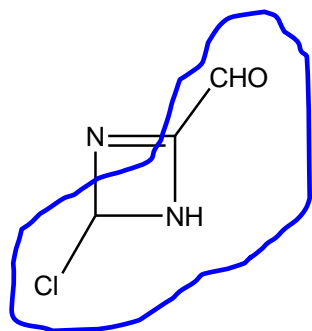
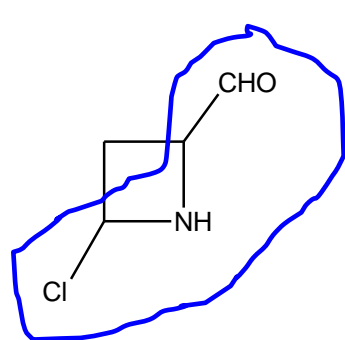
SciFinder结构绘制工具

The image shows the SciFinder Structure Editor window with various tools and features 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)
- 可变基团 (Variable Groups)
- R基团定义工具 (R-group Definition Tool)
- 重复基团工具 (Repeating Group Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 碳链工具 (Carbon Chain Tool)
- 模版工具 (Template Tool)
- 选择工具 (Selection Tool)
- 索套选择工具 (Lasso Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 原子锁定工具 (Atom Locking Tool)
- 旋转工具 (Rotation Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C-atom and Single Bond Restoration Tool)
- 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)
- 常见环, 多元环工具 (Common Rings, Polycyclic Rings Tool)

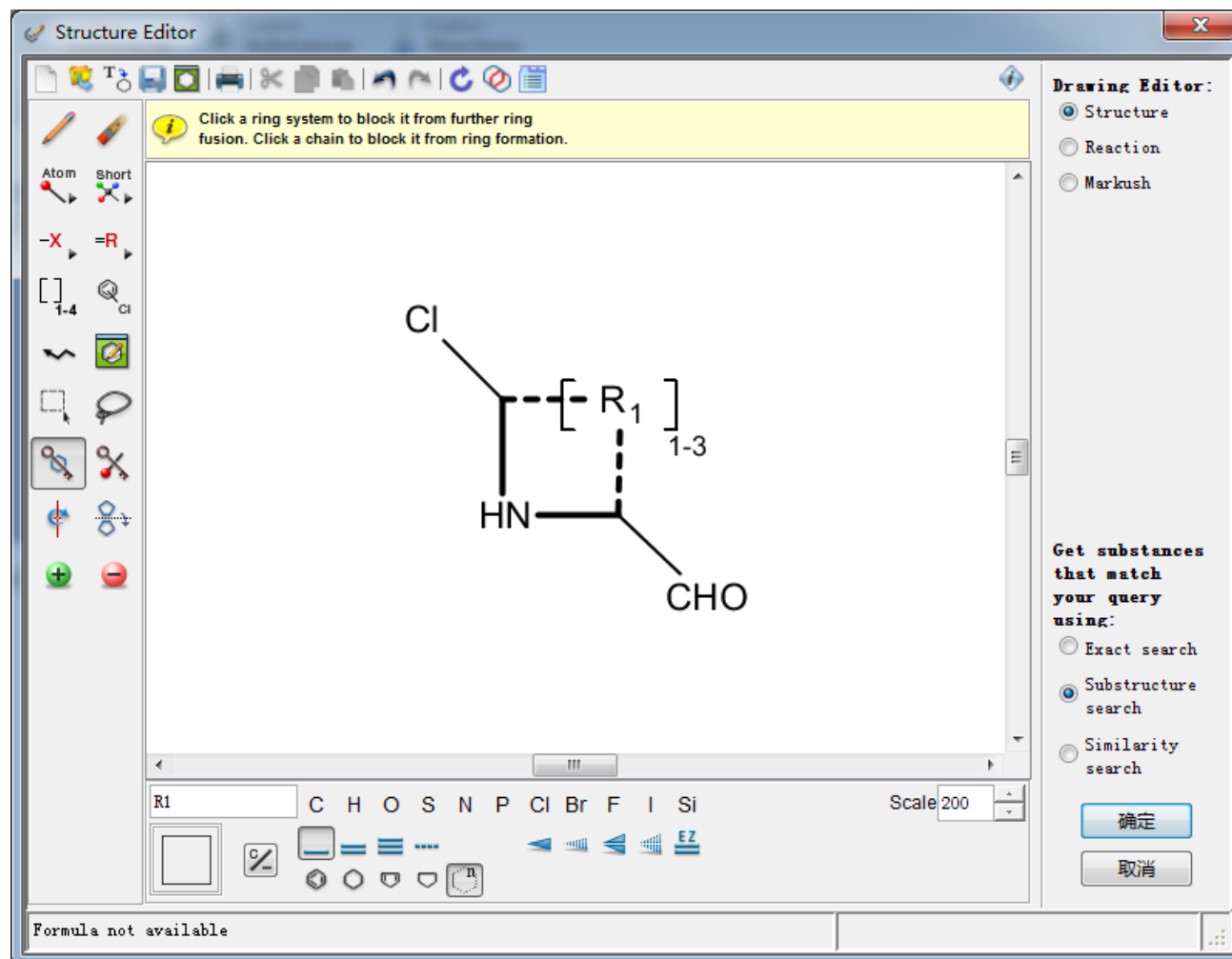
The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search and drawing options. The bottom of the window shows a command line and a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si).

想获得以下的一系列物质



○ ○ ○ ○ ○ ○

结构定义



用亚结构检索获得所有的物质

亚结构检索结果

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure substructure > substances (469)

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: Number of References ▾

Answers per Page [50] View: ||| ||| |||

0 of 469 Substances Selected

Page: 1 of 10

Analyze by: ?

