SciFinder Web

源于化学，超越化学的一站式检索平台

SciFinder Web 培训

CAS北京代表处
培训专员

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Mail:Della@igroup.com.cn
Tel:010-82335058-807

提纲

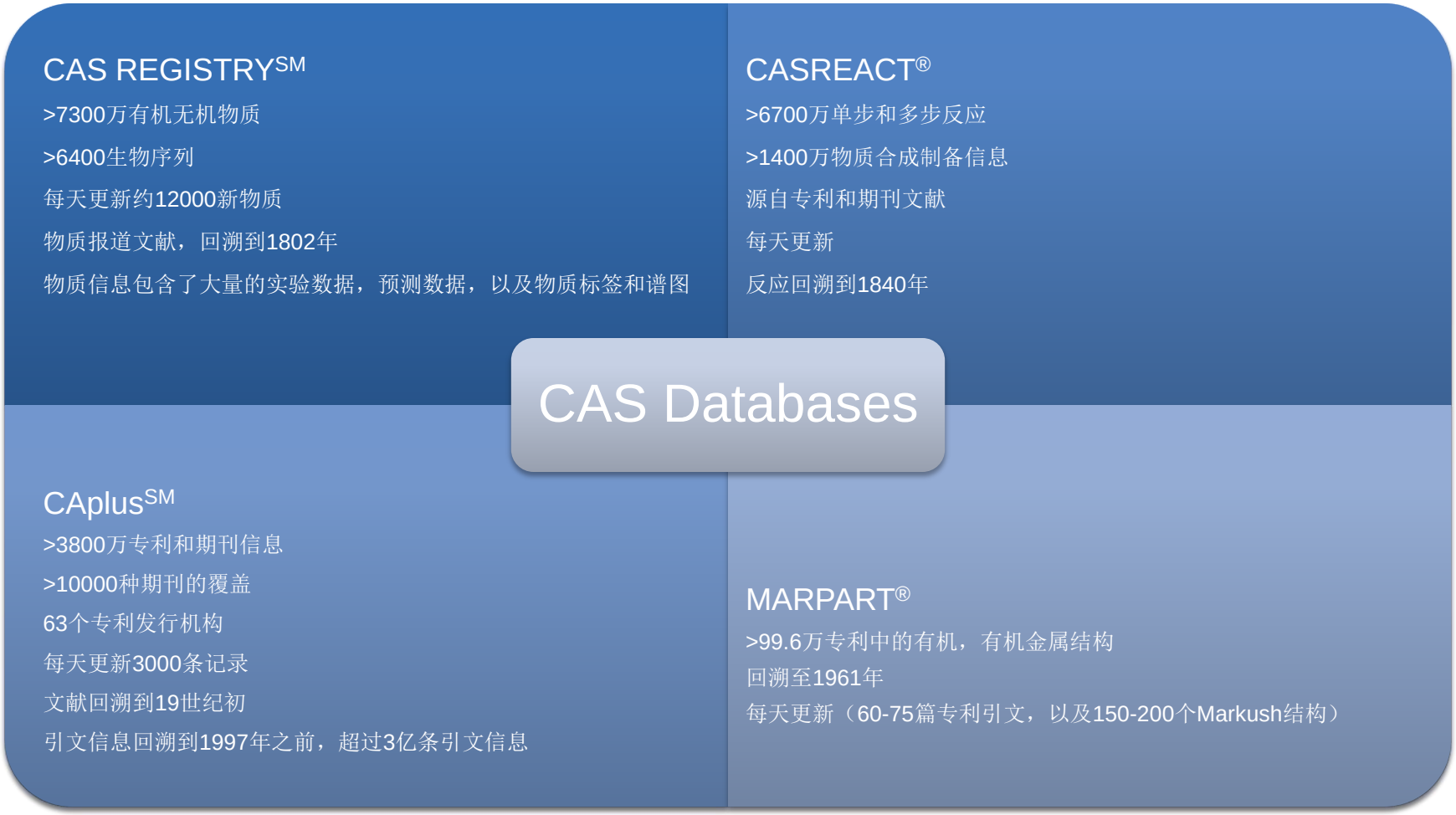
- 介绍
  - SciFinder Web内容
- **SciFinder Web中的检索**
  - SciFinder中的文献检索
  - SciFinder中的结构面板使用技巧
  - SciFinder中的物质结果及物质检索方法
  - SciFinder中的反应检索技巧
- **SciFinder Web的注册和常见问题**

美国化学文摘社—Chemical Abstract Service

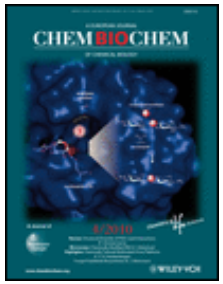
- ACS的分支机构，创立于1907年
- 致力于跟踪、索引并提炼全球化学相关的科技文献信息
- 最先创立了纸本《化学文摘》Chemical Abstracts TM
- 总部位于俄亥俄州的哥伦布市

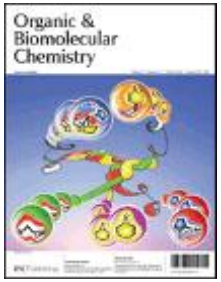
- 1300名员工，精通50多种语言。
- 关注索引上万种期刊和63家专利
- 客户覆盖全球1900所高校、500强公司以及所有主要的专利局。

