



# SciFinder<sup>®</sup>

The choice for chemistry research.<sup>™</sup>

## SciFinder Web使用介绍

刘衍兰

SciFinder培训专员

2015.5

# 提纲

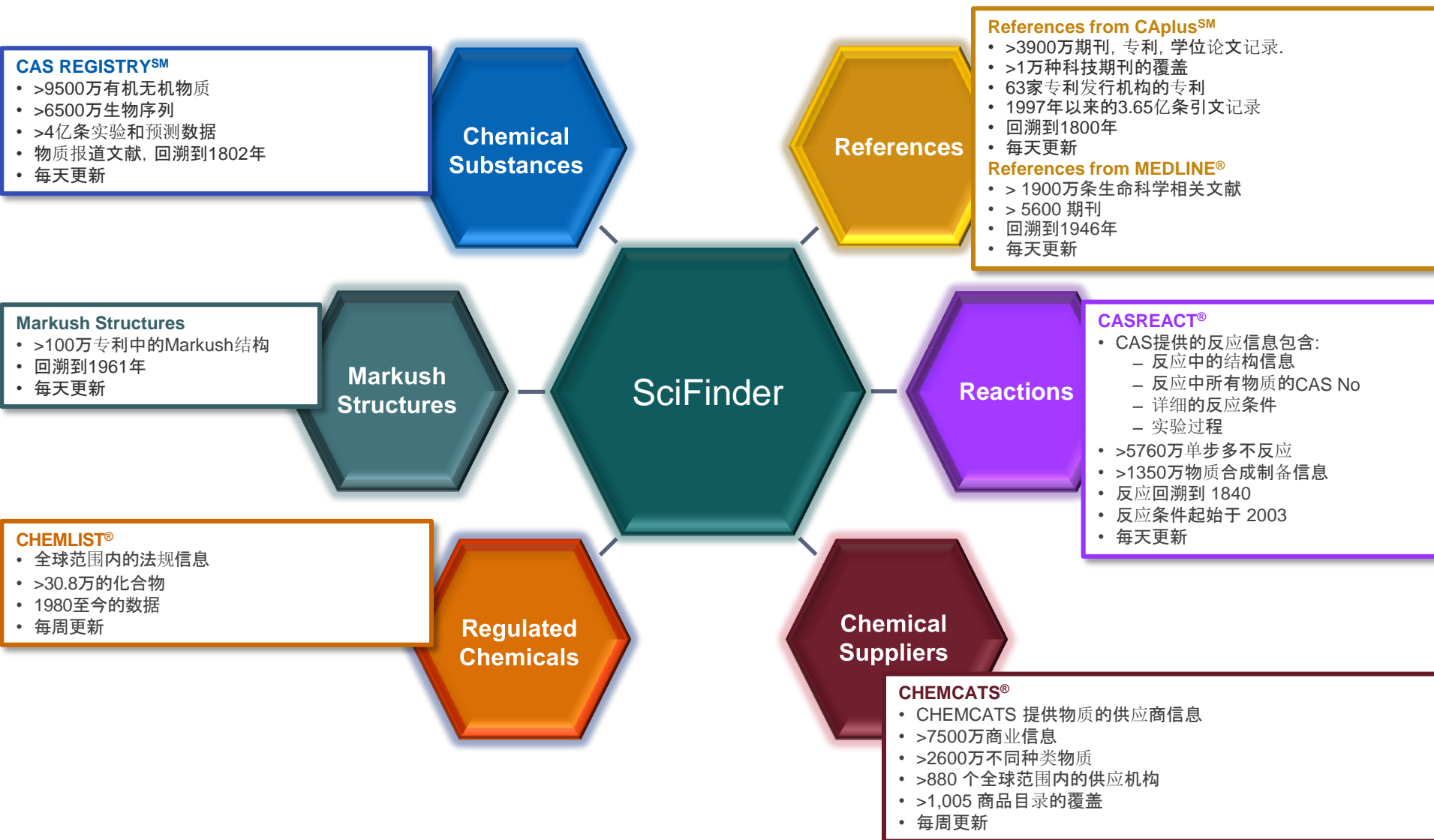
- 介绍
  - SciFinder Web中的内容
  - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索技巧
  - SciFinder Web中的反应检索及SciPlanner功能
- **SciFinder Web的注册和常见问题**

# 美国化学文摘社—Chemical Abstract Service

- 创建于1907年
- ACS的分支机构
- 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



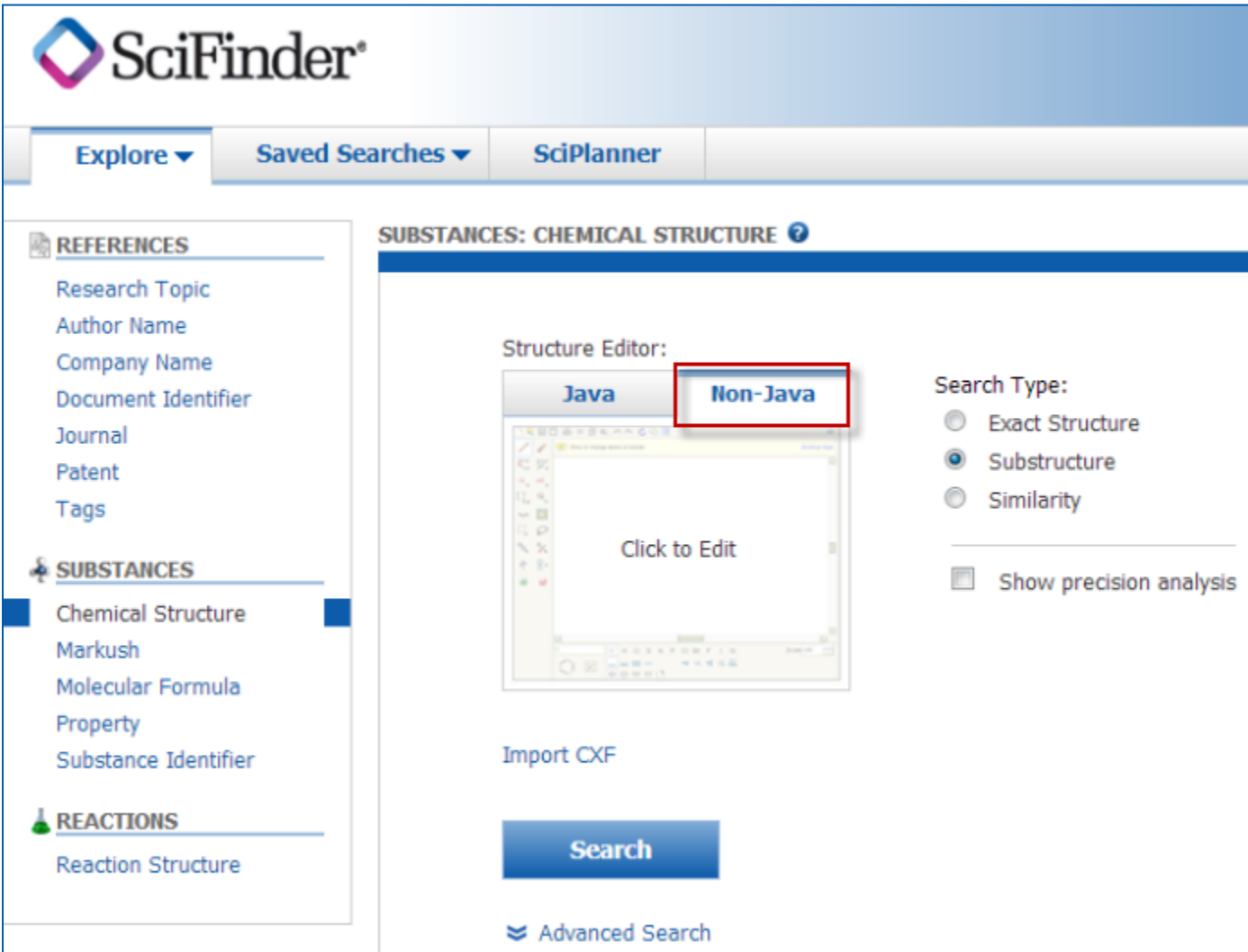
# SciFinder的覆盖内容



# 提纲

- 介绍
  - SciFinder Web中的内容
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# Non-Java结构面板



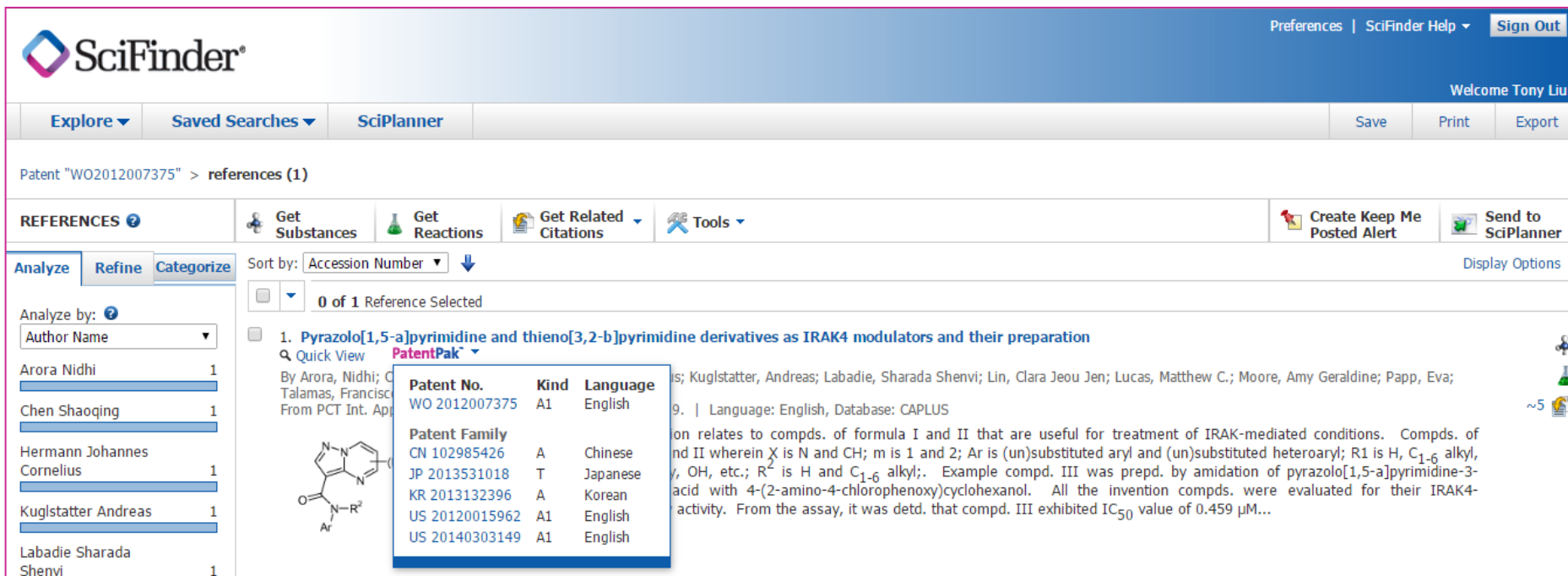
The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. A left-hand sidebar contains a menu with three main sections: 'REFERENCES' (with sub-items like Research Topic, Author Name, etc.), 'SUBSTANCES' (with sub-items like Chemical Structure, Markush, etc.), and 'REACTIONS' (with sub-item Reaction Structure). The 'SUBSTANCES' section is currently active. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. It features a 'Structure Editor' window with two tabs: 'Java' and 'Non-Java'. The 'Non-Java' tab is highlighted with a red box. Below the tabs, the editor area contains the text 'Click to Edit'. To the right of the editor, there are search options: 'Search Type' with radio buttons for 'Exact Structure', 'Substructure' (which is selected), and 'Similarity'. Below these is a checkbox for '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'.

# SciFinder和ChemDraw整合

The screenshot illustrates the integration of SciFinder into ChemBioDraw Ultra. The main window shows the chemical structure of Canagliflozin. A SciFinder search dialog is open, allowing for substance or reaction searches. The search results window displays two chemical structures with their respective CAS numbers and names:

- Structure 1:** CAS 928672-86-0, D-Galacti, 1,3-anhydro-1-C(3-[2-(4-fluorophenyl)-2-ethoxy]ethyl)-4-methylphenyl, (1S)
- Structure 2:** CAS 928672-86-0, D-Galacti, 1,3-anhydro-1-C(3-[2-(4-fluorophenyl)-2-ethoxy]ethyl)-4-methylphenyl, hydrate (2:1), (1S)

# PatentPak-自动的专利流程工具



SciFinder®

Preferences | SciFinder Help | Sign Out

Welcome Tony Liu

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

Patent "WO2012007375" > references (1)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Accession Number

0 of 1 Reference Selected

1. **Pyrazolo[1,5-a]pyrimidine and thieno[3,2-b]pyrimidine derivatives as IRAK4 modulators and their preparation**

By Arora, Nidhi; Talamas, Francisco; Kuglstatter, Andreas; Labadie, Sharada Shenvi; Lin, Clara Jeou Jen; Lucas, Matthew C.; Moore, Amy Geraldine; Papp, Eva;

From PCT Int. App.

| Patent No.           | Kind | Language |
|----------------------|------|----------|
| WO 2012007375        | A1   | English  |
| <b>Patent Family</b> |      |          |
| CN 102985426         | A    | Chinese  |
| JP 2013531018        | T    | Japanese |
| KR 2013132396        | A    | Korean   |
| US 20120015962       | A1   | English  |
| US 20140303149       | A1   | English  |

Chemical structure: C1=CN2C(=O)N(R2)C=C2N1

9. | Language: English, Database: CAPLUS

on relates to compds. of formula I and II that are useful for treatment of IRAK-mediated conditions. Compds. of and II wherein X is N and CH; m is 1 and 2; Ar is (un)substituted aryl and (un)substituted heteroaryl; R1 is H, C<sub>1-6</sub> alkyl, /, OH, etc.; R<sup>2</sup> is H and C<sub>1-6</sub> alkyl;. Example compd. III was prepd. by amidation of pyrazolo[1,5-a]pyrimidine-3-acid with 4-(2-amino-4-chlorophenoxy)cyclohexanol. All the invention compds. were evaluated for their IRAK4-activity. From the assay, it was detd. that compd. III exhibited IC<sub>50</sub> value of 0.459 μM...

Analyze by: Author Name

- Arora Nidhi 1
- Chen Shaoqing 1
- Hermann Johannes Cornelius 1
- Kuglstatter Andreas 1
- Labadie Sharada Shenvi 1

1. 主要专利机构的可检索的专利全文
2. 链接到多语种的专利族原文
3. 定位专利中化合物出现的页码
4. 专利中的化合物进行SciFinder检索



# 提纲

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# SciFinder中的文献记录

|  |                |                       |               |   |
|--|----------------|-----------------------|---------------|---|
| REFERENCE DETAIL   | Get Substances | Get Related Citations | Get Full Text | Send to SciPlanner  |
| <a href="#">Return</a>   |                |                       |               | ◀ Previous<br>  Next ▶  |
| <h2>1. Selective oxidation of <b>light</b> alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials</h2> <p>By: Cavani, F.; Trifiro, F.</p> <p>A review, with 202 refs., on the selective oxidn. of <b>light</b> (C<sub>≤6</sub>) alkanes to bulk and <b>industrial chems.</b>, 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 <b>light</b> 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.</p> |                |                       |               | <b>QUICK LINKS</b><br>0 Tags, 0 Comments  |
| <b>Indexing</b><br>Fossil Fuels, Derivatives, and Related Products (Section51-0)<br>Section cross-reference(s): 35, 45   |                |                       |               | <b>SOURCE</b><br><i>Catalysis Today</i><br>Volume51<br>Issue3-4<br>Pages561-580<br>Journal; General Review<br>1999<br>CODEN:CATTEA<br>ISSN:0920-5861<br>DOI:10.1016/S0920-5861(99)00041-3 |
| <b>Concepts</b><br>Redox reaction catalysts<br>catalyst-gas phase interactions in selective oxidn. of <b>light</b> alkanes to bulk and <b>industrial chems.</b><br>Alkaline earth oxides      Rare earth oxides<br>catalysts contg.; catalyst-gas phase interactions in selective oxidn. of <b>light</b> alkanes to bulk and <b>industrial chems.</b><br>Catalyst use; Properties; Uses  |                |                       |               |   |
| <b>Substances</b><br>12026-66-3<br>58834-75-6<br>catalyst-gas phase interactions in selective oxidn. of <b>light</b> alkanes to bulk and <b>industrial chems.</b><br>Catalyst use; Uses<br>1303-86-2 Boron oxide, uses<br>1332-29-2 Tin oxide<br>7631-86-9 Silica, uses  |                |                       |               |   |
|  |                |                       |               | <b>COMPANY/ORGANIZATION</b><br>Dipartimento di Chimica Industriale e dei Materiali<br>Bologna, Italy 40136  |
|  |                |                       |               | <b>ACCESSION NUMBER</b><br>1999:340014<br>CAN131:159478<br>CAPLUS   |
|  |                |                       |               | <b>PUBLISHER</b><br>Elsevier Science B.V.   |

### Citations

Bielanski, A; Oxygen in Catalysis 1991  
 Haber, J; ACS Symp Series 1996, 638, 20   
 Oyama, S; ACS Symp Series 1996, 638, 2   
 Lee, J; Catal Rev-Sci Eng 1988, 30, 249   
 Kung, H; Adv Catal 1994, 40, 1   
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 Vedrine, J; Catal Today 1996, 32, 115   
 Busca, G; Catal Today 1996, 32, 133   
 Cavani, F; Catalysis 1994, 11, 246   
 Albonetti, S; Catal Rev-Sci Eng 1996, 38, 413   
 Sokolovskii, V; Catal Rev-Sci Eng 1990, 32, 1   
 Delmon, B; Catalysts in Petroleum Refining and Petrochemical Industries 1995 1996  
 Burch, R; J Mol Catal A 1995, 100, 13   
 Schmidt, L; Chem Eng Sci 1994, 49, 3981   
 Kung, H; ACS Symp Series 1993, 523, 387  
 Trifiro, F; Selective Partial Oxidation of Hydrocarbons and Related Oxidations 1994  
 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： **Marine Drugs with anticancer** (海洋药物在抗肿瘤方面的研究进展)



The screenshot shows the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar menu is open, showing categories: REFERENCES, SUBSTANCES, and REACTIONS. Under REFERENCES, 'Research Topic' is selected. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing 'Marine Drugs with anticancer'. Below the input field, there are examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the main area, there is a link for '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 ▾
SciPlanner

Research Topic "Marine Drugs with anticancer"

**REFERENCES** ?

[Select All](#)   [Deselect All](#)

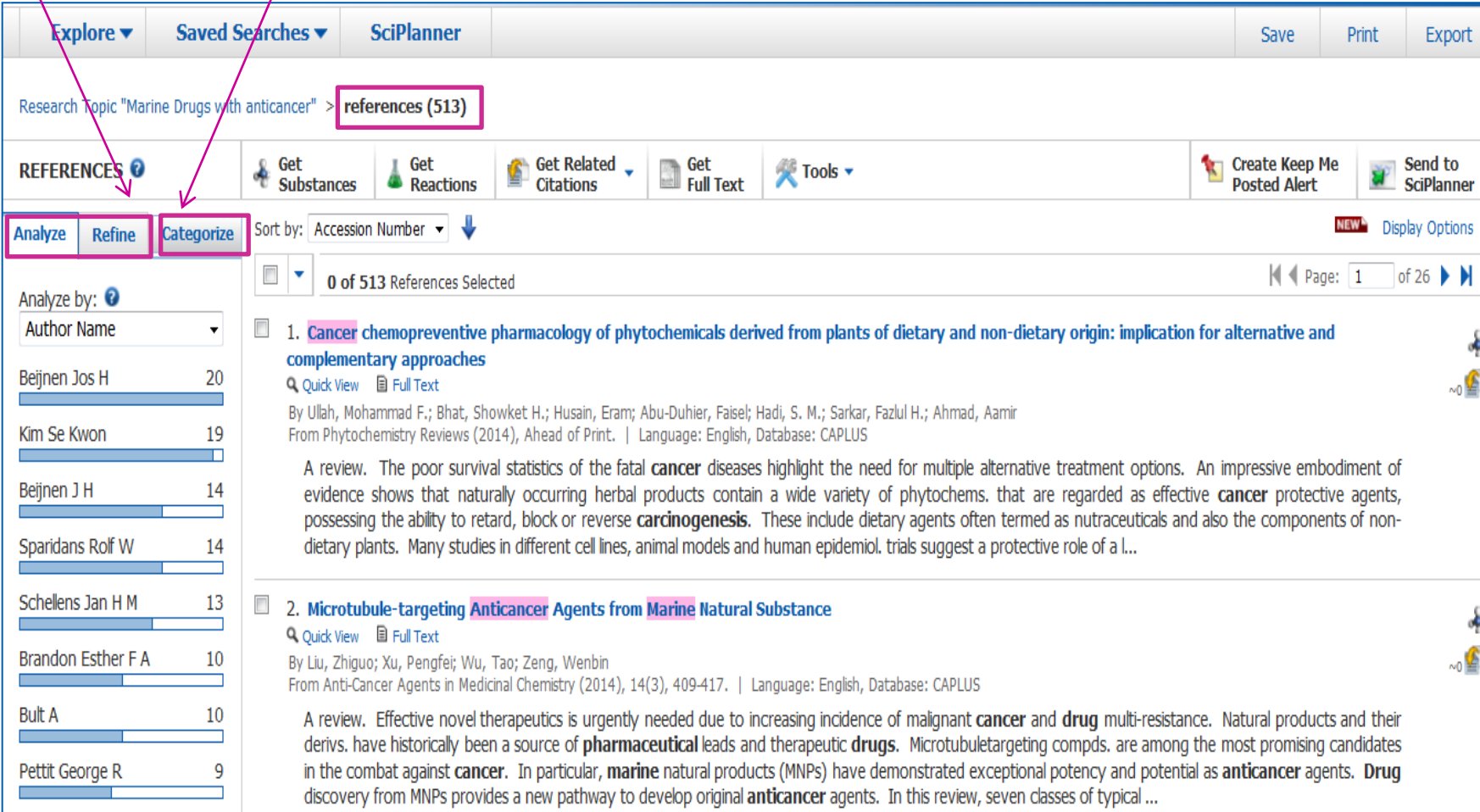
1 of 4 Research Topic Candidates Selected

|                                     |   | References |
|-------------------------------------|---|------------|
| <input checked="" type="checkbox"/> | 513 references were found containing the two <u>concepts "Marine Drugs" and "anticancer" closely associated with one another.</u> | 513        |
| <input type="checkbox"/>            | 1069 references were found where the two <u>concepts "Marine Drugs" and "anticancer" were present anywhere in the reference.</u>  | 1069       |
| <input type="checkbox"/>            | 4245 references were found containing the concept "Marine Drugs".   | 4245       |
| <input type="checkbox"/>            | 1005232 references were found containing the concept "anticancer".  | 1005232    |