Substance Role ▾

Preparation 155

Reactant or Reagent 123

Biological Study 15

Uses 11

Prophetic in Patents 8

Properties 6

Formation, Nonpreparative 2

Analytical Study 1

1. Substance Detail 54087-03-5

~33

O=Cc1cccc(Cl)n1

C₆ H₄ Cl N O

2. Substance Detail 1757-28-4

~19

O=Cc1cc(Cl)c[nH]1

C₅ H₄ Cl N O
1H-Pyrrole-2-carboxaldehyde, 5-chloro-

Experimental Properties

3. Substance Detail 81293-97-2

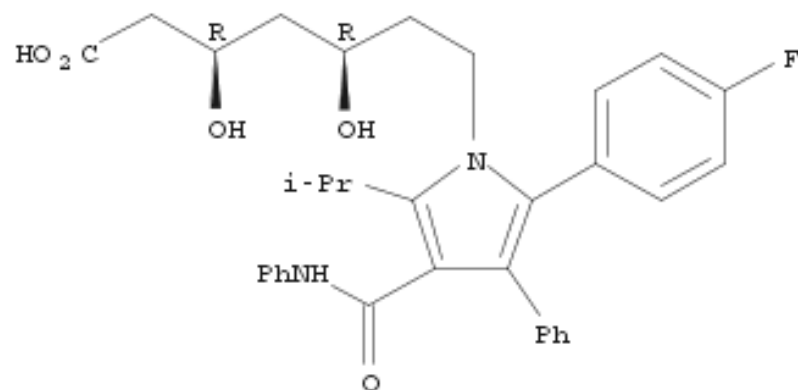
~11

O=Cc1c(Cl)c(Cl)n[nH]1

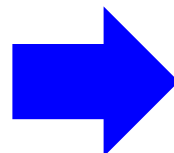
C₄ H₂ Cl₂ N₂ O
1H-Imidazole-2-carboxaldehyde, 4,5-dichloro-

案例研究

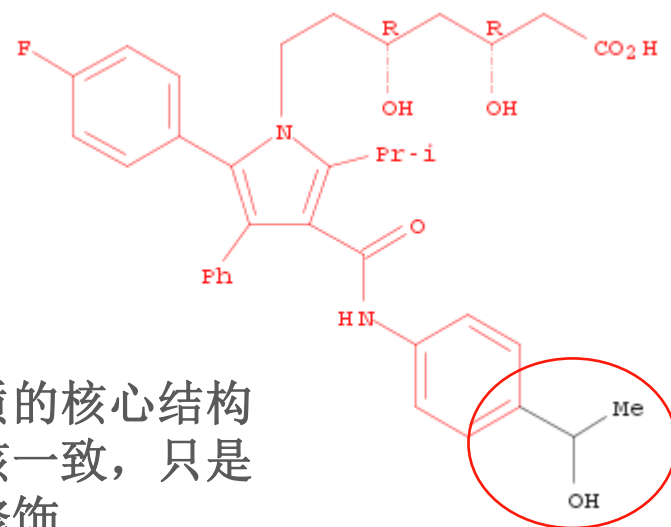
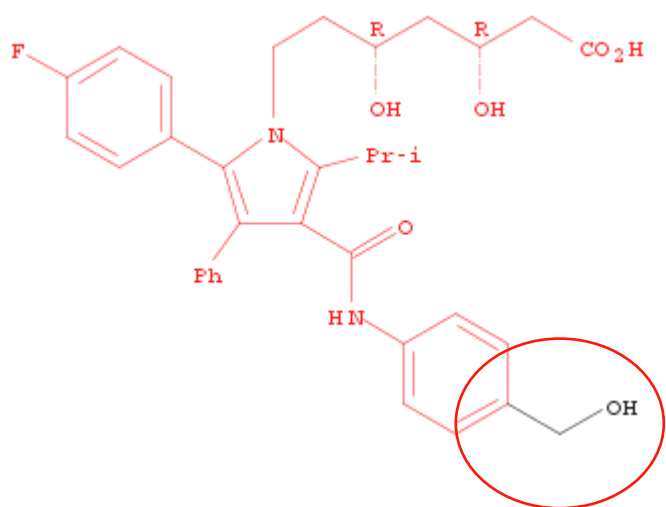
对某一结构进行改造，看是否有更好的新结构



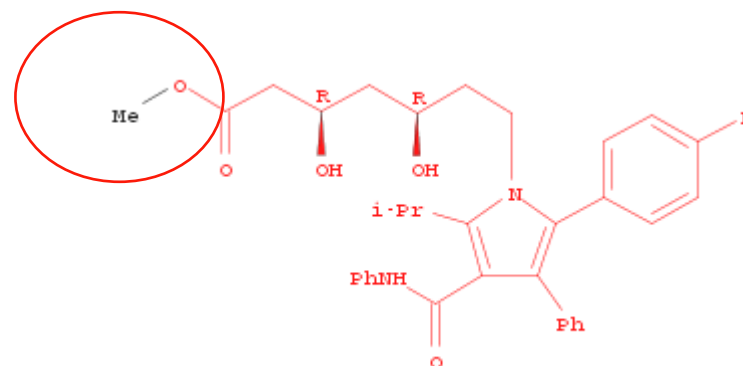
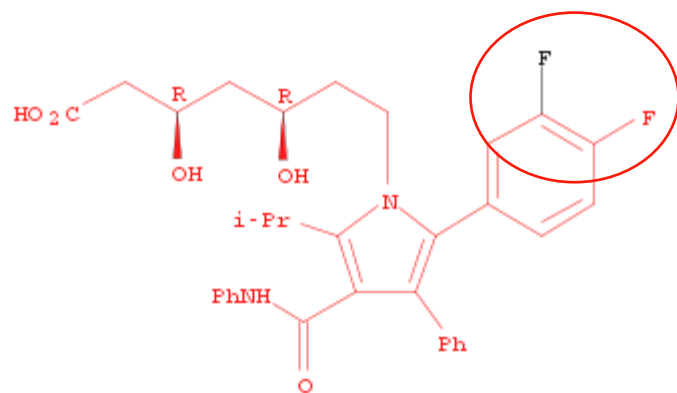
• 1/2 Ca