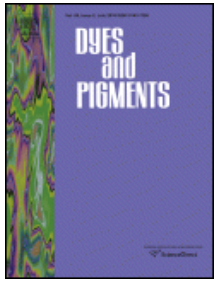
SciFinder Web中的几个主要数据库

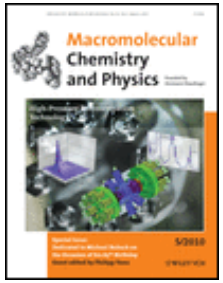


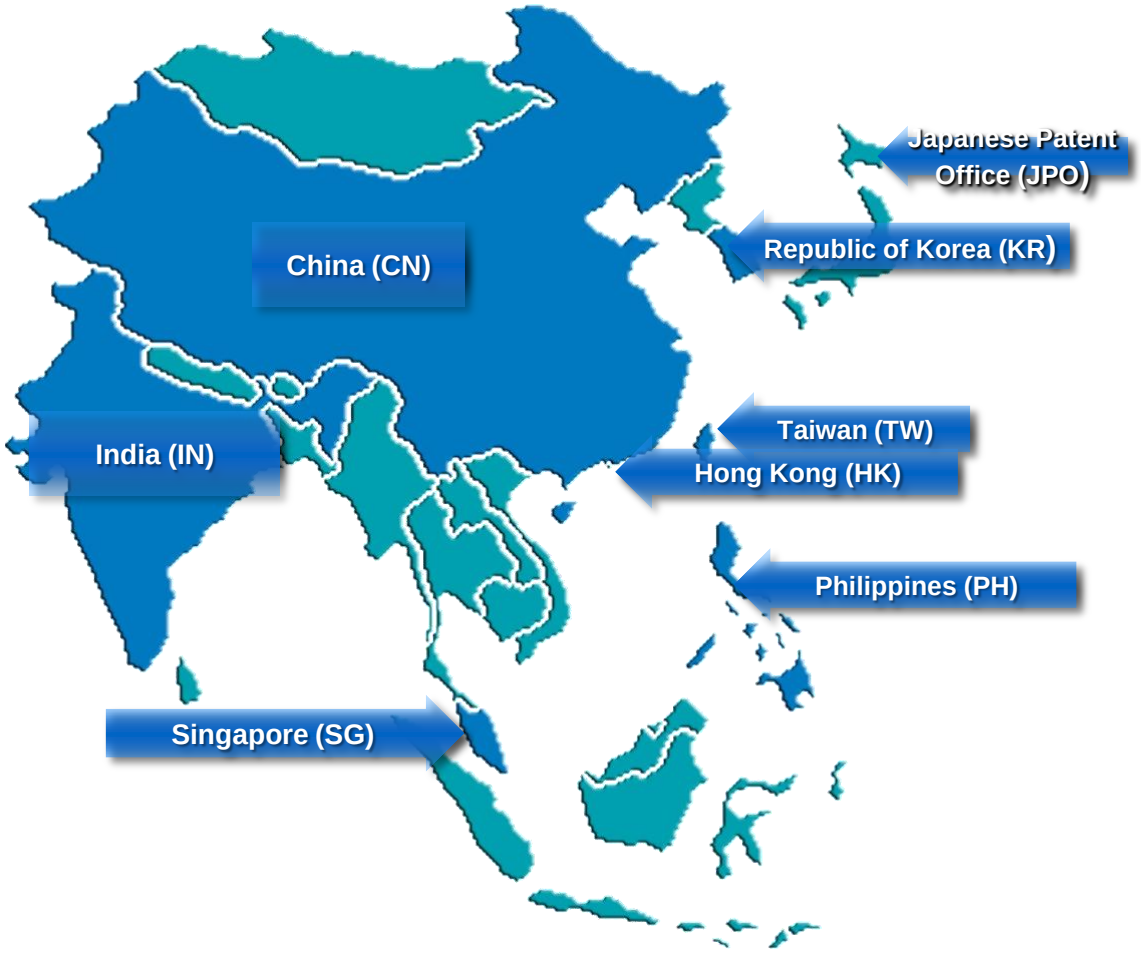
CAplus℠ 涵盖了上万种期刊及63个专利发行机构专利







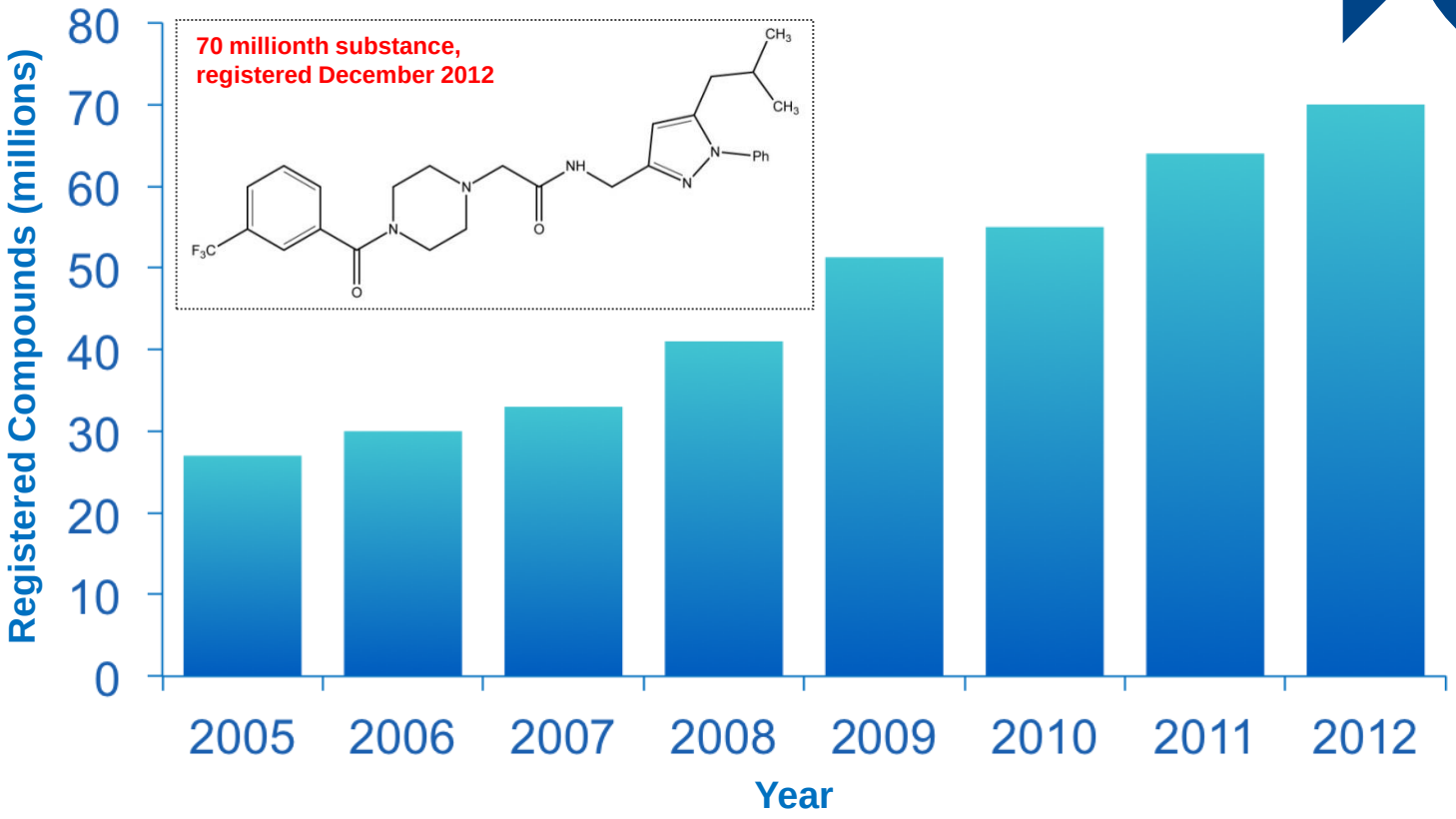




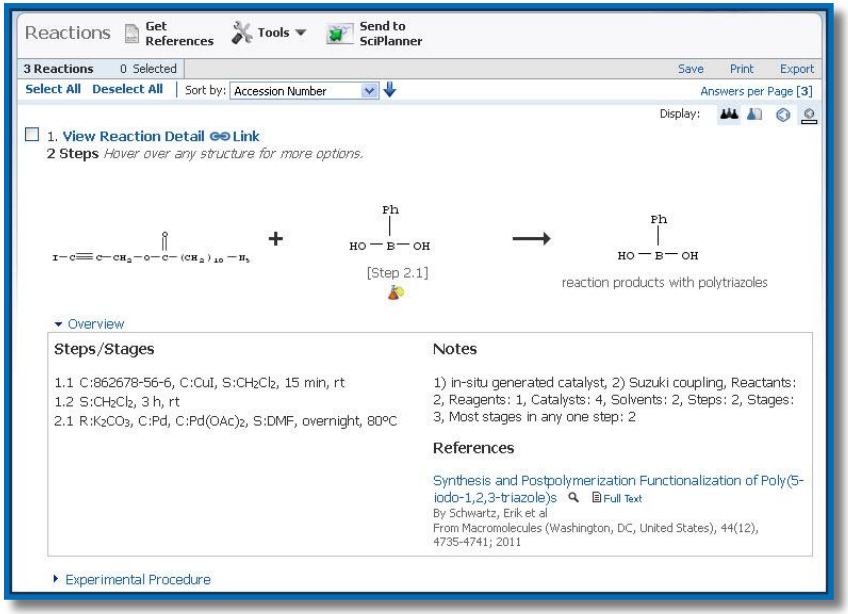
CAS Registry 是世界上最大的化学物质数据库

CAS REGISTRY

Currently
