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SciFinder Web使用介绍

----上海工程技术大学

SciFinder产品专员　朱传娴

2013.11.

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- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

美国化学文摘社—Chemical Abstract Service

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

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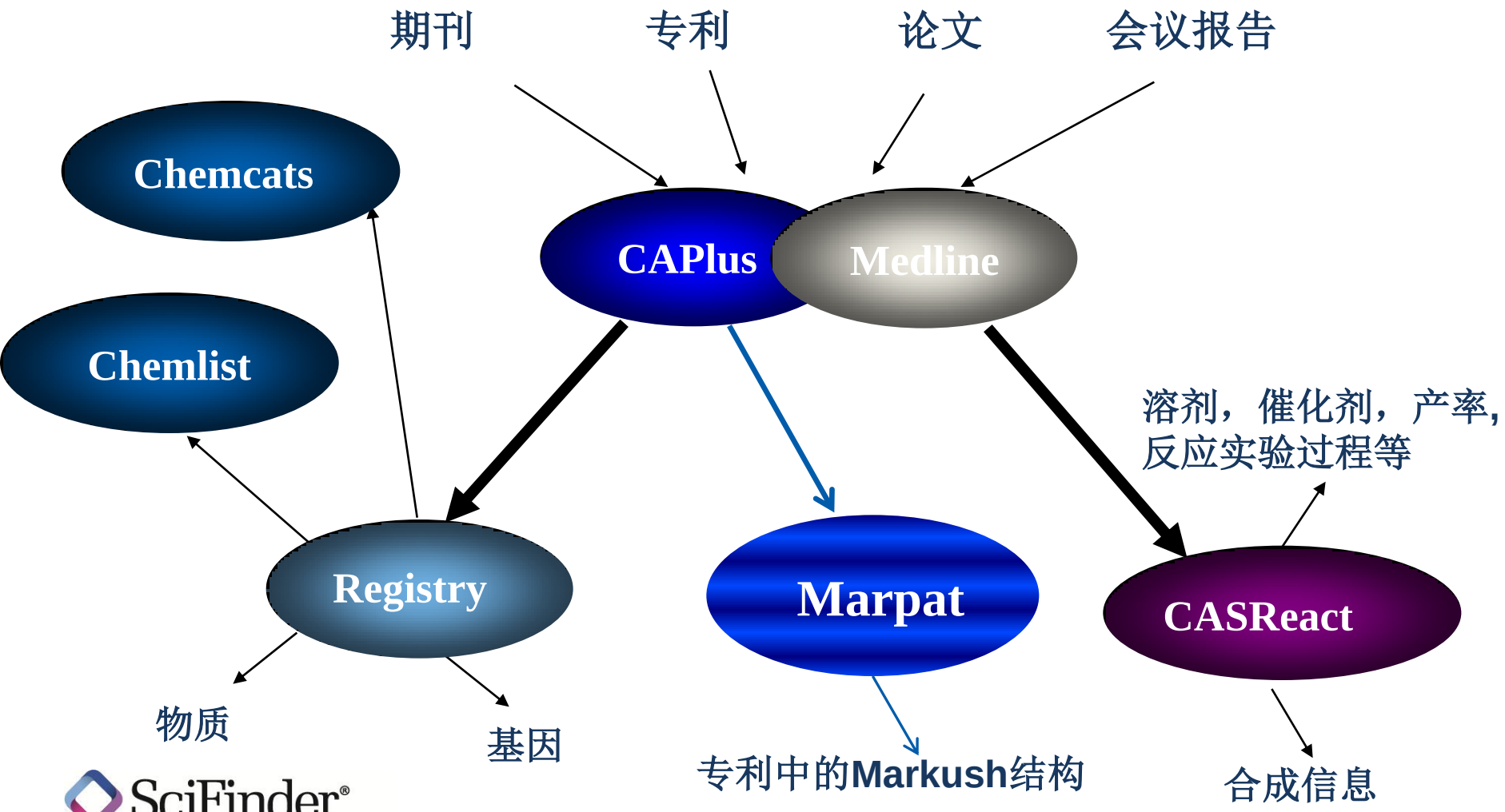

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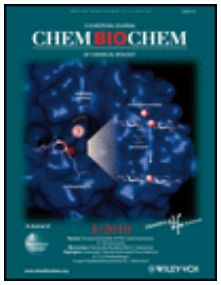

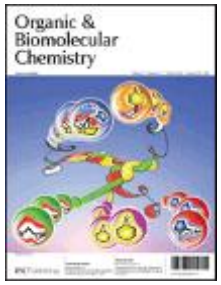

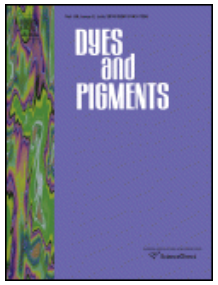

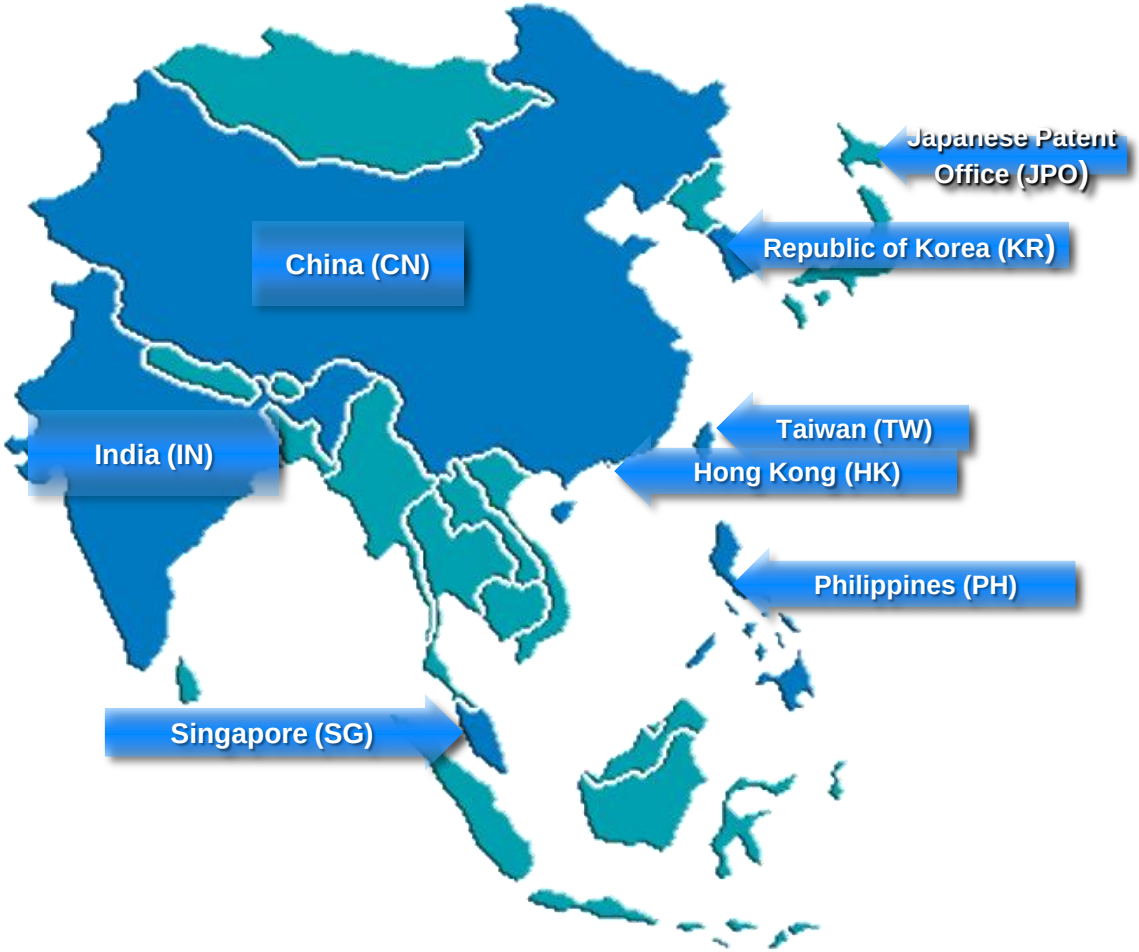

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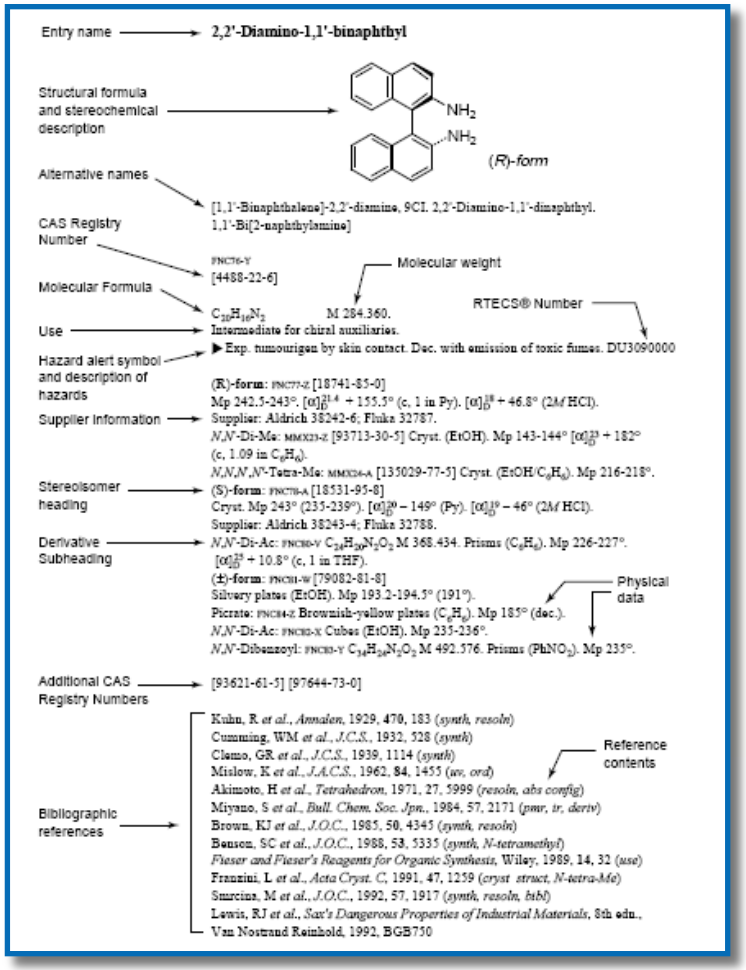

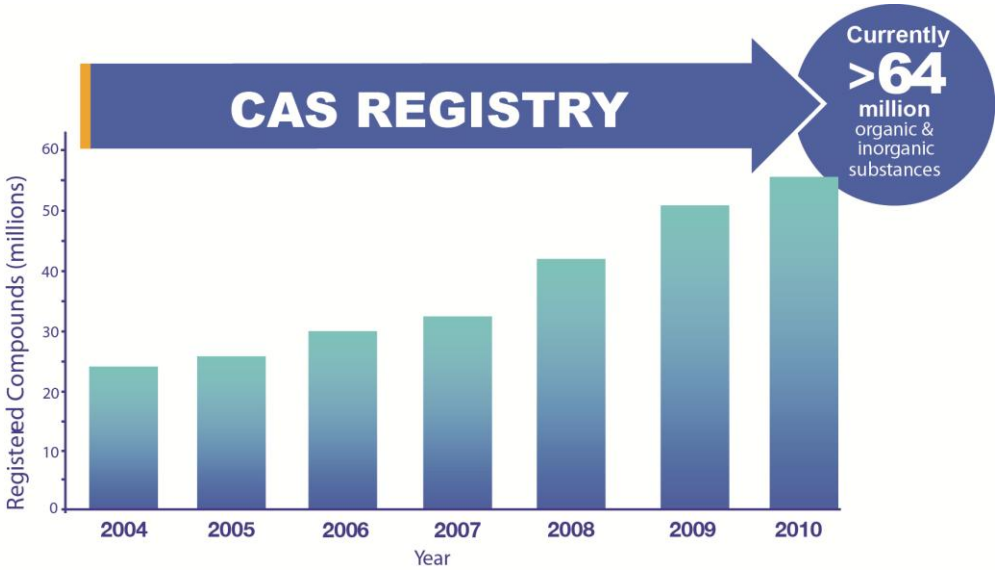

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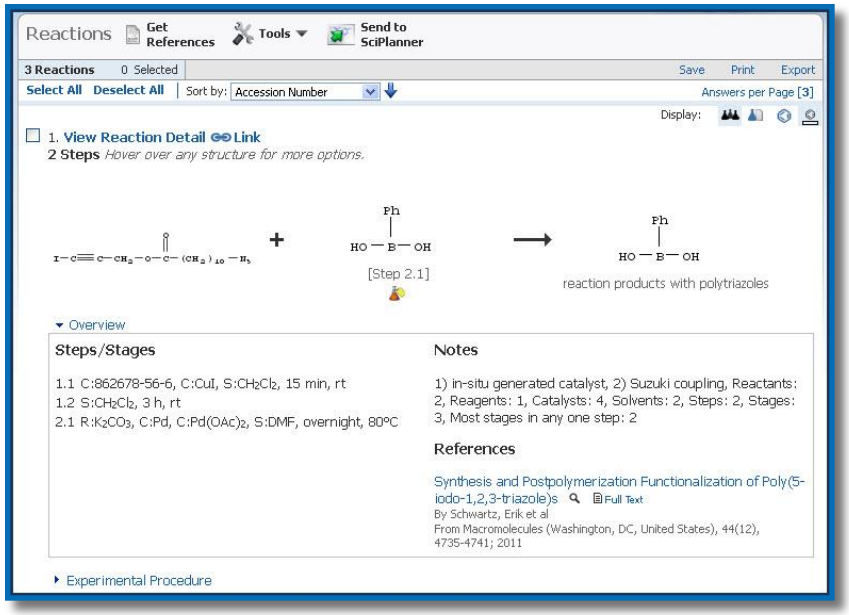