Substructure Search—用于检索结构的修饰物



这些物质的核心结构
都和母核一致，只是
多了些修饰



Atom Attachment直接限定感兴趣的修饰位点

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	487
<input type="checkbox"/> C	1049
<input type="checkbox"/> N	2
<input type="checkbox"/> Ca	2
<input type="checkbox"/> Al	2
<input type="checkbox"/> Si	1
<input type="checkbox"/> P	1
<input type="checkbox"/> A - Any (not H)	1057
<input type="checkbox"/> Ak - Alkyl chain	1034
<input checked="" type="checkbox"/> Cb - Carbocycle	10
<input type="checkbox"/> Q - Any (not C,H)	8
<input type="checkbox"/> Hy - Heterocycle	6
<input type="checkbox"/> M - Metal	4

对支链O的修饰研究

对苯环对位修饰研究

对特定定位点的修饰了解，帮助了解该位点都已经有了什么类型的修饰研究，便于开创新的修饰结构，也可配合文献调研，获得与构效关系有关的判断。

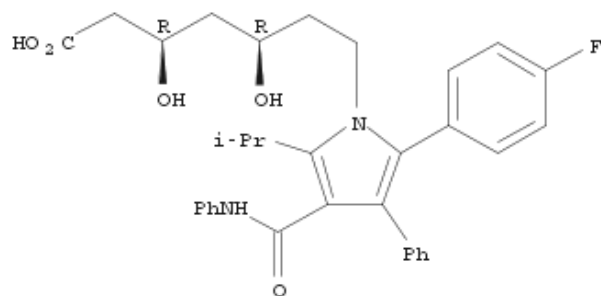
Substructure

Atom Attachments

Select All Deselect All

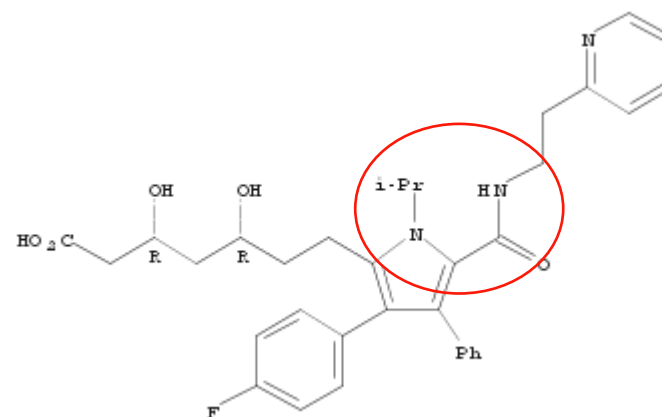
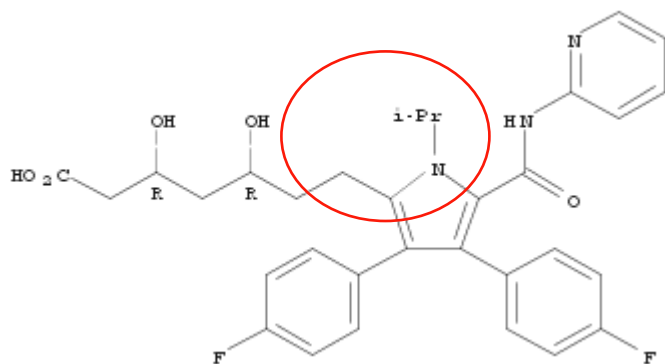
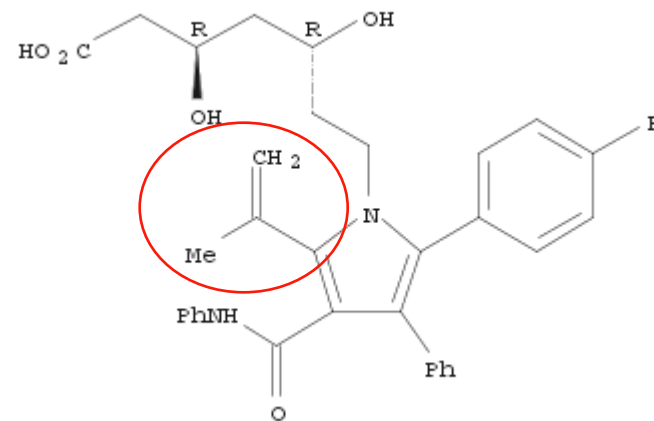
<input type="checkbox"/> H or None	1342
<input type="checkbox"/> C	109
<input type="checkbox"/> O	58
<input type="checkbox"/> N	29
<input type="checkbox"/> F	6
<input type="checkbox"/> A - Any (not H)	202
<input type="checkbox"/> Ak - Alkyl chain	109
<input checked="" type="checkbox"/> Q - Any (not C,H)	93
<input type="checkbox"/> X - Halogen	6