>71
million
organic &
inorganic
substances



CASREACT® 是检索化学反应最权威的来源



- **>5100万 单步和多步反应**
- **>1360万 物质合成制备信息**
- **源自专利和期刊**
- **可回溯到1840年**
- **每天更新**

CASREACT是世界上最大的，更新速度最快的反应数据库

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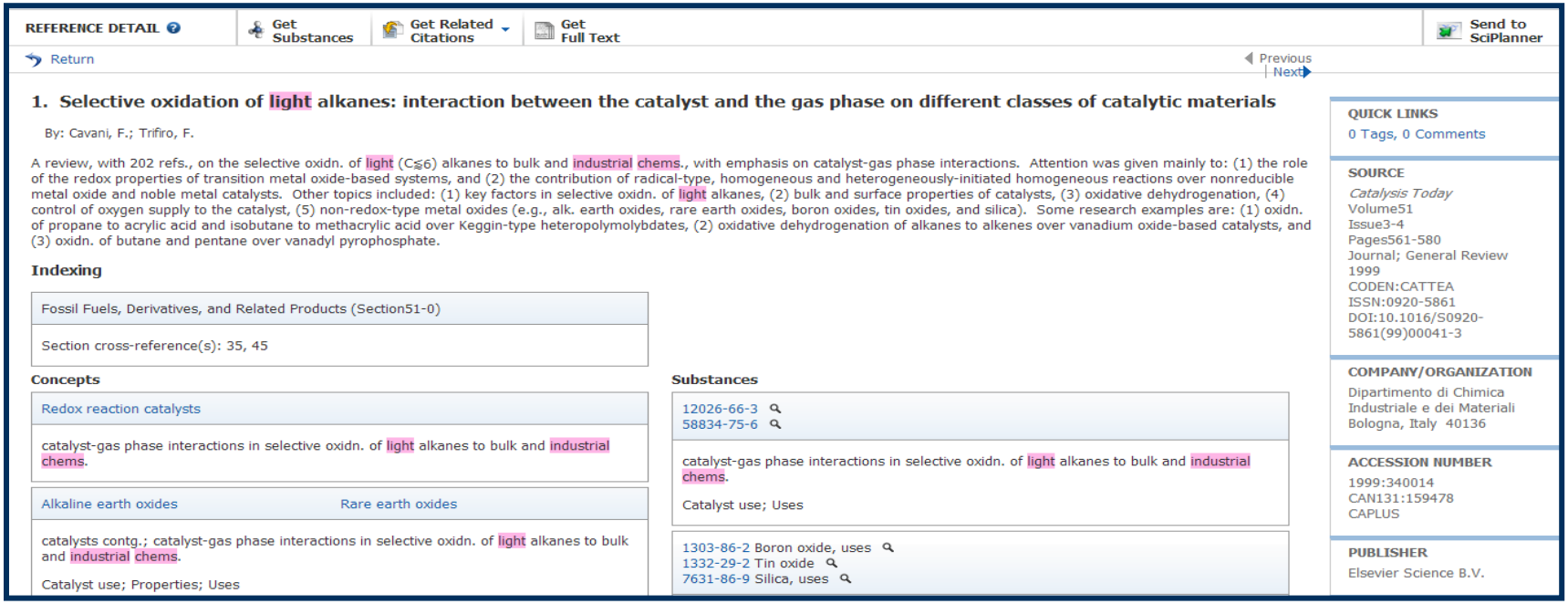
SciFinder Web登陆界面—http://scifinder.cas.org