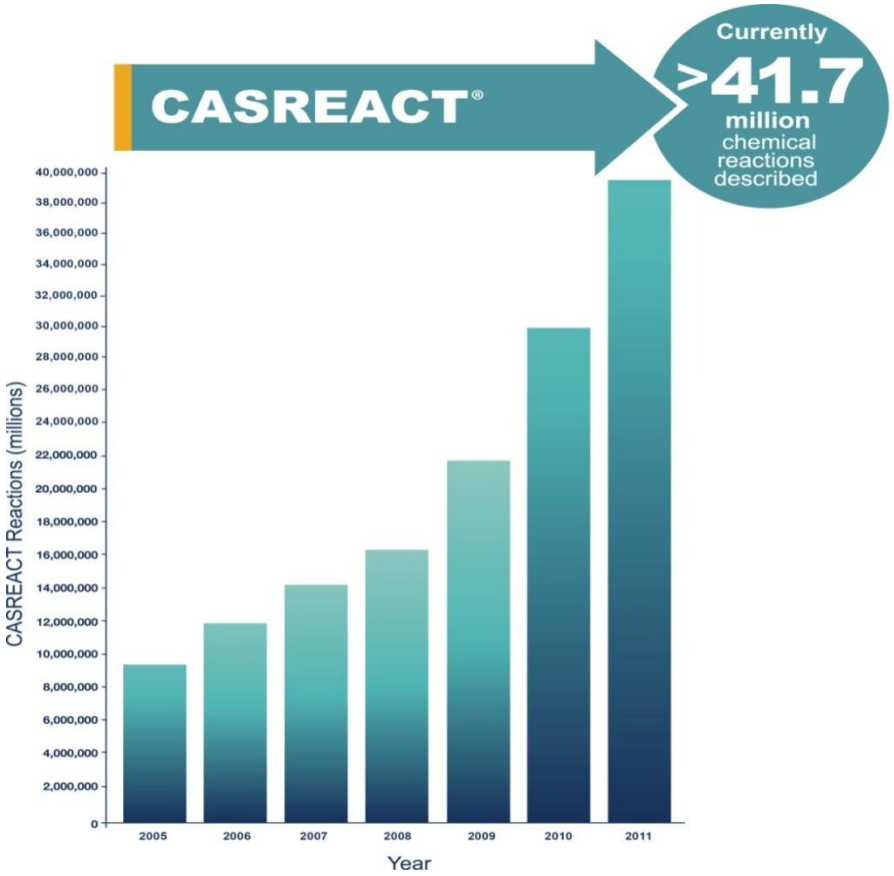

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MARPAT® —全球专利文献中的Markush结构库

```
L1   ANSWER 1 OF 1  MARPAT  COPYRIGHT 2007 ACS on STN
 Full Text
AN   142:204619  MARPAT
TI   Bioactive compositions for enhancement of drug comprising triazines
IN   Sahouani, Hassan; Scherrer, Robert A.; Jumaa, Mouhannad; Zarraga, Isidro
     Angelo Eleazar; Vogel, Kim M.; Vogel, Dennis E.; Zou, Wei
PA   3M Innovative Properties Company, USA
SO   PCT Int. Appl., 28 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  A61K009-00
CC   63-5 (Pharmaceuticals)
FAN.CNT 2
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
PI   WO 2005011629     A1    20050210      WO 2004-US24515  20040729
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     AU 2004261243     A1    20050210      AU 2004-261243   20040729
     CA 2533128        A1    20050210      CA 2004-2533128  20040729
     EP 1651185        A1    20060503      EP 2004-779530   20040729
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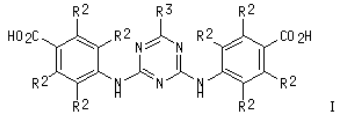

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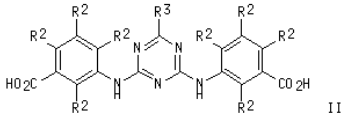

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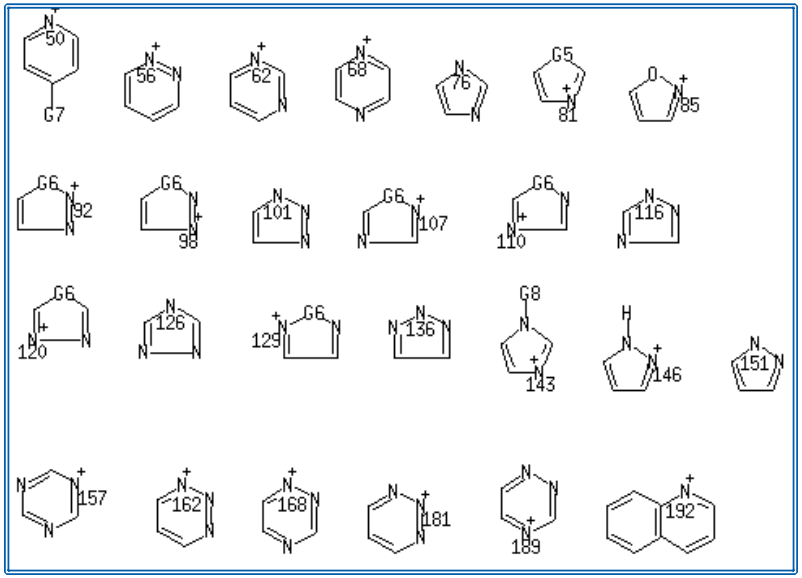

MARPAT帮助最大程度的找到结构相关专利文献

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  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

SciFinder Web的注册和登陆

SciFinder Web的系统要求：

Windows用户支持IE 8.x或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，www.java.com）

在图书馆相关页面上找到
SciFinder Web注册用的网址

首页 书目检索 学科导航 本校论文 读者论坛 FAQ 科技查新 联系我们 English

今天是:2013年10月29日 星期二

SciFinder数据库使用指南

发布时间：2013-10-18 浏览次数：222

经过一系列的调研、试用和培训活动，图书馆正式引进SciFinder数据库，欢迎广大师生使用。SciFinder的前身是美国《化学文摘》（Chemical Abstracts，简称CA）。CA是世界最大的化学文摘库，也是目前世界上应用最广泛，最为重要的化学、化工及相关学科的检索工具。CA创刊于1907年，由CAS编辑出版，被誉为“打开世界化学化工文献的钥匙”。CA的内容几乎涉及了化学家感兴趣的所有领域。随着网络技术的发展，1995年CAS推出了SciFinder联机检索数据库。自推出以来，SciFinder一直都是全世界的科学家进行化学课题研究、成果查阅、学术期刊浏览、以及把握科技发展前沿的最得力工具。与CA相比，SciFinder具有更丰富的内容和更强大的功能。SciFinder数据库收录的文献资料来自全球200多个国家和地区的60多种语言，包括1万多份期刊、63家专利机构的专利、评论、会议录、论文、技术报告和图书中的各种化学研究成果。SciFinder 比其他科学资源有更多的期刊和专利链接，能够帮助您在研究过程中更有效率，更有创意。

数据库使用方式：学生及教师使用我校邮箱地址注册个人账号及密码。注册成功后，在校园网IP范围内用个人账号和密码登录和使用化学文摘网页版。

使用步骤：

1、请点击进行账号注册，注册流程可参看注册指南.pdf。

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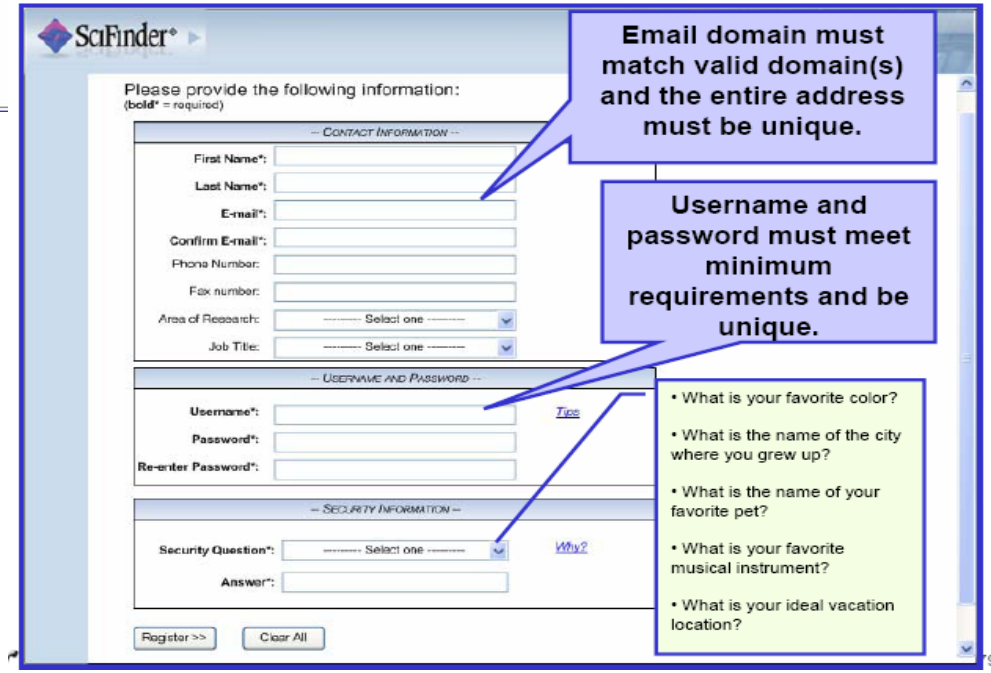
点击URL创建SciFinder Web账号

开始创建SciFinder Web帐号

创建ID不能用代理服务器的IP地址

一人只能注册一个账号



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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、 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

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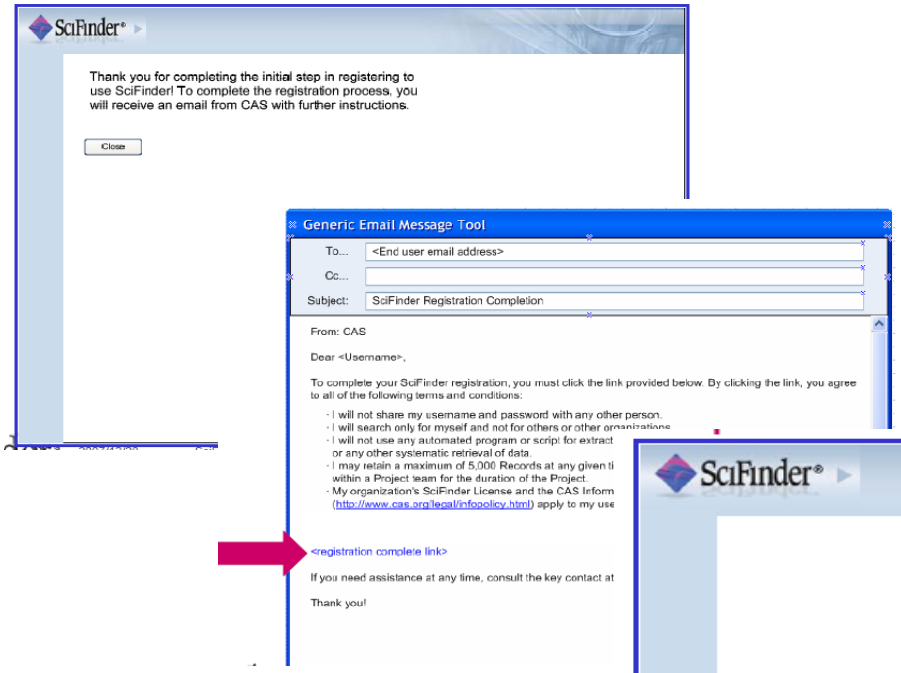
对新ID的Email确认



40分钟内查收邮件，注意垃圾邮箱
48小时内点击邮件中的确认链接

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Http://origin-scifinder.cas.org

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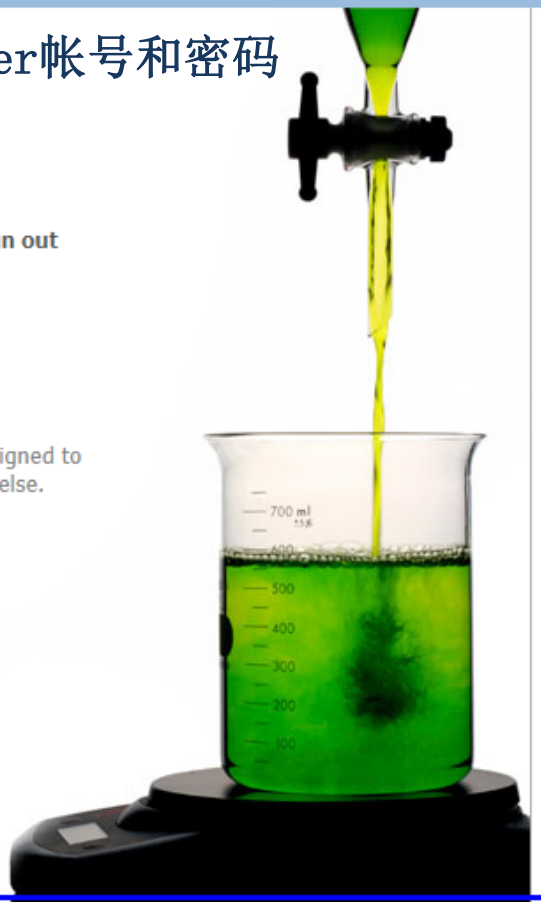

News & Updates

Welcome to SciFinder

A New Non-Java Structure Editor is Now Available in SciFinder

SciFinder now features a non-Java version of the CAS Structure Editor, a new option for your substance and reaction searching! Start searching with the new editor today. Plus, we've added a new option to Analyze reaction answer sets by reagent, along with other enhancements. See all that's new in the latest release.

Learn about this year's Nobel Prize-winning chemistry research with SciFinder

By now you've heard that Martin Karplus, Michael Levitt and Arieh Warshel were awarded the 2013 Nobel Prize in Chemistry. But did you know that much of their Nobel Prize-winning research can be found in SciFinder? Check out a few examples of their most highly cited articles.

Watch Part 3 of Our New Science in the News Podcast on Molecular Gastronomy

In part 3 of our Science in the News podcast on molecular gastronomy, find out why SciFinder is essential to food chemistry research. Watch it now and don't forget to catch all three parts of

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在线帮助

Contents Search - Search - Go

- Getting Started
- Searching for References
- Searching for Substances
- Searching for Reactions
- Finding Commercial Sources
- Using Keep Me Posted (KMP) Alerts
- Organizing Information in SciPlanner
- Viewing Session History
- Transitioning to the Web version of SciFin
- SciFinder Preferences
- System Information
- Terminology
- 日本語 (Japanese)

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Getting Started : Introduction

Introduction

To help you get started, see the suggested workflows for:

Working with **References** | Working with **Substances** | Working with **Reactions**

Because the information in SciFinder is uniquely integrated, you can start your exploration with a search for references, substances, or reactions, and then easily retrieve related information from any of the other areas.

What's New in SciFinder