- ◆ “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 "Marine Drugs with anticancer" > **references (513)**

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: Accession Number ▾

NEW Display Options

0 of 513 References Selected

Page: 1 of 26

- Cancer chemopreventive pharmacology of phytochemicals derived from plants of dietary and non-dietary origin: implication for alternative and complementary approaches**  
 Quick View | Full Text  
 By Ullah, Mohammad F.; Bhat, Showket H.; Husain, Eram; Abu-Duhier, Faisal; Hadi, S. M.; Sarkar, Fazlul H.; Ahmad, Aamir  
 From *Phytochemistry Reviews* (2014), Ahead of Print. | Language: English, Database: CAPLUS  
 A review. The poor survival statistics of the fatal **cancer** diseases highlight the need for multiple alternative treatment options. An impressive embodiment of evidence shows that naturally occurring herbal products contain a wide variety of phytochems. that are regarded as effective **cancer** protective agents, possessing the ability to retard, block or reverse **carcinogenesis**. These include dietary agents often termed as nutraceuticals and also the components of non-dietary plants. Many studies in different cell lines, animal models and human epidemiol. trials suggest a protective role of a l...
- Microtubule-targeting Anticancer Agents from Marine Natural Substance**  
 Quick View | Full Text  
 By Liu, Zhiguo; Xu, Pengfei; Wu, Tao; Zeng, Wenbin  
 From *Anti-Cancer Agents in Medicinal Chemistry* (2014), 14(3), 409-417. | Language: English, Database: CAPLUS  
 A review. Effective novel therapeutics is urgently needed due to increasing incidence of malignant **cancer** and **drug** multi-resistance. Natural products and their derivs. have historically been a source of **pharmaceutical** leads and therapeutic **drugs**. Microtubuletargeting compds. are among the most promising candidates in the combat against **cancer**. In particular, **marine** natural products (MNPs) have demonstrated exceptional potency and potential as **anticancer** agents. **Drug** discovery from MNPs provides a new pathway to develop original **anticancer** agents. In this review, seven classes of typical ...

| Author Name        | Count |
|--------------------|-------|
| Beijnen Jos H      | 20    |
| Kim Se Kwon        | 19    |
| Beijnen J H        | 14    |
| Sparidans Rolf W   | 14    |
| Schellens Jan H M  | 13    |
| Brandon Esther F A | 10    |
| Bult A             | 10    |
| Pettit George R    | 9     |

SciFinder提供强大的文献处理工具，帮助处理文献

# SciFinder提供的引文排序— Citing Reference

Explore ▾
Saved Searches ▾
SciPlanner
Save
Print
Export

Research Topic "Marine Drugs with anticancer" > **references (513)**

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

Analyze Refine Categorize

Analyze by: ?

Author Name ▾

Beijnen Jos H 20

Kim Se Kwon 19

Beijnen J H 14

Sparidans Rolf W 14

Schellens Jan H M 13

Brandon Esther F A 10

Bult A 10

Pettit George R 9

Jimeno Jose 8

Sort by: Citing References ▾

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

1. **Drug discovery from marine natural products**

By Molinski, Tadeusz F.; Dalisay, Doralyn S.; Lievens, Sarah L.; Saludes, Jonel P.  
 From Nature Reviews Drug Discovery (2009), 8(1), 69-85. | Language: English, Database: CAPLUS

A review. **Drug** discovery from **marine** natural products has enjoyed a renaissance in the past few years. Ziconotide (Prialt; Elan **Pharmaceuticals**), a peptide originally discovered in a tropical cone snail, was the first **marine**-derived compd. to be approved in the United States in Dec. 2004 for the treatment of pain. Then, in Oct. 2007, trabectedin (Yondelis; PharmaMar) became the first **marine anticancer drug** to be approved in the European Union. Here, we review the history of **drug** discovery from **marine** natural products, and by describing selected examples, we examine the factors that contrib...

2. **Marine-derived fungi: a chemically and biologically diverse group of microorganisms**

By Bugni, Tim S.; Ireland, Chris M.  
 From Natural Product Reports (2004), 21(1), 143-163. | Language: English, Database: CAPLUS

A review. A diverse array of secondary metabolites have been isolated and characterized from **marine**-derived fungi. The structures and biol. activities of these metabolites are presented. Addnl, some basic principles of mycol. are covered. Overall, 273 structures are presented and the review contains 162 refs.

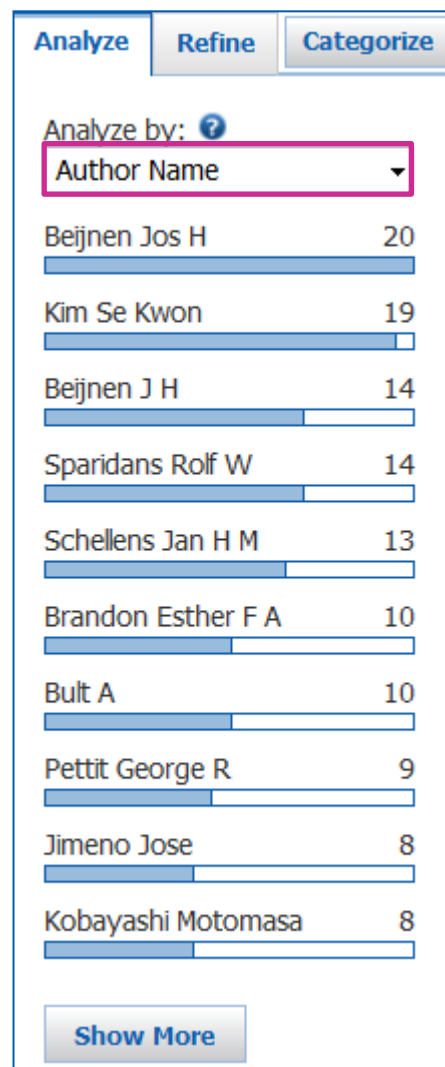
3. **Antiproliferative activity of ecteinascidin 743 is dependent upon transcription-coupled nucleotide-excision repair**

By Takebayashi, Yuji; Pourquier, Philippe; Zimonjic, Drazen B.; Nakayama, Kentaro; Emmert, Steffen; Ueda, Takahiro; Urasaki, Yoshimasa; Kanzaki, Arsuko; Akiyama, Shin-Ichi; Popescu, Nicholas; et al

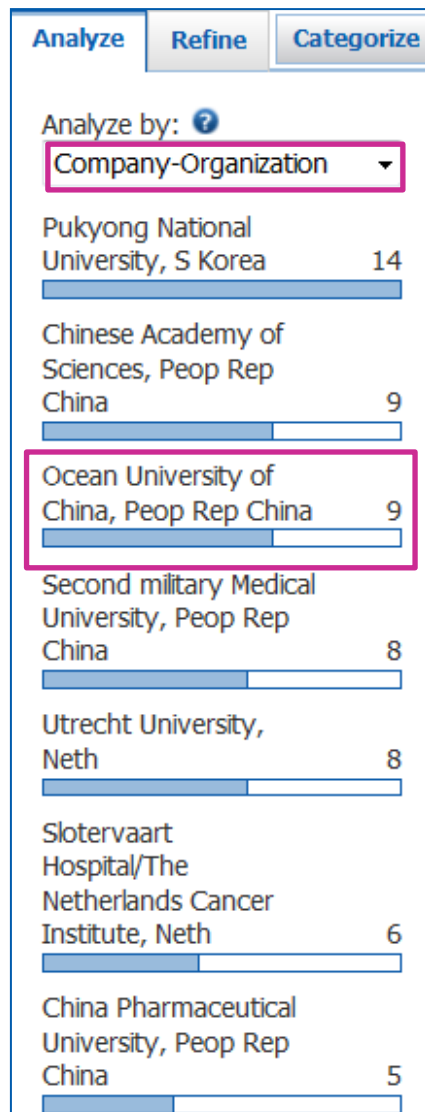
NEW Display Options  
Page: 1 of 26

# SciFinder中的Analyze

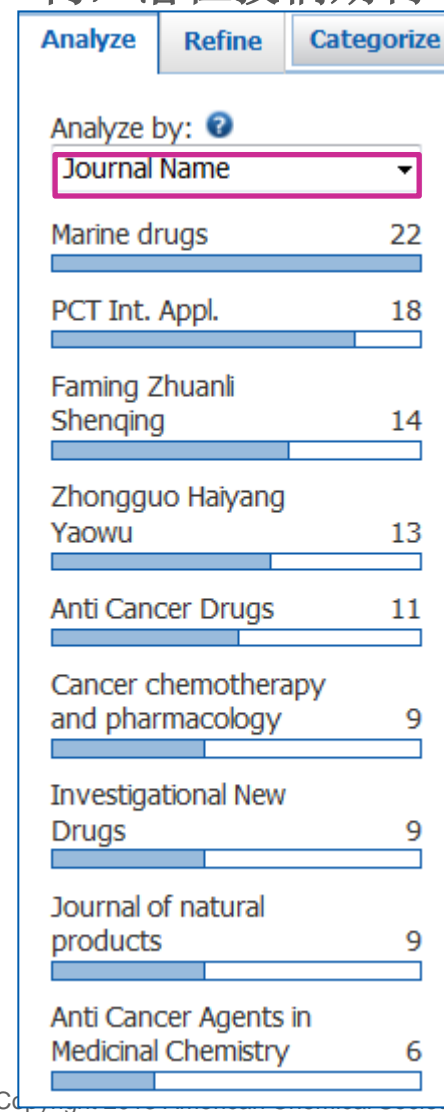
领域内主要研究人员，专家



主要研究机构，合作伙伴，竞争对手



主要出版杂志，机构，潜在投稿期刊





# SciFinder中的Analyze- Index Term

索引词 (Index Term)：可以帮助我们大致了解文献的内容

Analyze
Refine
Categorize

Analyze by: Index Term

|                                  |     |
|----------------------------------|-----|
| Antitumor agents                 | 331 |
| Natural products, pharmaceutical | 160 |
| Human                            | 157 |
| Neoplasm                         | 102 |
| Humans                           | 66  |
| Pharmacology                     | 66  |
| Animals                          | 63  |
| Antineoplastic Agents            | 55  |
| Apoptosis                        | 54  |
| Drug Discovery                   | 54  |

Show More

**Analyze - Index Term**

2668 Items
2 Selected
Export

Sort by: Frequency
Page: 1 of 20

Select bars to view only those references within the current answer set.

|  |     |
|--|-----|
| <input checked="" type="checkbox"/> Antitumor agents                 | 331 |
| <input checked="" type="checkbox"/> Natural products, pharmaceutical | 160 |
| <input type="checkbox"/> Human                                       | 157 |
| <input type="checkbox"/> Neoplasm                                    | 102 |
| <input type="checkbox"/> Humans                                      | 66  |
| <input type="checkbox"/> Pharmacology                                | 66  |
| <input type="checkbox"/> Animals                                     | 63  |
| <input type="checkbox"/> Antineoplastic Agents                       | 55  |
| <input type="checkbox"/> Apoptosis                                   | 54  |
| <input type="checkbox"/> Drug Discovery                              | 54  |

Apply

Cancel

# SciFinder中的Refine

## 文献类型限定：获得最新综述类文献

Analyze
Refine
Categorize

Refine by: ?

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

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Document Type(s)

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

Refine



0 of 219 References Selected
Page: 1 of 11

1. **Cancer** chemopreventive pharmacology of phytochemicals derived from plants of dietary and non-dietary origin: implication for alternative and complementary approaches

[Quick View](#) [Full Text](#)

By Ullah, Mohammad F.; Bhat, Showket H.; Husain, Eram; Abu-Duhier, Faisal; Hadi, S. M.; Sarkar, Fazlul H.; Ahmad, Aamir  
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A review. The poor survival statistics of the fatal **cancer** diseases highlight the need for multiple alternative treatment options. An impressive embodiment of evidence shows that naturally occurring herbal products contain a wide variety of phytochems. that are regarded as effective **cancer** protective agents, possessing the ability to retard, block or reverse **carcinogenesis**. These include dietary agents often termed as nutraceuticals and also the components of non-dietary plants. Many studies in different cell lines, animal models and human epidemiol. trials suggest a protective role of a l...

  

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3. **Marine Bromopyrrole Alkaloids: Synthesis and Diverse Medicinal Applications**

[Quick View](#) [Full Text](#)

By Rane, Rajesh; Sahu, Niteshkumar; Shah, Chetan; Karpoomath, Rajshekhhar  
 From *Current Topics in Medicinal Chemistry (Sharjah, United Arab Emirates)* (2014), 14(2), 253-273. | Language: English, Database: CAPLUS

A review. **Marine** organisms have been found to be a very rich source of bioactive mols. Among **marine** organisms, sponges have been proven to be excellent producers of secondary metabolites. More than 5,300 compds. have been isolated from sponges with around 200 new mols. reported each year. Bromopyrrole alkaloids constitute a family of exclusively **marine** alkaloids and represent a fascinating example of the large variety of compds. formed by **marine** sponges which exhibit different biol. activities such as antifeedent, **anti**-biofilm, **anticancer**, antiinflammatory, antimicrobial, immunomodulatory,...

# SciFinder 中的Categorize

REFERENCES ?

Analyze Refine **Categorize**

Analyze by: ?

Author Name

|                    |    |
|--------------------|----|
| Beijnen Jos H      | 20 |
| Kim Se Kwon        | 19 |
| Beijnen J H        | 14 |
| Sparidans Rolf W   | 14 |
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| Pettit George R    | 9  |
| Jimeno Jose        | 8  |
| Kobayashi Motomasa | 8  |

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1. **Cancer chemopreventive pharmacology of phytochemicals derived from plants of dietary and non-dietary origin: implication for alternative and complementary approaches**

Quick View Full Text

By Ullah, Mohammad F.; Bhat, Showket H.; Husain, Eram; Abu-Duhier, Faisal; Hadi, S. M.; Sarkar, Fazlul H.; Ahmad, Aamir  
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2. **Microtubule-targeting Anticancer Agents from Marine Natural Substance**

Quick View Full Text

By Liu, Zhiguo; Xu, Pengfei; Wu, Tao; Zeng, Wenbin  
 From Anti-Cancer Agents in Medicinal Chemistry (2014), 14(3), 409-417. | Language: English, Database: CAPLUS

A review. Effective novel therapeutics is urgently needed due to increasing incidence of malignant **cancer** and **drug** multi-resistance. Natural products and their derivs. have historically been a source of **pharmaceutical** leads and therapeutic **drugs**. Microtubuletargeting compds. are among the most promising candidates in the combat against **cancer**. In particular, **marine** natural products (MNPs) have demonstrated exceptional potency and potential as **anticancer** agents. **Drug** discovery from MNPs provides a new pathway to develop original **anticancer** agents. In this review, seven classes of typical ...



---

3. **Marine Bromopyrrole Alkaloids: Synthesis and Diverse Medicinal Applications**

Quick View Full Text

By Rane, Rajesh; Sahu, Niteshkumar; Shah, Chetan; Karpoomath, Rajshekhhar  
 From Current Topics in Medicinal Chemistry (Sharjah, United Arab Emirates) (2014), 14(2), 253-273. | Language: English, Database: CAPLUS

A review. **Marine** organisms have been found to be a very rich source of bioactive mols. Among **marine** organisms, sponges have been proven to be excellent

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.      2. Select index terms of interest.

| Category Heading | Category                     | Index Terms   | Selected Terms   |
|------------------|------------------------------|---|--|
| All              | Substances in medicine (979) | Page: 1 of 10<br>Select All   Deselect All<br><input type="checkbox"/> Antitumor agents 48<br><input type="checkbox"/> Natural products, pharmaceutical 31<br><input checked="" type="checkbox"/> Yondelis 24<br><input type="checkbox"/> Peptides 20<br><input type="checkbox"/> Alkaloids 19<br><input type="checkbox"/> Apoptosis 16<br><input type="checkbox"/> Aplidin 15<br><input type="checkbox"/> Doxorubicin 11<br><input type="checkbox"/> Paclitaxel 11<br><input type="checkbox"/> Cytarabine 9<br><input type="checkbox"/> Didemnin B 9<br><input type="checkbox"/> Isoquinoline 9<br><input type="checkbox"/> Kahalalide F 9<br><input type="checkbox"/> Cell division 8<br><input type="checkbox"/> Vinblastine 8 | Click 'x' to remove the category from 'Selected Terms'<br>* Biotechnology > Substances in medicine (1 Terms) |

Biotechnology > Substances in medicine > 1 Index Term(s) Selected

OK   Cancel

曲贝替定

# SciFinder中的KMP

随时跟踪科研最新进展

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Sort by: Accession Number

0 of 513 References Selected

1. **Cancer chemopreventive pharmacology of phytochemicals derived from plants of dietary and non-dietary origin: implication for alternative and complementary approaches**  
 Quick View | Full Text  
 By Ullah, Mohammad F.; Bhat, Showket H.; Husain, Eram; Abu-Duhier, Faisal; Hadi, S. M.; Sarkar, Fazlul H.; Ahmad, Aamir  
 From Phytochemistry Reviews (2014), Ahead of Print. | Language: English, Database: CAPLUS  
 A review. The poor survival statistics of the fatal **cancer** diseases highlight the need for multiple alternative treatment options. An impressive embodiment of evidence shows that naturally occurring herbal products contain a wide variety of phytochems. that are regarded as effective **cancer** protective agents, possessing the ability to retard, block or reverse **carcinogenesis**. These include dietary agents often termed as nutraceuticals and also the components of non-dietary plants. Many studies in different cell lines, animal models and human epidemiol. trials suggest a protective role of a L...

2. **Microtubule-targeting Anticancer Agents from Marine Natural Substance**  
 Quick View | Full Text  
 By Liu, Zhiguo; Xu, Pengfei; Wu, Tao; Zeng, Wenbin  
 From Anti-Cancer Agents in Medicinal Chemistry (2014), 14(3), 409-417. | Language: English, Database: CAPLUS  
 A review. Effective novel therapeutics is urgently needed due to increasing incidence of malignant **cancer** and **drug** multi-resistance. Natural products and their derivs. have historically been a source of **pharmaceutical** leads and therapeutic **drugs**. Microtubuletargeting compds. are among the most promising candidates in the combat against **cancer**. In particular, **marine** natural products (MNPs) have demonstrated exceptional potency and potential as **anticancer** agents. **Drug** discovery from MNPs provides a new pathway to develop original **anticancer** agents. In this review, seven classes of typical ...

### Create Keep Me Posted Profile

**Title: \***  \* Required

**Description:**

Characters Remaining: 1024

**Duration**  
Expires On: Apr 07, 2015 [Change](#)

**Frequency**  
Send updates once every

Exclude previously retrieved references.