SciFinder中的文献记录



REFERENCE DETAIL | Get Substances | Get Related Citations | Get Full Text | Send to SciPlanner

Return | Previous | Next

1. Selective oxidation of light alkanes: interaction between the catalyst and the gas phase on different classes of catalytic materials

By: Cavani, F.; Trifiro, F.

A review, with 202 refs., on the selective oxidn. of light (C≤6) alkanes to bulk and industrial chems., with emphasis on catalyst-gas phase interactions. Attention was given mainly to: (1) the role of the redox properties of transition metal oxide-based systems, and (2) the contribution of radical-type, homogeneous and heterogeneously-initiated homogeneous reactions over nonreducible metal oxide and noble metal catalysts. Other topics included: (1) key factors in selective oxidn. of light alkanes, (2) bulk and surface properties of catalysts, (3) oxidative dehydrogenation, (4) control of oxygen supply to the catalyst, (5) non-redox-type metal oxides (e.g., alk. earth oxides, rare earth oxides, boron oxides, tin oxides, and silica). Some research examples are: (1) oxidn. of propane to acrylic acid and isobutane to methacrylic acid over Keggin-type heteropolymolybdates, (2) oxidative dehydrogenation of alkanes to alkenes over vanadium oxide-based catalysts, and (3) oxidn. of butane and pentane over vanadyl pyrophosphate.

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-0)

Section cross-reference(s): 35, 45

Concepts

Redox reaction catalysts

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Alkaline earth oxides | Rare earth oxides

catalysts contg.; catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Properties; Uses

Substances

12026-66-3
58834-75-6

catalyst-gas phase interactions in selective oxidn. of light alkanes to bulk and industrial chems.

Catalyst use; Uses

1303-86-2 Boron oxide, uses
1332-29-2 Tin oxide
7631-86-9 Silica, uses

QUICK LINKS
0 Tags, 0 Comments

SOURCE
Catalysis Today
Volume51
Issue3-4
Pages561-580
Journal; General Review
1999
CODEN:CATTEA
ISSN:0920-5861
DOI:10.1016/S0920-5861(99)00041-3

COMPANY/ORGANIZATION
Dipartimento di Chimica Industriale e dei Materiali
Bologna, Italy 40136

ACCESSION NUMBER
1999:340014
CAN131:159478
CAPLUS

PUBLISHER
Elsevier Science B.V.

Citations

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
Vedrine, J; Catal Today 1997, 33, 3
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

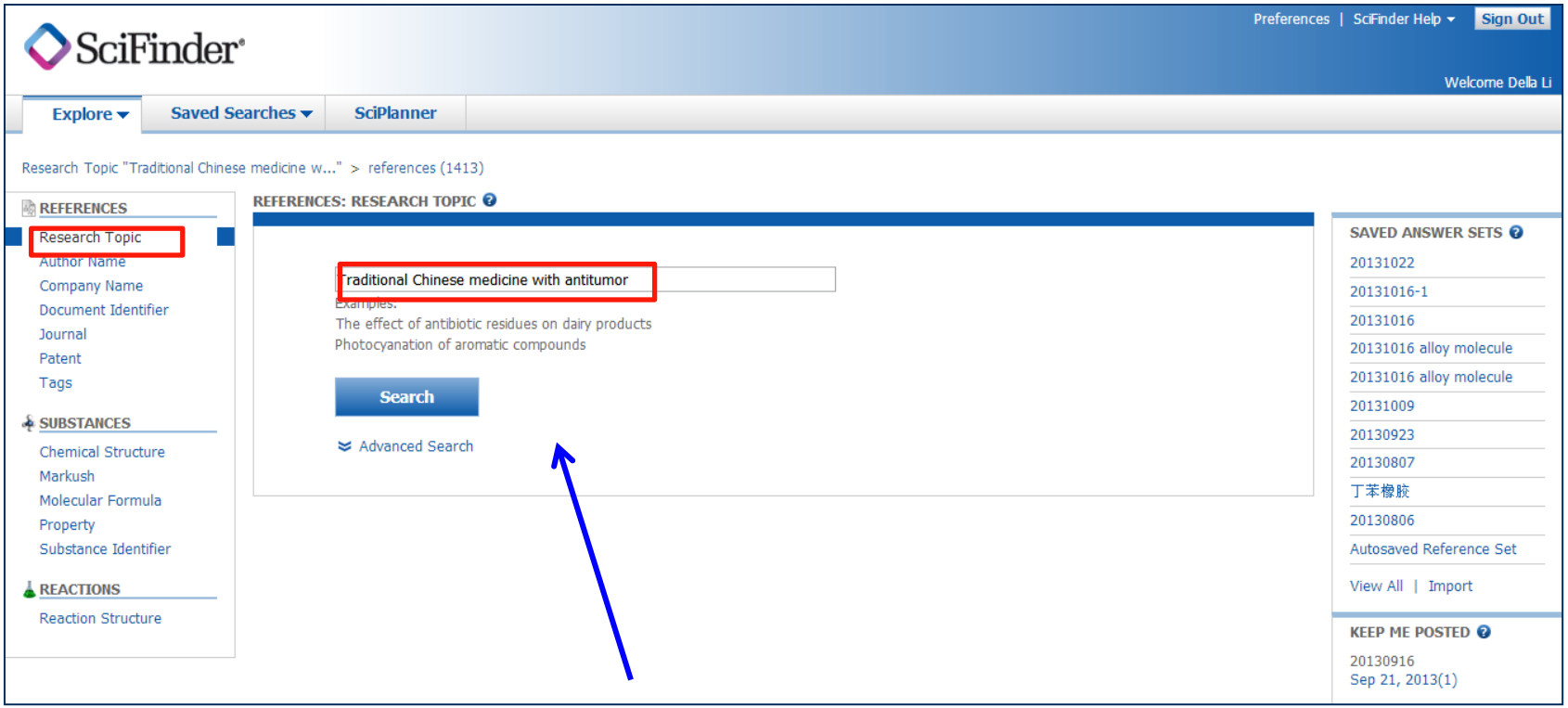
- 主题检索
- 作者名检索
- 机构名检索
- 文献标示符检索
- 从物质，反应获得文献