Similarity Search—用于检索结构的类似物



• 1/2 Ca

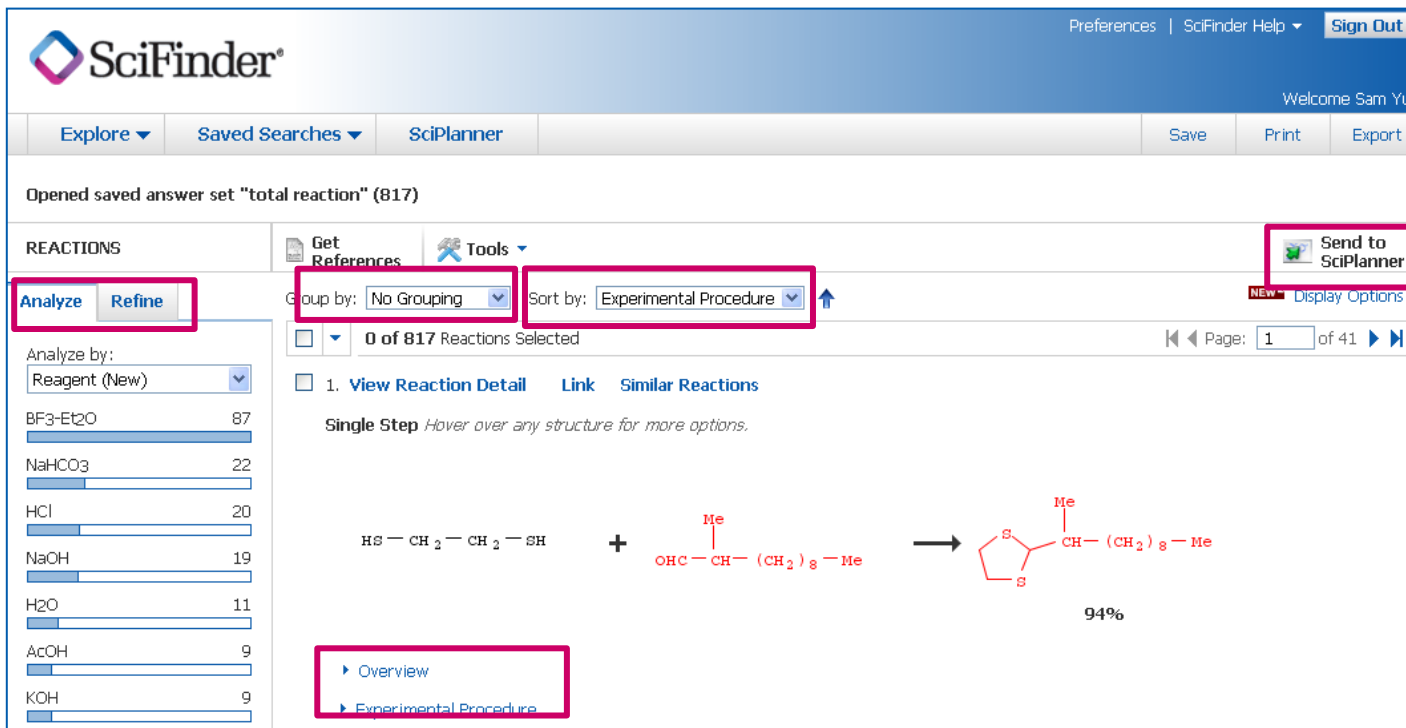
结构都存在相似性，
但是又和原结构有
不同的地方



提纲

- 介绍
 - SciFinder Web中的内容
 - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索技巧
 - SciFinder Web中的反应记录及反应检索技巧
- **SciFinder Web的注册和常见问题**

SciFinder Web中的反应记录



SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Opened saved answer set "total reaction" (817)

REACTIONS

Get References | Tools

Analyze | Refine

Analyze by:
 Reagent (New)