The June 2013 release features a new, streamlined interface that was created in close collaboration with scientists. See the Quick Tour for a brief, 10-minute presentation of the new design.

SciFinder **Quick Tour**

See CAS Content at a Glance for the most recent database statistics.

Learning resources

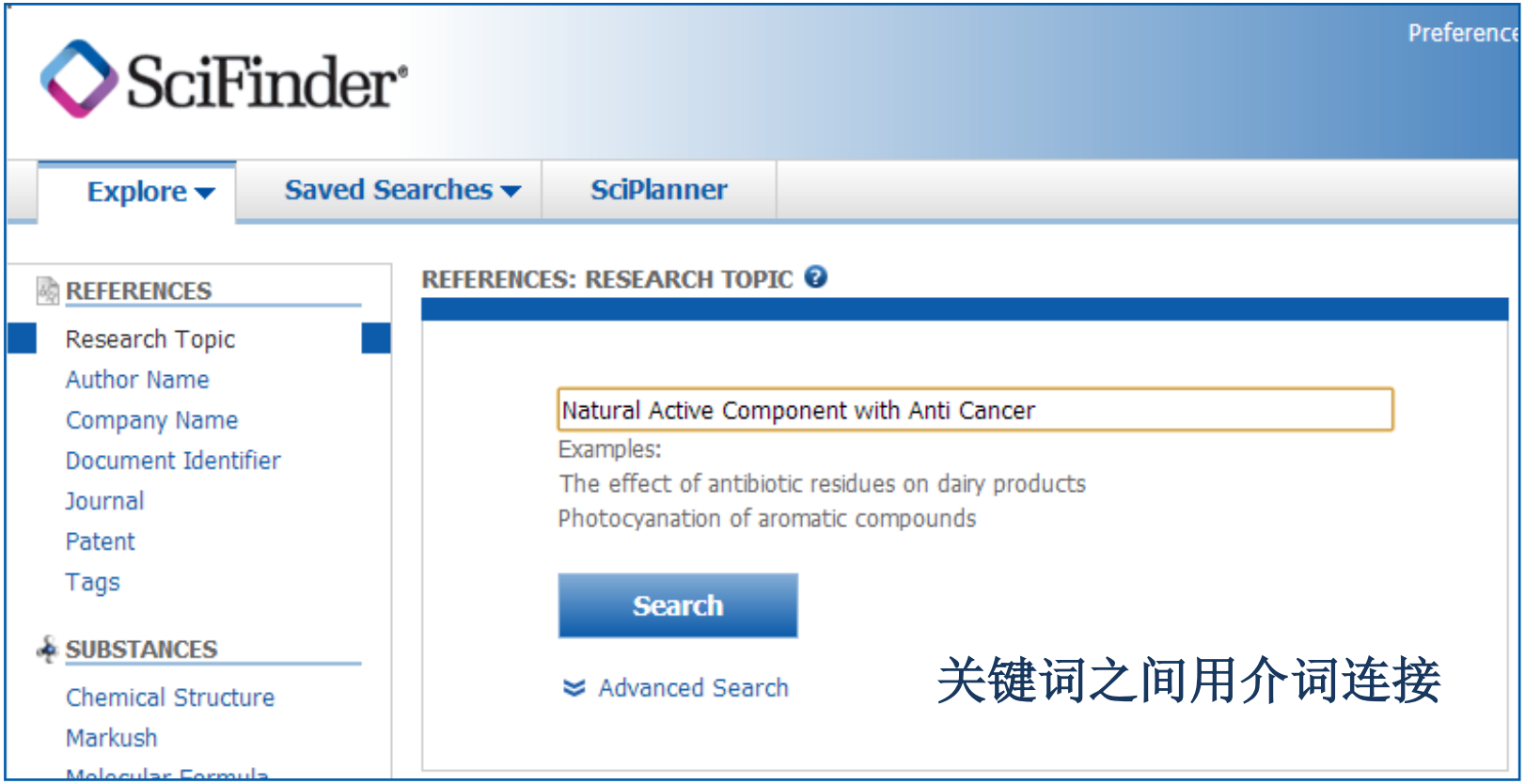
提 纲

- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

文献检索—主题

主题检索： 具有抗癌作用的天然活性成分

关键词： **Natural Active Component 、 Anti Cancer**



关键词之间用介词连接

主题检索的候选项

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Research Topic "Natural Active Component with ..."

只有104篇文献吗？

REFERENCES

Select All Deselect All

1 of 4 Research Topic Candidates Selected

		References
☑	104 references were found containing the two concepts **"Natural Active Component"** and **"Anti Cancer"** closely associated with one another.	104
☐	235 references were found where the two concepts **"Natural Active Component"** and **"Anti Cancer"** were present anywhere in the reference.	235
☐	2840 references were found containing the concept **"Natural Active Component"**.	2840
☐	968272 references were found containing the concept **"Anti Cancer"**.	968272

Get References

“Concept”表示做了同意词的扩展

“Closely associated with one another”表示同时出现在一个句子中

“were present anywhere in the reference”表示同时出现在一段话中

文献检索结果

文献分析工具

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Research Topic "Natural Active Component with ..." > **references (104)**

REFERENCES

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Analyze | Refine | Categorize

Sort by: Accession Number

Answers per Page [20] Display:

Analyze by: Author Name

- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

Liu Li 3

Shi Qiang 3

0 of 104 References Selected

Page: 1 of 6

1. **A method for preparing dandelion tea [Machine Translation].** Full Text

By Fu, Zunan

From Faming Zhuanli Shenqing (2013), CN 103330035 A 20131002. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The invention discloses a method for prepg. Dandelion Tea, comprises the following steps: (1) selecting materials for use; (2) after cleaning and drying, cut into pieces for use; (3) sterilizing at high temp.; (4) de-enzyming; (5) baking, baking **component** in two stages; (6) kneading, completed by mech. kneading twice; (7) loosing, mech. loosing; (8) fine selecting and packaging. the invention due to the adoption of pure **natural** Dandelion Leaf tea as raw materials, adding other adjuvants, Dandelion in pharmacol. provided thereon with antibacterial, endogen...

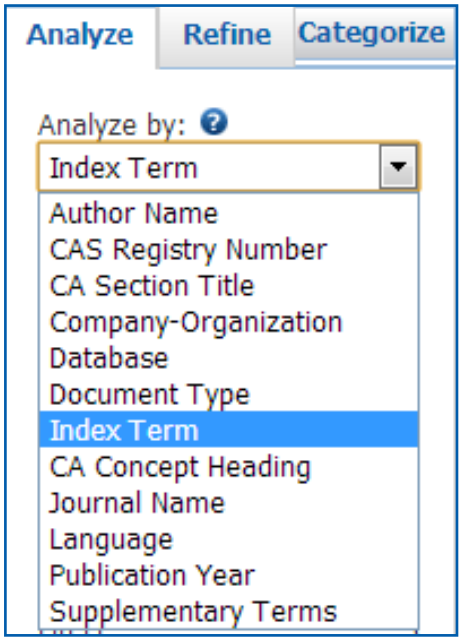
2. **Composition capable of reducing human blood sugar with natural product extract as effective component** Full Text

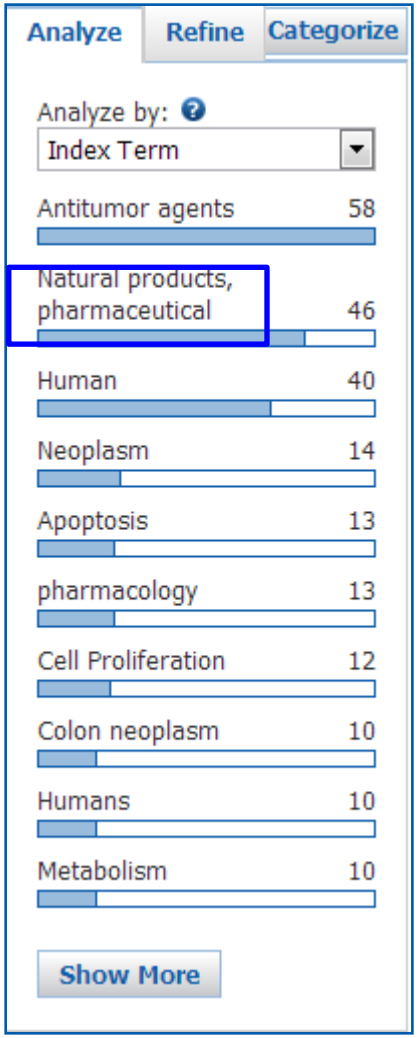
By Zhao, Shijun

From Faming Zhuanli Shenqing (2013), CN 103284045 A 20130911. | Language: Chinese, Database: CAPLUS

The invention discloses a compn. capable of **reducing** human blood sugar with **natural** product ext. as effective

文献检索结果的Analyze





Index Term基于内容的分析工具，发现 **natural products, Pharmaceutical** 这个和天然活性成分很相关的词

是否用这个词去检索，效果会更好？

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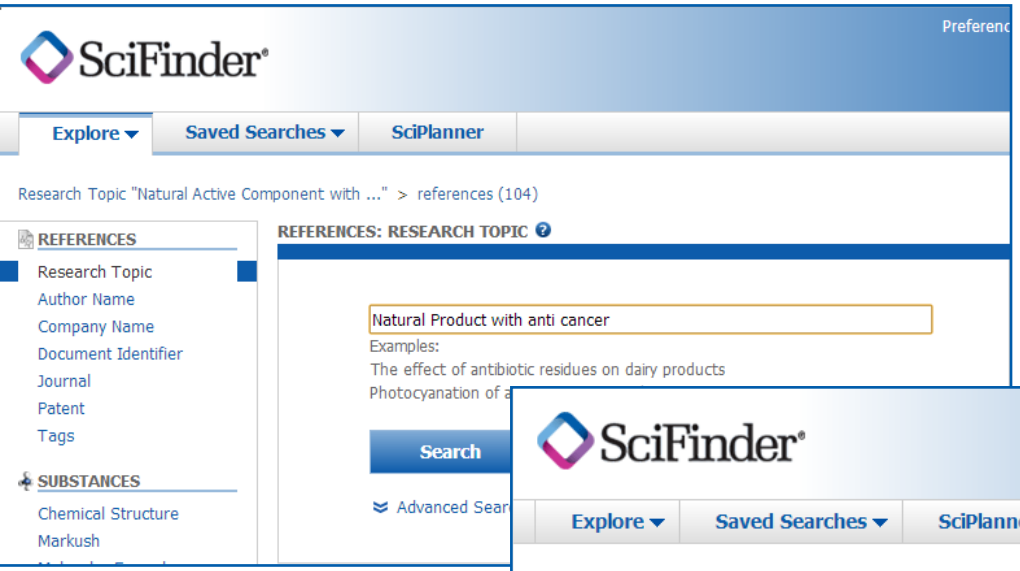
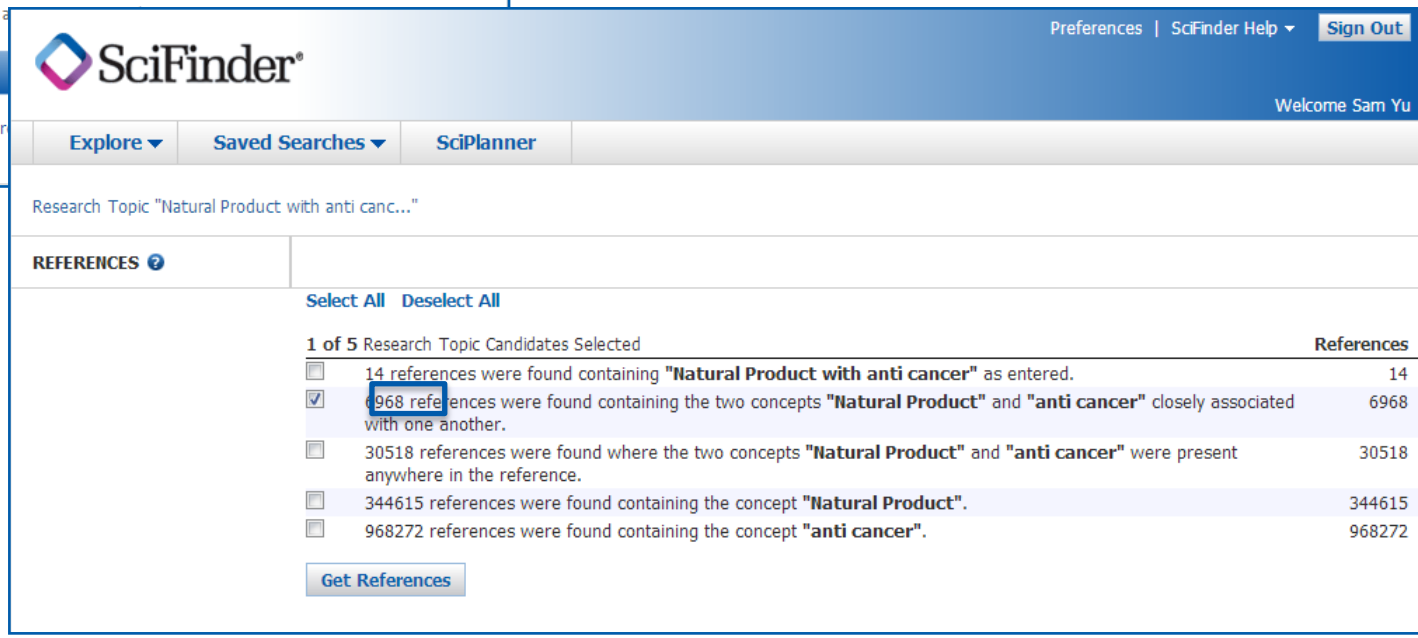
尝试新的检索



新的检索式：

Natural Product with anti cancer



更换检索词后，
结果放大了70倍

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SciFinder中的结果

SciFinder

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Research Topic "Natural Product with anti canc..." > references (6968)

REFERENCES

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

Analyze | Refine | Categorize

Sort by: Accession Number

Answers per Page [20] Display:

0 of 6968 References Selected

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Analyze by: Author Name

Liu Li	46
Newman David J	41
Cheng Yiyu	39
Ge Zhiwei	39
Shui Wenbo	37

1. Semisynthesis process for natural active compound betulinic acid [M
By Peng, Xuedong; Zhang, Mei; Zhao, Jinshao; Yan, Yongyi
From Faming Zhuanli Shenqing (2013), CN 103351418 A 20131016. | Langu
[Machine Translation of Descriptors]. This invention relates to a semisyn **anticancer natural product**, using betulin extd. from bark of birch protecting 3-hydroxyl of betulin using arom. acyl chloride, oxidizing 28- deprotecting in an alk. soln. to obtain betulinic acid crude **product**. ethanol to obtain purified betulinic acid with content and purity of above

2. Migrastatin analogues inhibit canine mammary cancer cell migration
By Majchrzak, Kinga; Lo Re, Daniele; Gajewska, Malgorzata; Bulkowska, Malgorz
Tomasz; Murphy, Paul V.; Krol, Magdalena

5. Advances in research on the effects of traditional Chinese medicines on platinum antitumor drugs
Full Text
By Zhang, Pei; Lu, Mengying; Liu, Quan; Bai, Ruizhen; Zhang, Zunjian; Xu, Fengguo
From Yaoxue Jinzhan (2013), 37(5), 207-214. | Language: Chinese, Database: CAPLUS