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中的主题检索

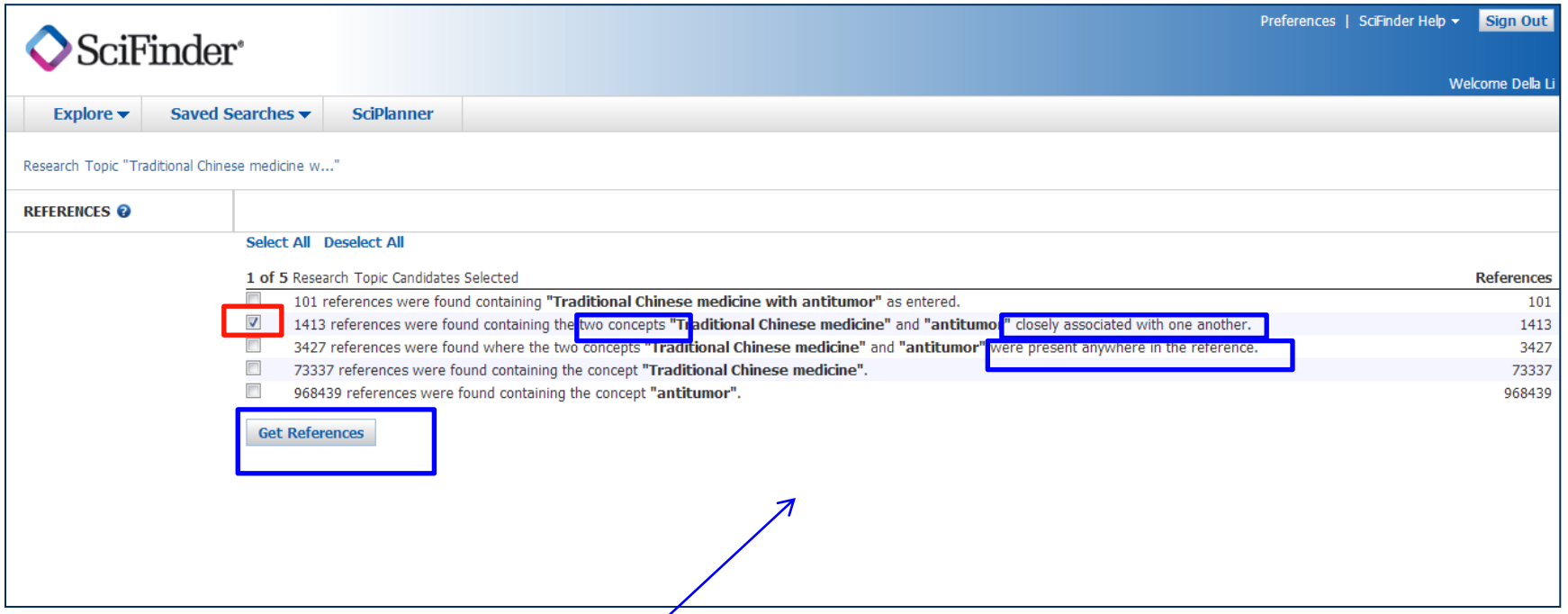
主题词： Traditional Chinese medicine with antitumor