BF ₃ -Et ₂ O	87
NaHCO ₃	22
HCl	20
NaOH	19
H ₂ O	11
AcOH	9
KOH	9

Group by: No Grouping | Sort by: Experimental Procedure

0 of 817 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

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

HS-CH2-CH2-SH + CC(C)CCCCCCCC=O → CC(C)CCCCCCCC1SCCSC1

94%

Overview | Experimental Procedure

Send to SciPlanner

Display Options

Page: 1 of 41

1. 反应分组功能
2. 反应排序功能
3. 反应后处理功能
4. 反应全景及实验过程
5. SciPlanner

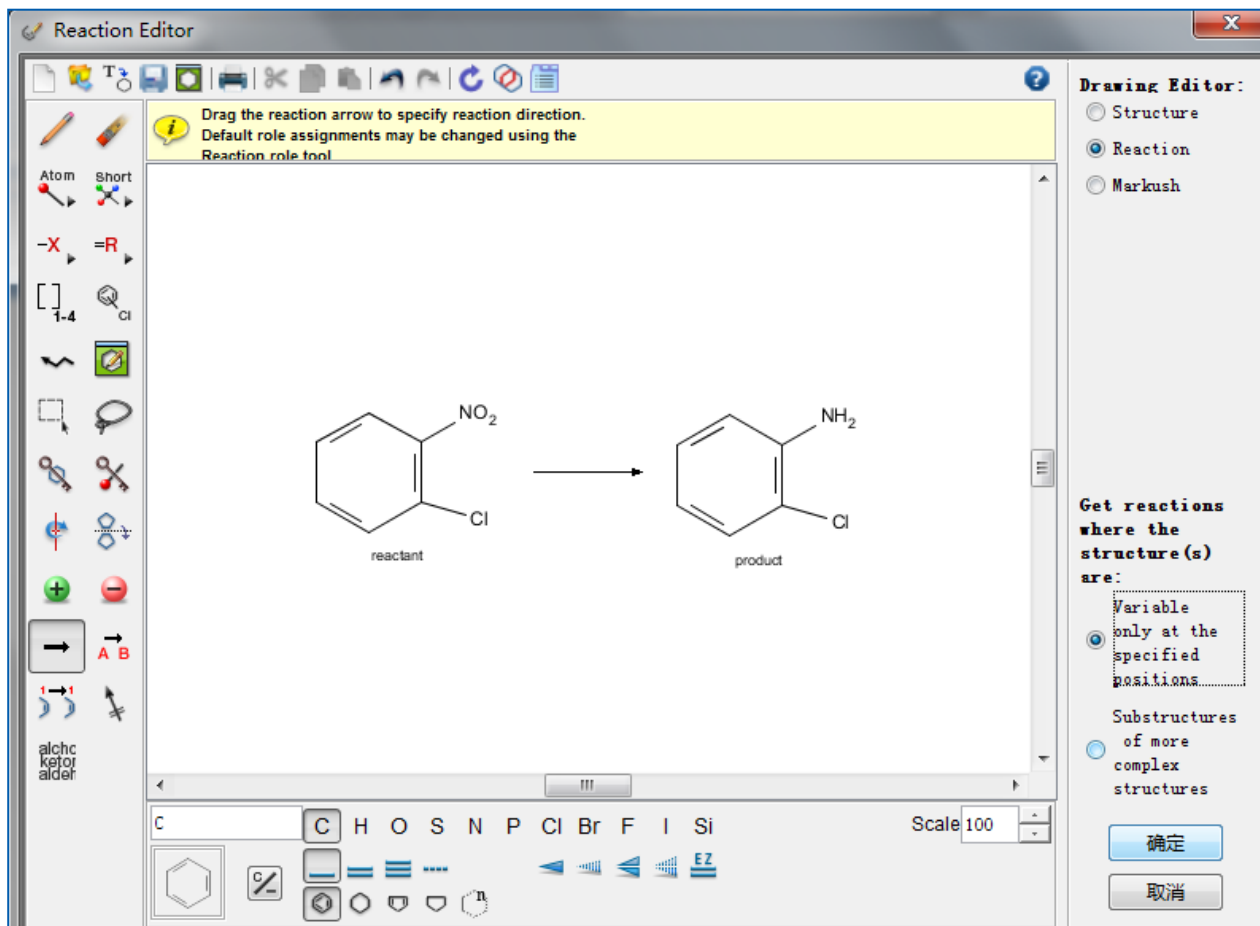
SciFinder中的反应定义工具

The screenshot shows the 'Reaction Editor' window in SciFinder. The interface includes a toolbar on the left with various drawing tools, a central canvas for drawing, and a right-hand panel with 'Drawing Editor' options and search criteria. 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 the reaction arrow.
- 反应角色工具** (Reaction Role Tool): Points to the tool that adds roles (R, S) to the reaction arrow.
- 反应位置标记工具** (Reaction Position Labeling Tool): Points to the tool that adds position labels (1, 2) to the reaction arrow.
- 反应官能团列表** (Reaction Functional Group List): Points to the list of functional groups (alchc, ketor, alder) at the bottom of the toolbar.

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' (radio button) and 'Substructures of more complex structures' (radio button). At the bottom right are '确定' (OK) and '取消' (Cancel) buttons.

SciFinder反应检索



Allow variability only as specified: 仅在特定位点发生变化

Substructure: 亚结构检索，允许有更多取代情况

反应检索界面

[Explore ▾](#)
[Saved Searches ▾](#)
[SciPlanner](#)

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

REACTIONS: REACTION STRUCTURE ?

Structure Editor:

Java

Non-Java

reactant

product

Click image to change structure or view detail.

[Import CXF](#)

Search

Search Type:

☒ Allow variability only as specified
 ☐ Substructure

Java Structure Editor

Having issues with Java? Switch to the Non-Java editor.
 To switch between editors, click the tabs above the structure editor box.

精确反应检索结果

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Tony Liu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Reaction Structure structure variable only at spe... > reactions (335)

REACTIONS ?

Get References | Tools

Analyze | Refine

Group by: No Grouping | Sort by: Relevance

0 of 335 Reactions Selected

Analyze by: Reagent (New)

H ₂	196
N ₂ H ₄ ·H ₂ O	23
H ₂ O	17
NaOH	17
CO	15
KOH	15
Me ₂ CHOH	8

1. View Reaction Detail | Link | Similar Reactions

Single Step Hover over any structure for more options.

~90 | 100% | ~119

Overview

Group by Document 按照出处文献分类显示

SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Tony Liu

Explore | Saved Searches | SciPlanner

Save | Print | Export

Reaction Structure structure variable only at spe... > reactions (335)

REACTIONS ?

Get References | Tools

Analyze | Refine

Analyze by: Reagent (New)

H₂ 196
N₂H₄+H₂O 23
H₂O 17
NaOH 17
CO 15
KOH 15
Me₂CHOH 8
NaBH₄ 8
NH₄Cl 8

Group by: Document
No Grouping
Document
Transformation

Sort by: Relevance

1. Selective hydrogenation of o-chloronitrobenzene over tin dioxide supported platinum-ruthenium bimetallic nanocatalysts without solvent

1 Reaction Similar Reactions

Single Step Hover over any structure for more options.

~90

100%

~119

Overview

2. Selective hydrogenation of nitroaromatics by ceria nanorods

1 Reaction Similar Reactions

Single Step Hover over any structure for more options.

来自同一篇文献的反应都被整合到一起并集中显示

Group by Transformation 按照反应类型分类显示

The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. Below this, a breadcrumb trail indicates the current search results for 'reactions (335)'. The main content area is titled 'REACTIONS' and includes a 'Get References' button and a 'Tools' dropdown. A sidebar on the left allows for refining the search by reagent, with a list of reagents and their corresponding reaction counts: H₂ (196), N₂H₄-H₂O (23), H₂O (17), NaOH (17), CO (15), KOH (15), Me₂CHOH (8), NaBH₄ (8), and NH₄Cl (8). The main results area shows a list of reaction types, each with a checkbox, a title, a count of reactions, and a chemical equation. The 'Group by' dropdown is set to 'Transformation', and the 'Sort by' dropdown is set to 'Frequency'. The results are as follows:

Reaction Type	Count	Chemical Equation
1. Reduction of Nitro Compounds to Amines	331 Reactions	$R-NO_2 \longrightarrow R-NH_2$
2. Dehalogenation of Aromatic Compounds	36 Reactions	$Ar-X \xrightarrow{cat.} Ar-H$
3. Reduction of Alkyl Halides/ Dehalogenation	36 Reactions	$R-X \longrightarrow R-H$
4. Reduction of Nitro Compounds to Hydroxylamines	3 Reactions	$R-NO_2 \longrightarrow R-\overset{H}{N}-OH$

同一类反应被整合到一起并以通式结构集中显示；
仅适用于单步反应，未被分类的反应显示在结果集最后

获得有实验步骤的反应结果集

[Explore](#)
[Saved Searches](#)
[SciPlanner](#)

Reaction Structure structure variable only at spe... > **reactions (335)**

REACTIONS
[Get References](#)
[Tools](#)

Analyze
Refine

Analyze by: [?](#)
Reagent (New)

H ₂	196
N ₂ H ₄ ·H ₂ O	23
H ₂ O	17
NaOH	17
CO	15
KOH	15
Me ₂ CHOH	8

Group by: No Grouping Sort by: **Experimental Procedure**

- Relevance
- Accession Number
- Experimental Procedure**
- Number of Steps
- Product Yield
- Publication Year

0 of 335 Reactions Selected

1. [View Reaction Detail](#)

Single Step Hover over any structure for more options.