Platinum complexes had a broad spectrum of **antitumor** activity and played an important role in the chemotherapy of malignant **tumors**. However, their clin. applications were limited due to the serious toxic and side effects such as nephrotoxicity, gastrointestinal toxicity, ototoxicity, hematopoietic system toxicity, nervous system toxicity, etc. Recently, some Traditional Chinese Medicines showed great potentials to enhance the efficacy and diminish the side effects when used in combination with platinum **antitumor** drugs. The advances in research on the effects of Traditional Chinese Medicines...

6. Progress in research of the natural product Oroxylin A
Full Text
By Guo, Ying; Qu, Jing-tian; Zhao, Xin; Wang, Hong
From Liaoning Zhongyi Zazhi (2012), 39(12), 2512-2515. | Language: Chinese, Database: CAPLUS
The **natural product** Oroxylin A has a wide range of biol. activities, such as **anti-tumor**, neuroprotective, **anti**-inflammatory, tocolytic and **anti**-pruritic activity. Currently it has evoked great interests in the world. In this paper, it reviewed the researches on the extn., synthesis, biol. activities and mol. mechanism of Oroxylin A in recent years.

7. Nucleoside analogue as an anticancer compound
Full Text
By Kate, Abhijeet Sudhir; George, Saji David; Sonawane, Shailendra; Periyasamy, Giridharan
From PCT Int. Appl. (2013), WO 2013144894 A1 20131003. | Language: English, Database: CAPLUS
The invention relates to a compd. of I. The invention includes all isomeric forms and tautomeric forms I and pharmaceutically acceptable salts and derivs. such as esters and ethers. The invention further relates to the processes for isolation and prodn. of the compd. of formula (1) by fermn. of the marine actinomycetes strain PM0895117/MTCC 5675. The invention also relates to the pharmaceutical compns. contg. I as an active ingredient and use in medicines for the treatment of **cancer**.

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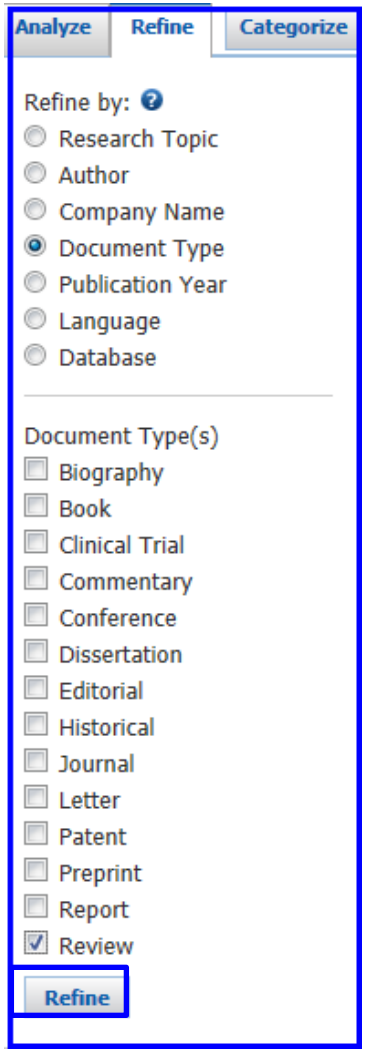

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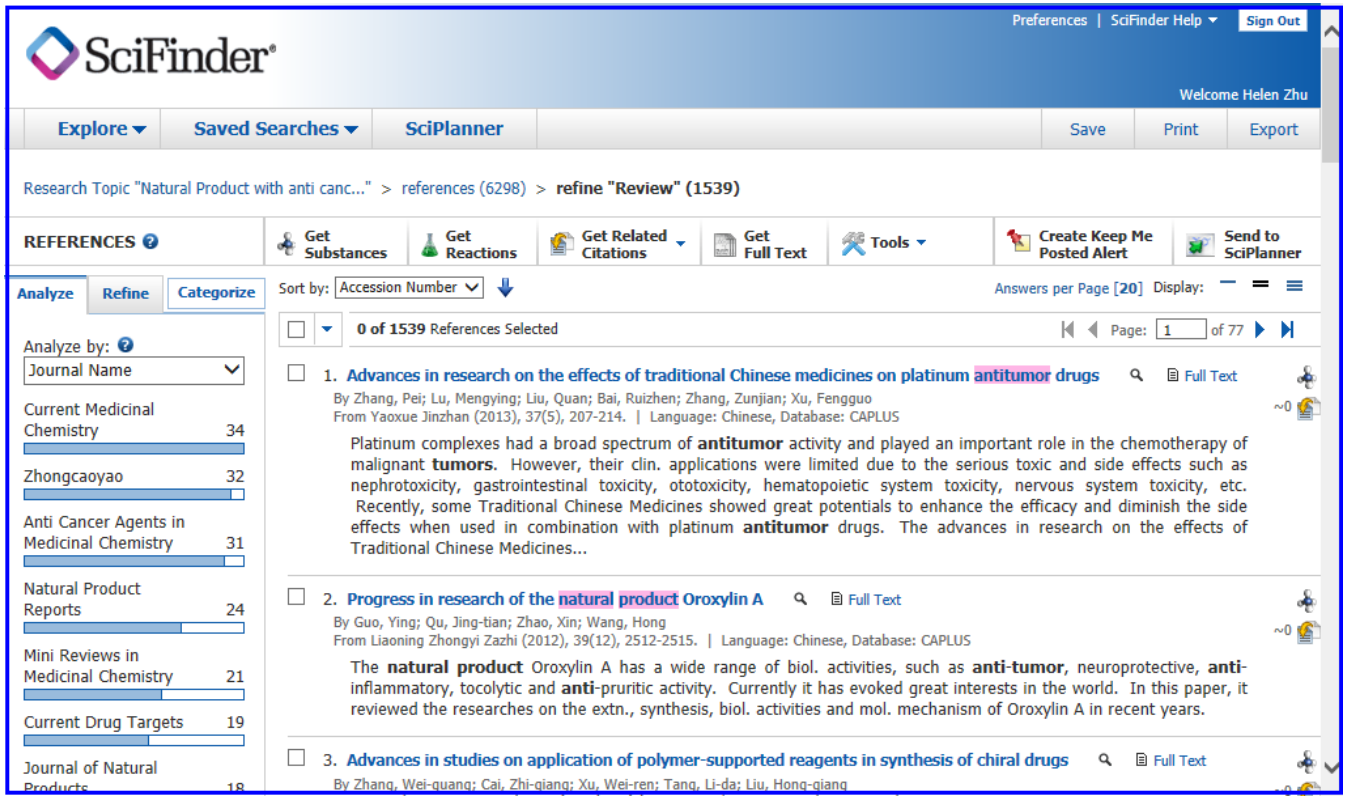

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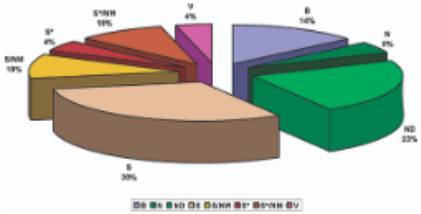
Anti Cancer Agents in Medicinal Chemistry	31
Natural Product Reports	24
Mini Reviews in Medicinal Chemistry	21
Current Drug Targets	19
Journal of Natural Products	18

1. **as Sources of New Drugs over the Last 25 Years** Full Text
By Newman, David J.; Cragg, Gordon M.
From Journal of Natural Products (2007), 70(3), 461-477. | Language: English, Database: CAPLUS
1291



A review. This review is an updated and expanded version of two prior reviews that were published in this journal in 1997 and 2003. In the case of all approved agents the time frame has been extended to include the 25½ years from 01/1981 to 06/2006 for all diseases worldwide and from 1950 (earliest so far identified) to 06/2006 for all approved **antitumor** drugs worldwide. We have continued to utilize our secondary subdivision of a "**natural product** mimic" or "NM" to join the original primary divisions. From the data presented, the utility of **natural products** as sources of novel structures,...

2. **P-glycoprotein: from genomics to mechanism** Full Text
By Ambudkar, Suresh V.; Kimchi-Sarfaty, Chava; Sauna, Zuben E.; Gottesman, Michael M.
From Oncogene (2003), 22(47), 7468-7485. | Language: English, Database: CAPLUS
481

A review. Resistance to chem. different **natural product anti-cancer** drugs (multidrug resistance, or MDR) results from decreased drug accumulation, resulting from expression of one or more ATP-dependent efflux pumps. The first of these to be identified was P-glycoprotein (P-gp), the **product** of the human MDR1 gene, localized to chromosome

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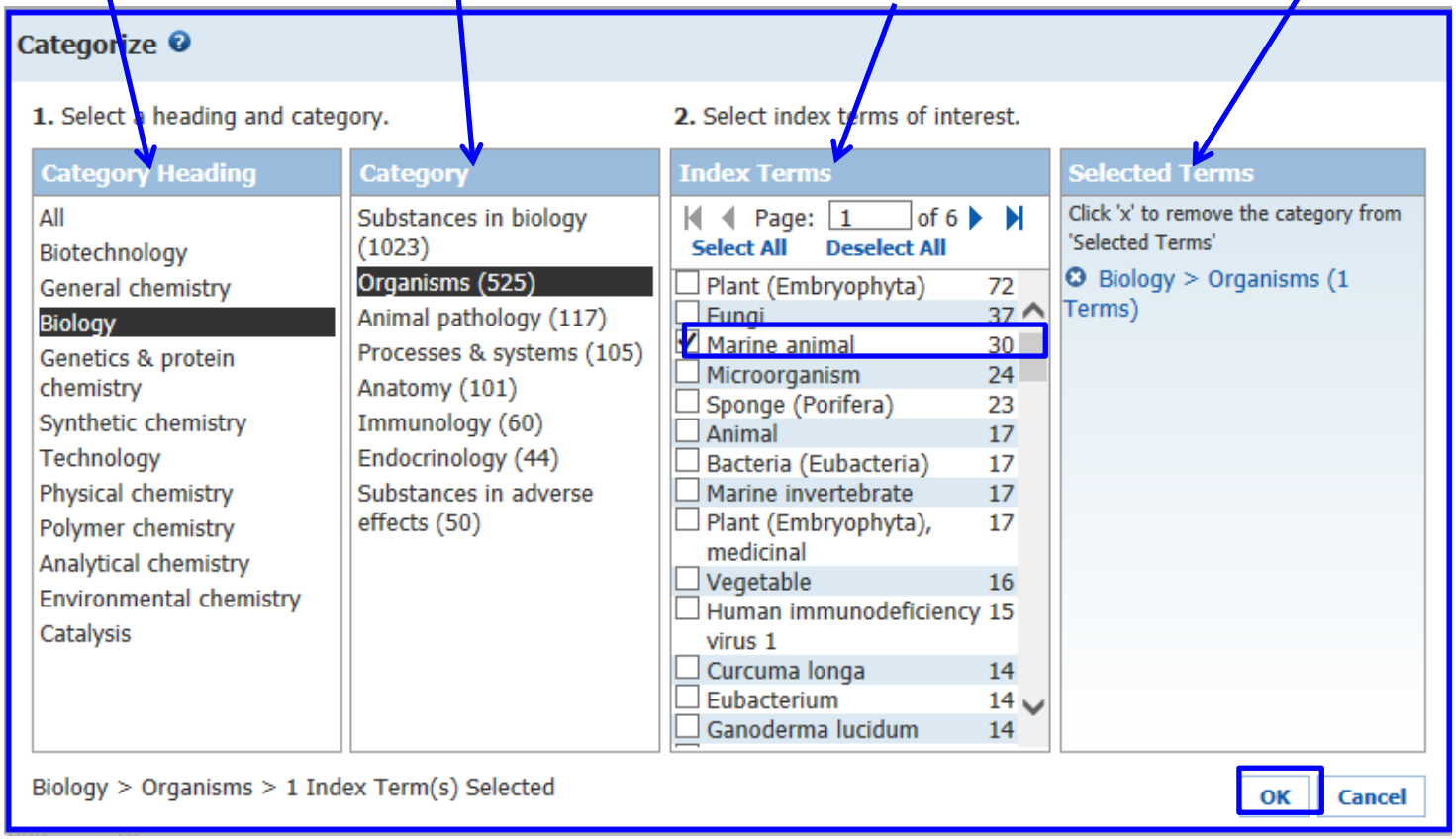

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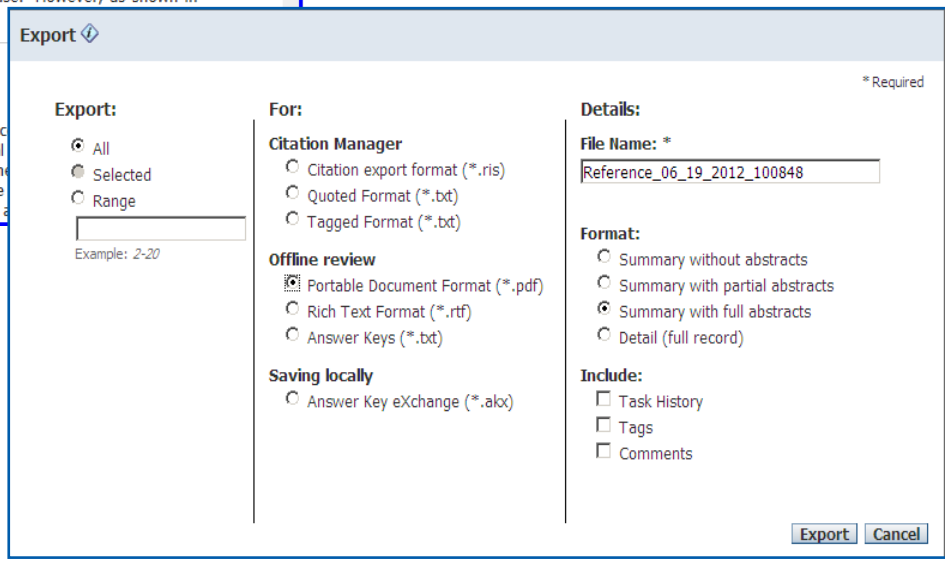

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2. Drug development from marine natural products

By: Molinski, Tadeusz F.; Dalisay, Doralyn S.; Lievens, Sarah L.; Saludes, Jonel P.

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 contribute to new discoveries and the difficulties assocd. with translating marine-derived compds. into clin. trials. Providing an outlook into the future, we also examine the advances that may further expand the promise of drugs from the sea.

Indexing

Pharmacology (Section1-0)

Concepts 重要概念

Antitumor agents

antimitotic; drug development from marine natural products

Drug design
Human
Natural products, pharmaceutical
Drug discovery
Marine animal
Neoplasm
Snail

drug development from marine natural products

Substances 重要物质

114899-77-3 Yondelis

drug development from marine natural products

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

107452-89-1 Prialt

ziconotide; drug development from marine natural products

Natural product occurrence; Pharmacological activity; Therapeutic use; Biological study; Occurrence; Uses

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SOURCE

Nature Reviews Drug Discovery