术语之间最好用英文的介词如 **of, with, beyond, in, on, as** 等连接；

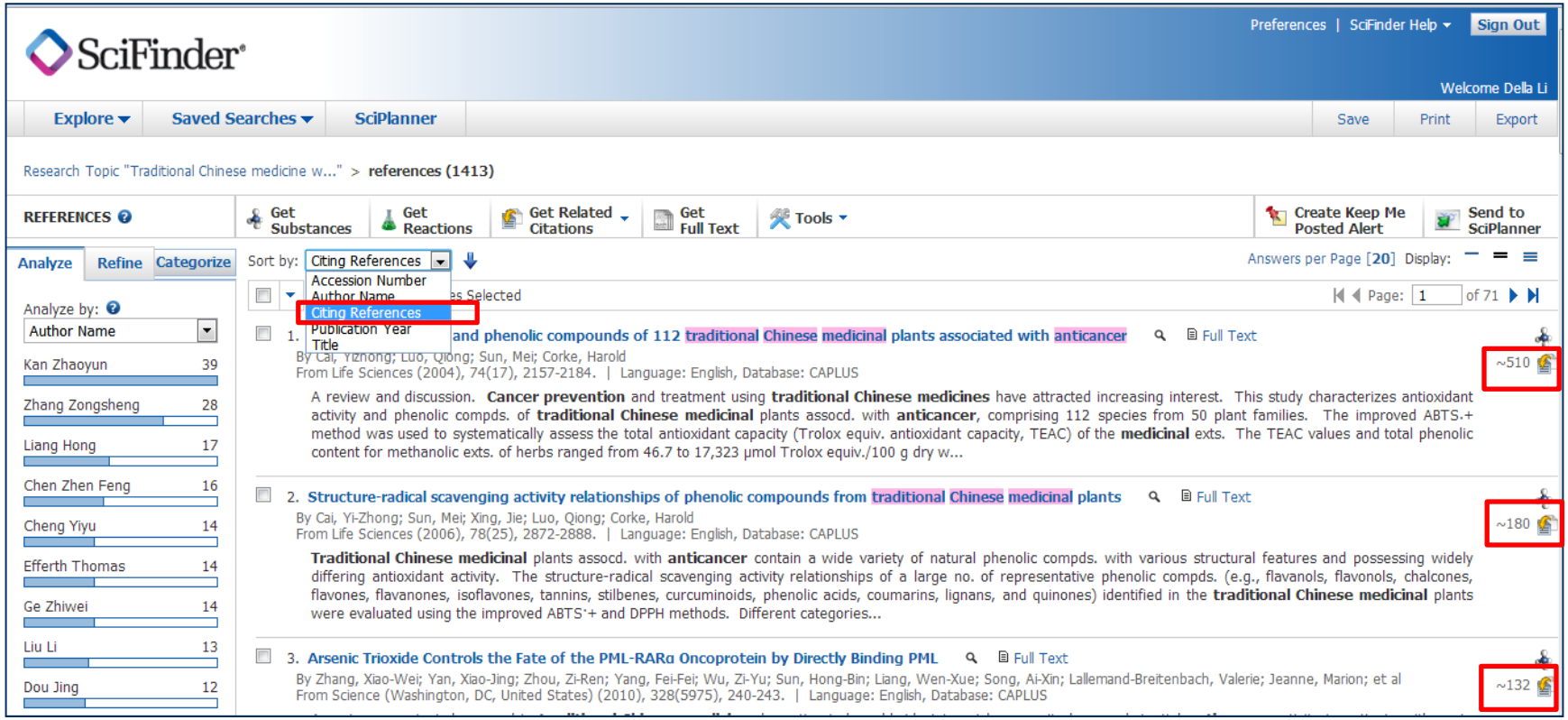
最多输入 5 个术语，2~3个左右最好

SciFinder中的候选选项



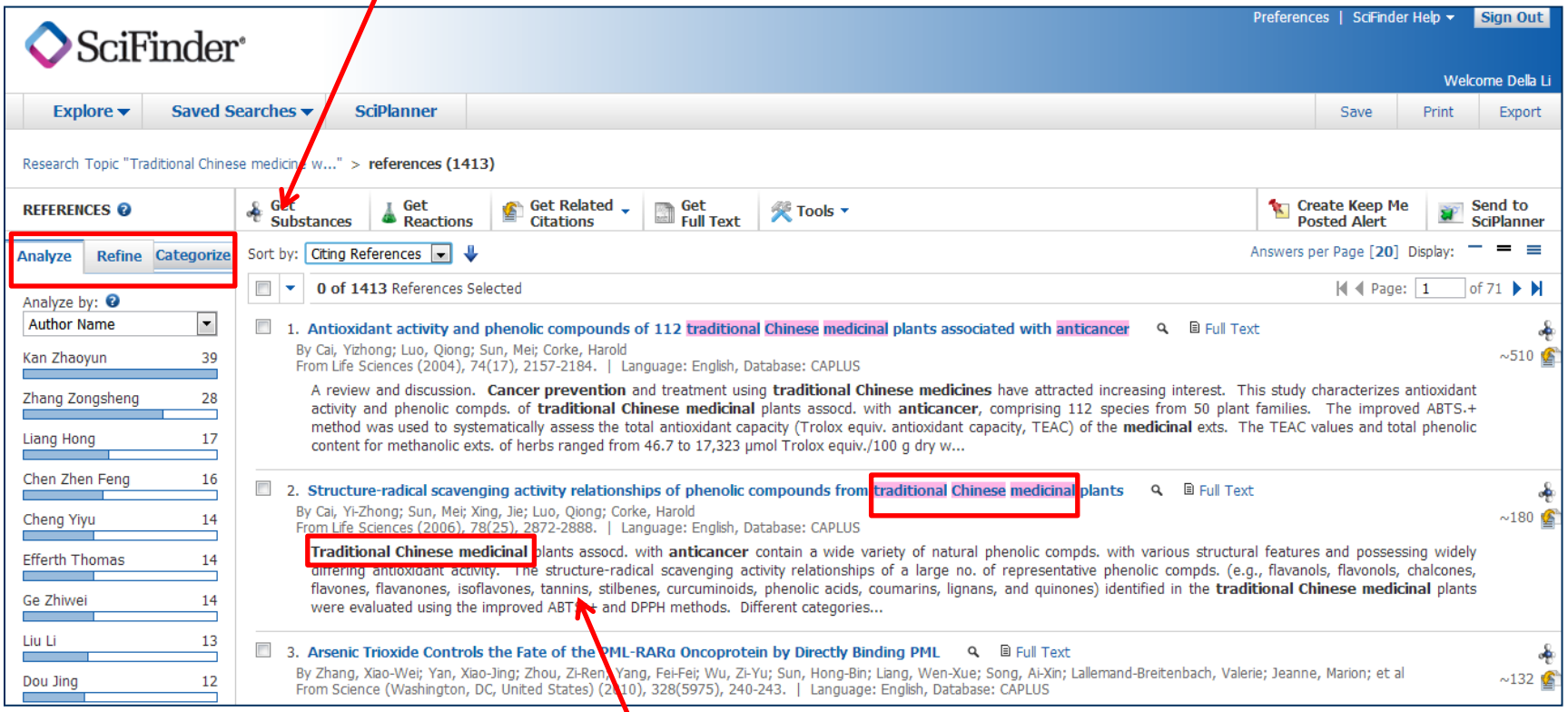
关键词拼写上的变化及同义词都会会被检索到
通常,第二项有“concept”和“closely associated with one another” 的选项是更好的选择