[Overview](#)
[Experimental Procedure](#)

1. [View Reaction Detail](#)

Single Step Hover over any structure for more options.

[Overview](#)

[Experimental Procedure](#)

General/Typical Procedure: **Reflux Conditions (Table 1)**. To a solution of 2.0 mmol of substrate **Preparation and Isolation of Fe₃O₄ Nanoparticles**. A solution of Fe(acac)₃ 0.02 mmol (7.1 mg) and hydrazine hydrate (2 mmol) in methanol (1.5 mL) was placed into a 10 mL microwave vial and heated at 150 °C for 1 minutes. The resulting mixture was cooled at room temperature and after 20-30 min the black precipitate was retrieved with magnetic separation or centrifugation (5000 rpm, 5 min). The solid was washed 3 times with fresh methanol and dried overnight in a drying oven at 70 °C. The obtained Fe₃O₄ nanocrystals were characterized by means of X-ray powder diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM).¹⁶ **Reflux Conditions (Table 1)**. To a solution of 2.0 mmol of substrate in ethanol (1.5 mL) were added 3.6 mmol (1.2 equiv, 0.175 mL) of N₂H₄·H₂O and 3 mol % Fe(acac)₃. The mixture was placed into a 10 mL round-bottom flask and heated at reflux for the desired time (Table 1). When the nitroarene was consumed the reaction mixture was cooled to room temperature. Then, the solvent was evaporated under reduced pressure and the crude product purified by flash chromatography (hexane/ethyl acetate). Careful solvent evaporation yielded the pure aniline. **Aniline (Table 1, entry 1): Table 4. Reduction of Nitroarenes with Hydrazine Hydrate Catalyzed by in-situ Generated Fe₃O₄ Nanocrystals under Microwave Irradiation**^a Entry 3 Yield 97%.

反应结果集的分析限定工具

Analyze
Refine

Analyze by: ?

Reagent (New)

- Author Name
- Catalyst
- Company-Organization
- Complete Iterations
- Document Type
- Experimental Procedure
- Journal Name
- Language
- Number of Steps
- Product Yield
- Publication Year
- Reagent (New)
- Solvent

C₂H₆ 5

CH₄ 4

ClCH₂CH₂Cl 4

Na 4

Show More

反应分析类型:

作者姓名	出版语言
催化剂	出版年代
机构名称	反应步数
文献类型	产率
期刊名称	试剂
实验步骤	溶剂

反应的限定功能:

反应式
产率
反应步数
反应类型
排除的反应类型
不参与反应的基团

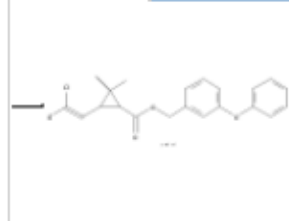
Analyze
Refine

Refine by: ?

- ☒ Reaction Structure
- ☐ Product Yield
- ☐ Number of Steps
- ☐ Reaction Classification
- ☐ Excluding Reaction Classification
- ☐ Non-participating functional groups

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Search type: **Allow variability only as specified**

Refine

提纲

- 介绍
 - SciFinder Web中的内容
 - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
 - SciFinder Web中的文献记录及主题检索
 - SciFinder Web中的物质结果及物质检索技巧
 - SciFinder Web中的反应记录及反应检索技巧
- **SciFinder Web的注册和常见问题**

SciFinder Web的注册和登陆

SciFinder Web的系统要求

Windows用户支持IE 9. x或者FireFox 2. x

Mac 用户支持 Firefox 和 Safari

Java 安装（初次使用结构时自动安装，建议安装Java 7）

在图书馆相关页面上找到SciFinder Web注册用的网址

鉴于360浏览器以及360安全卫士会对SciFinder的使用造成一定的影响，建议大家最好不要使用360浏览器。

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分类查询

超期公告

新书通报

热门书刊

提示:

查询我校图书馆馆藏书刊信息。

中文资源

西文资源

服务指南

- 爱思唯尔 (EIS) 电子书
- SciFinder Academic
- Web of Science
- Thieme药学期刊

- Emerald管理学全文期刊库
- ACS数据库
- EBSCOhost
- Wiley Online Libra...

- The Cochrane Libra...
- Springer全文期刊数据库
- Thomson Reuters In...
- RSC英国皇家化学学会期刊



论文提交



新生入馆教育

通知公告
资源动态

- 图书馆开展读者协会会员教育培训 14-10-21
- SciFinder网络培训通知 14-10-21
- SciFinder Web 使用培训 14-10-20
- 读者协会招募志愿者 14-10-20
- EPS数据库培训通知 14-10-09
- ACS、Annual Reviews、Thi... 14-10-08
- 图书馆“十·一”期间开馆通知 14-09-25
- 米内网数据库培训讲座通知 14-09-22