Volume8
Issue1
Pages69-85
Journal; General Review
2009
CODEN:NRDDAG
ISSN:1474-1776
DOI:10.1038/nrd2487

COMPANY/ORGANIZATION

Department of Chemistry and Biochemistry and Skaggs School of Pharmacy and Pharmaceutical Sciences
University of California, San Diego
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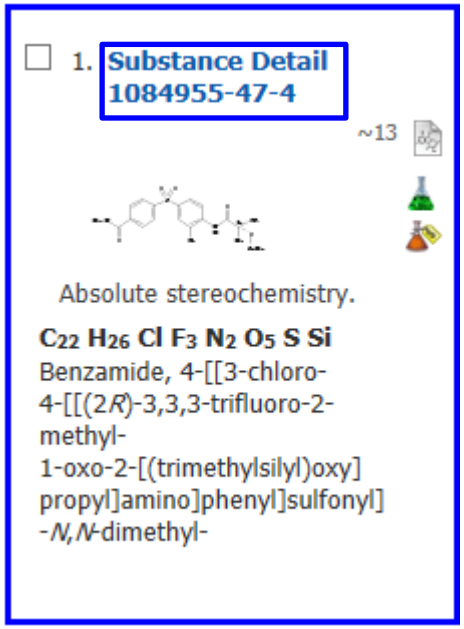

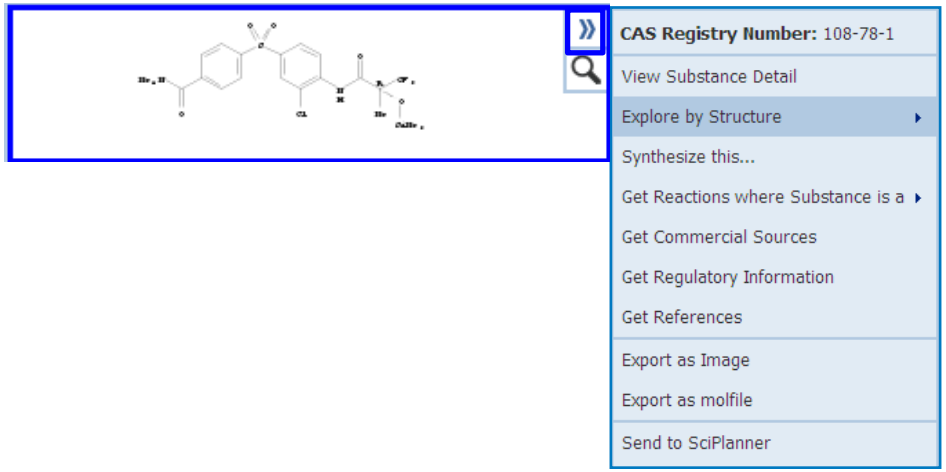

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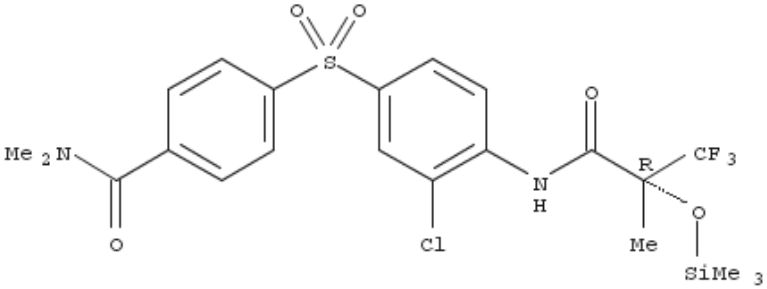
CAS Registry Number: 1084955-47-4

$C_{22}H_{26}ClF_3N_2O_5SSi$

Benzamide, 4-[[3-chloro-4-[[(2*R*)-3,3,3-trifluoro-2-methyl-1-oxo-2-[(trimethylsilyl)oxy]propyl]amino]phenyl]sulfonyl]-*N*,*N*-dimethyl-

AZD 7545

Deleted CAS Registry Numbers: 670276-04-7



Absolute stereochemistry.

Source of Registration: CA

~13 References

物质信息来源

Document Types: Journal, Patent

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Biological Study	✓	✓	✓	✓
Preparation		✓		
Properties		✓		✓
Uses	✓	✓	✓	

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Enzymes (all) >>>> Pyruvate dehydrogenase kinase	4

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

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	104	pH 1 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 2 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 3 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 4 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 5 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 6 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 7 Temp: 25 °C	(1)	
Bioconcentration Factor	104	pH 8 Temp: 25 °C	(1)	
Bioconcentrat				
Bioconcentrat				

Chemical Pr

Koc	
Koc	

Density Properties	Value	Condition	Note	Top
Density	1.314±0.06 g/cm3	Temp: 20 °C Press: 760 Torr	(1)	
Molar Volume	419.1±3.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(1)	

Lipinski and Related Properties	Value	Condition	Note	Top
Freely Rotatable Bonds	7		(1)	
H Acceptors	7		(1)	
H Donors	1		(1)	
H Donor/Acceptor Sum	8		(1)	
logP	2.956±0.651	Temp: 25 °C	(1)	
Molecular Weight	551.05		(1)	

Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See spectrum		(2)	
Proton NMR Spectrum	See spectrum		(2)	

Structure-related Properties	Value	Condition	Note	Top
Polar Surface Area	101 A2		(1)	

Thermal Properties	Value	Condition	Note	Top
Boiling Point	630.3±55.0 °C	Press: 760 Torr	(1)	
Enthalpy of Vaporization	93.23±3.0 kJ/mol	Press: 760 Torr	(1)	

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- Reaction Structure

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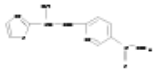
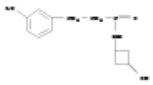


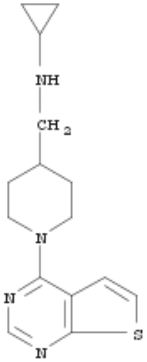
$C_{12}H_{14}N_4S_2$
3-Pyridinecarbothioamide, 6-[[1-(2-thiazolyl)propyl]amino]-

2. Substance Detail 1462241-00-4



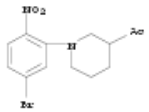
$C_{13}H_{16}BrNO_2$
Benzenepropanamide, 3-bromo-*N*-(3-hydroxycyclobutyl)-

3. Substance Detail 1462240-99-8



$C_{15}H_{20}N_4S$
4-Piperidinemethanamine, *N*-cyclopropyl-1-thieno[2,3-*d*]pyrimidin-4-yl-

4. Substance Detail 1462240-97-6



$C_{13}H_{15}BrN_2O_3$
Ethanone, 1-[1-(5-bromo-2-nitrophenyl)-3-piperidinyl]-

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6. Substance Detail

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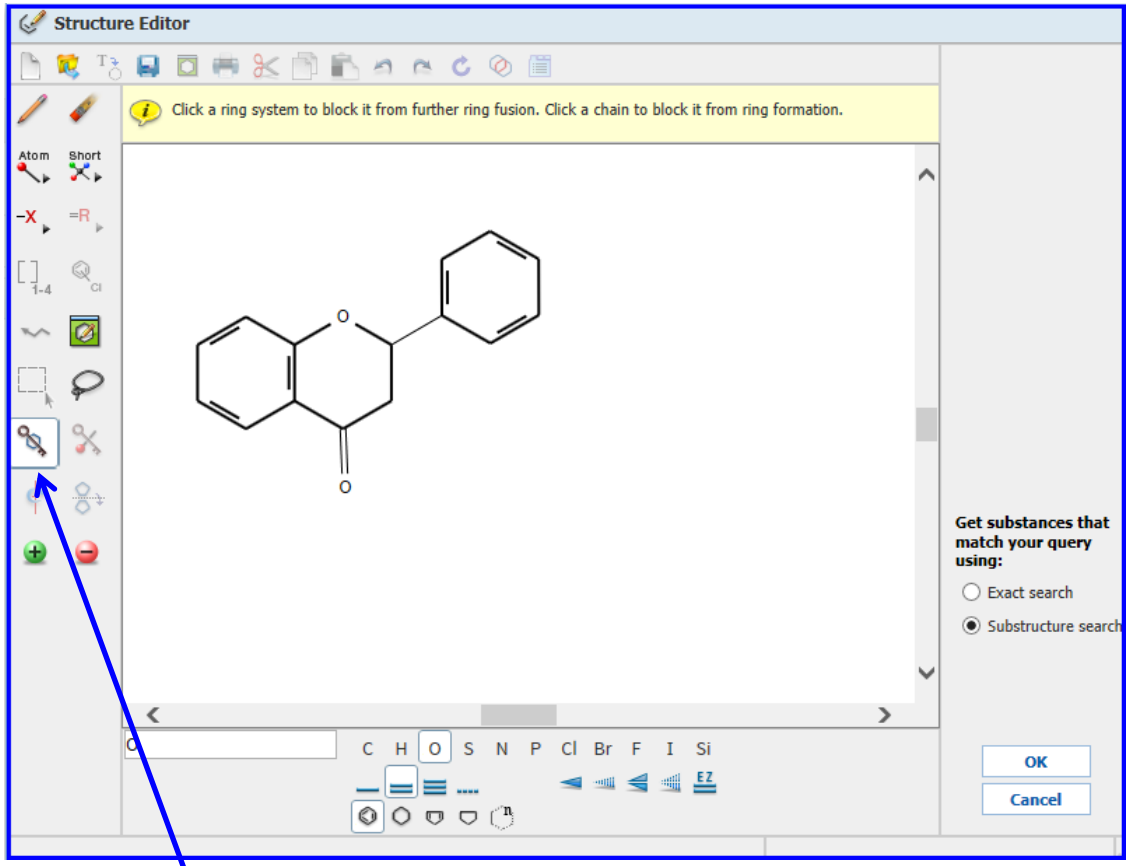

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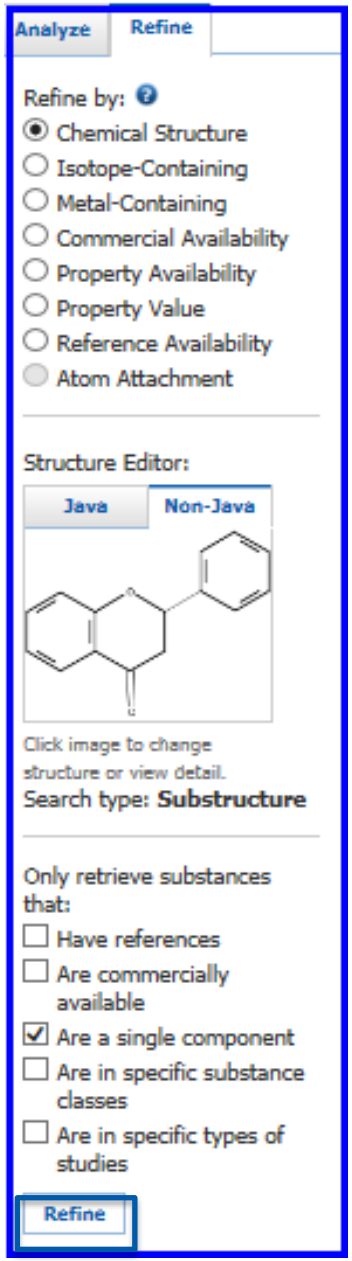

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Uses	1857
Properties	1615
Reactant or Reagent	1574
Occurrence	805
Analytical Study	436
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Formation, Nonpreparative	172
Prophetic in Patents	40

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1. Substance Detail 958734-07-1 ~1
$C_{15}H_{12}O_4$
4*H*-1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-2,3-dihydro-

2. Substance Detail 1438763-28-0 ~1
Absolute stereochemistry.
$C_{17}H_{16}O_2$
4*H*-1-Benzopyran-4-one, 2-(4-ethylphenyl)-2,3-dihydro-, (2*R*)-

3. Substance Detail 21785-09-1 ~133
$C_{16}H_{14}O_3$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-2-phenyl-
Spectra
Experimental Properties

4. Substance Detail 72984-48-6 ~20
Absolute stereochemistry.,Rotation (-).
$C_{16}H_{14}O_3$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-7-methoxy-2-phenyl-, (2*S*)-
Experimental Properties

5. Substance Detail 725263-73-0 ~14
Absolute stereochemistry.,Rotation (+).
$C_{16}H_{14}O_3$

6. Substance Detail 62252-06-6 ~7
$C_{15}H_{12}O_4$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-7-

7. Substance Detail 138474-12-1 ~2
Absolute stereochemistry.
$C_{15}H_{12}O_4$

8. Substance Detail 1256571-17-1 ~2
Absolute stereochemistry.
$C_{15}H_{12}O_4$

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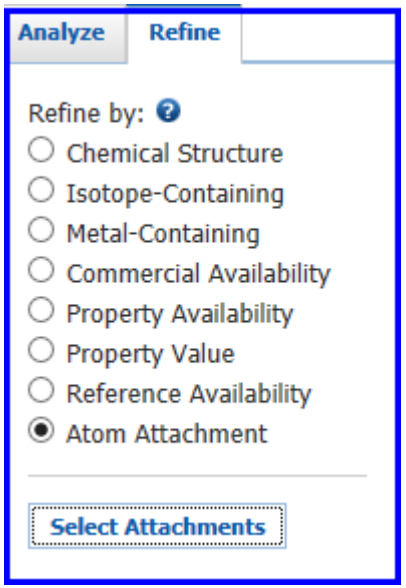

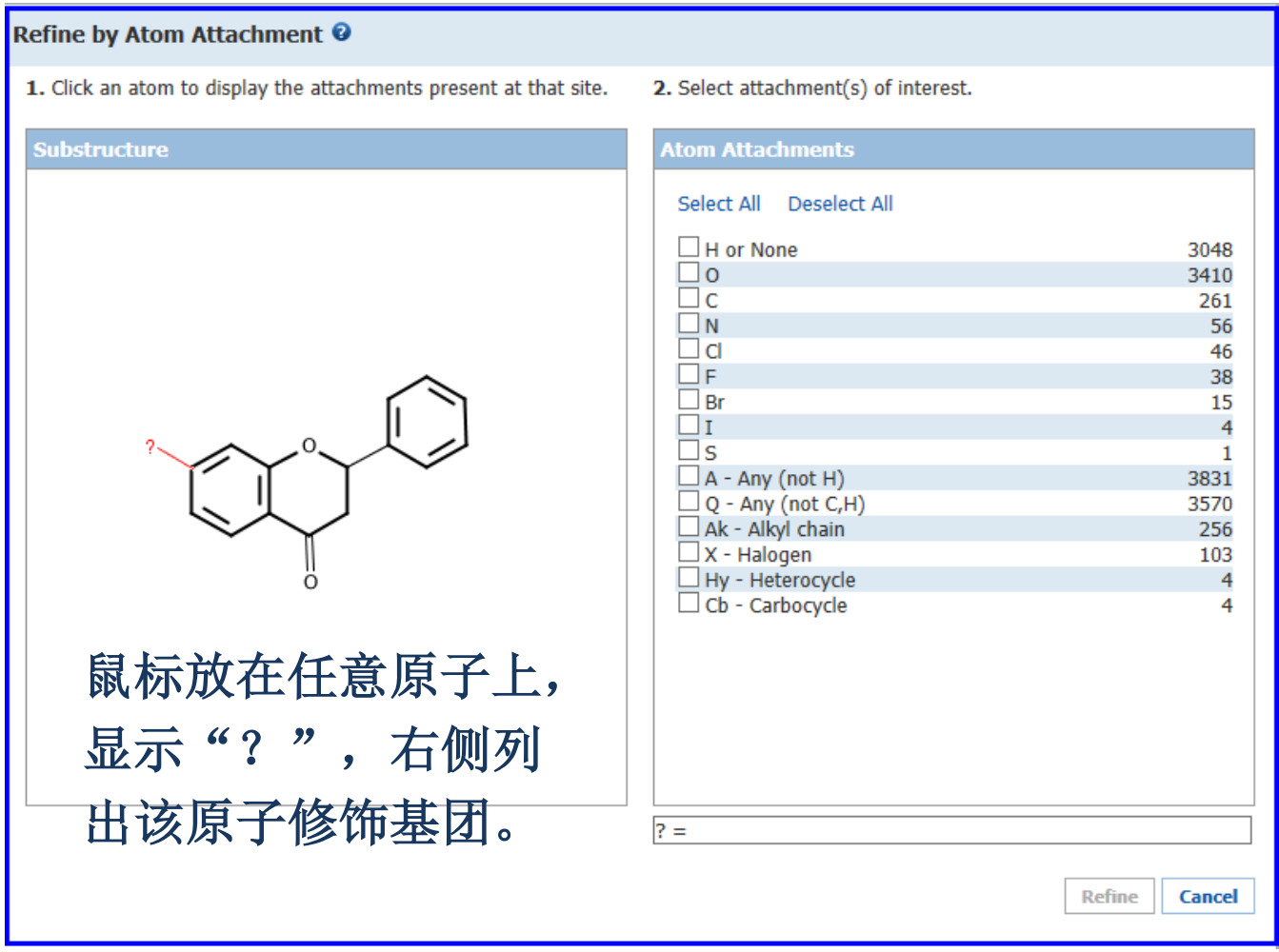

鼠标放在任意原子上，显示“？”，右侧列出该原子修饰基团。

Atom Attachemnt：

了解结构中原子修饰情况。

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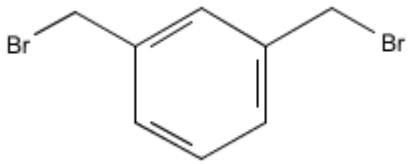