SciFinder中的引文排序



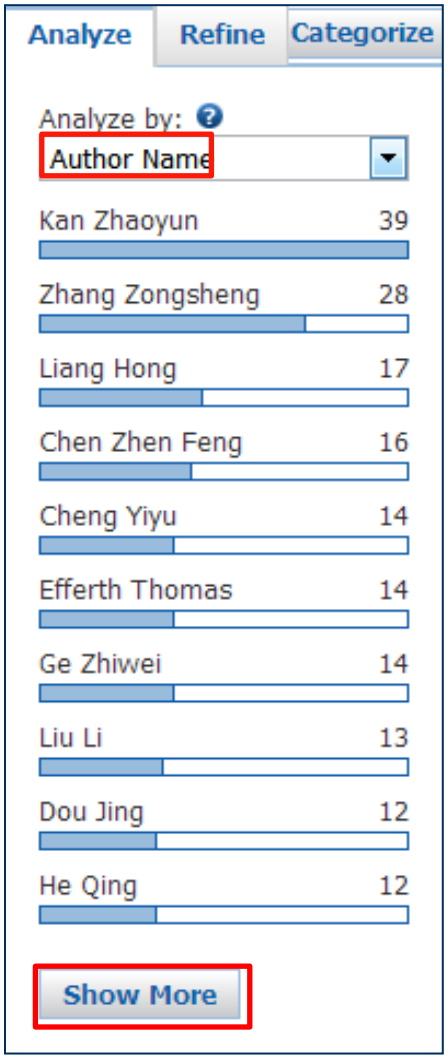
选择sort by里的citing reference 可以获得被引用次数最多的文献