[Create](#) [Cancel](#)

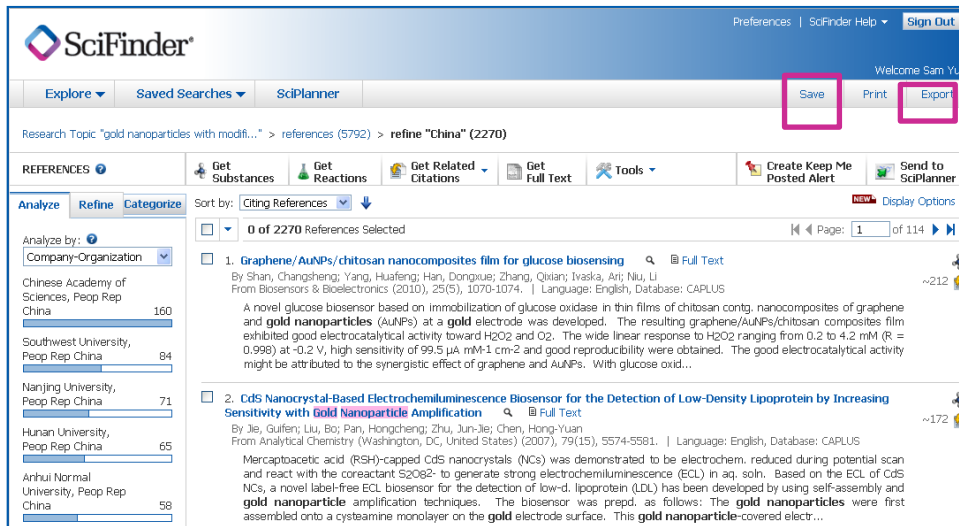
**Search:**  
Explore references by research topic: **Marine Drugs with anticancer**

**Candidates Selected:**  
References which contain the two concepts "Marine Drugs" and "anticancer" closely associated with one another

设置有效期

设置提醒频率

# 结果集的保存



SciFinder® Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

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 | Display Options

0 of 2270 References Selected | Page: 1 of 114

1. **Graphene/AuNPs/chitosan nanocomposites film for glucose biosensing** | Full Text | ~212  
 By Shan, Changsheng; Yang, Huaifeng; Han, Dongxue; Zhang, Qitian; Ivaska, Art; Niu, Li  
 From Biosensors & Bioelectronics (2010), 25(5), 1070-1074. | Language: English, Database: CAPLUS  
 A novel glucose biosensor based on immobilization of glucose oxidase in thin films of chitosan contg. nanocomposites of graphene and gold nanoparticles (AuNPs) at a gold electrode was developed. The resulting graphene/AuNPs/chitosan composites film exhibited good electrocatalytic activity toward H<sub>2</sub>O<sub>2</sub> and O<sub>2</sub>. The wide linear response to H<sub>2</sub>O<sub>2</sub> ranging from 0.2 to 4.2 mM (R = 0.998) at -0.2 V, high sensitivity of 99.5 μA mM<sup>-1</sup> cm<sup>-2</sup> and good reproducibility were obtained. The good electrocatalytic activity might be attributed to the synergistic effect of graphene and AuNPs. With glucose oxid...

2. **CdS Nanocrystal-Based Electrochemiluminescence Biosensor for the Detection of Low-Density Lipoprotein by Increasing Sensitivity with Gold Nanoparticle Amplification** | Full Text | ~172  
 By Jie, Gufen; 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  
 Mercaptoacetic acid (RSH)-capped CdS nanocrystals (NCs) was demonstrated to be electrochem. reduced during potential scan and react with the coreactant S<sub>2</sub>O<sub>8</sub><sup>2-</sup> to generate strong electrochemiluminescence (ECL) in aq. soln. Based on the ECL of CdS NCs, a novel label-free ECL biosensor for the detection of low-d. lipoprotein (LDL) has been developed by using self-assembly and gold nanoparticle amplification techniques. The biosensor was prepd. as follows: The gold nanoparticles were first assembled onto a cysteamine monolayer on the gold electrode surface. This gold nanoparticle-covered electr...

**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

### Save This Answer Set

\* Required

**Save:**

All answers

Only selected answers

**Title: \***

**Description:**

OK Cancel

**Save:**  
保存在服务器上，可登陆后查看

### Export

\* Required

**Export:**

All

Selected

Range

Example: 2-20

**For:**

**Citation Manager**

Citation export format (\*.ris)

Quoted Format (\*.bt)

Tagged Format (\*.bt)

**Offline review**

Portable Document Format (\*.pdf)

Rich Text Format (\*.rtf)

Answer Keys (\*.bt)

**Saving locally**

Answer Key eXchange (\*.alox)

**Details:**

**File Name: \***

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

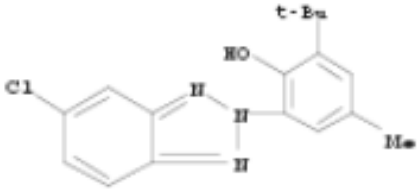
- 介绍
  - SciFinder Web中的内容
  - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索技巧
  - SciFinder Web中的反应检索及SciPlanner功能
- **SciFinder Web的注册和常见问题**



# SciFinder中的物质结果界面

1. 3896-11-5

~2057 
~54 



**C17 H18 Cl N3 O**  
 Phenol, 2-(5-chloro-2*H*-benzotriazol-2-yl)-6-(1,1-dimethylethyl)-4-methyl-

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

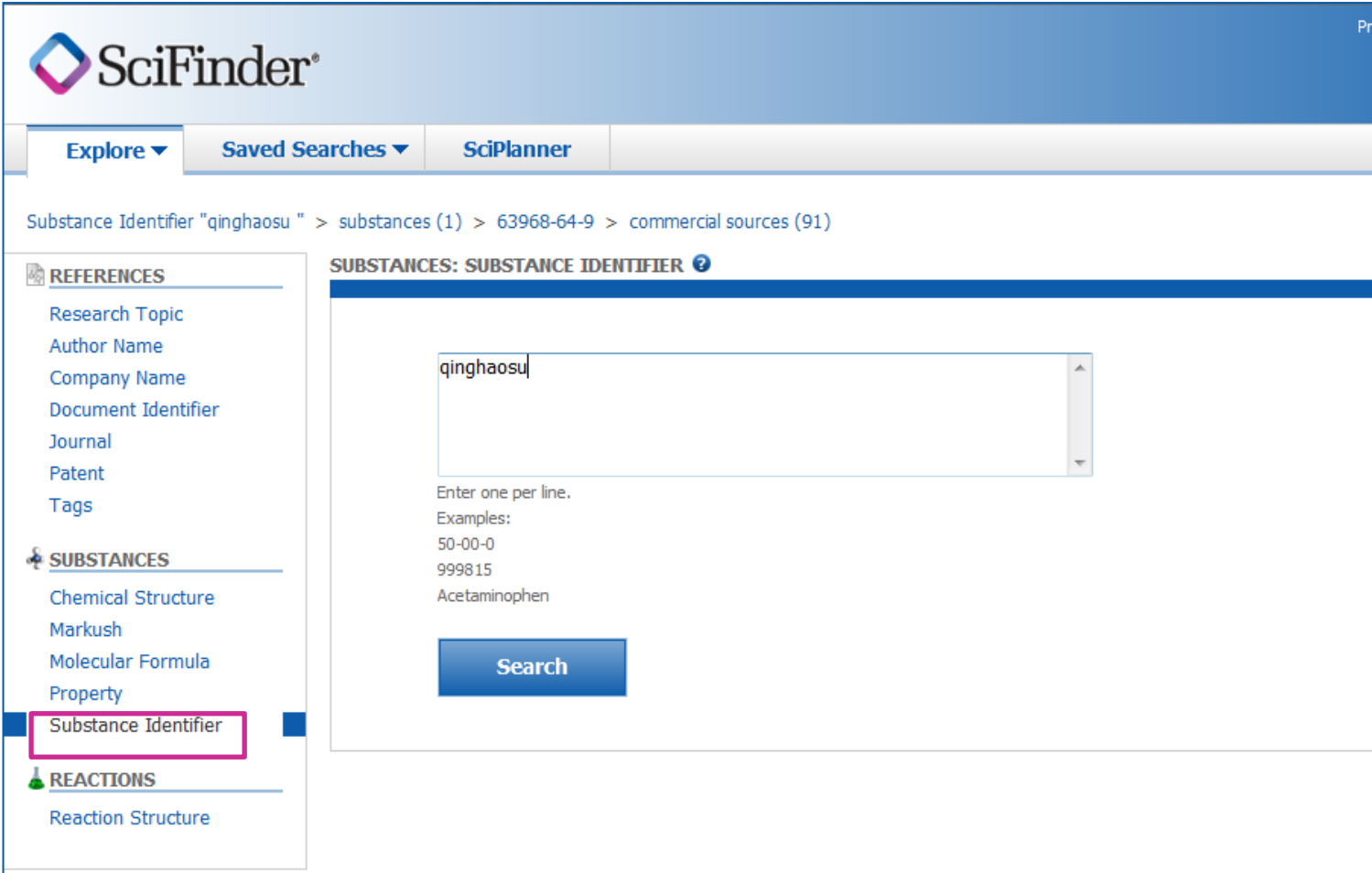
一个完整的物质结果界面包含：

- 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

# 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**

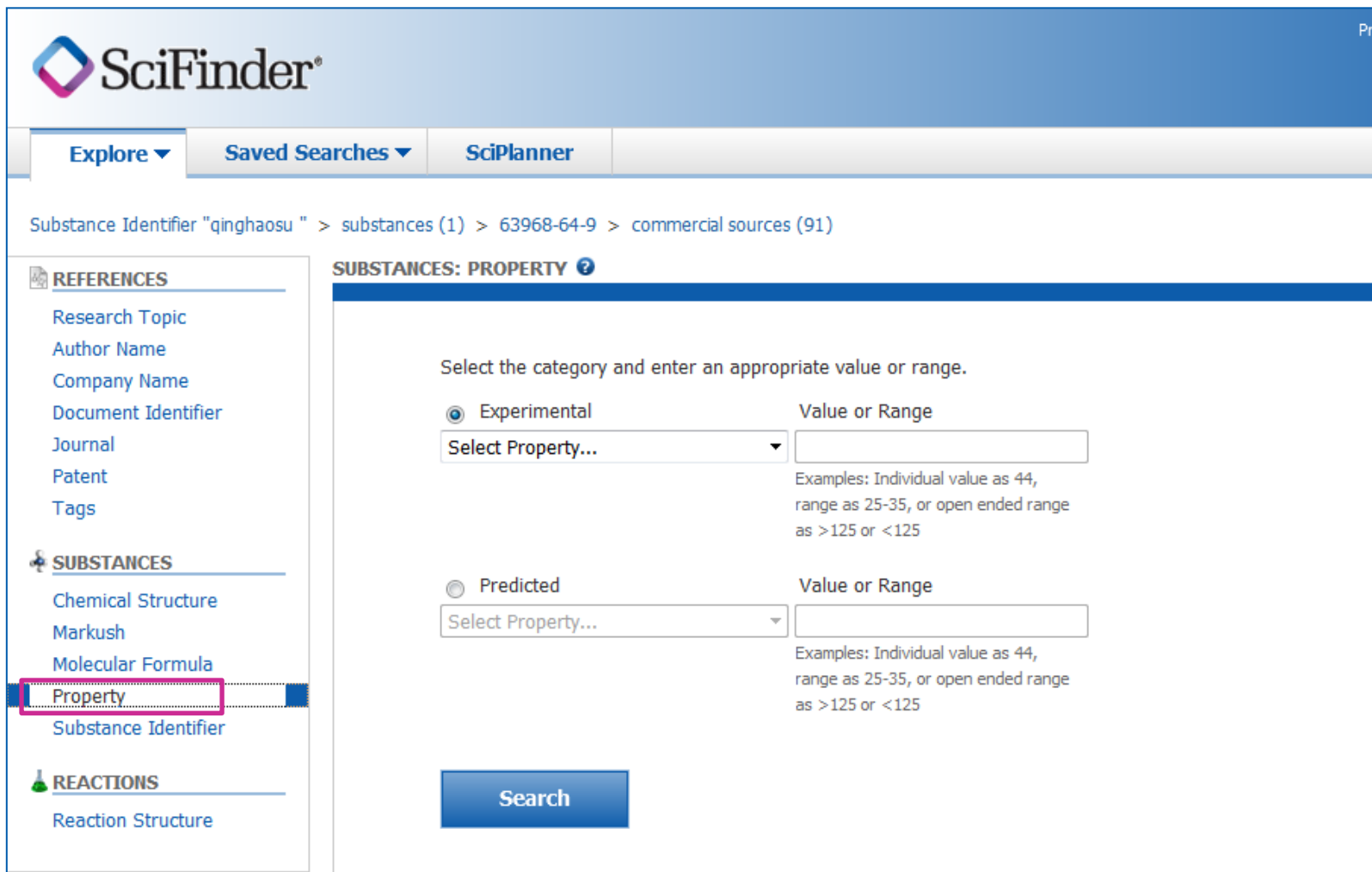
qinghaosu

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



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

Select Property...

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

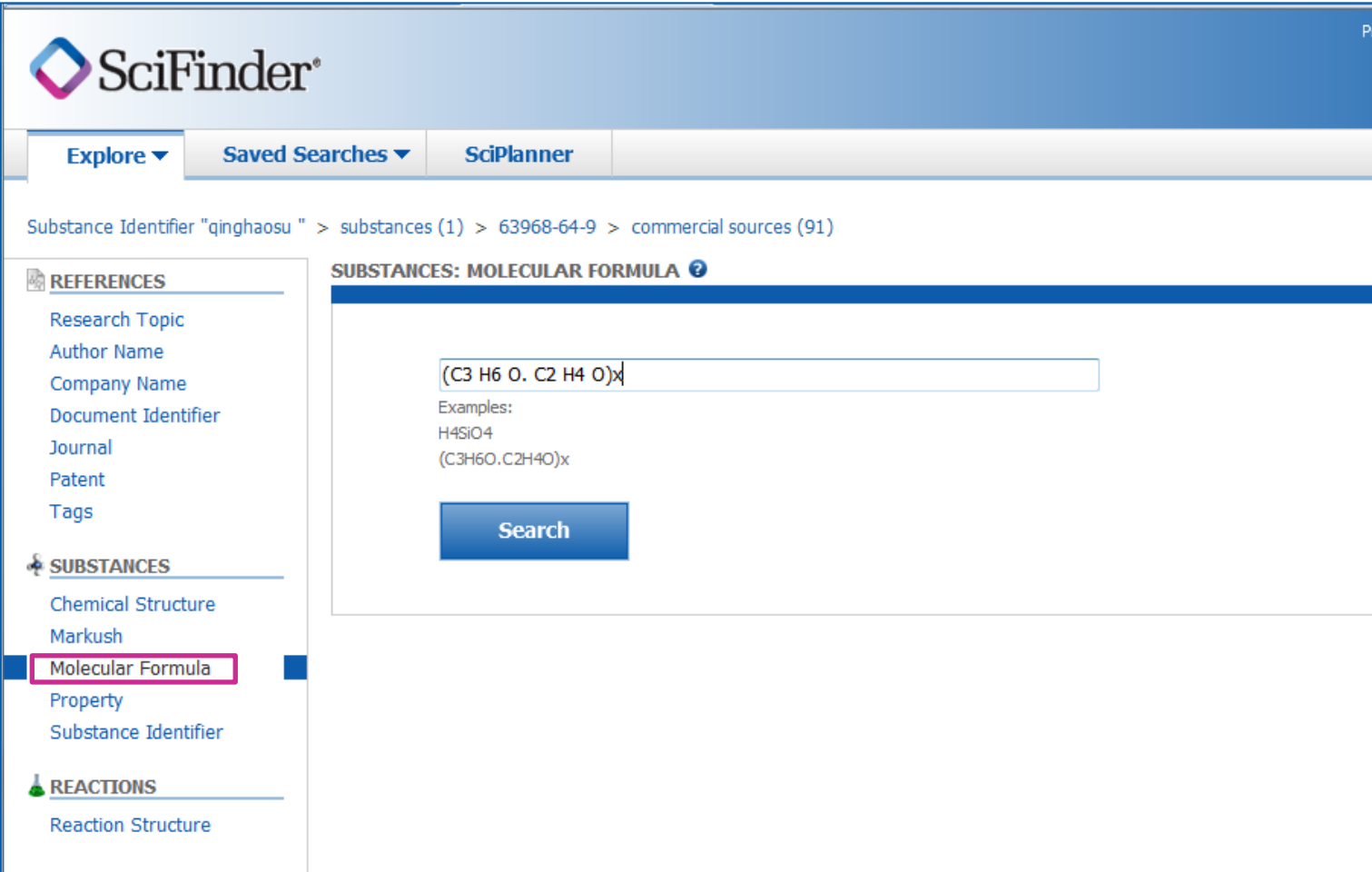
Predicted

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



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: MOLECULAR FORMULA ?**

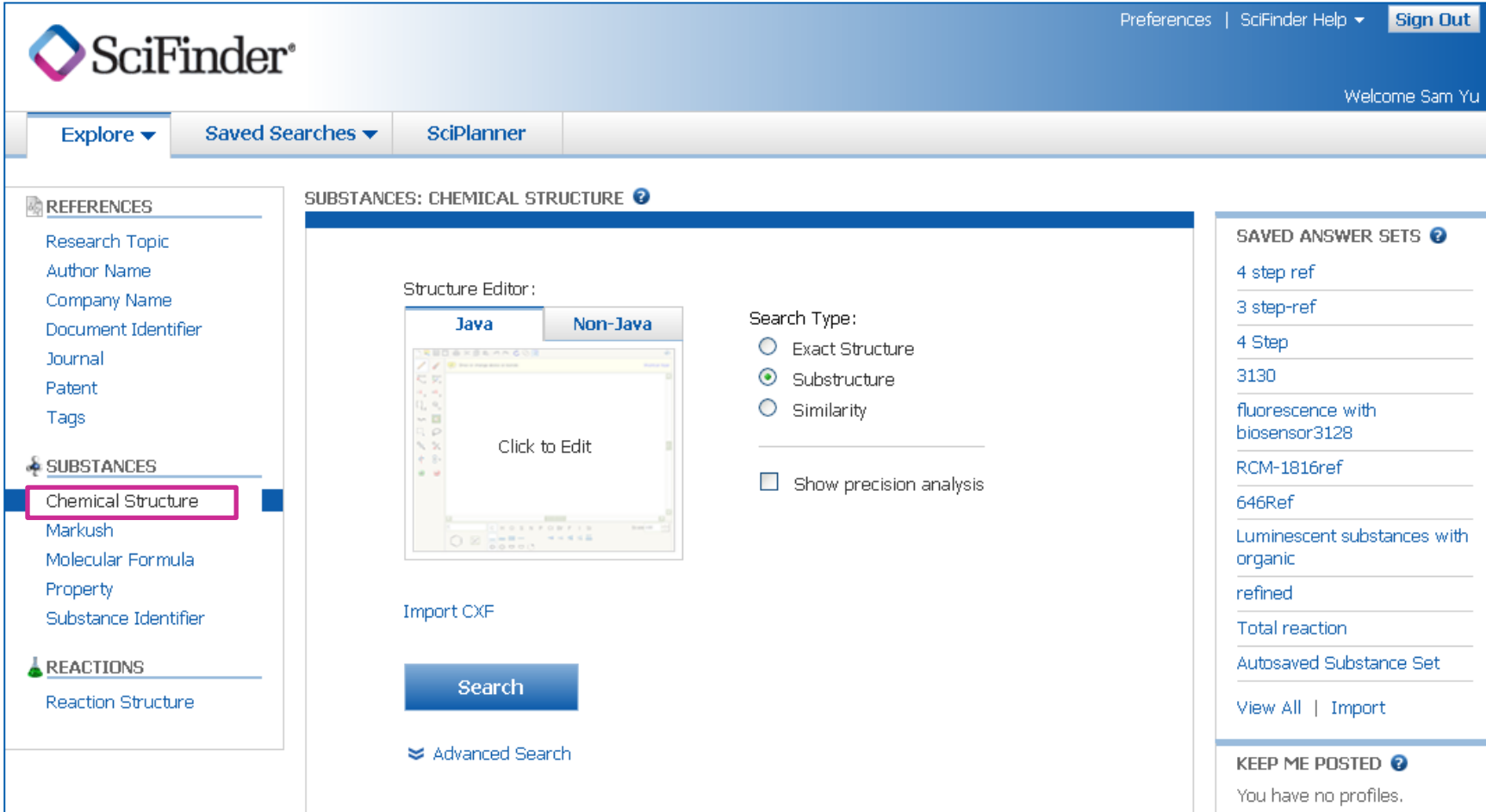
(C3 H6 O. C2 H4 O)x

Examples:  
 H4SiO4  
 (C3H6O.C2H4O)x

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



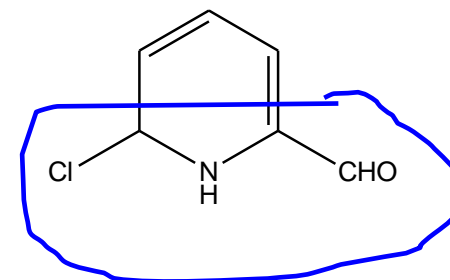
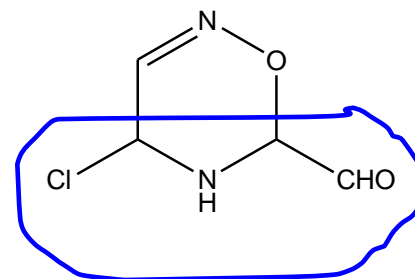
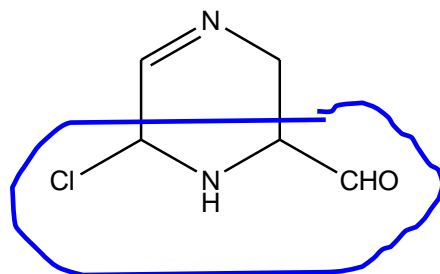
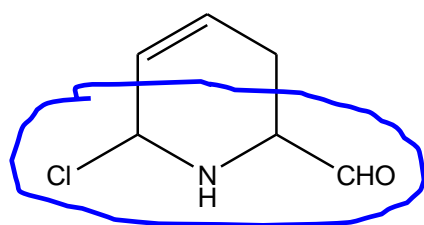
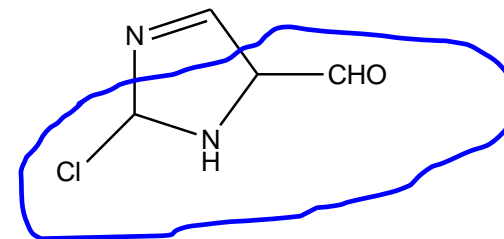
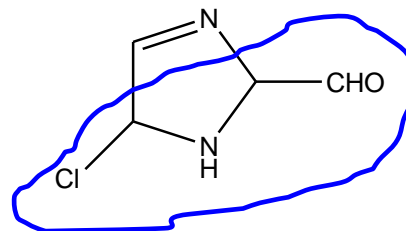
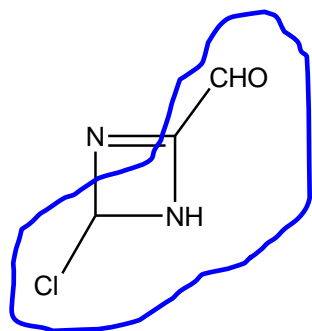
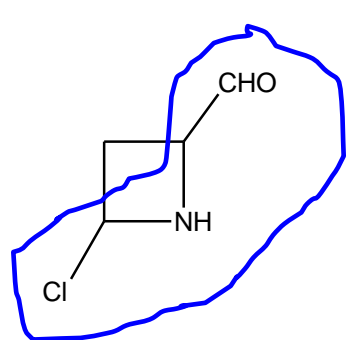
The screenshot displays the SciFinder web interface for chemical structure search. At the top, the SciFinder logo is on the left, and navigation links for 'Preferences', 'SciFinder Help', and 'Sign Out' are on the right. A user greeting 'Welcome Sam Yu' is visible in the top right corner. Below the header is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE'. On the left, a sidebar menu lists 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier). The 'Chemical Structure' option is highlighted with a red box. Below the sidebar, the 'REACTIONS' section includes 'Reaction Structure'. The central workspace features a 'Structure Editor' with 'Java' and 'Non-Java' tabs, a 'Click to Edit' button, and an 'Import CXF' option. To the right of the editor, the 'Search Type' section includes radio buttons for 'Exact Structure', 'Substructure' (selected), and 'Similarity', along with a checkbox for 'Show precision analysis'. A blue 'Search' button is located below the editor. At the bottom of the workspace, there is an 'Advanced Search' link. On the right side of the interface, the 'SAVED ANSWER SETS' section lists several saved sets: '4 step ref', '3 step-ref', '4 Step', '3130', 'fluorescence with biosensor3128', 'RCM-1816ref', '646Ref', 'Luminescent substances with organic refined', 'Total reaction', and 'Autosaved Substance Set'. At the bottom of this section, there are 'View All' and 'Import' links. Below the saved sets, the 'KEEP ME POSTED' section indicates 'You have no profiles.'