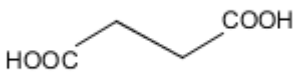
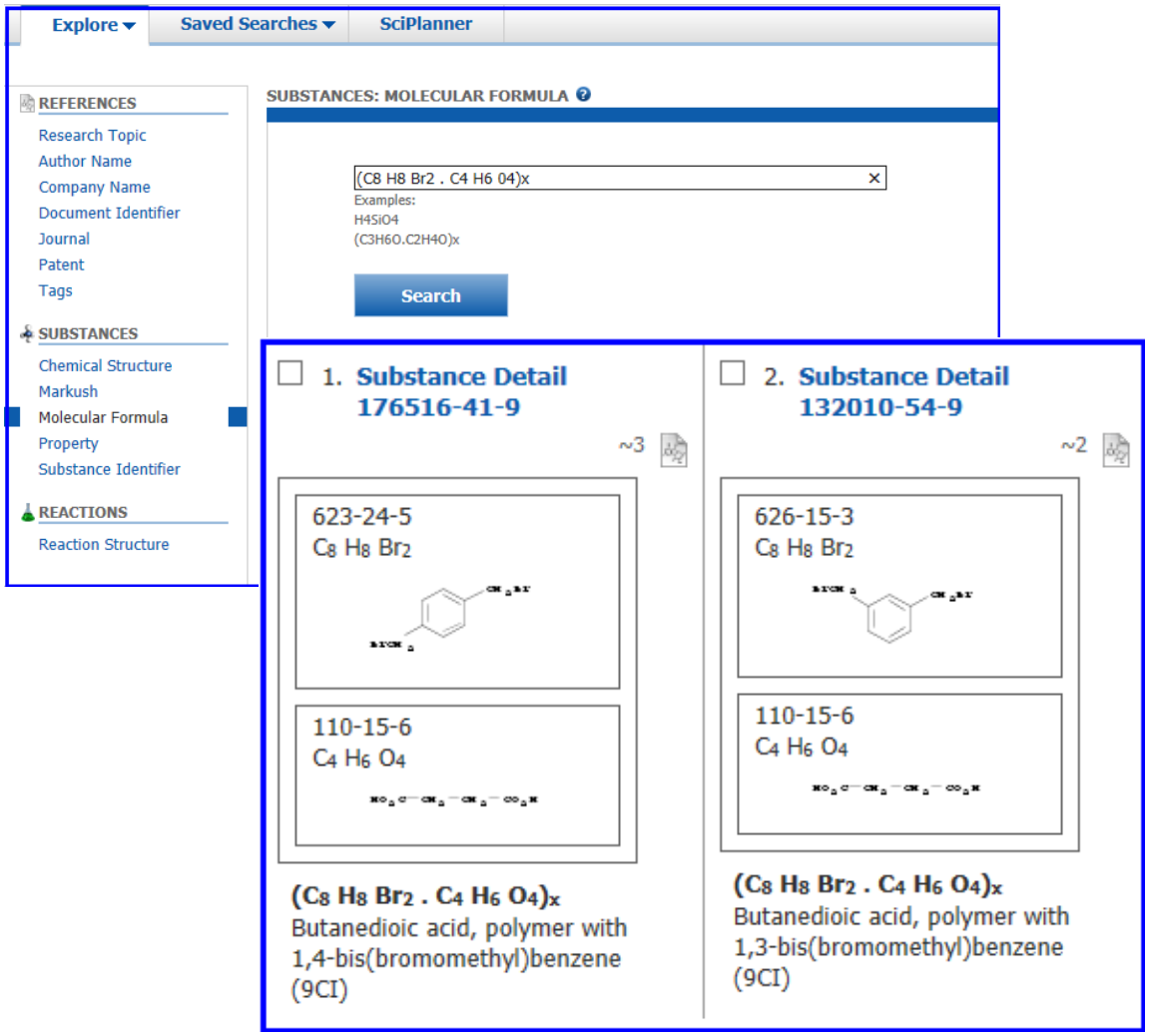
物质检索—分子式

已知起始原料的聚合物





（C8 H8 Br2 . C4 H6 O4）x



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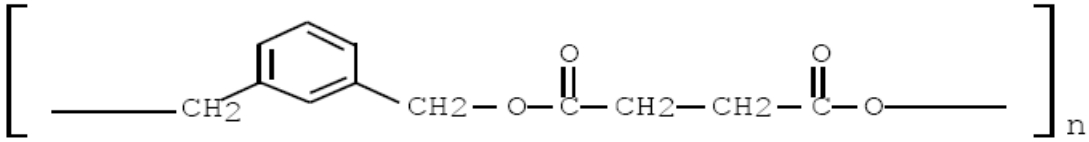
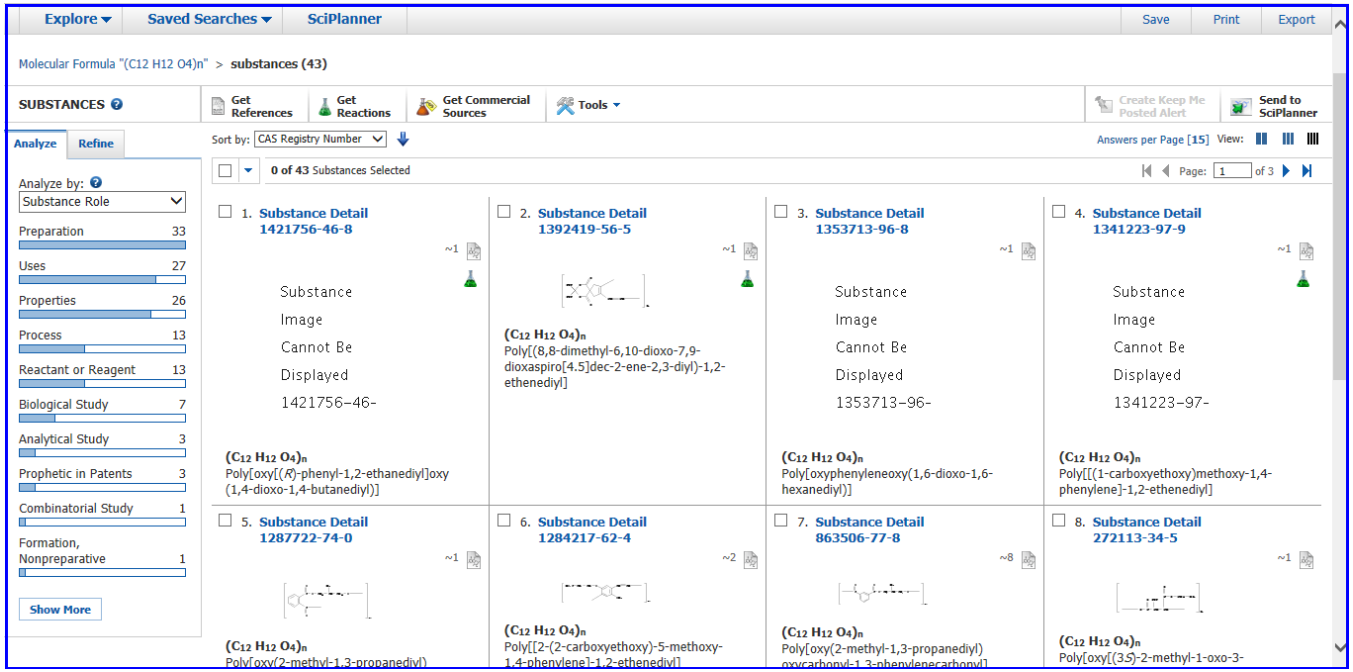
物质检索—分子式

已知重复单元的聚合物



(C12 H12 O4)n



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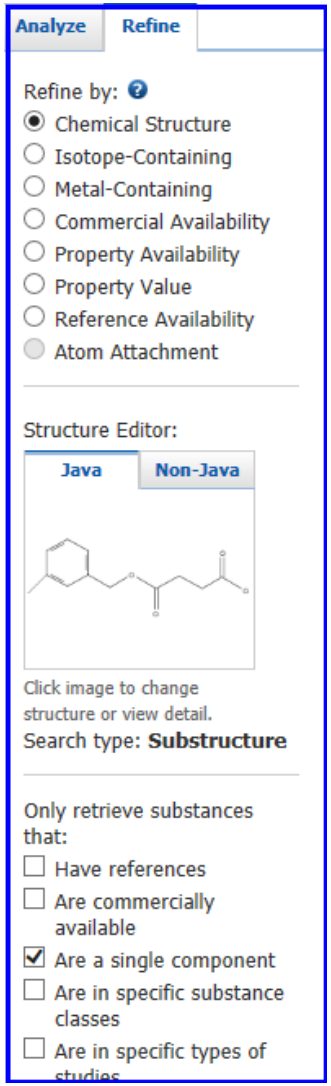

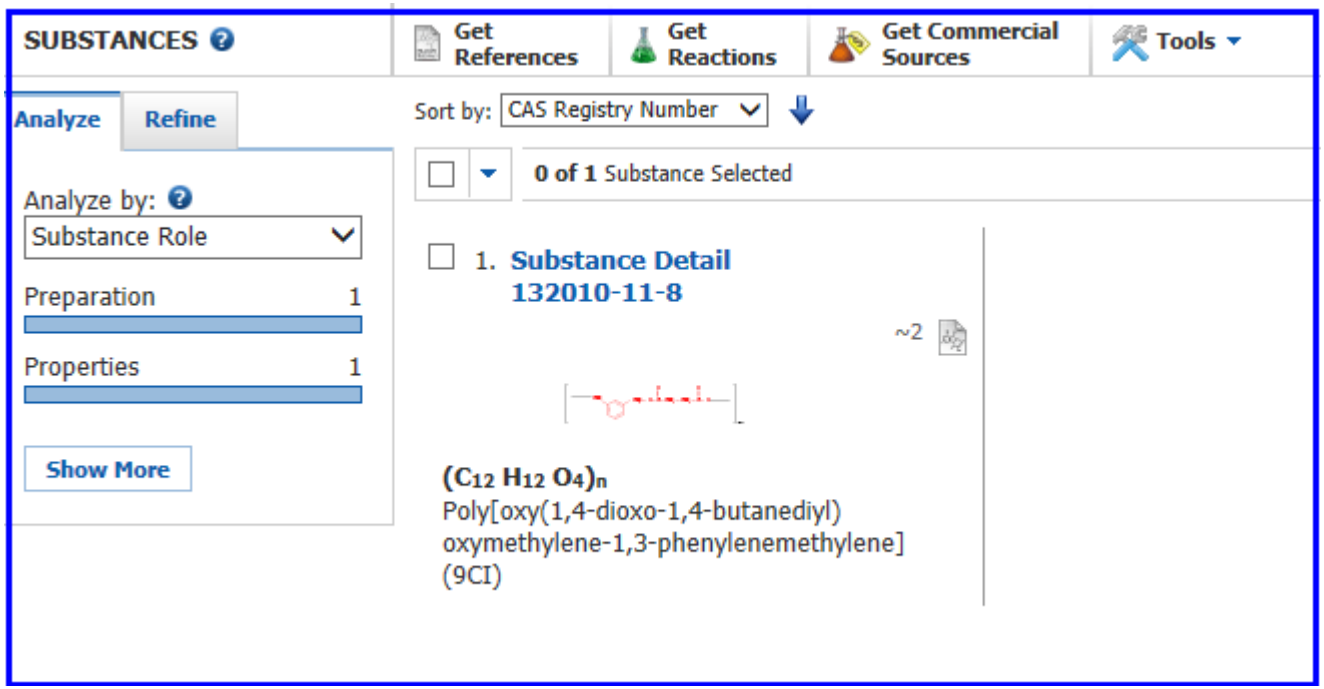

利用结构特征进行**Refine**，迅速查找需要的物质

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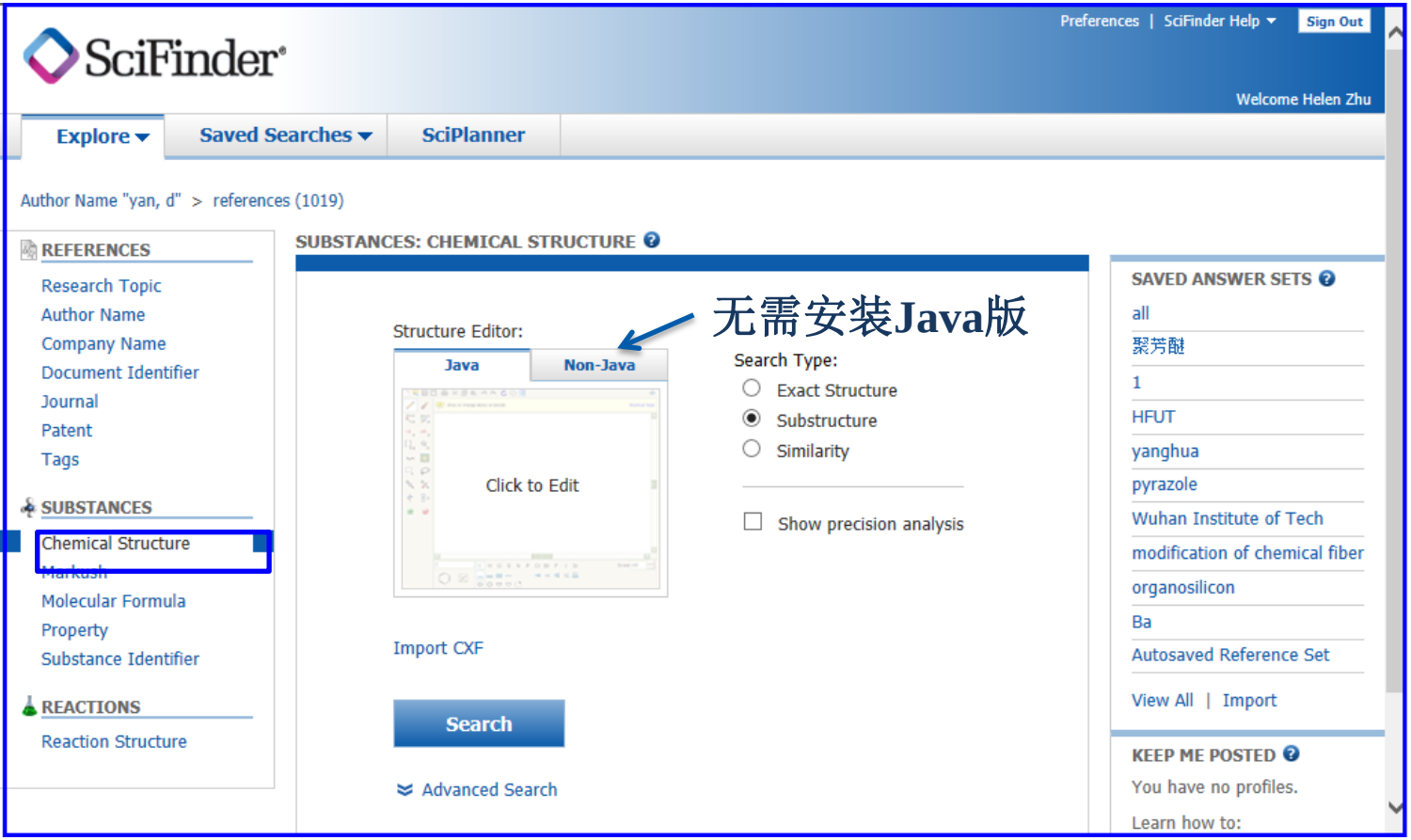
物质检索--结构



点击画图版来进行结构输入，初次使用时需要安装Java插件

64位系统：需同时安装32位和64位Java

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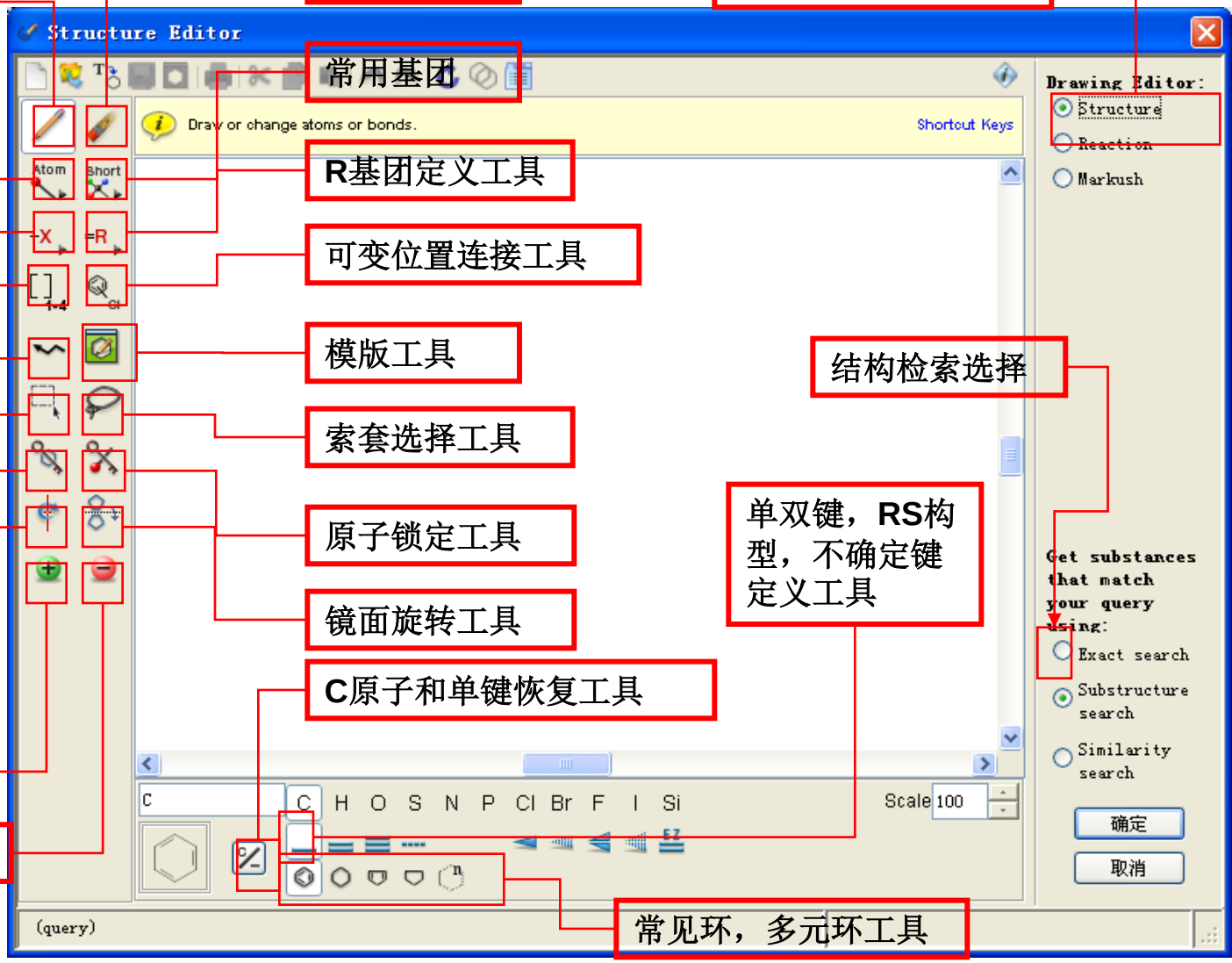
SciFinder结构绘制工具



铅笔

橡皮

结构和反应切换功能

元素周期表

常用基团

R基团定义工具

可变基团

可变位置连接工具

重复基团工具

模版工具

结构检索选择

碳链工具

索套选择工具

选择工具

原子锁定工具

单双键，RS构型，不确定键定义工具

环锁定工具

镜面旋转工具

旋转工具

C原子和单键恢复工具

正电子

负电子

常见环，多元环工具

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Structure Editor

Add to Editor

Enter CAS Registry Number, SMILES, or InChI:

196618-13-0

Examples:

50-00-0

CCCO

InChI=1S/C3H8O/c1-2-3-4/h4H, 2-3H2, 1H3

达菲的CAS No.

Shortcut Keys

Drawing Editor:

Structure

Reaction

Markush

Structure Editor

Drag the lasso around a structure to select it.

存为模板

调用模板

Save As Template...

Please enter a template name

dafei

确定

取消

Templates

Polycarbocyclic

O-containing

Nucleic Acid

NOS-containing

N-containing

Monocarbocyclic

Misc

Cycloalkane

Coordination

Carbohydrate

Bicarbocyclic

Amino Acid

Alkaloid

User Defined

dafei

Close

Get substances that match your query using:

Exact search

Substructure search

Similarity search

确定

取消

C H O S N P Cl Br F I Si

Scale 100

312.41

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精确结构检索

精确结构检索：

获得结构本身、盐及混合物

Explore ▾ | Saved Searches ▾ | SciPlanner

Substance Identifier "AZD 7545 " > substances (1) > 1084955-47-4

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: CHEMICAL STRUCTURE

Search Type:
- Exact Structure
- Substructure
- Similarity

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Sort by: Relevance | Answers per Page [15] | View:

0 of 25 Substances Selected | Page: 1 of 2

1. Substance Detail 196618-13-0 ~1245
Absolute stereochemistry.,Rotation (-).
$C_{16}H_{28}N_2O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-
Experimental Properties

2. Substance Detail 204255-11-8 ~552
196618-13-0
$C_{16}H_{28}N_2O_4$
Absolute stereochemistry.,Rotation (-).
7664-38-2
H_3O_4P
$C_{16}H_{28}N_2O_4 . H_3O_4P$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-, phosphate (1:1)

3. Substance Detail 756819-03-1 ~4
196618-13-0
$C_{16}H_{28}N_2O_4$
Absolute stereochemistry.,Rotation (-).
7664-93-9
H_2O_4S
$C_{16}H_{28}N_2O_4 . x H_2O_4S$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-, sulfate

4. Substance Detail 204255-09-4 (Component: 196618-13-0) ~3
Absolute stereochemistry.,Rotation (-).
$C_{16}H_{28}N_2O_4 . Cl H$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, hydrochloride (1:1), (3*R*,4*R*,5*S*)-

Stereo Candidates

5 Candidates 1 Selected

Select All Deselect All

Stereo Candidates
- [x] Absolute stereo match
- [ ] Absolute stereo mirror image
- [ ] Relative stereo match
- [ ] Stereo that doesn't match query
- [ ] No stereo in answer structure

Get Substances

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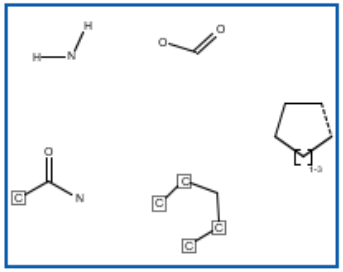
亚结构检索

作用机理

编辑本段

帕拉米韦是Babu等在分析唾液酸、扎那米韦、奥司他韦与NA的互相作用机制及构效关系的基础上设计并合成的环戊烷衍生物，与环连接的基团有亲水的羧基和胍基以及疏水的异戊基和乙酰氨基，4个极性不同的基团分别作用于流感病毒NA结构中不同的活性位点区域。羧基部分与NA活性位点的3个精氨酸残基Arg118，Arg292，

SUBSTANCES: CHEMICAL STRUCTURE



Click image to change structure or view detail.

Import CXF

Search

Advanced Search ☐ Always Show

Search Type:

- ○ Exact Structure
- ◉ Substructure
- ○ Similarity

☐ Show precision analysis

Formula Weight	☐ Return only substances in this formula weight range: Min: Max:	
Characteristics	☑ Single component	单组分物质
	☐ Commercially available	
	☐ Included in references	
Classes	☐ Alloys	
	☐ Coordination compounds	
	☐ Incompletely defined	
	☐ Mixtures	
	☐ Polymers	
	☑ Organics, and others not listed	有机物质

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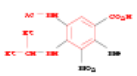
亚结构检索

0 of 704 Substances Selected

1. **Substance Detail**
127971-59-9

~1

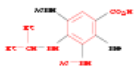


$C_{15}H_{21}N_3O_5$
Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-

Experimental Properties

2. **Substance Detail**
127971-80-6

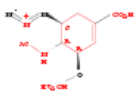
~1



$C_{17}H_{25}N_3O_4$
Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-

3. **Substance Detail**
182367-45-9

~1



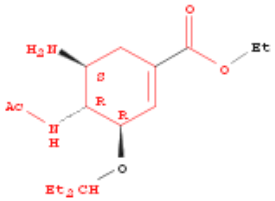
Relative stereochemistry.

$C_{14}H_{22}N_4O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3α,4β,5α)-(9CI)

4. **Substance Detail**
182367-47-1

达菲核心成分

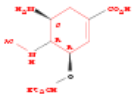
~1