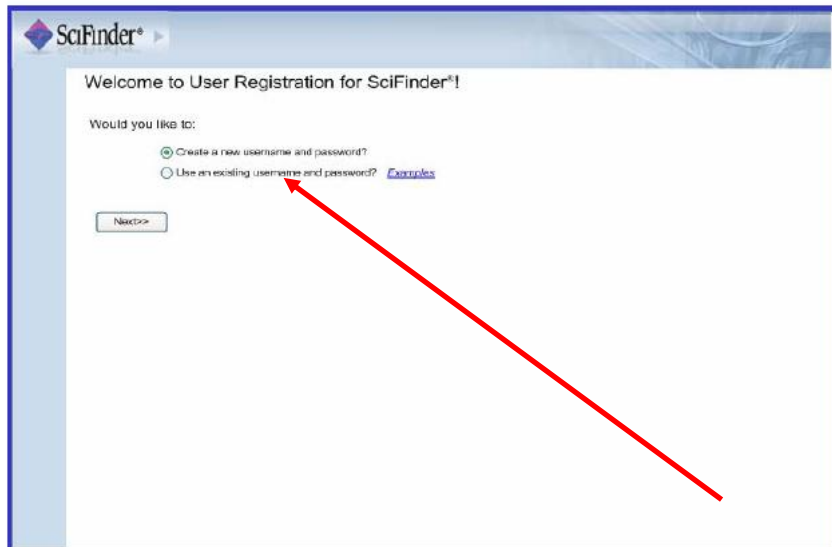
[MORE ▶](#)

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59

点击URL创建SciFinder Web账号



Welcome to User Registration for SciFinder®!

Would you like to:

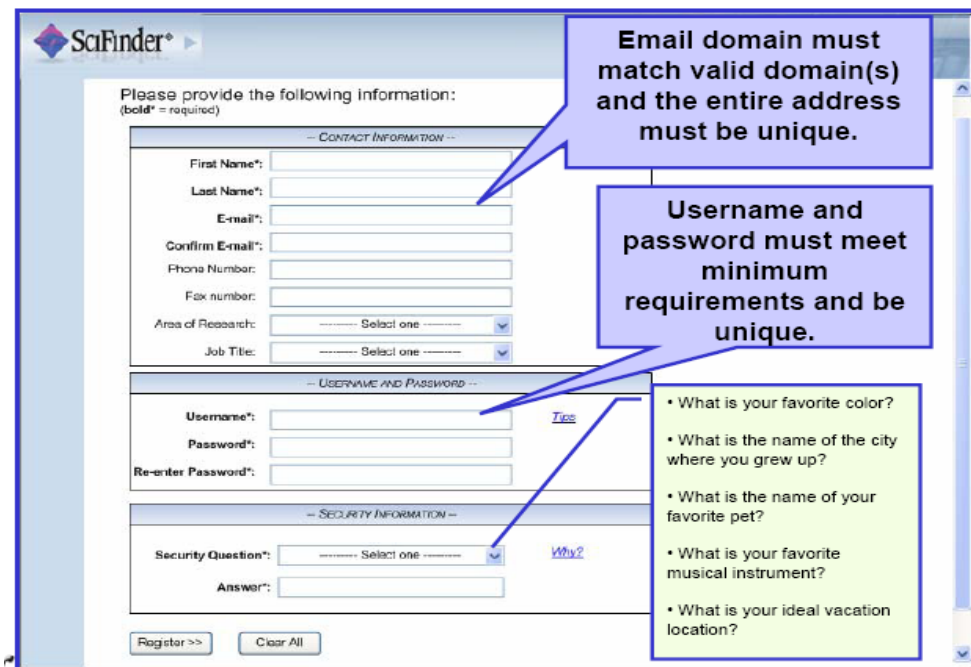
☒ Create a new username and password?

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

[Next >>](#)

请用邮箱注册，一人只能注册一个账号

开始创建SciFinder Web帐号



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*:

Callouts:

- 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?

[Why?](#)

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

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：

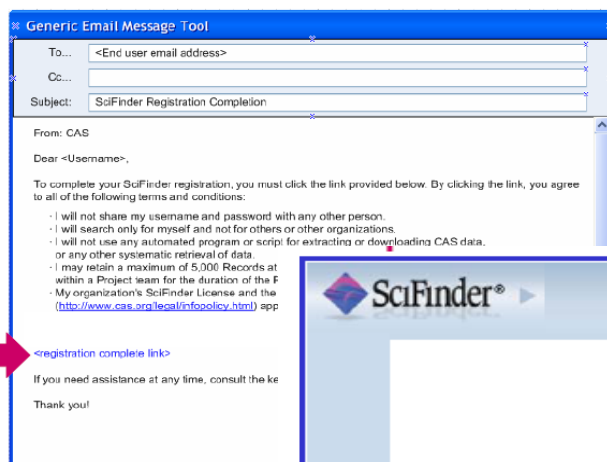
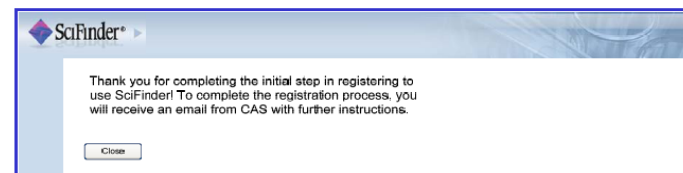
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