# SciFinder结构绘制工具

The screenshot shows the SciFinder Structure Editor interface with various tools highlighted by red boxes and Chinese labels. The interface includes a toolbar on the left, a central drawing area, and a right-hand panel with search options. 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 (Repeat 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 recovery tool)
- 负电子 (Electron)
- 结构检索选择 (Structure search selection)
- 单双键, RS构型, 不确定键定义工具 (Single/double bond, RS configuration, uncertain bond definition tool)
- 常见环, 多元环工具 (Common rings, multi-membered rings tool)

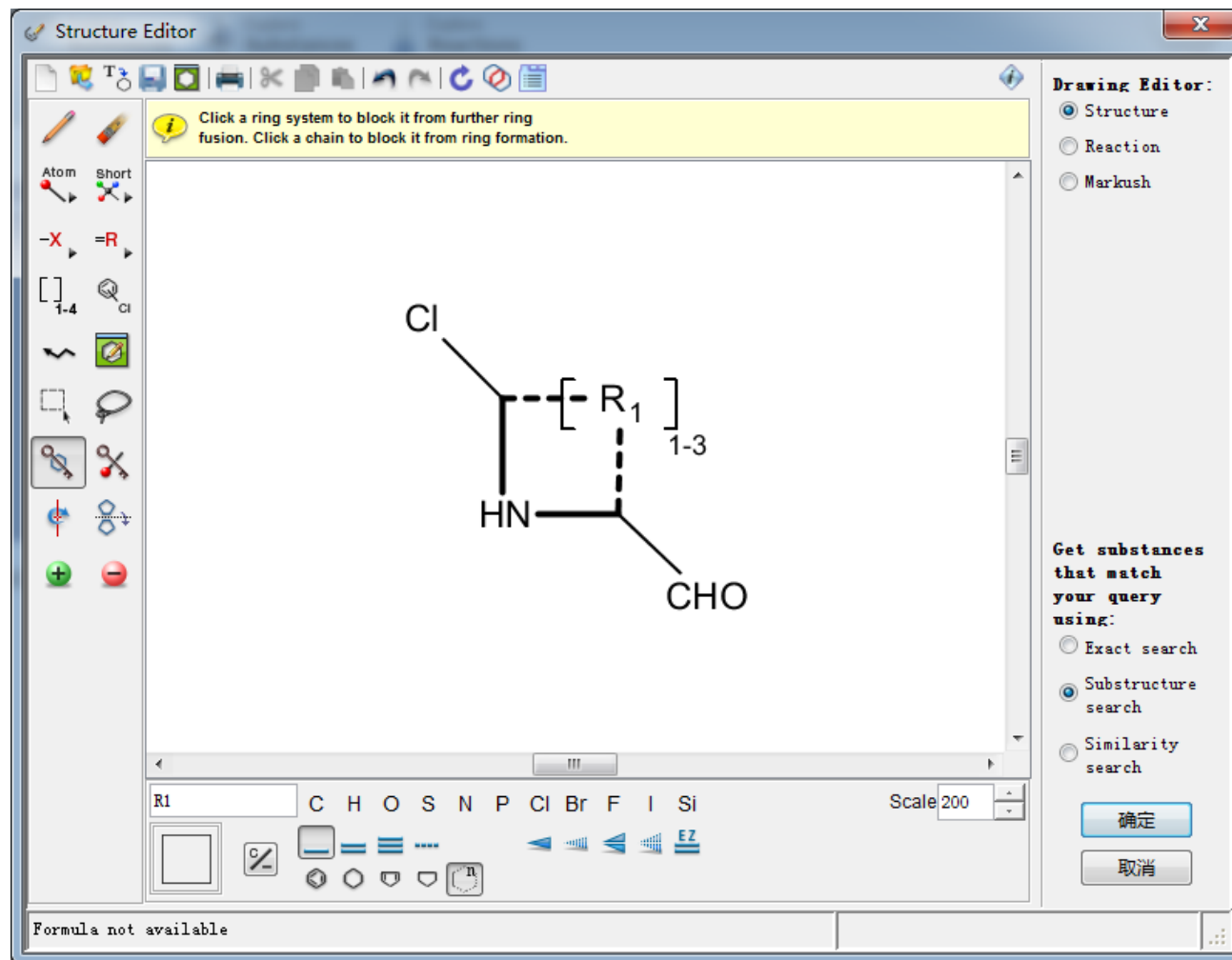
# 想获得以下的一系列物质



○ ○ ○ ○ ○ ○




# 结构定义



用亚结构检索获得所有的物质

# 亚结构检索结果


Preferences | SciFinder Help Sign Out

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

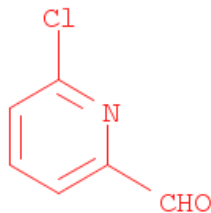
Prophetic in Patents 8

Properties 6

Formation, Nonpreparative 2

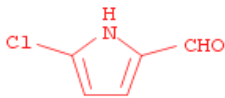
Analytical Study 1

1. Substance Detail  
54087-03-5



**C<sub>6</sub> H<sub>4</sub> Cl N O**

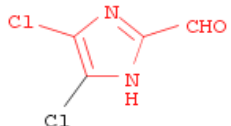
2. Substance Detail  
1757-28-4



**C<sub>5</sub> H<sub>4</sub> Cl N O**  
1H-Pyrrole-2-carboxaldehyde, 5-chloro-

Experimental Properties

3. Substance Detail  
81293-97-2



**C<sub>4</sub> H<sub>2</sub> Cl<sub>2</sub> N<sub>2</sub> O**  
1H-Imidazole-2-carboxaldehyde, 4,5-dichloro-

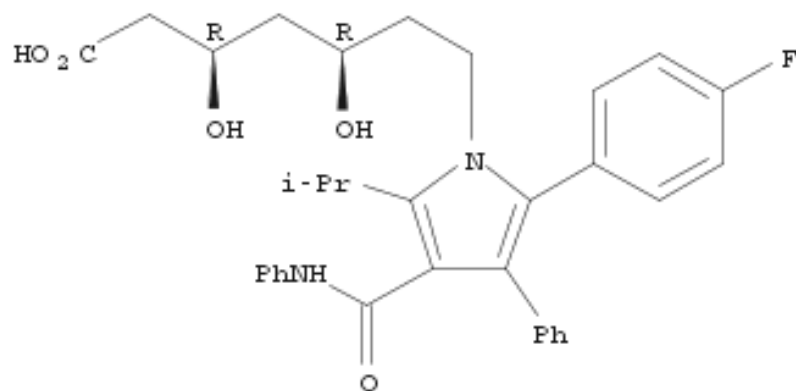
CAS is a division of the American Chemical Society.

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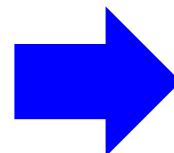
34

# 案例研究

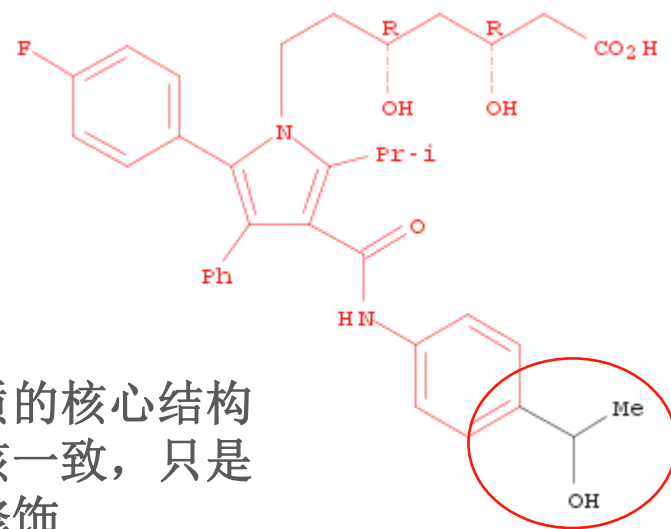
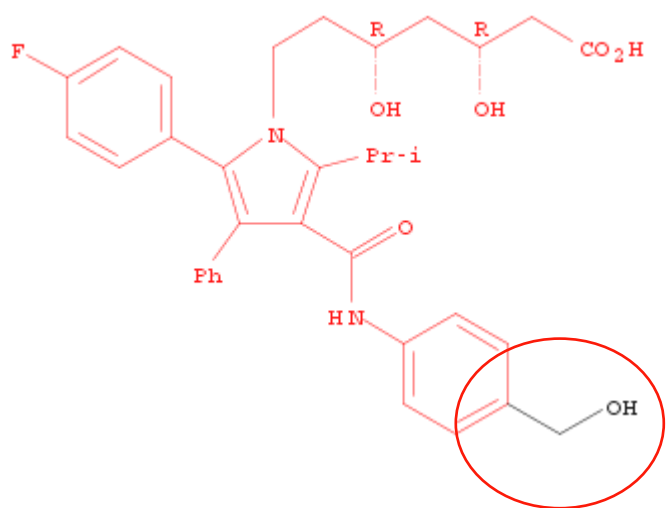
对某一结构进行改造，看是否有更好的新结构



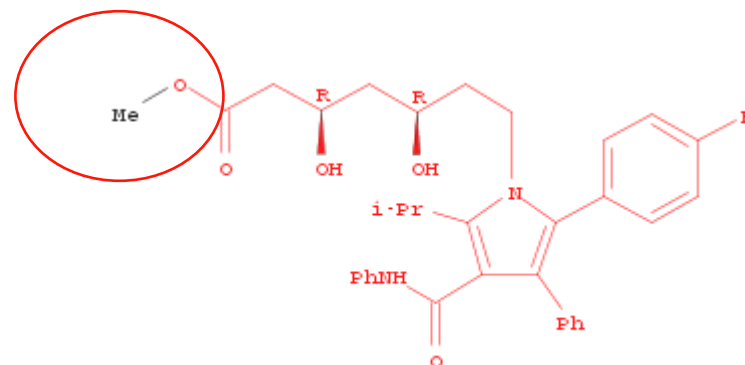
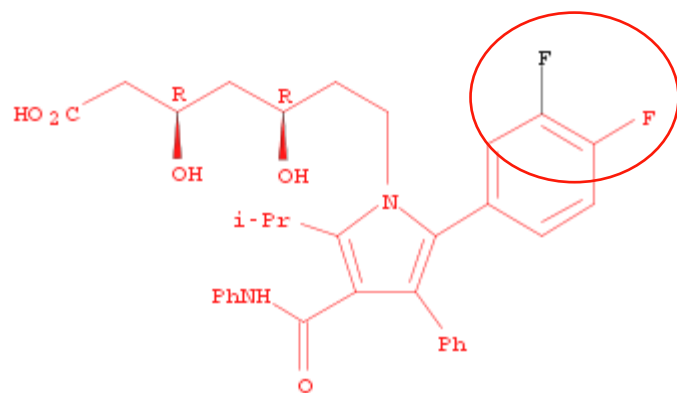
• 1/2 Ca



# Substructure Search—用于检索结构的修饰物



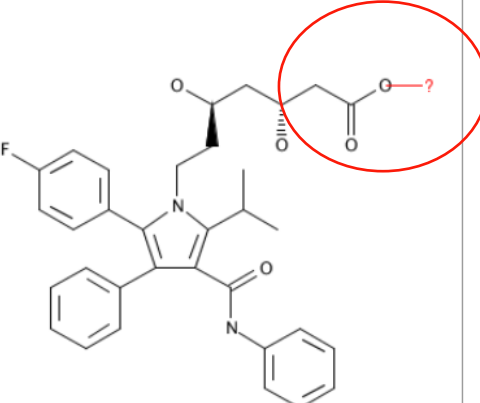
这些物质的核心结构都和母核一致，只是多了些修饰



# 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

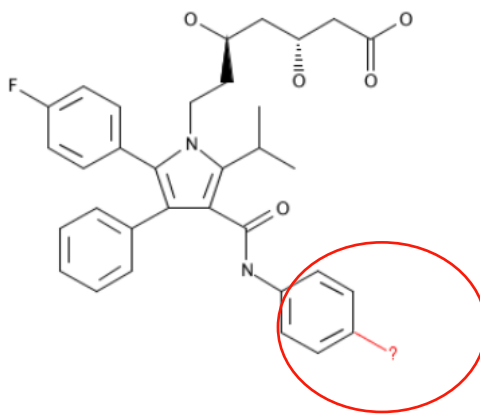
|   |      |
|---|------|
| <input type="checkbox"/> H or None                  | 487  |
| <input type="checkbox"/> C                          | 1049 |
| <input type="checkbox"/> N                          | 2    |
| <input type="checkbox"/> Ca                         | 2    |
| <input type="checkbox"/> 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**

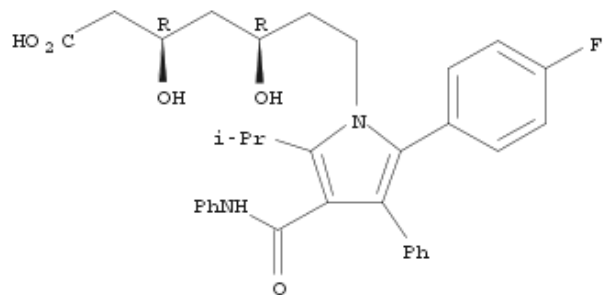


**Atom Attachments**

Select All   Deselect All

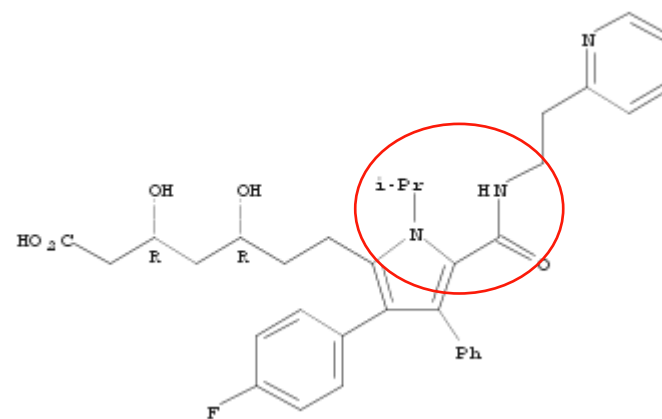
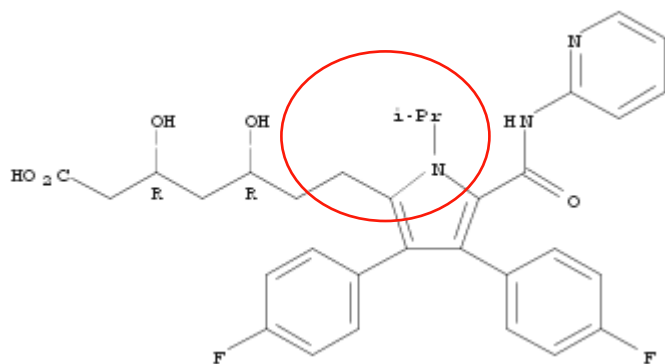
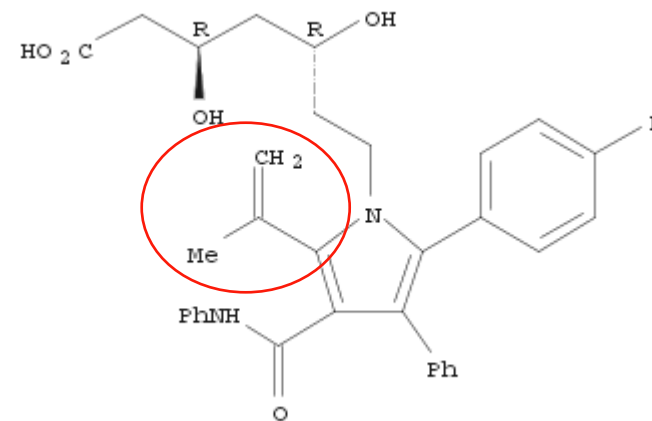
|   |      |
|---|------|
| <input type="checkbox"/> H or None                    | 1342 |
| <input type="checkbox"/> C                            | 109  |
| <input type="checkbox"/> O                            | 58   |
| <input type="checkbox"/> N                            | 29   |
| <input type="checkbox"/> 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

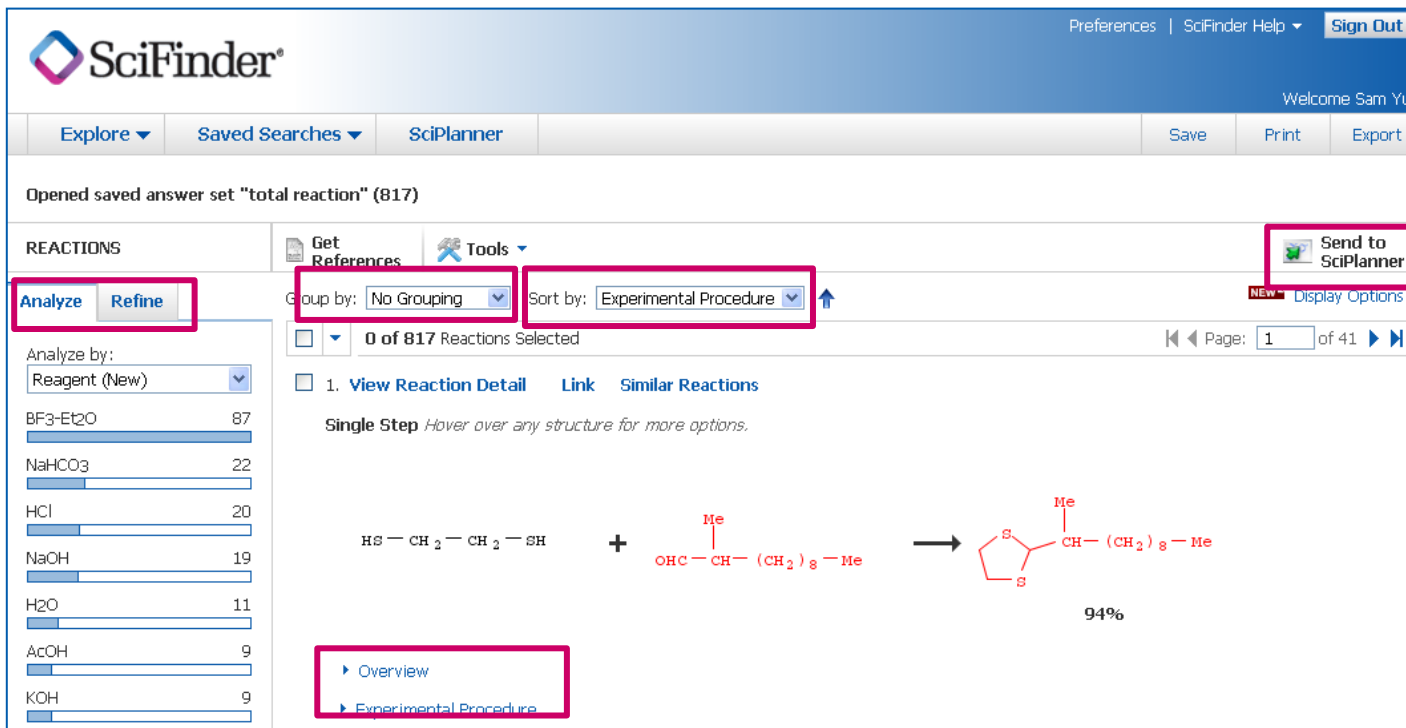
结构都存在相似性，  
但是又和原结构有  
不同的地方



# 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中的反应检索及SciPlanner功能
- **SciFinder Web的注册和常见问题**

# SciFinder Web中的反应记录



SciFinder<sup>®</sup> Preferences | SciFinder Help | Sign Out

Welcome Sam Yu

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

Opened saved answer set "total reaction" (817)