$C_{16}H_{28}N_2O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3α,4β,5α)-(9CI)

5. **Substance Detail**
182367-71-1

~2

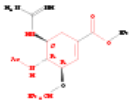


Relative stereochemistry.

$C_{14}H_{24}N_2O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3*R*,4*R*,5*S*)-*rel*-

6. **Substance Detail**
182367-73-3

~1



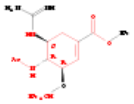
Relative stereochemistry.

$C_{17}H_{30}N_4O_4$
1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3*R*,4*R*,5*S*)-*rel*-

7. **Substance Detail**
182367-74-4

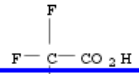
~1

182367-73-3
$C_{17}H_{30}N_4O_4$



Relative stereochemistry.

76-05-1
$C_2HF_3O_2$



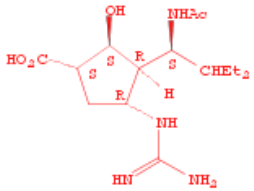
182368-47-4

~1

1. **Substance Detail**
330600-85-6

帕拉米韦

~286



$C_{15}H_{28}N_4O_4$
Cyclopentanecarboxylic acid, 3-[(1*S*)-1-(acetylamino)-2-ethylbutyl]-4-[(aminoiminomethyl)amino]-2-hydroxy-, (1*S*,2*S*,3*R*,4*R*)-

亚结构检索：获得包含全部片段结构的所有物质

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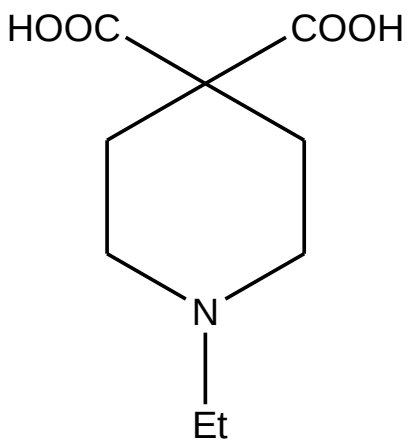
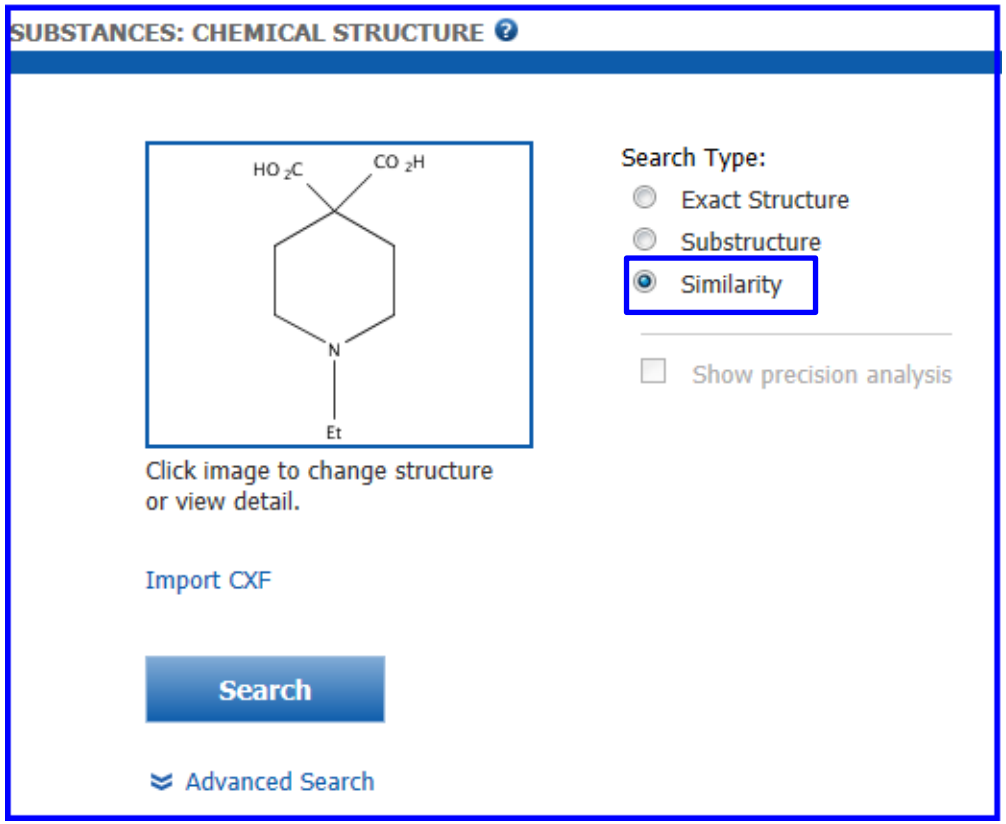
结构检索—结构相似的检索

SciFinder中的相似结构检索，帮助获得在结构上存在相似的物质。



Chemical Structure exact > **substances (0)**



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相似结构检索

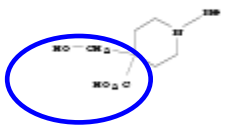
Select All Deselect All

1 of 6 Similarity Candidates Selected

		Substances
☐	≥ 99 (most similar)	0
☐	95-98	0
☐	90-94	0
☑	85-89	11
☐	80-84	30
☐	75-79	127
☐	70-74	435
☐	65-69	1287
☐	0-64 (least similar)	4617

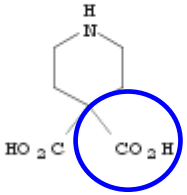
Get Substances

Score: 88
1. **Substance Detail**
1267985-98-7



$C_8H_{15}NO_3$
4-Piperidinecarboxylic acid, 4-(hydroxymethyl)-1-methyl-

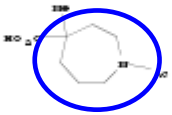
Score: 83
13. **Substance Detail**
121880-27-1



$C_7H_{11}NO_4$
4,4-Piperidinedicarboxylic ac

Score: 78
17. **Substance Detail**
1027511-99-4

~0



$C_{10}H_{17}NO_3$
1*H*-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-

相似结构检索：

取代基位置变化
取代基变化
母体结构变化

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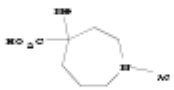
无文献的物质

Score: 78

17. **Substance Detail**
1027511-99-4

~0



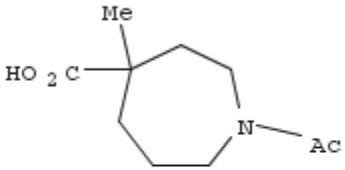
$C_{10}H_{17}NO_3$
1*H*-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-

17.

CAS Registry Number: 1027511-99-4 *Score:* 78

$C_{10}H_{17}NO_3$

1*H*-Azepine-4-carboxylic acid, 1-acetylhexahydro-4-methyl-



Source of Registration: Chemical Catalog
Supplier: AstaTech, Inc.

~0 References

很多无文献的物质是有试剂供应商提供给CAS申请登记号，
并有证据表明其存在

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结构检索小结

- 精确结构检索：
  获得物质的盐，聚合物，混合物，配合物等，母体结构不能修改，不能修饰

- 亚结构检索：
  所画的结构必须存在，母体结构不能修改，但可以被修饰

- 相似结构检索：
  母体结构可以修改，也可以被修饰，用相似度来控制获得的结果

提 纲

- 介绍
  - SciFinder Web中的内容
  - SciFinder Web的注册和登陆
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献检索
  - SciFinder Web中的物质检索
  - SciFinder Web中的Markush检索
  - SciFinder Web中的反应检索
- **SciFinder Web使用常见问题和网络资源**

- **具体物质[Specific Substance]：**

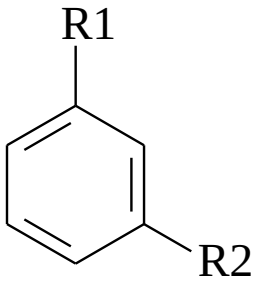
  以具体化学结构所陈述的特定物质，会被标示CAS No.

- **预测性物质[Prophetic Substance]：**

  使用Markush结构所陈述的预测物质，一个Markush可以陈述上百或上千的化学物质

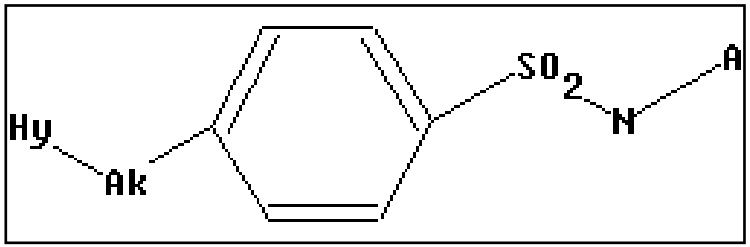
  Patent 中所陈述的预测物质，不会被标示CAS No.

  Markush检索，能检索到通过结构检索检不到的专利

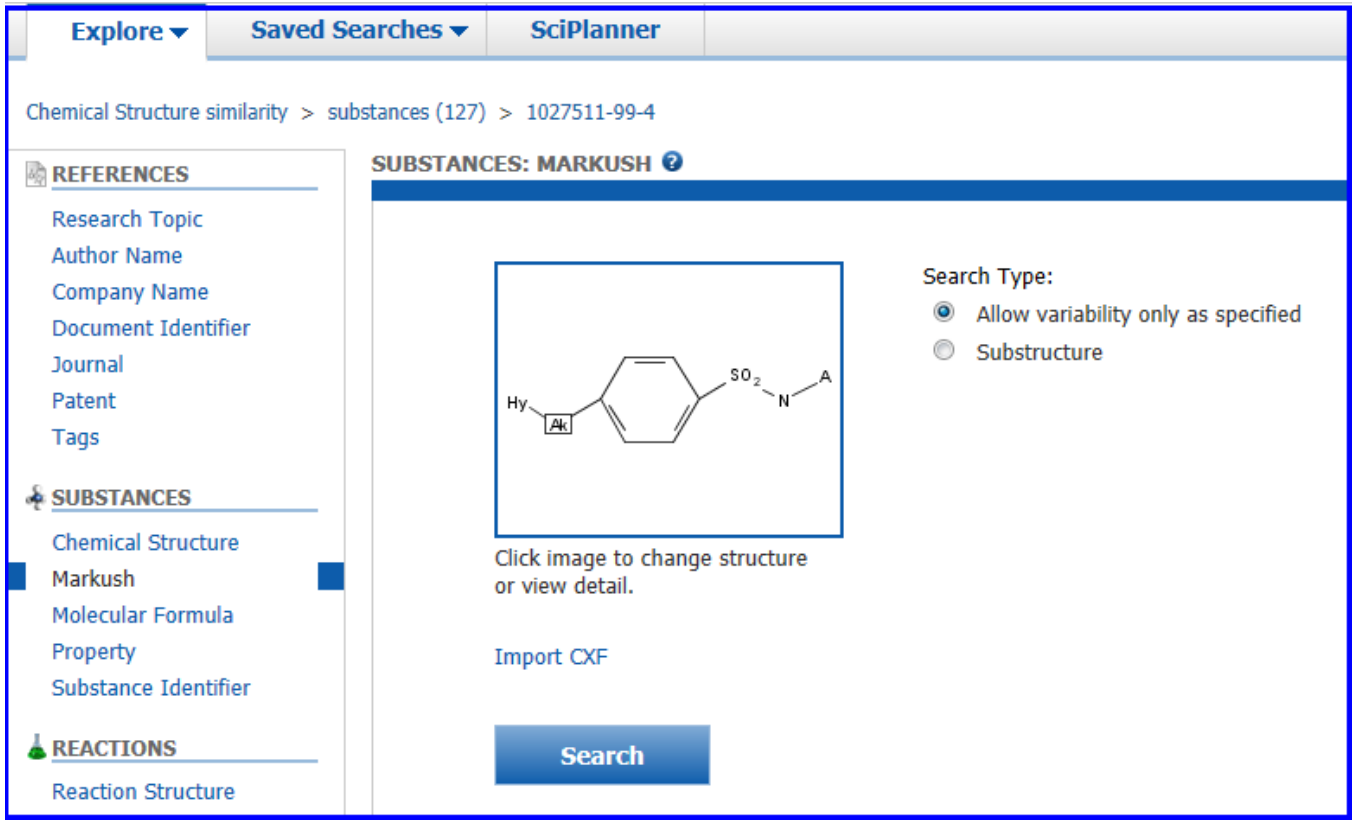


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH_2–halogen, —CH(–CH_3)–halogen,



SciFinder中的Markush检索能帮助做初步的专利评估。



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Markush structure variable only at spe... > references (119)

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Patent 119

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Answers per Page [20] Display:

0 of 119 References Selected

Page: 1 of 6

1. **Substituted piperidine derivatives as a GPR119 agonist useful in treatment of metabolism related diseases and their preparation** Full Text

By Yang, Jin; Kim, Jinwoong; Lee, Hankyu; Kim, Jaehyun; Son, Changmo; Lee, Kyuhwan; Choi, Hyungho; Kim, Daehoon; Choi, Hyosun; Rhee, Jaekeol

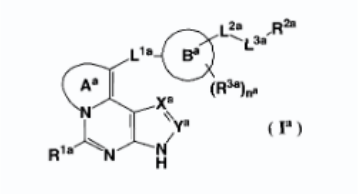
From PCT Int. Appl. (2013), WO 2013105753 A1 20130718. | Language: English, Database: CAPLUS

The invention is related to substituted piperidine derivs. of formula I as a GPR119 agonist useful in treatment of metab. related diseases such as diabetes or obesity and their prepn. The invention compds. I, wherein A is (un)substituted Ph or heterocyclic group; R^1 is $COOR_3$, or a (un)substituted heterocyclic group; R^2 and R^3 are each independently a straight or branched chain, or a(un)substituted C_{1-5} alkyl group; m is 0, 1, 2, 3; n is 1, 2, 3; their pharmaceutically acceptable salts are claimed. Compd. II was prepd. by multi-step procedure (procedure given). The invention compds. were eva...

2. **Preparation of tricyclic heterocyclic compounds as JAK inhibitors** Full Text

By Hayashi, Keishi; Watanabe, Tsuneo; Toyama, Koji; Kamon, Junji; Minami, Masataka; Uni, Miyuki; Nasu, Mariko

From PCT Int. Appl. (2013), WO 2013024895 A1 20130221. | Language: English, Database: CAPLUS