密码设置小技巧：

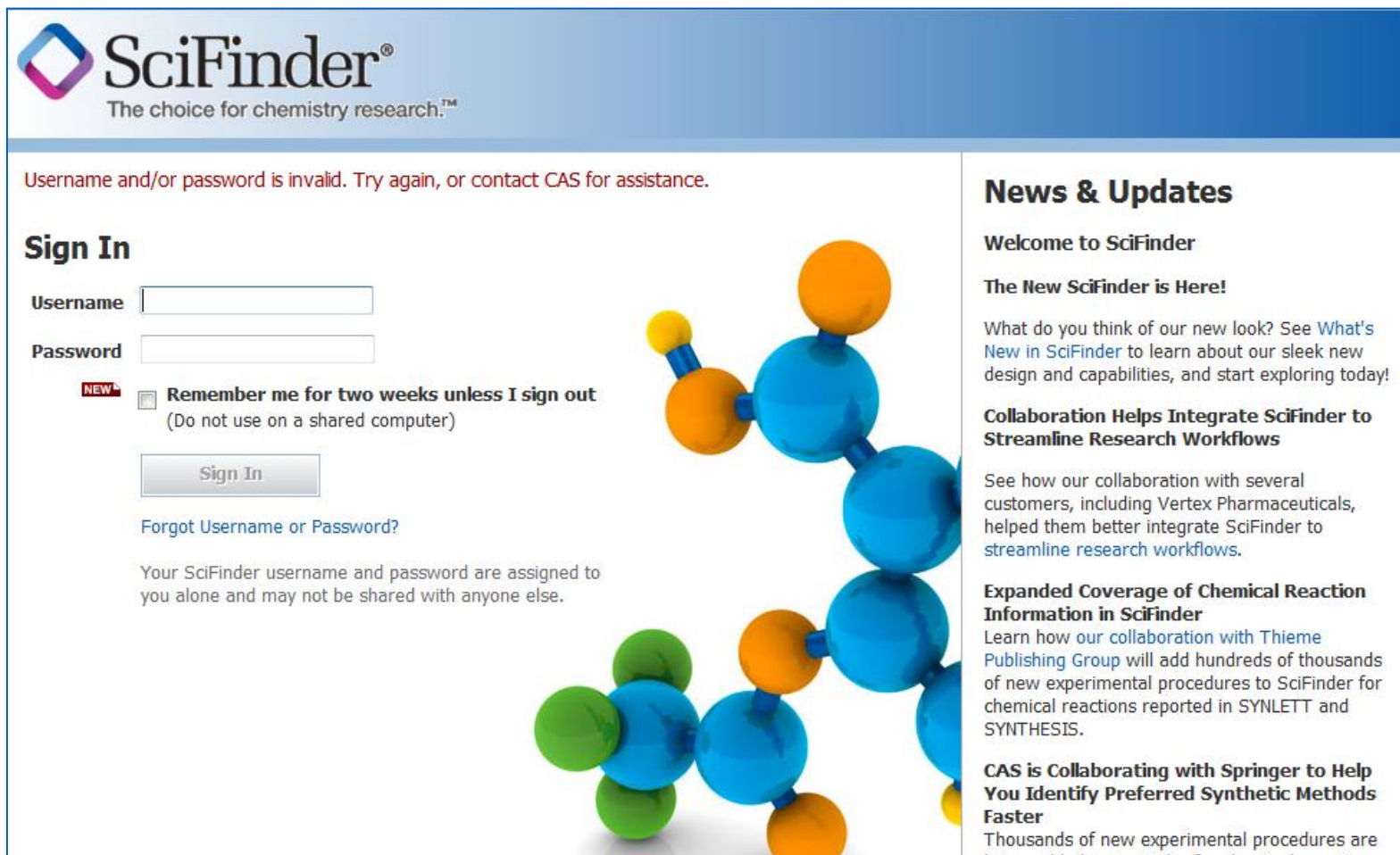
- 1：不要和账号中有重复的字符
- 2：密码格式最好是abc@123

对新ID的Email确认

48小时内，需要点击邮件中的确认链接



SciFinder Web 常见问题



SciFinder®
The choice for chemistry research.™

Username and/or password is invalid. Try again, or contact CAS for assistance.

Sign In

Username

Password

NEW ☐ Remember me for two weeks unless I sign out
(Do not use on a shared computer)

[Forgot Username or Password?](#)

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

News & Updates

Welcome to SciFinder

The New SciFinder is Here!

What do you think of our new look? See [What's New in SciFinder](#) to learn about our sleek new design and capabilities, and start exploring today!

Collaboration Helps Integrate SciFinder to Streamline Research Workflows

See how our collaboration with several customers, including Vertex Pharmaceuticals, helped them better integrate SciFinder to streamline research workflows.

Expanded Coverage of Chemical Reaction Information in SciFinder

Learn how our collaboration with [Thieme Publishing Group](#) will add hundreds of thousands of new experimental procedures to SciFinder for chemical reactions reported in SYNLETT and SYNTHESIS.

CAS is Collaborating with Springer to Help You Identify Preferred Synthetic Methods Faster

Thousands of new experimental procedures are being added to SciFinder for chemical reactions.

账号或密码错误，请在username处填写，截图，并与图书馆联系

SciFinder Web 常见问题

任何需要反馈给图书馆的问题，都请点击测试IP地址的链接

<http://www.cas.org/cgi-bin/casip>



Your IP address comes across to CAS as: 210.32.9.45

将页面截图下来，一并发给图书馆

SciFinder Web网络在线资源平台

www.igroup.com.cn/cas



The screenshot shows the SciFinder website interface. At the top, there is a banner with the CAS logo (A division of the American Chemical Society) and a molecular structure visualization. Below the banner, there is a sidebar on the left with navigation links: 常见问题, 资源下载, 新闻与公告, 在线演示, 网络培训, and 加入我们. The main content area is titled 'CAS资源下载' and lists several resources for download, including 'SciFinder 快速参考手册', '案例研究' (with sub-items like 特鲁瓦达-首个艾滋病预防药物, 纳米材料药物研究, 准晶体, 肝素, 反应定义工具案例, SciFinder新界面-自修复材料, N-二甲基亚硝胺NDMA, case study 没食子酸丙酯, case study-肉毒毒素, 转基因食品案例), and 'SciFinder新功能' (with sub-items like 生物活性及靶点分析, SciFinder R15新功能).

资源下载: **PDF文件**

在线演示: **Flash演示**

网络培训: 不定期的网络专题培训

Comprehensive Content

Sophisticated Analysis

Unprecedented Results



Thank You

刘衍兰

SciFinder 培训专员

Mail: tony@igroup.com.cn

QQ答疑群: 275247551