REACTIIONS

Get References | Tools

Analyze | Refine

Group by: No Grouping | Sort by: Experimental Procedure

Send to SciPlanner

0 of 817 Reactions Selected

1. View Reaction Detail | Link | Similar Reactions

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

$\text{HS}-\text{CH}_2-\text{CH}_2-\text{SH} + \text{Me}-\text{CH}(\text{OH})-(\text{CH}_2)_8-\text{Me} \rightarrow \text{Product} \quad 94\%$

Overview | Experimental Procedure

Analyze by: Reagent (New)

|                                    |    |
|------------------------------------|----|
| BF <sub>3</sub> -Et <sub>2</sub> O | 87 |
| NaHCO <sub>3</sub>                 | 22 |
| HCl                                | 20 |
| NaOH                               | 19 |
| H <sub>2</sub> O                   | 11 |
| AcOH                               | 9  |
| KOH                                | 9  |

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

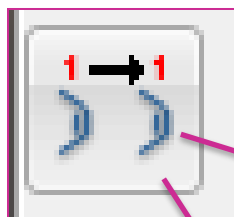


# SciFinder中的反应定义工具

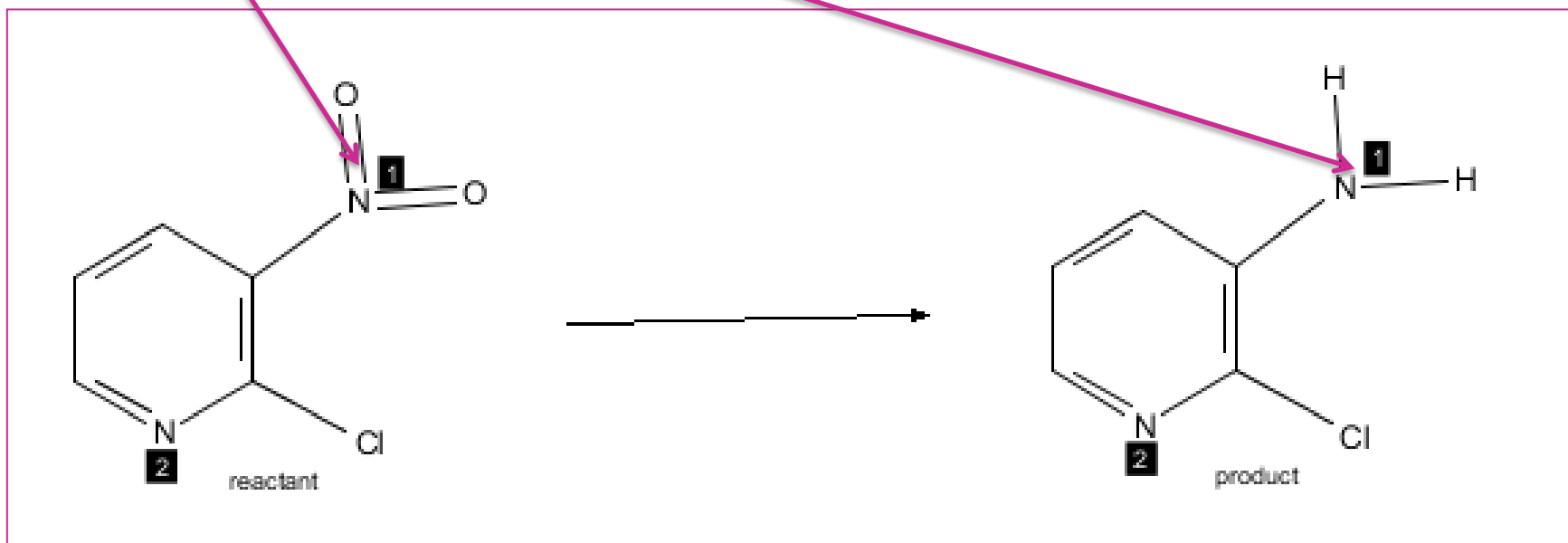
The image shows the 'Reaction Editor' window in SciFinder. The interface is divided into several sections:

- Left Toolbar:** Contains various drawing tools for atoms, bonds, and reaction symbols. Annotations with red boxes and lines point to:
  - 反应箭头:** Points to the reaction arrow icon.
  - 反应原子标记工具:** Points to the atom labeling tool (A, B).
  - 反应官能团列表:** Points to the functional group list (alchc, ketor, alder).
- Central Drawing Area:** A large white space for drawing chemical structures. A yellow banner at the top says 'Draw or change atoms or bonds.' and 'Shortcut Keys' is visible on the right.
- Right Panel:**
  - Drawing Editor:** Radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'.
  - Get reactions where the structure(s) are:**
    - Radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures' (selected).
  - Buttons for '确定' (OK) and '取消' (Cancel).
- Bottom:** A chemical element palette (C, H, O, S, N, P, Cl, Br, F, I, Si) and a 'Scale 100' dropdown.

# 反应精准性定义工具—原子标记工具



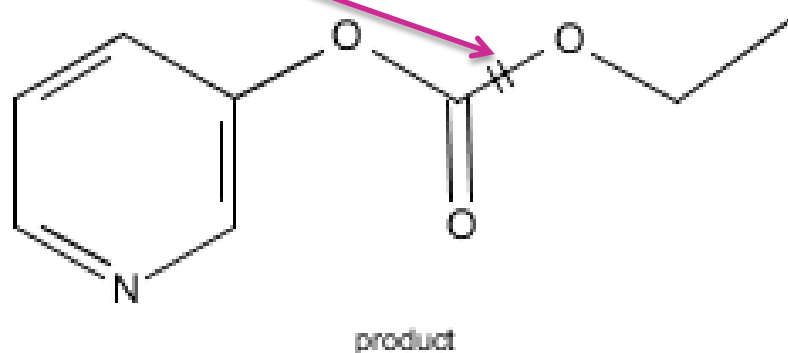
原子标记工具标记反应前后必须匹配的原子，主要用于反应中心的定义



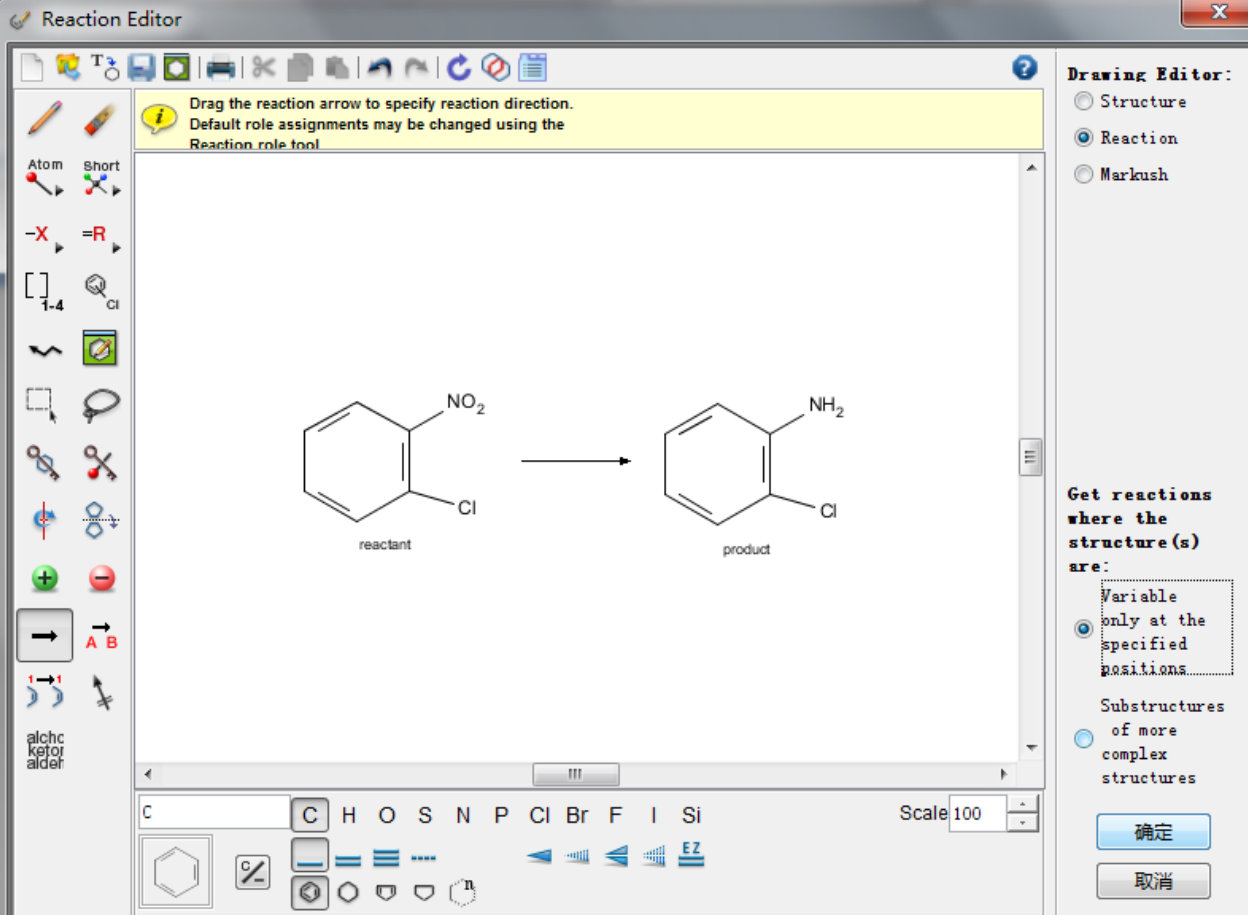
# 反应精准性定义工具—键标记工具



键标记工具，用于标记反应过程中必须发生变化的键



# SciFinder 反应检索



Reaction Editor

Drag the reaction arrow to specify reaction direction.  
 Default role assignments may be changed using the Reaction role tool.

reactant → product

Structure  
 Reaction  
 Markush

Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

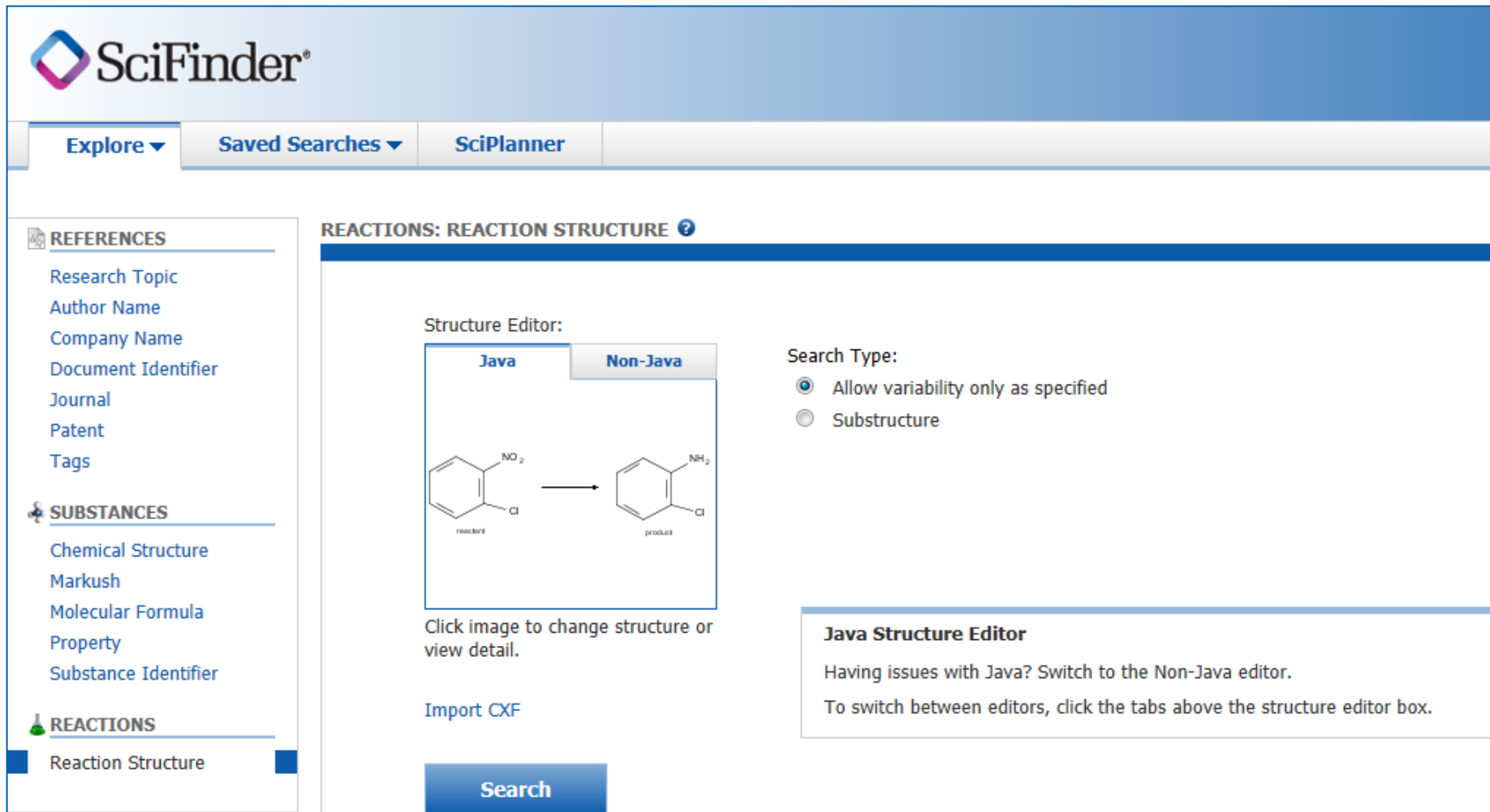
确定  
 取消

C H O S N P Cl Br F I Si Scale 100

**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



The screenshot shows the SciFinder web interface for searching reaction structures. At the top, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". On the left, a sidebar menu is visible with sections for "REFERENCES" (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and "SUBSTANCES" (Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier). Below these is a "REACTIONS" section with a "Reaction Structure" option highlighted.

The main content area is titled "REACTIONS: REACTION STRUCTURE" and contains a "Structure Editor" box. This editor has two tabs: "Java" (selected) and "Non-Java". Inside the editor, a chemical reaction is shown: a benzene ring with a nitro group (NO<sub>2</sub>) and a chlorine atom (Cl) at the 1 and 2 positions (labeled "reactant") is converted to a benzene ring with an amino group (NH<sub>2</sub>) and a chlorine atom (Cl) at the 1 and 2 positions (labeled "product").


Below the structure editor, there is a "Click image to change structure or view detail." instruction and an "Import CXF" link. A large blue "Search" button is positioned at the bottom of the editor area.

To the right of the structure editor, the "Search Type" options are:
 

- Allow variability only as specified
- Substructure

A callout box titled "Java Structure Editor" provides instructions: "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

Preferences | SciFinder Help ▾ | [Sign Out](#)

Welcome Tony Liu

[Explore ▾](#)
[Saved Searches ▾](#)
[SciPlanner](#)
[Save](#)
[Print](#)
[Export](#)

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

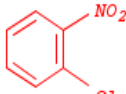
**REACTIONS** ?
 Get References
 Tools ▾
 Send to SciPlanner

Analyze **Refine**
Group by: No Grouping ▾ Sort by: Relevance ▾ ↓
NEW [Display Options](#)

▾ 0 of 335 Reactions Selected
⏪ ⏩ Page: 1 of 14 ⏪ ⏩

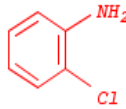
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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



~90

→



**100%**  
~119

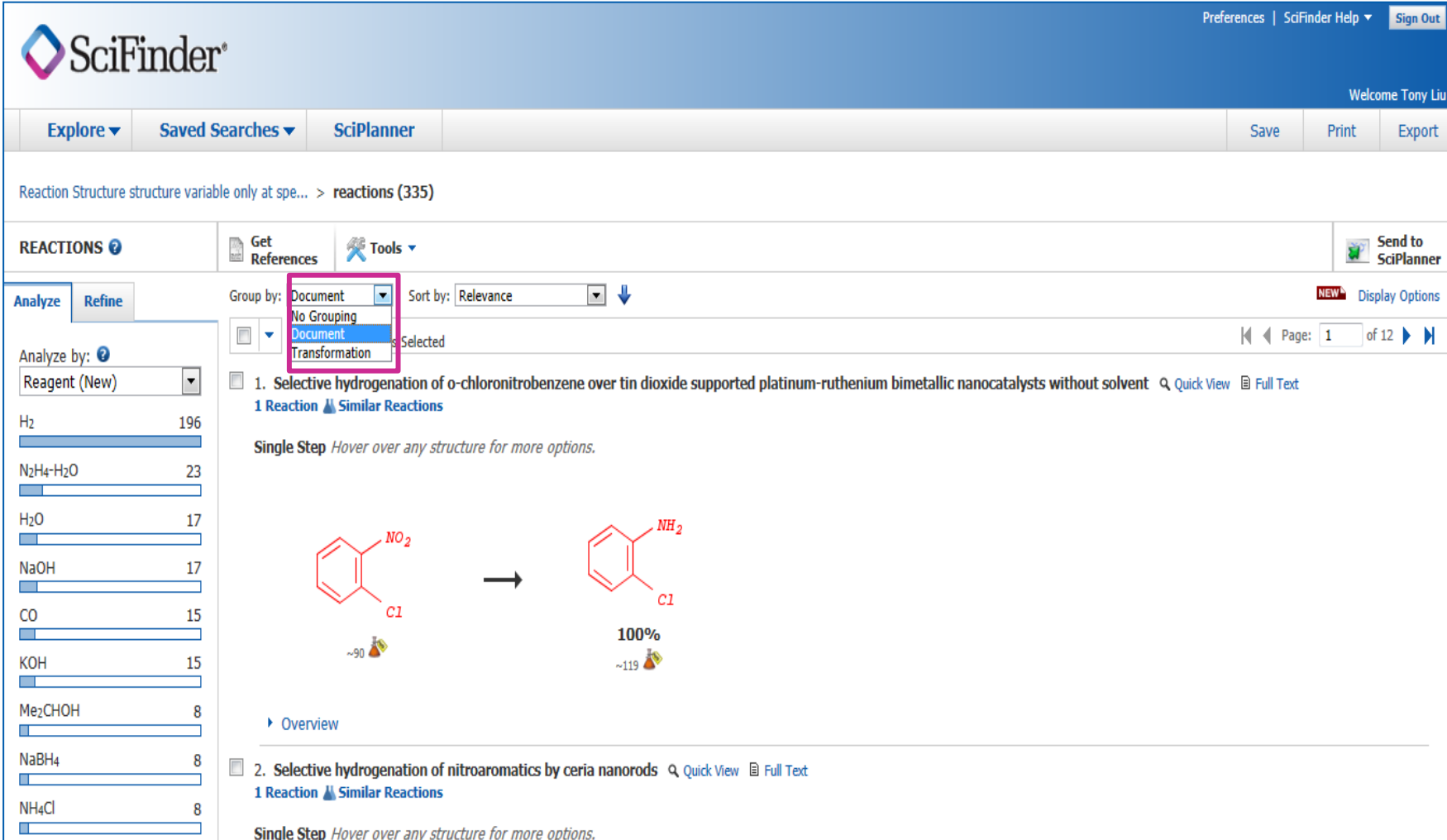
▸ Overview

Analyze by: ?