Title compds. I [A^a = 5- to 6-membered heteroaryl contg. one or two N atom; X^a = H or CR^{9a}; R^{1a} = H, halo, alkyl or haloalkyl; ring B^a = cycloalkane, cycloalkene, 3- to 14-membered nonarom. heterocycle, arom. carbocycle or 5- to 10-membered arom. heterocycle; R^{2a} = H, halo, azido, cycloalkyl, etc.; L^{1a} = single bond, alkylene, alkenylene or alkynylene; L^{2a} = single bond, alkylene, alkenylene, or alkynylene; L^{3a} = single bond, O, S, etc.; Ya = CR^{10a}; n = 0, 1 or 2, R^{3a} = hydroxy, amino, carboxy, carbamoyl, each of R^{9a} and R^{10} independently = H, halogen, cyano, carbamoyl, etc.], and their pharma...

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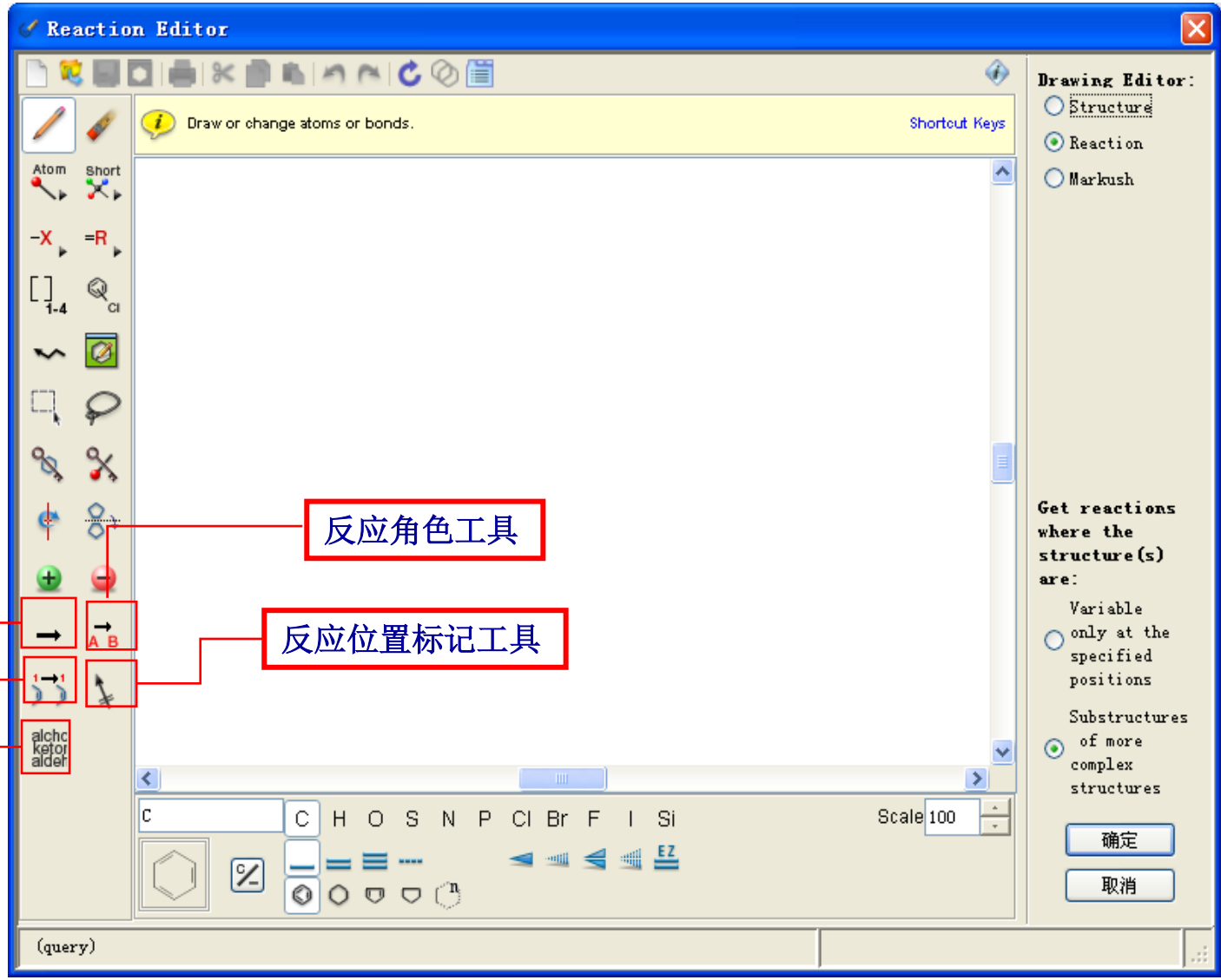

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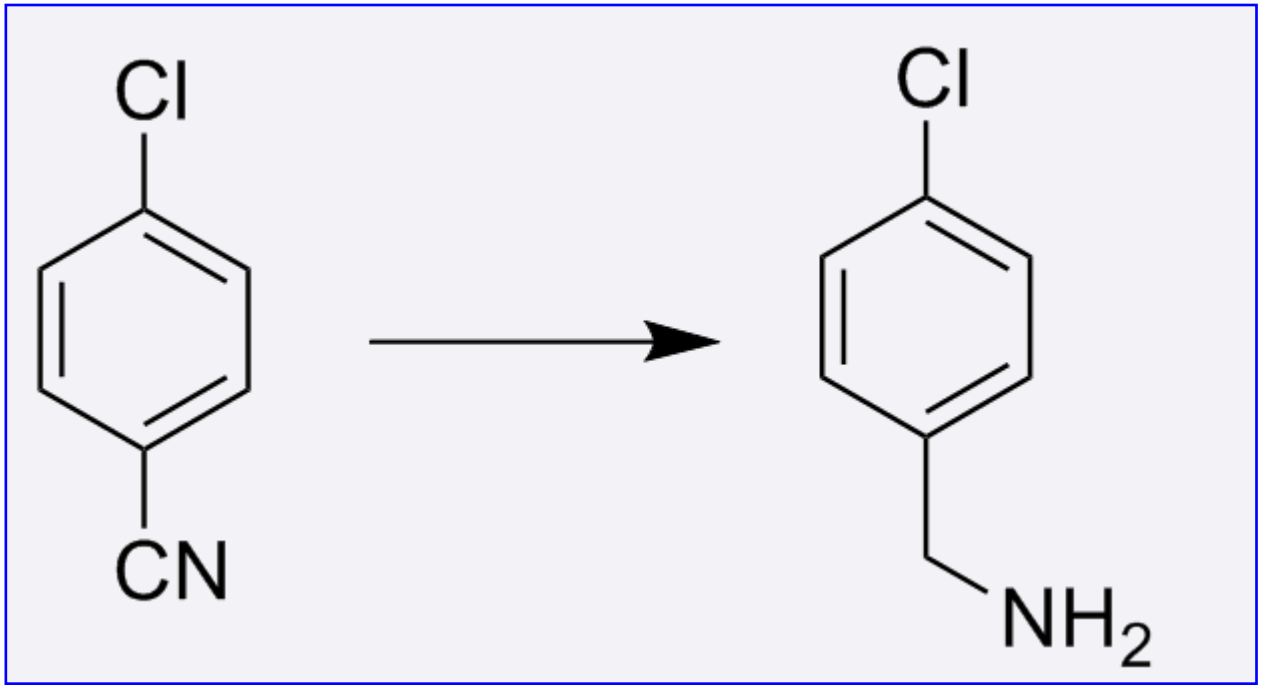

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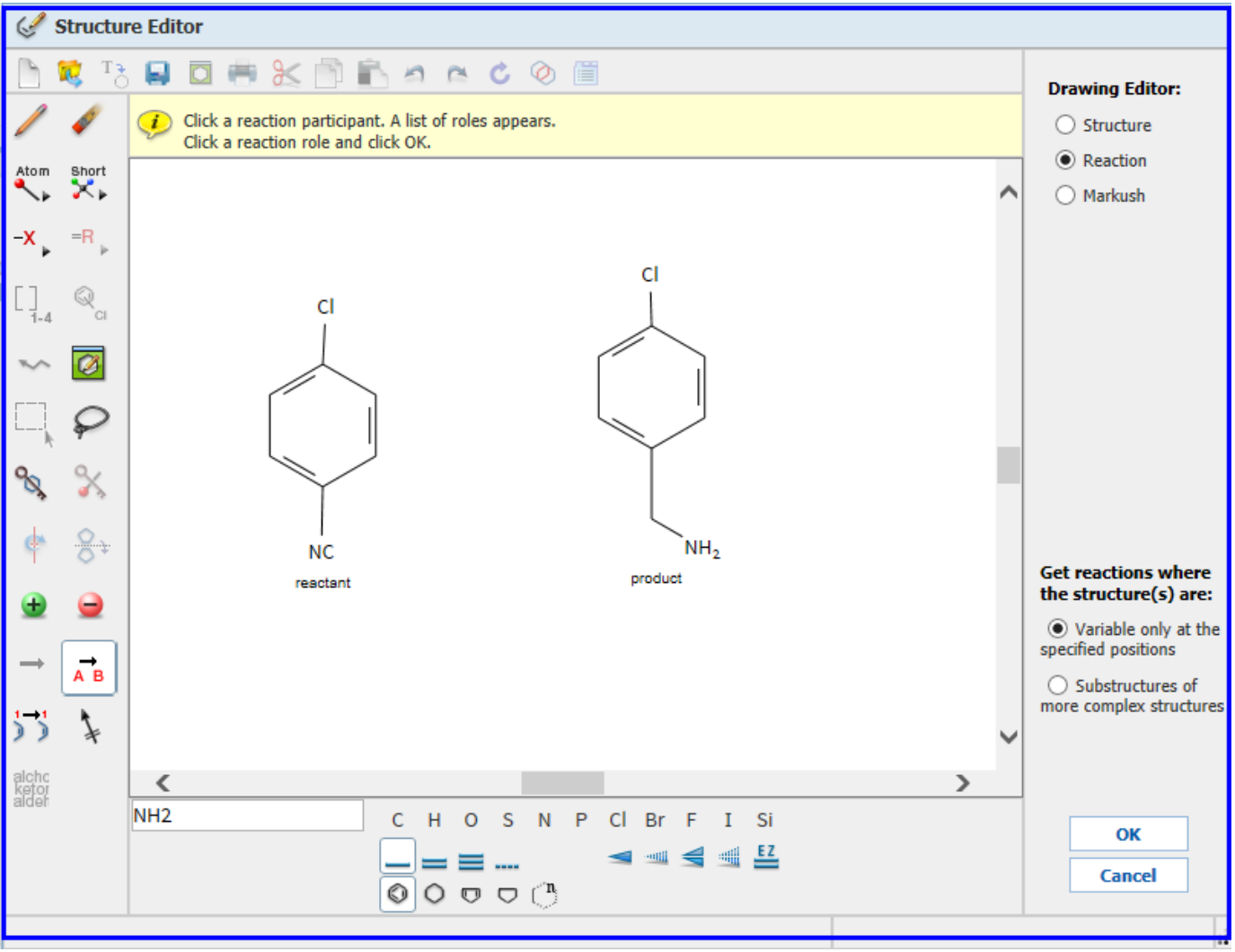

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Reaction Structure structure variable only at spe... > **reactions (20)**

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No Grouping
Document
Transformation

Selected

Analyze by: Reagent (New)

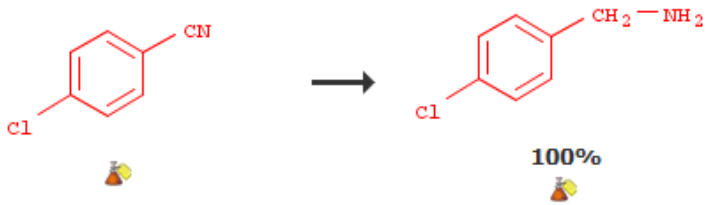
H_2	5
HCl	5
NaOH	4
SmI_2	3
F_3CCO_2H	2
H_2O	2
KOH	2
$NaBD_4$	2
$NaBH_4$	2
NH_3	2

Show More

1. View Reaction Detail | Link | Similar Reactions

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

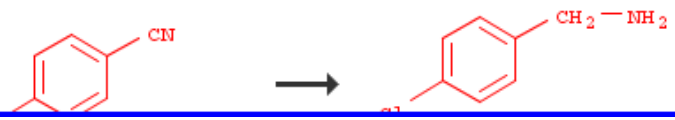
浏览记录，发现很多反应来自同一篇文献，通过反应分类进行合并。



Overview

2. View Reaction Detail | Link | Similar Reactions

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



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反应检索结果

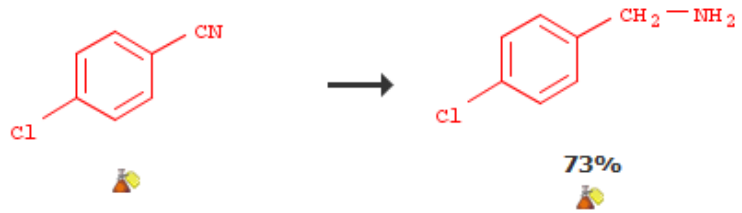
文献题目

命中反应数

9. **Selective Ruthenium-Catalyzed Transfer Hydrogenations of Nitriles to Amines with 2-Butanol** Full Text

2 Reactions Similar Reactions

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



Overview

Steps/Stages

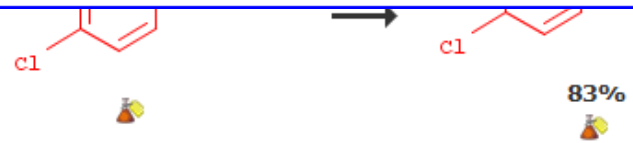
1.1 R:*s*-BuOH, C:52462-29-0, C:$(Ph_2PCH_2CH_2)_2$, 5 min, rt
1.2 R:NaOH, 5 min, rt
1.3 rt; 20 min, 120°C

Notes

GC yield; 2-butanol also used as solvent (stage 1), Reactants: 1, Reagents: 2, Catalysts: 2, Steps: 1, Stages: 3, Most stages in any one step: 3

References

Selective Ruthenium-Catalyzed Transfer Hydrogenations of Nitriles to Amines with 2-Butanol Full Text
By Werkmeister, Svenja et al
From Chemistry - A European Journal, 19(14), 4437-4440; 2013



Overview

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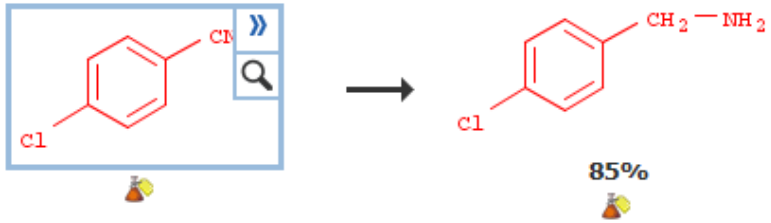
Experimental Procedure

8. **View Reaction Detail** **Link** **Similar Reactions**

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



- Overview
- Experimental Procedure

General/Typical Procedure: In a typical procedure, in a 100 ml conical flask mounted over a magnetic stirrer, fitted with reflux condenser and a mercury trap, was placed a mixture of nitrile (9.8 mmol), anhyd. nickel (II) chloride (9.8 mmol) and dry ethanol (20 ml). Sodium borohydride (29.4 mmol) was added very cautiously while stirring the solution vigorously. The progress of the reaction was monitored by TLC using benzene : ethyl acetate (90: 10, v/v) as eluent. After the complete disappearance of the nitrile (~5 min), the reaction mixture was filtered through a celite pad after ~ 15 min. The filtered nickel boride precipitate was washed with ethanol (2 x 10 ml). The combined filtrate was diluted with water (150 ml) and extracted with ethyl acetate (3 x 10 ml). The combined extract was dried over anhyd. $MgSO_4$, filtered and concentrated on a rotary vacuum evaporator. After drying under vacuum, the product was purified by column chromatogaphy over silica gel (20 x 2 cm; 100-200 mesh) using benzene: ethyl acetate as the eluent. Eluate was concentrated under reduced pressure to afford the products which were analysed by IR, NMR and mass spectra as most of these are known products.[10] **2d**, yield 85%

不用阅读全文，直接获得包含实验过程的反应记录

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Reaction Structure structure variable only at spe... > **reactions (20)**

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H_2	5
HCl	5
NaOH	4
SmI_2	3
F_3CCO_2H	2
H_2O	2
KOH	2
$NaBD_4$	2

0 of 20 Reactions Selected

1. **Reduction of Nitriles to Amines**
   20 Reactions

   $R-C\equiv N \longrightarrow R^{\diagup}\!\!\!\!\diagdown NH_2$

2. **Dehalogenation of Aromatic Compounds**
   2 Reactions

   $Ar-X \xrightarrow{cat.} Ar-H$

3. **Reduction of Alkyl Halides/ Dehalogenation**
   2 Reactions

   $R-X \longrightarrow R-H$

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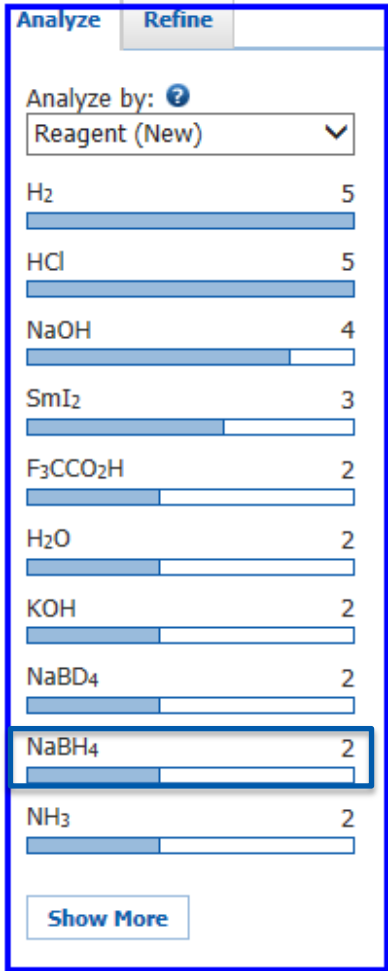

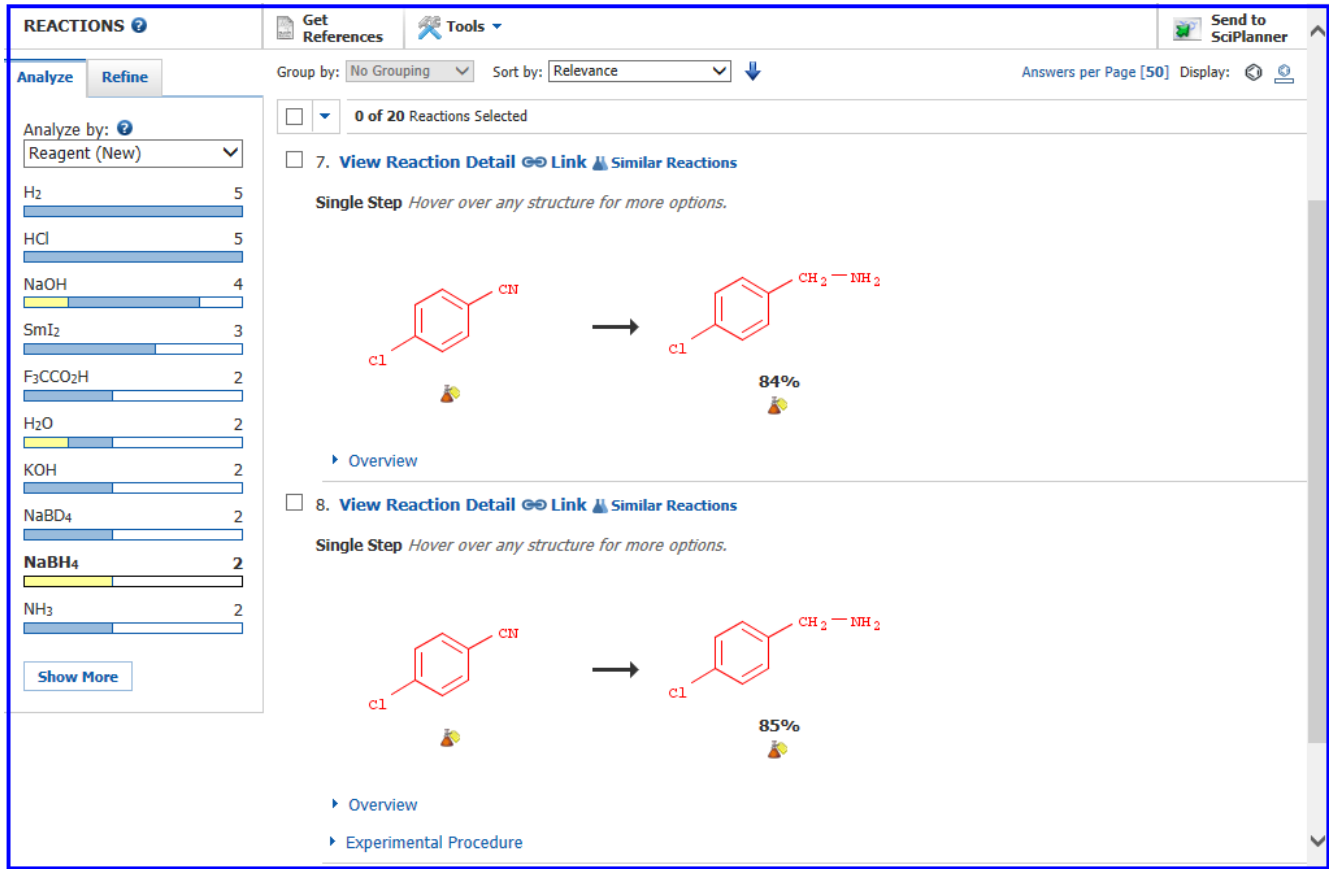

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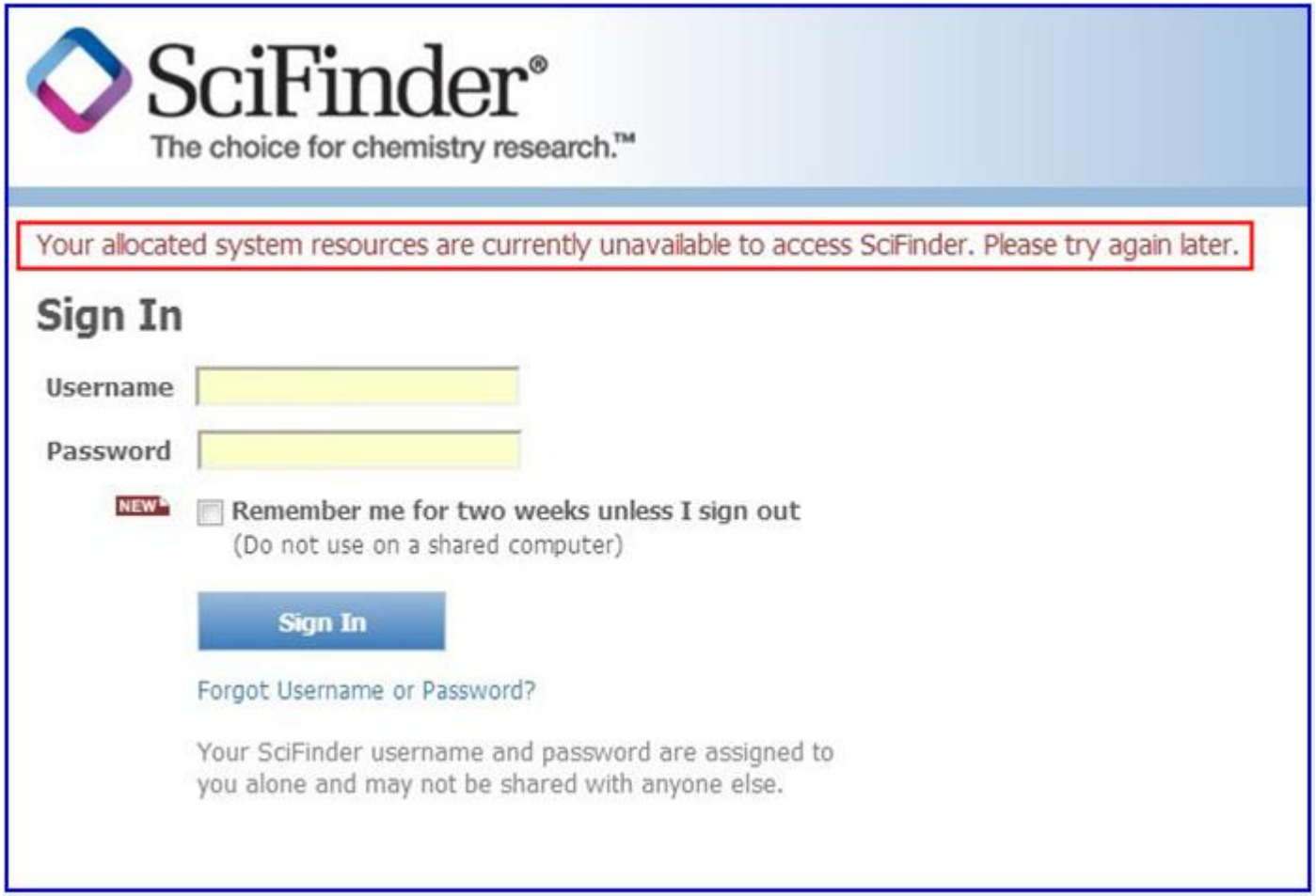

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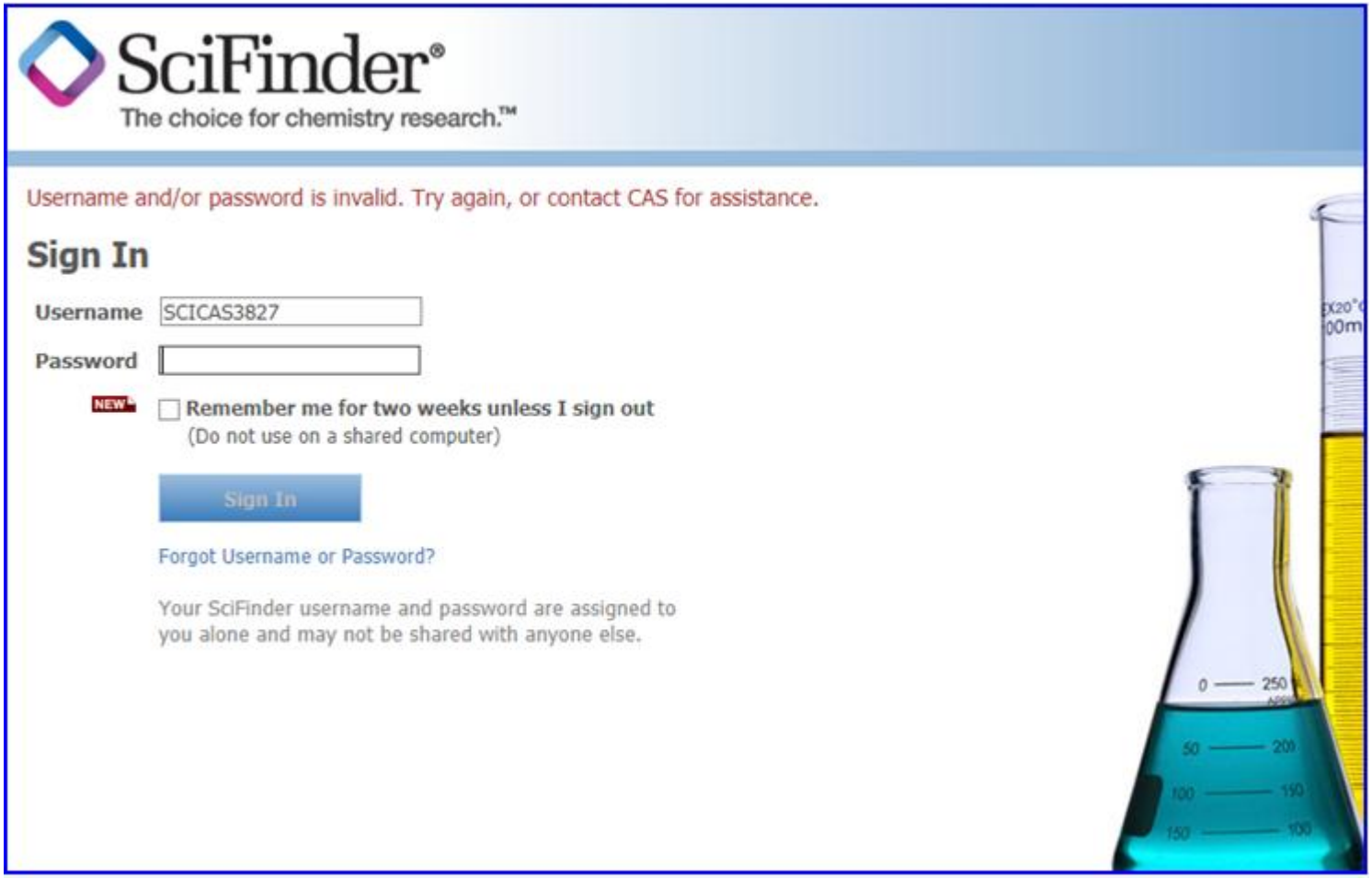

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