Reagent (New) ▾

|   |     |
|---|-----|
| H <sub>2</sub>                                  | 196 |
| N <sub>2</sub> H <sub>4</sub> -H <sub>2</sub> O | 23  |
| H <sub>2</sub> O                                | 17  |
| NaOH  | 17  |
| CO  | 15  |
| KOH   | 15  |
| Me <sub>2</sub> CHOH                            | 8   |

# Group by Document 按照出处文献分类显示



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

REACTIONS Get References Tools Send to SciPlanner

Analyze Refine Group by: Document Sort by: Relevance NEW Display Options

Analyze by: Reagent (New)

|   |     |
|---|-----|
| H <sub>2</sub>                                  | 196 |
| N <sub>2</sub> H <sub>4</sub> +H <sub>2</sub> O | 23  |
| H <sub>2</sub> O                                | 17  |
| NaOH  | 17  |
| CO  | 15  |
| KOH   | 15  |
| Me <sub>2</sub> CHOH                            | 8   |
| NaBH <sub>4</sub>                               | 8   |
| NH <sub>4</sub> Cl                              | 8   |

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

1 Reaction Similar Reactions

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

O=[N+]([O-])c1ccccc1Cl → Nc1ccccc1Cl

~90 100%

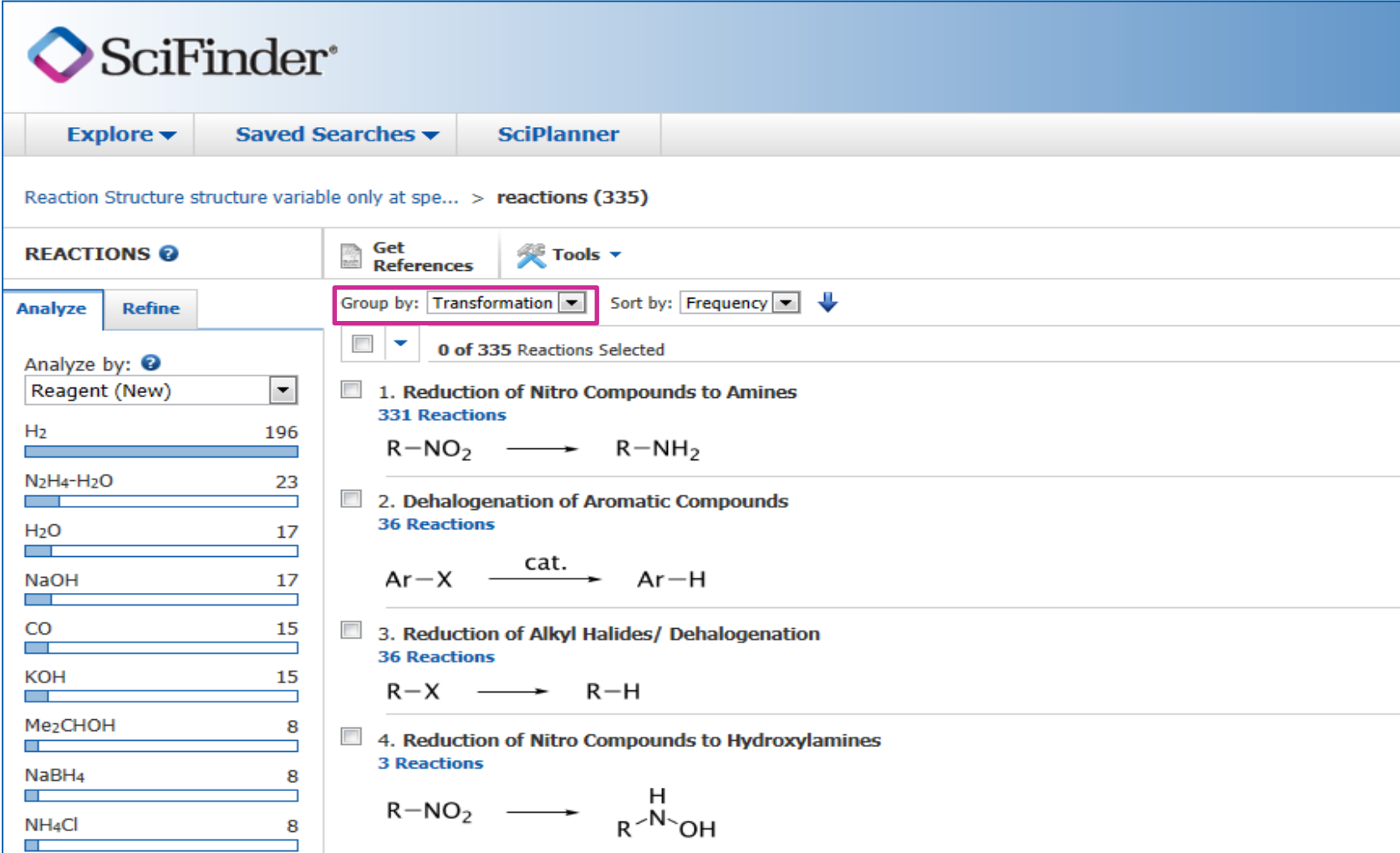
2. Selective hydrogenation of nitroaromatics by ceria nanorods Quick View Full Text

1 Reaction Similar Reactions

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

来自同一篇文章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 interface with the following elements:

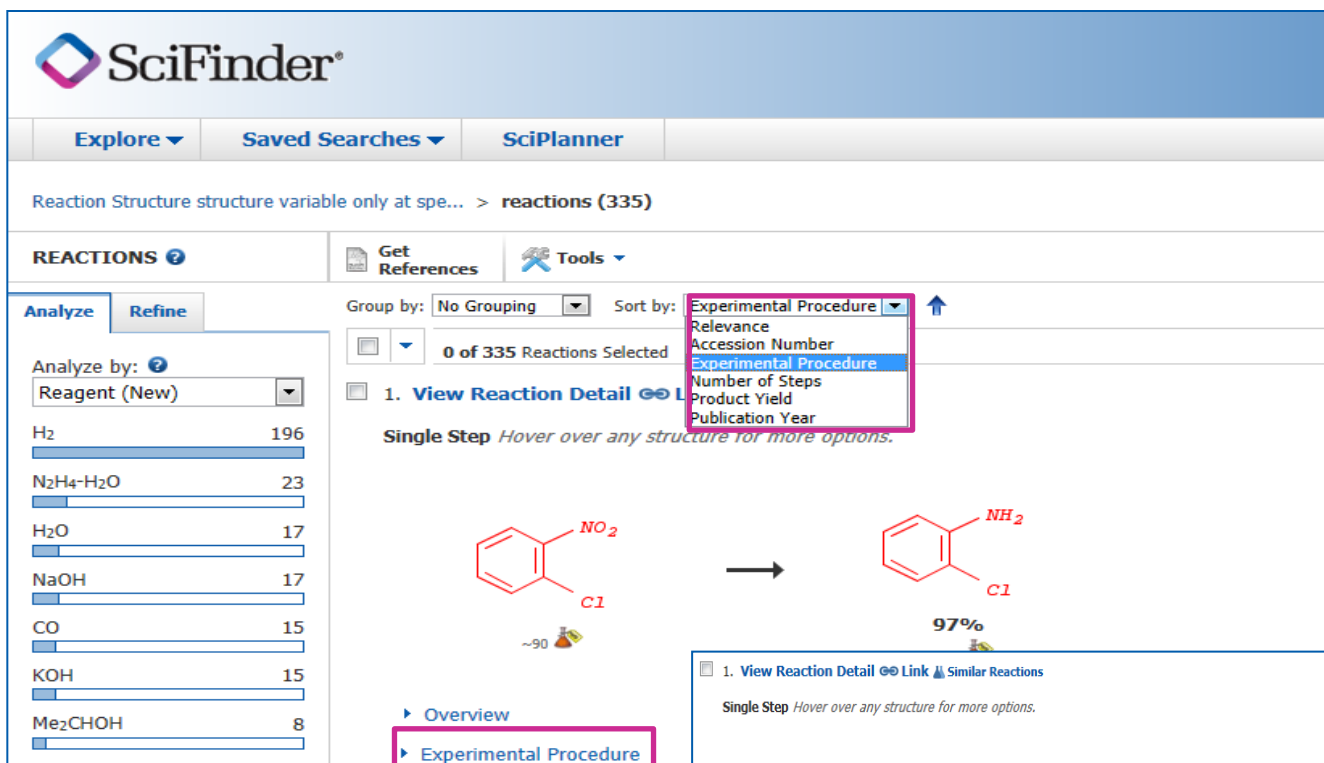
- Navigation:** Explore, Saved Searches, SciPlanner.
- Path:** Reaction Structure structure variable only at spe... > reactions (335)
- Tools:** Get References, Tools.
- Grouping and Sorting:** Group by: Transformation (highlighted in a red box), Sort by: Frequency.
- Analysis Panel (Left):** Analyze by: Reagent (New).
 

| Reagent   | Count |
|---|-------|
| H <sub>2</sub>                                  | 196   |
| N <sub>2</sub> H <sub>4</sub> -H <sub>2</sub> O | 23    |
| H <sub>2</sub> O                                | 17    |
| NaOH  | 17    |
| CO  | 15    |
| KOH   | 15    |
| Me <sub>2</sub> CHOH                            | 8     |
| NaBH <sub>4</sub>                               | 8     |
| NH <sub>4</sub> Cl                              | 8     |
- Reaction Results (Right):**
  - 0 of 335 Reactions Selected
  - 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



SciFinder<sup>®</sup>

Explore ▾ Saved Searches ▾ SciPlanner

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

REACTIONS ⓘ

Get References Tools ▾

Group by: No Grouping ▾ Sort by: Experimental Procedure ▾ ↑

0 of 335 Reactions Selected

1. View Reaction Detail ⓘ Link

Single Step Hover over any structure for more options.

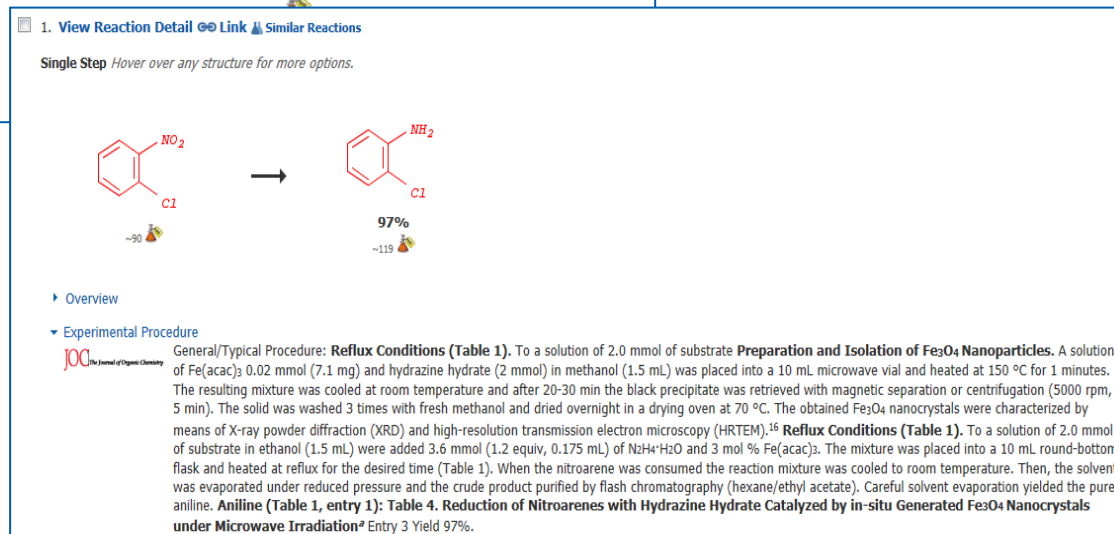
Analyze by: ⓘ

Reagent (New) ▾

|   |     |
|---|-----|
| H <sub>2</sub>                                  | 196 |
| N <sub>2</sub> H <sub>4</sub> ·H <sub>2</sub> O | 23  |
| H <sub>2</sub> O                                | 17  |
| NaOH  | 17  |
| CO  | 15  |
| KOH   | 15  |
| Me <sub>2</sub> CHOH                            | 8   |

Overview

Experimental Procedure



1. View Reaction Detail ⓘ Link Similar Reactions

Single Step Hover over any structure for more options.

Overview

Experimental Procedure

**JOC** The Journal of Organic Chemistry

General/Typical Procedure: **Reflux Conditions (Table 1)**. To a solution of 2.0 mmol of substrate **Preparation and Isolation of Fe<sub>3</sub>O<sub>4</sub> Nanoparticles**. A solution of Fe(acac)<sub>3</sub> (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 Fe<sub>3</sub>O<sub>4</sub> nanocrystals were characterized by means of X-ray powder diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM).<sup>16</sup> **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 N<sub>2</sub>H<sub>4</sub>·H<sub>2</sub>O and 3 mol % Fe(acac)<sub>3</sub>. 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 Fe<sub>3</sub>O<sub>4</sub> Nanocrystals under Microwave Irradiation<sup>a</sup> 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

|                                      |   |
|--------------------------------------|---|
| C <sub>2</sub> H <sub>6</sub>        | 5 |
| CH <sub>4</sub>                      | 4 |
| ClCH <sub>2</sub> CH <sub>2</sub> Cl | 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

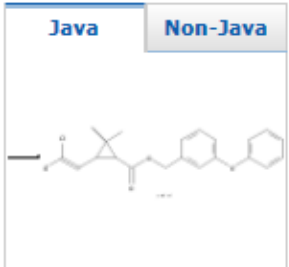
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

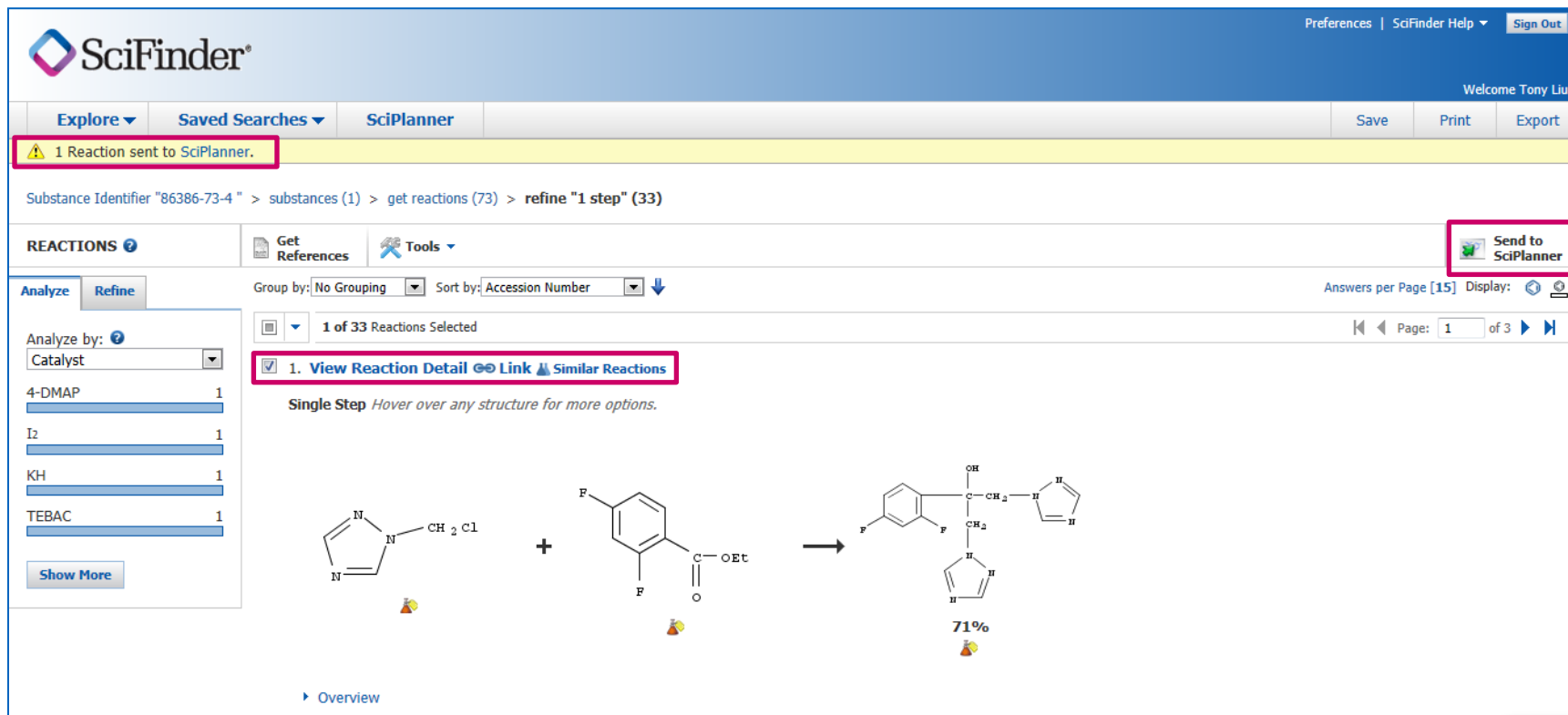


Click image to change structure or view detail.  
 Search type: **Allow variability only as specified**

Refine

# SciPlanner-反应路线设计, 创建反应路线报告

## 案例: 氟康唑合成路线设计

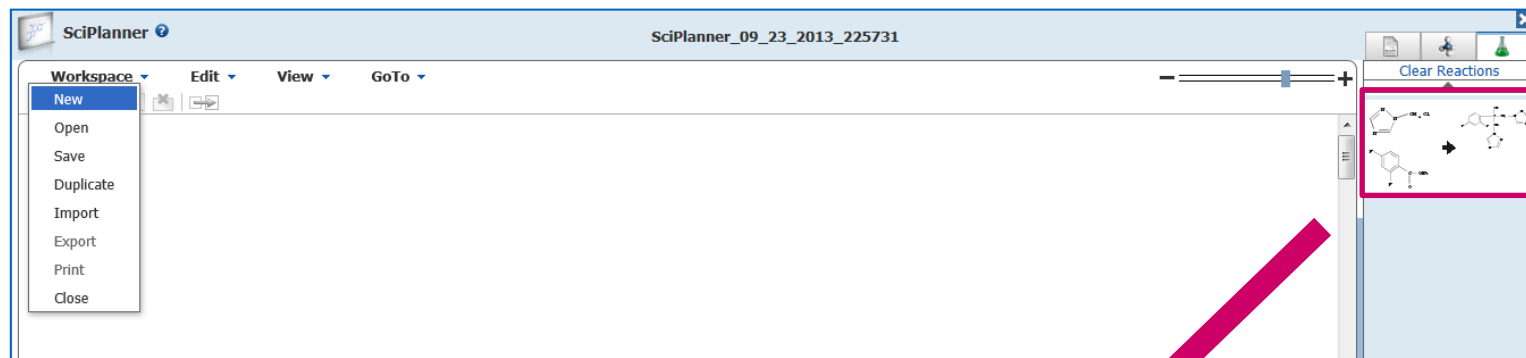


The screenshot displays the SciFinder SciPlanner interface. At the top, the SciFinder logo and navigation tabs (Explore, Saved Searches, SciPlanner) are visible. A yellow notification bar states "1 Reaction sent to SciPlanner." Below this, the breadcrumb trail reads: "Substance Identifier '86386-73-4' > substances (1) > get reactions (73) > refine '1 step' (33)".

The main interface is divided into several sections:

- REACTIIONS**: Includes "Get References" and "Tools" buttons. A "Send to SciPlanner" button is highlighted with a red box.
- Analyze/Refine**: A sidebar on the left allows for refining the search. Under "Analyze by:", "Catalyst" is selected. A list of catalysts is shown: 4-DMAP (1), I<sub>2</sub> (1), KH (1), and TEBAC (1). A "Show More" button is at the bottom.
- Reaction List**: Shows "1 of 33 Reactions Selected". A red box highlights the first reaction: "1. View Reaction Detail Link Similar Reactions".
- Reaction Detail**: Displays a "Single Step" reaction. The reactants are N-(chloromethyl)imidazole and ethyl 2,4-difluorobenzoate. The product is Fluconazole, with a yield of 71% indicated below the structure.

# 检索结果编辑平台



SciPlanner SciPlanner\_09\_23\_2013\_225731

Workspace Edit View GoTo

Clear Reactions

鼠标直接拖拽至编辑平台

Reaction scheme showing the synthesis of a complex molecule from two starting materials (2,4-difluorobenzoyl chloride and 1-(chloromethyl)imidazole) and a product molecule.

## 选择感兴趣的中间体的反应路线并发送到SciPlanner

The screenshot displays the SciPlanner interface with a workspace containing a chemical reaction scheme. A context menu is open over a chemical structure, listing several actions. The 'Synthesize this...' option is highlighted with a red box. The reaction scheme shows a 2,4-difluorobenzoyl chloride derivative reacting with a 1,2,4-triazole derivative to form a complex product.

Workspace: SciPlanner  
SciPlanner\_09\_23\_2013\_225731

Workspace Edit View GoTo

CAS Registry Number: 108928-00-3

- 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

Clear Reactions

SciFinder® Preferences | SciFinder Help | Sign Out

Welcome Tony Liu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

⚠ 1 Reaction sent to SciPlanner.

Substance Identifier "86386-73-4" > substances (1) > get reactions (73) > refine "1 step" (33) > get reactions (4)

REACTIONS ⓘ Get References Tools ▾ **Send to SciPlanner**

Analyze Refine Group by: No Grouping Sort by: Accession Number ↓ Answers per Page [15] Display: ⚙

Analyze by: ⓘ  
Catalyst ▾  
*No reactions available*

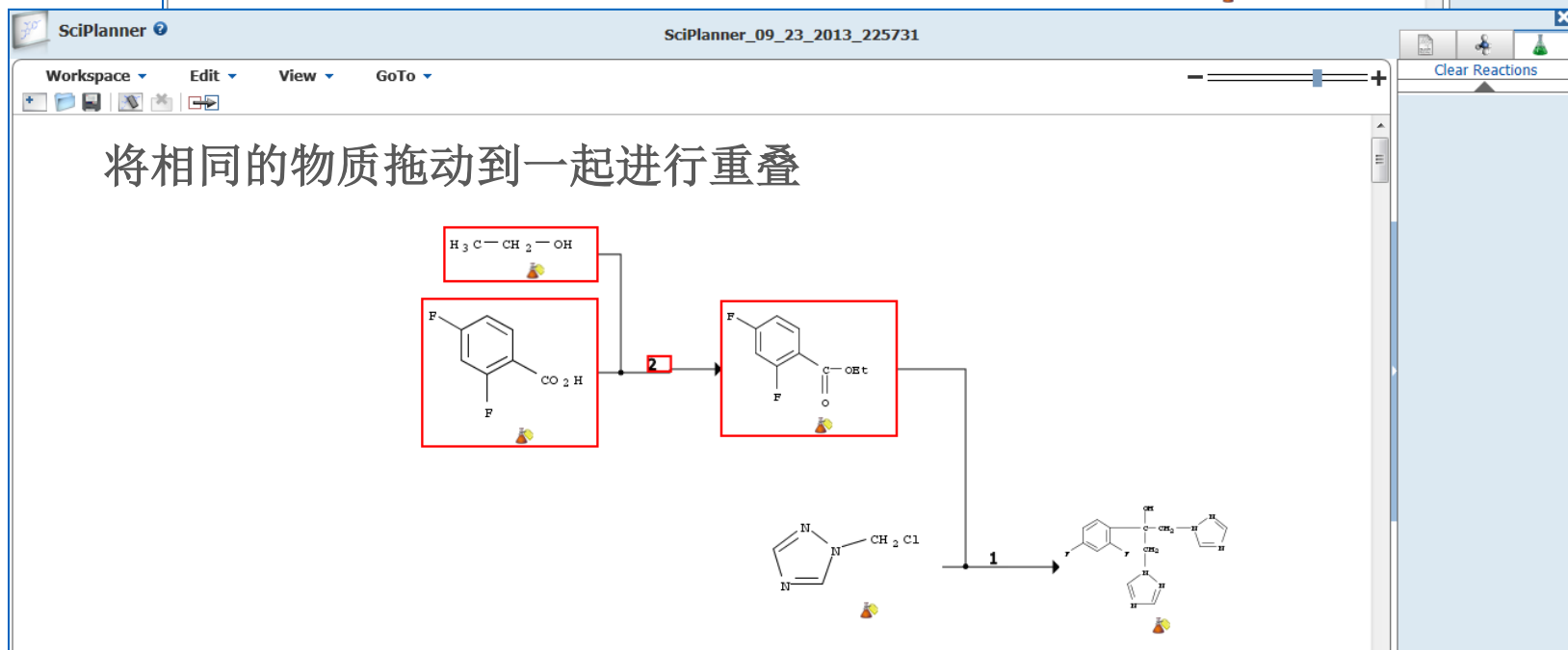
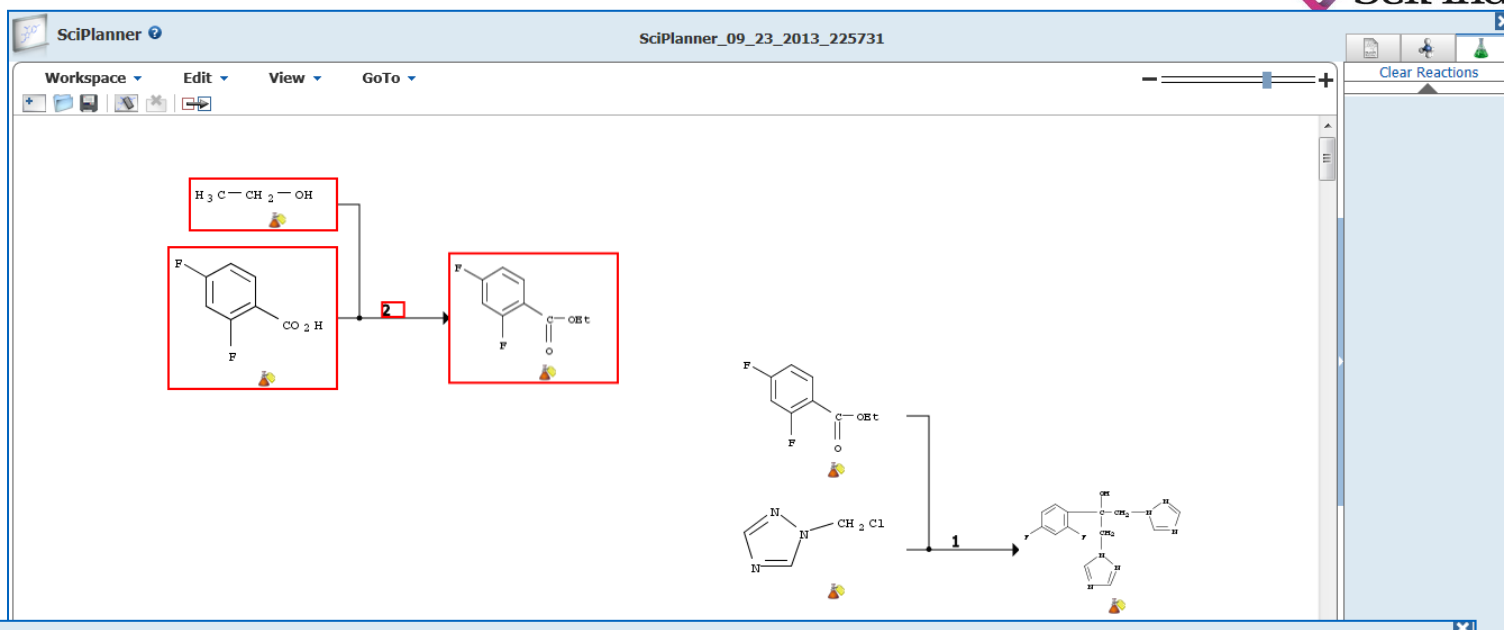
1 of 4 Reactions Selected

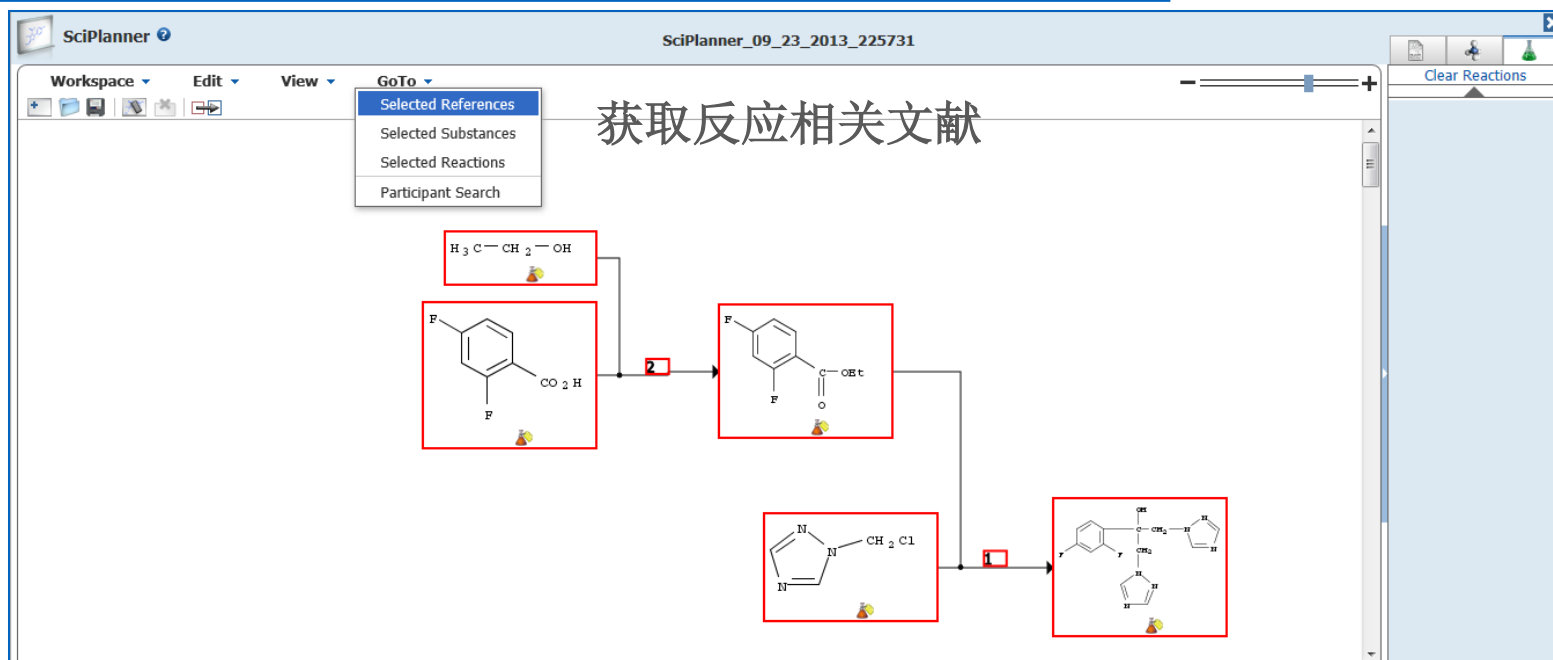
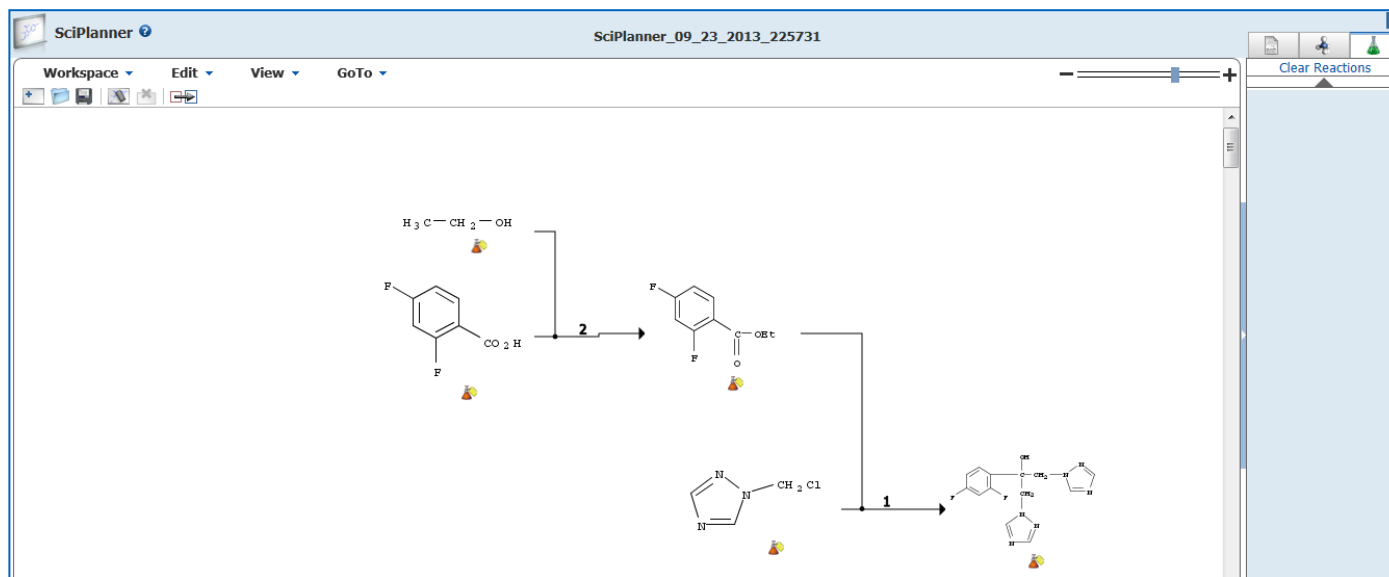
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

The reaction shows 2,4-difluorobenzoic acid reacting with ethanol (H<sub>3</sub>C-CH<sub>2</sub>-OH) to produce ethyl 2,4-difluorobenzoate. The reactants are shown on the left, separated by a plus sign, and the product is on the right, with a reaction arrow pointing to it.

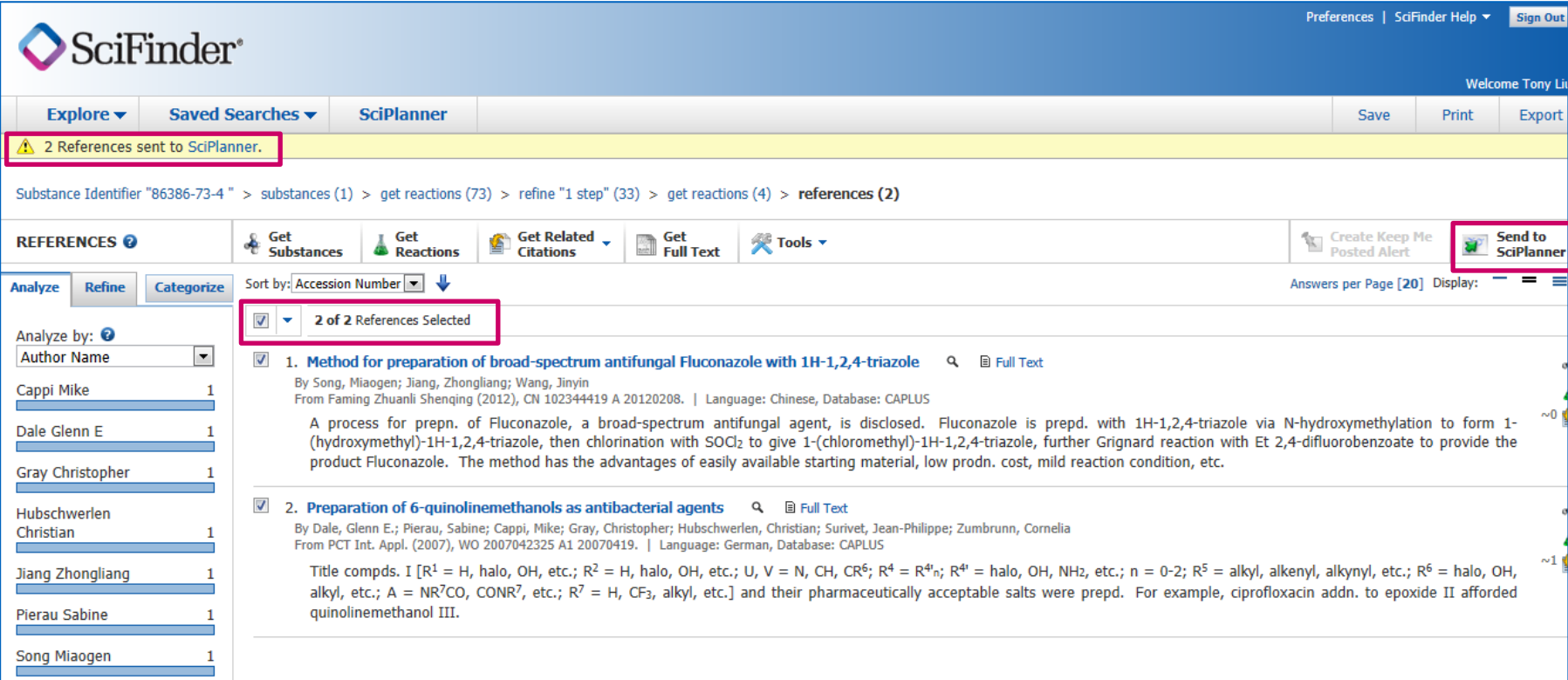
[Overview](#)  
[Experimental Procedure](#)







# 选择文献信息发送到SciPlanner



The screenshot shows the SciFinder web interface. At the top right, there are links for "Preferences", "SciFinder Help", and "Sign Out". Below the SciFinder logo, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". A yellow notification bar at the top left states "2 References sent to SciPlanner." The breadcrumb trail reads: "Substance Identifier '86386-73-4' > substances (1) > get reactions (73) > refine '1 step' (33) > get reactions (4) > references (2)".

The main content area is titled "REFERENCES" and includes several action buttons: "Get Substances", "Get Reactions", "Get Related Citations", "Get Full Text", and "Tools". On the right side of this area, there are buttons for "Create Keep Me Posted Alert" and "Send to SciPlanner", which is highlighted with a red box. Below the buttons, there are tabs for "Analyze", "Refine", and "Categorize". The "Sort by" dropdown is set to "Accession Number". A summary bar indicates "2 of 2 References Selected".

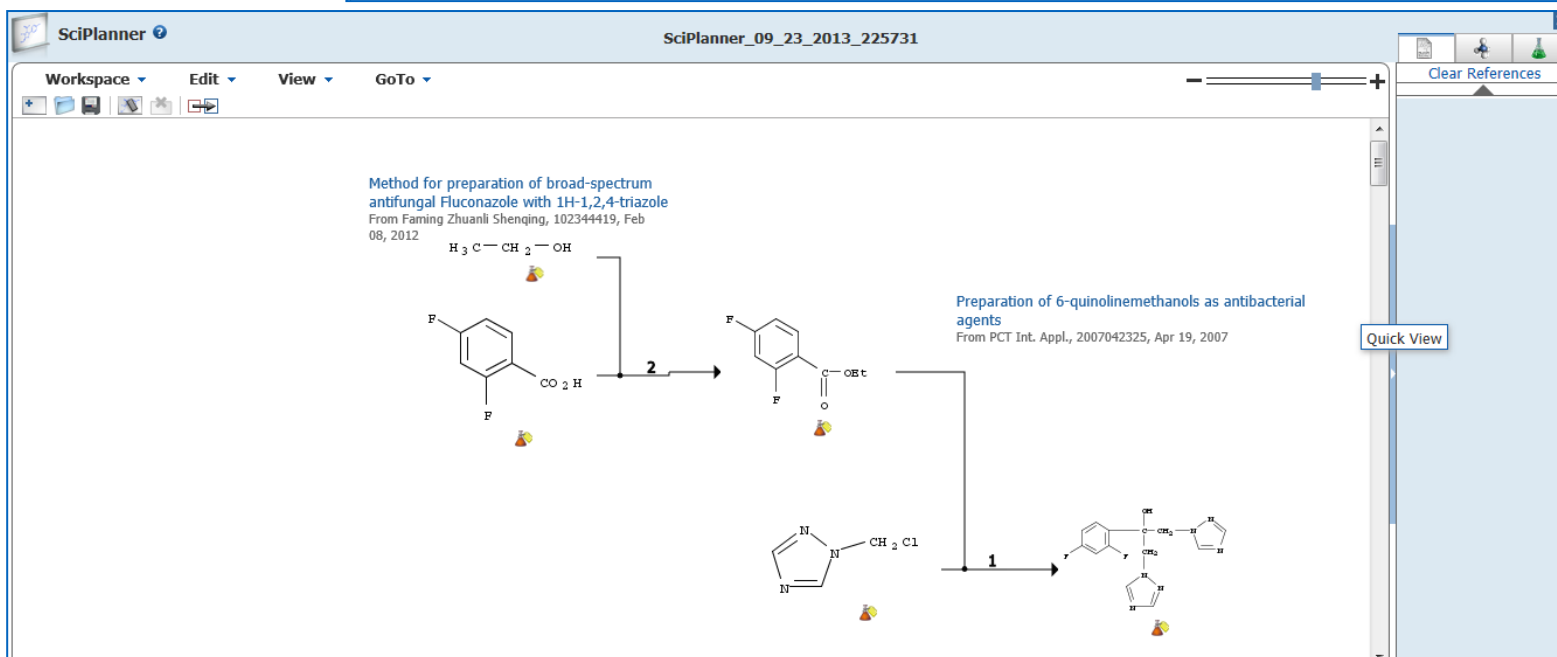
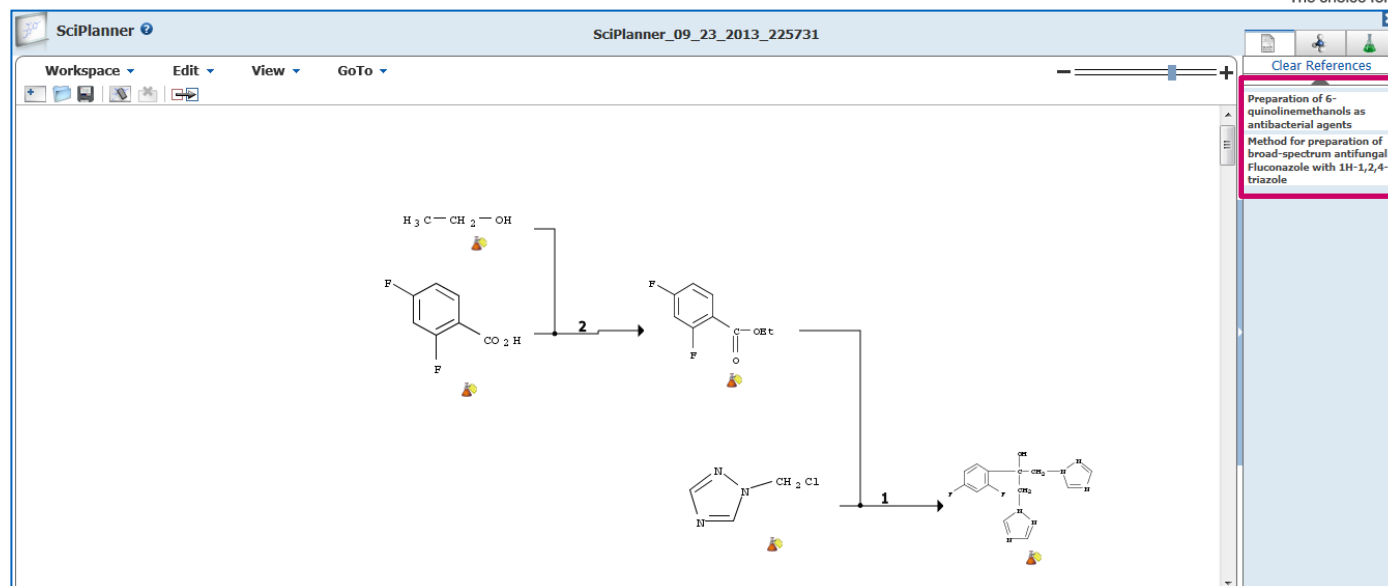
On the left side, there is an "Analyze by:" section with a dropdown menu set to "Author Name". Below this is a list of authors with their respective counts:

| Author Name            | Count |
|------------------------|-------|
| Cappi Mike             | 1     |
| Dale Glenn E           | 1     |
| Gray Christopher       | 1     |
| Hubschwerlen Christian | 1     |
| Jiang Zhongliang       | 1     |
| Pierau Sabine          | 1     |
| Song Miaogen           | 1     |

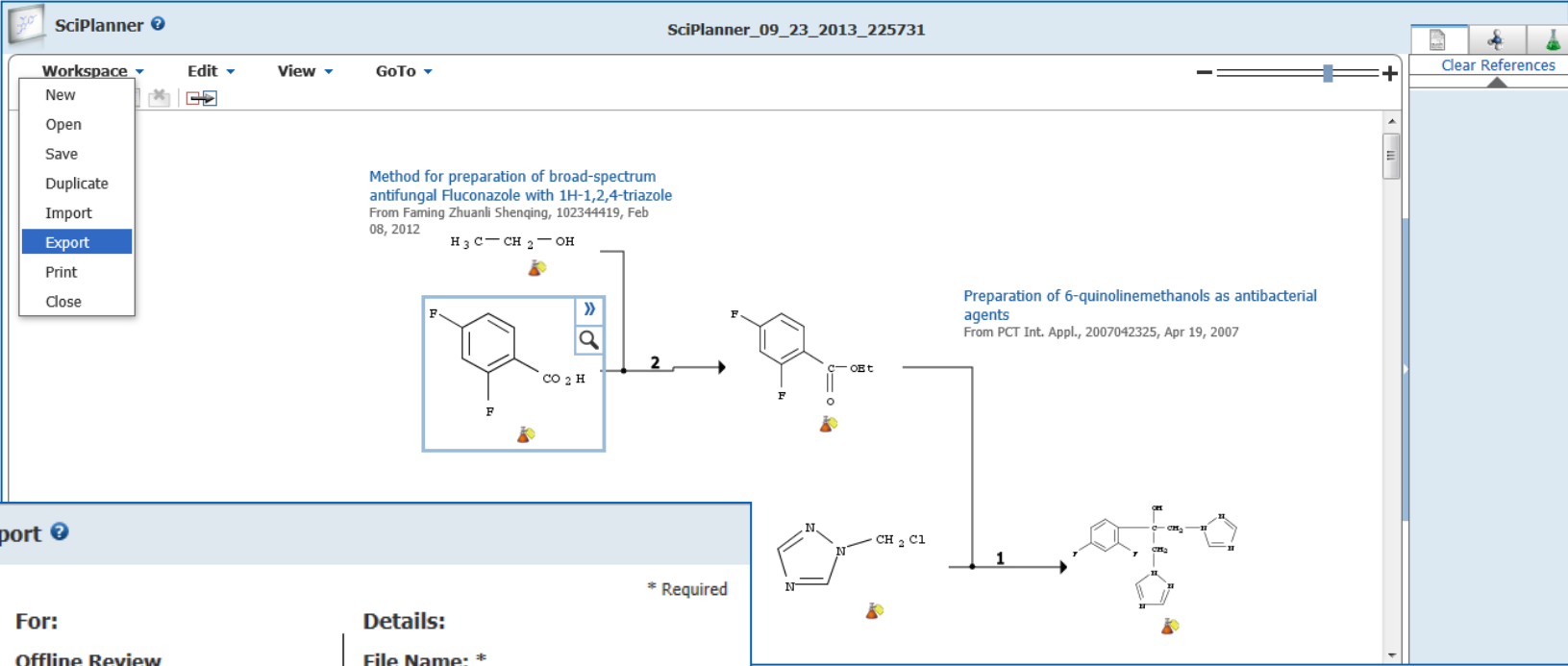
The main list of references shows two entries, both selected with checkboxes:

- 1. Method for preparation of broad-spectrum antifungal Fluconazole with 1H-1,2,4-triazole**  
 By Song, Miaogen; Jiang, Zhongliang; Wang, Jinyin  
 From Faming Zhuanyi Shenqing (2012), CN 102344419 A 20120208. | Language: Chinese, Database: CAPLUS  
 A process for prepn. of Fluconazole, a broad-spectrum antifungal agent, is disclosed. Fluconazole is prepd. with 1H-1,2,4-triazole via N-hydroxymethylation to form 1-(hydroxymethyl)-1H-1,2,4-triazole, then chlorination with SOCl<sub>2</sub> to give 1-(chloromethyl)-1H-1,2,4-triazole, further Grignard reaction with Et 2,4-difluorobenzoate to provide the product Fluconazole. The method has the advantages of easily available starting material, low prodn. cost, mild reaction condition, etc.
- 2. Preparation of 6-quinolinemethanols as antibacterial agents**  
 By Dale, Glenn E.; Pierau, Sabine; Cappi, Mike; Gray, Christopher; Hubschwerlen, Christian; Surivet, Jean-Philippe; Zumbrunn, Cornelia  
 From PCT Int. Appl. (2007), WO 2007042325 A1 20070419. | Language: German, Database: CAPLUS  
 Title compds. I [R<sup>1</sup> = H, halo, OH, etc.; R<sup>2</sup> = H, halo, OH, etc.; U, V = N, CH, CR<sup>6</sup>; R<sup>4</sup> = R<sup>4n</sup>; R<sup>4n</sup> = halo, OH, NH<sub>2</sub>, etc.; n = 0-2; R<sup>5</sup> = alkyl, alkenyl, alkynyl, etc.; R<sup>6</sup> = halo, OH, alkyl, etc.; A = NR<sup>7</sup>CO, CONR<sup>7</sup>, etc.; R<sup>7</sup> = H, CF<sub>3</sub>, alkyl, etc.] and their pharmaceutically acceptable salts were prepd. For example, ciprofloxacin addn. to epoxide II afforded quinolinemethanol III.

添加相应的  
文献信息



# 检索结果的保存与导出



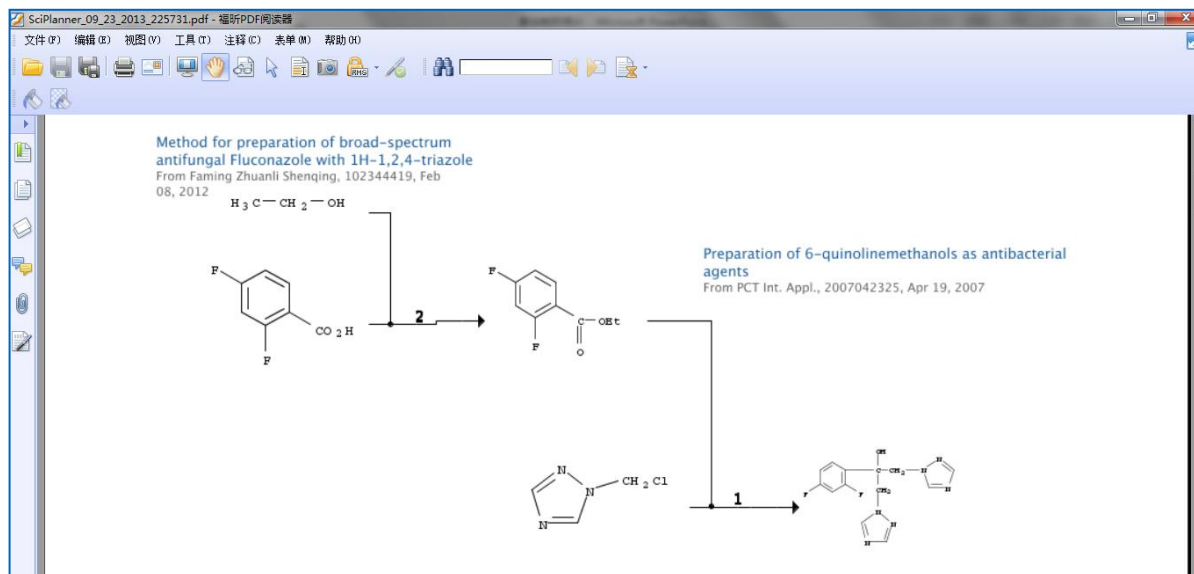
The screenshot displays the SciPlanner interface with a chemical reaction scheme. The reaction involves the synthesis of 6-quinolinemethanols from 2-chloromethylimidazole and a substituted benzene derivative. The interface includes a menu bar (Workspace, Edit, View, GoTo) and a 'Workspace' dropdown menu with options: New, Open, Save, Duplicate, Import, **Export**, Print, and Close. The main workspace shows two reaction steps: Step 1 (labeled '1') and Step 2 (labeled '2').

The **Export** dialog box is open, showing the following options:

- For:**
  - Portable Document Format (\*.pdf)
  - Citations (\*.ris)
  - Image (\*.png)
- Saving Locally:**
  - SciPlanner eXchange (\*.pkx)
- Details:**
  - File Name:** \* (Required)
  - Title:**
- Include:**
  - SciPlanner Image
  - Reaction Details
  - Substance Details
  - Reference Details

Buttons for **Export** and **Cancel** are located at the bottom of the dialog.

## Export功能输出反应路线报告



## 1. 反应路线信息

SciFinder® Page 2

| Reaction | Stages  | Notes   | Yield |
|----------|---|---|-------|
| 1        | 1.1 R:Mg, C:l <sub>2</sub> , S:THF, rt → reflux; 3 h, reflux<br>1.2 S:THF, < 50°C; 15 h, rt<br>1.3 R:NH <sub>4</sub> Cl, S:H <sub>2</sub> O | Grignard reaction, optimization study, optimized on time, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 3<br><br><b>Transformation:</b><br>1. Conversion of Carboxylic Derivatives to Ketones or Alcohols with Organometallic Compounds | 71%   |

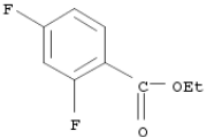
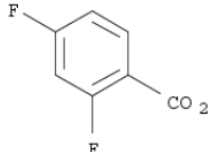
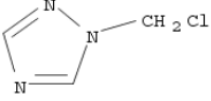
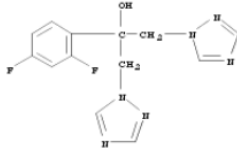
**References**  
[Method for preparation of broad-spectrum antifungal Fluconazole with 1H-1,2,4-triazole](#)  
 By Song, Miaogen et al  
 From Faming Zhuangli Shenqing, 102344419, 08 Feb 2012

## 2. 反应条件信息

### 3. 反应物质信息

SciFinder® Page 3

**Substance Information**

|   |   |  |
|---|---|--|
| <p><b>108928-00-3</b></p>  <p><chem>CCOC(=O)c1cc(F)cc(F)c1</chem></p> <p><math>C_9H_8F_2O_2</math><br/>Benzoic acid, 2,4-difluoro-, ethyl ester</p> <p><b>Related Info:</b>   ~ 42 References<br/> <a href="#">Reactions</a><br/> <a href="#">Commercial Sources</a><br/> <a href="#">Regulatory Information</a></p> | <p><b>1583-58-0</b></p>  <p><chem>OC(=O)c1cc(F)cc(F)c1</chem></p> <p><math>C_7H_4F_2O_2</math><br/>Benzoic acid, 2,4-difluoro-</p> <p><b>Related Info:</b>   ~ 337 References<br/> <a href="#">Reactions</a><br/> <a href="#">Commercial Sources</a><br/> <a href="#">Regulatory Information</a></p> | <p><b>64-17-5</b></p> <p><chem>CCO</chem></p> <p><math>C_2H_6O</math><br/>Ethanol</p> <p><b>Related Info:</b>   ~ 380582 References<br/> <a href="#">Reactions</a><br/> <a href="#">Commercial Sources</a><br/> <a href="#">Regulatory Information</a></p> |
| <p><b>84387-62-2</b></p>  <p><chem>CN1CN=CN1CCl</chem></p> <p><math>C_3H_4ClN_3</math><br/>1<i>H</i>-1,2,4-Triazole, 1-(chloromethyl)-</p>   | <p><b>86386-73-4</b></p>   |  |

# 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中的反应检索及SciPlanner功能
- **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。

# 登陆图书馆主页


沈阳药科大学图书馆  
 SHENYANG PHARMACEUTICAL UNIVERSITY LIBRARY

[首页](#) | [开馆时间](#) | [咨询服务](#) | [数字资源](#) | [教学培训](#) | [移动图书馆](#) | [VPN访问](#) | [学校首页](#) | [老版首页](#)

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一站式检索

题名 ▼

查询

简单查询

组合查询

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

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 ▶](#)



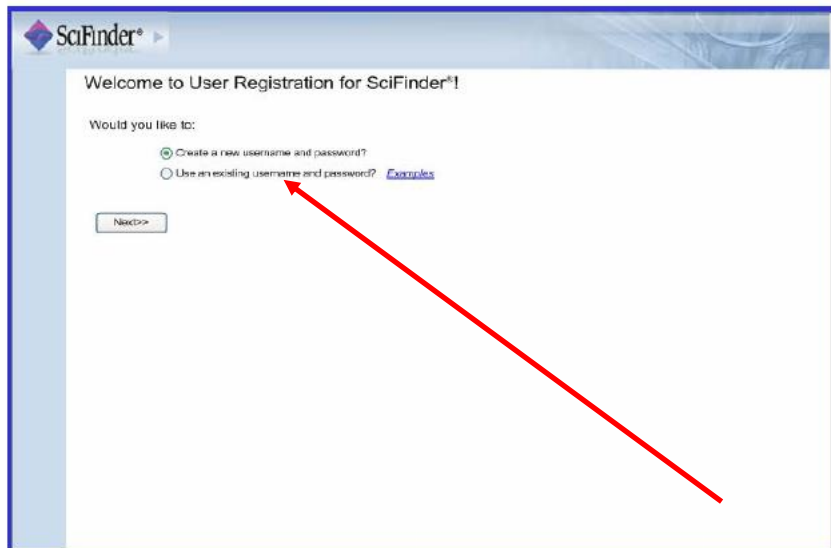
## 论文提交



## 新生入馆教育

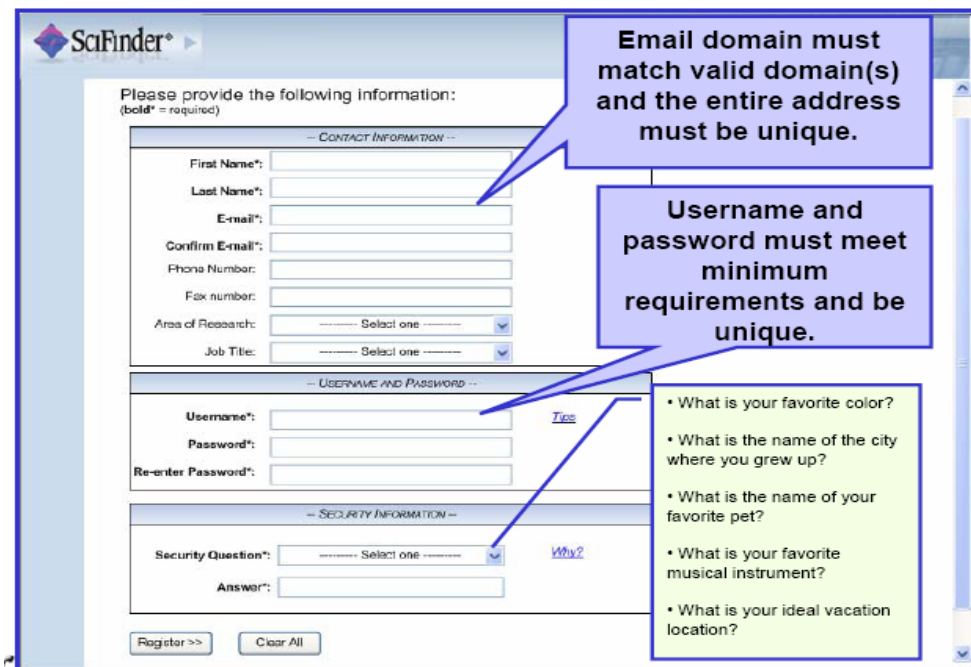


# 点击URL创建SciFinder Web账号



请用邮箱注册，一人只能注册一个账号

开始创建SciFinder Web帐号



**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：

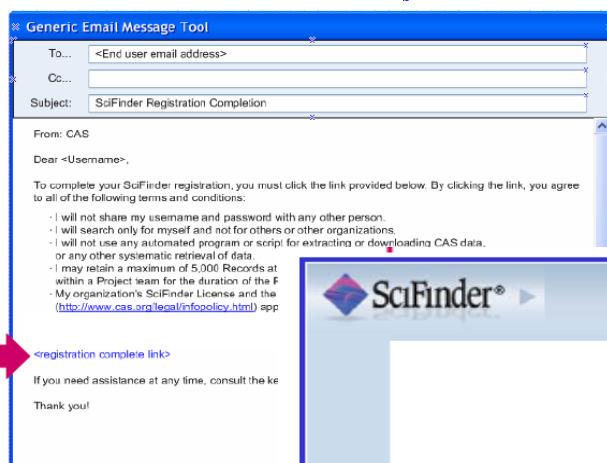
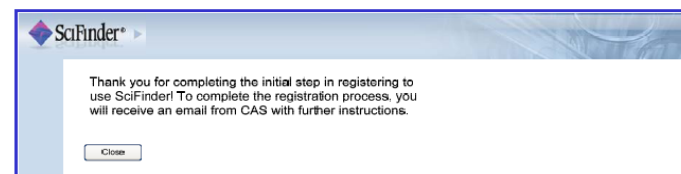
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、\*）

### 密码设置小技巧：

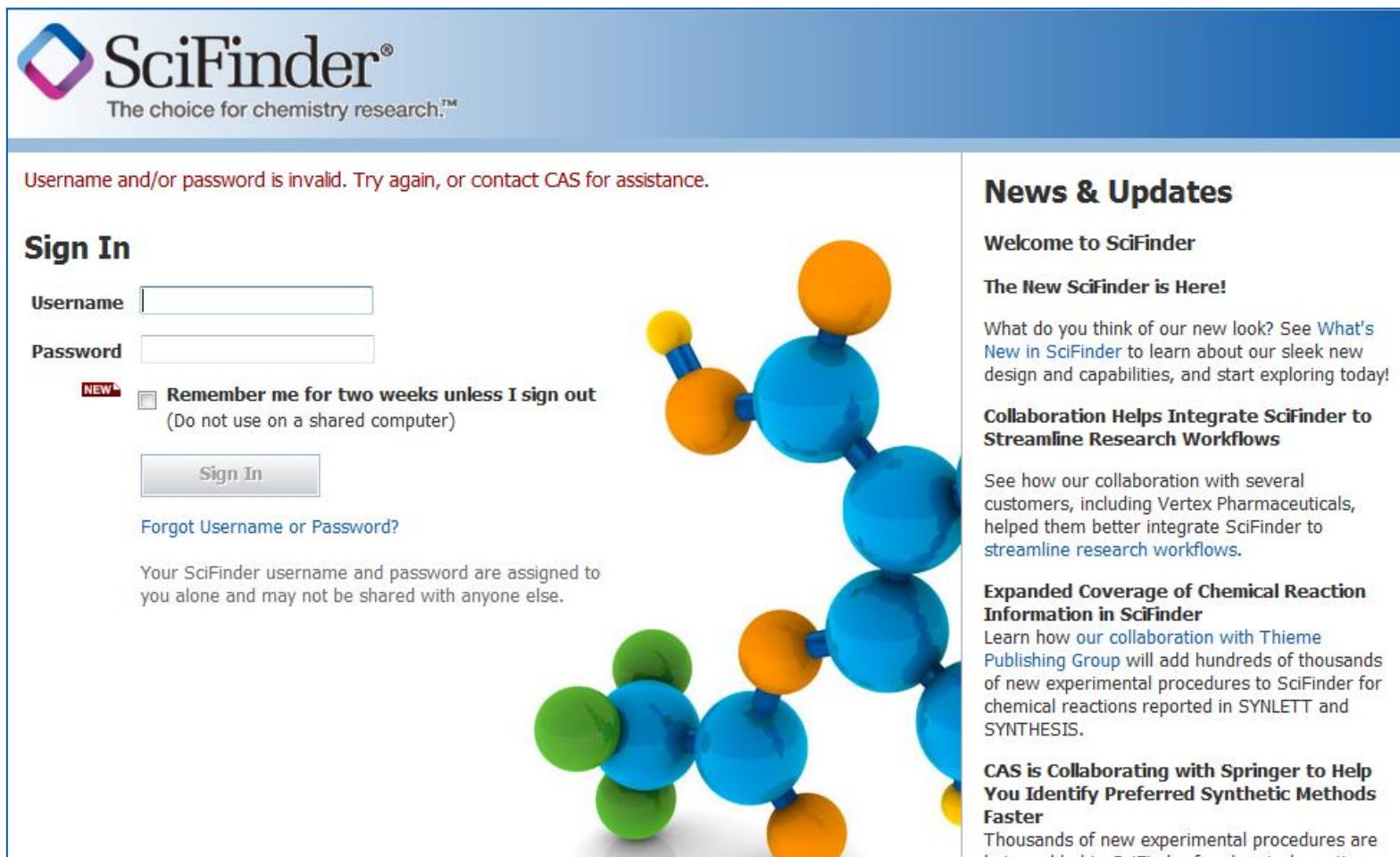
- 1：不要和账号中有重复的字符
- 2：密码格式最好是abc@123

# 对新ID的Email确认

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. On the left is a vertical navigation menu with the following items: 常见问题, 资源下载, 新闻与公告, 在线演示, 网络培训, 加入我们. The main content area is titled 'CAS资源下载' and contains three sections: 'SciFinder 快速参考手册 NEW' with a link to 'SciFinder 快速参考手册'; '案例研究 NEW' with links to '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', and '转基因食品案例'; and 'SciFinder新功能' with links to '生物活性及靶点分析' and '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](mailto:tony@igroup.com.cn)

QQ答疑: 340109774