SciFinder中的文献筛选工具

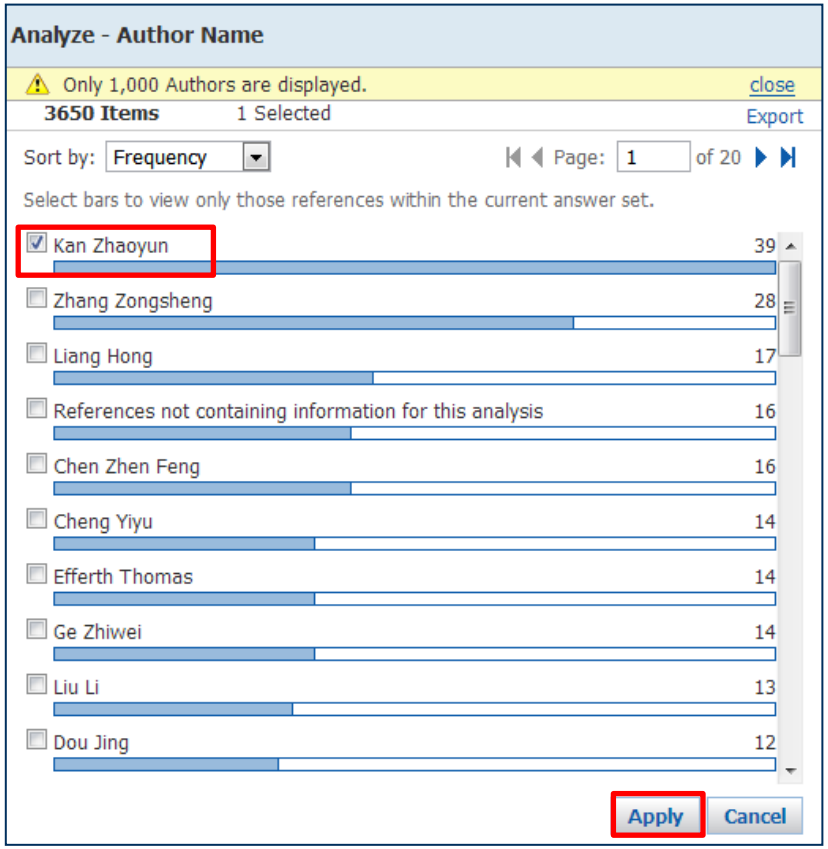


关键词高亮显示

Analyse-作者姓名分析

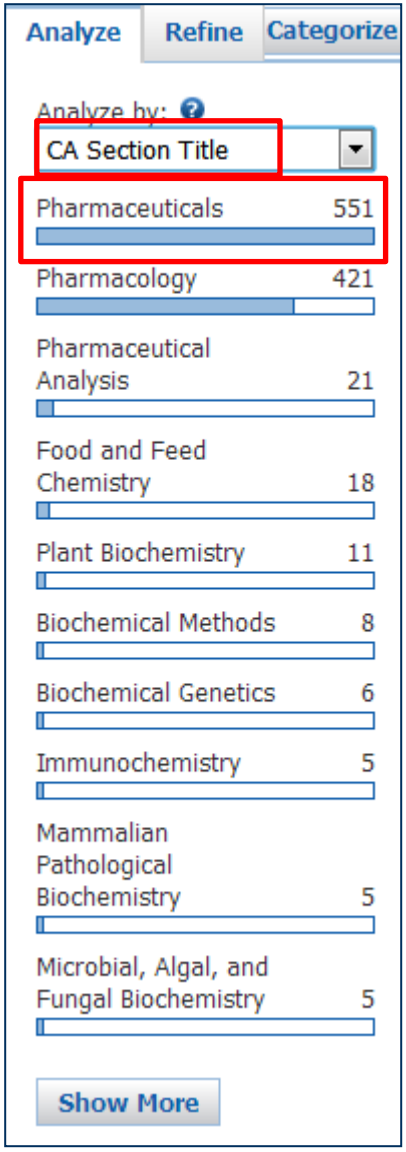


Kan Zhaoyun在此领域发表了39篇文献



点击Apply获得相应作者的文献

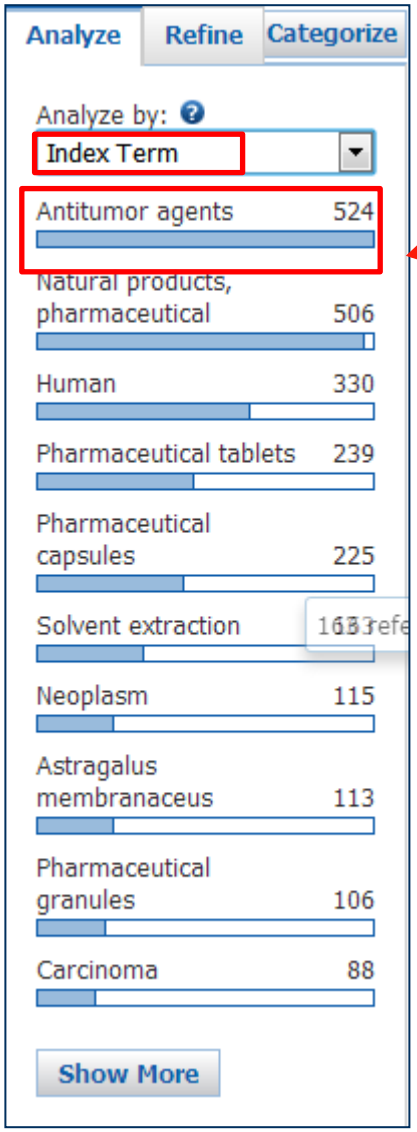
Analyse-CA Section Title分析



CA Section Title帮助分析主要的应用领域

抗肿瘤中药主要应用的领域有：
制药，药理，药物分析，食品
和饲料化学等等

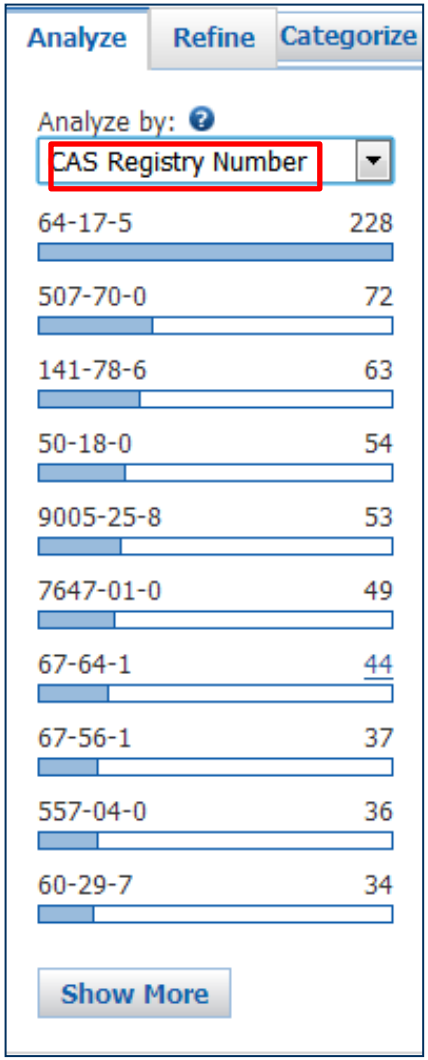
Analyse-索引词分析



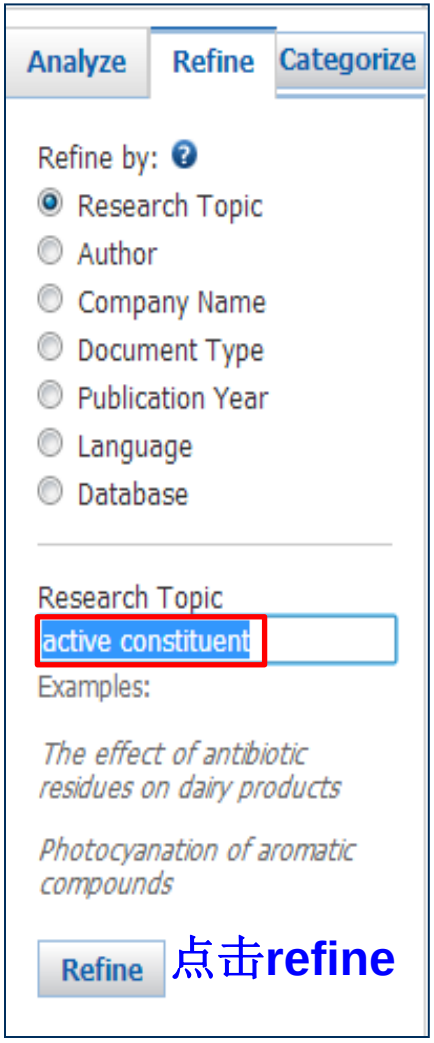
Index Term帮助分析文献中出现的重要内容

直接点击感兴趣的
内容获得相应文献

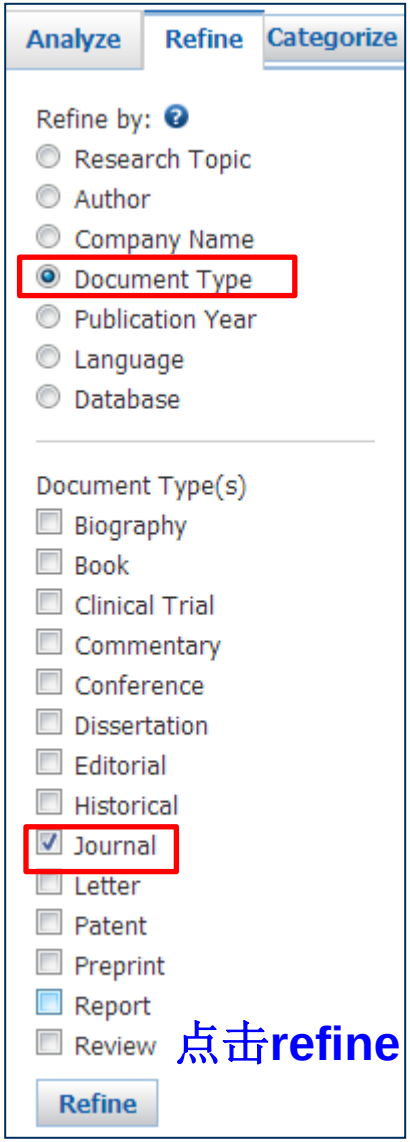
Analyse-机构名称，期刊名称，CAS No分析



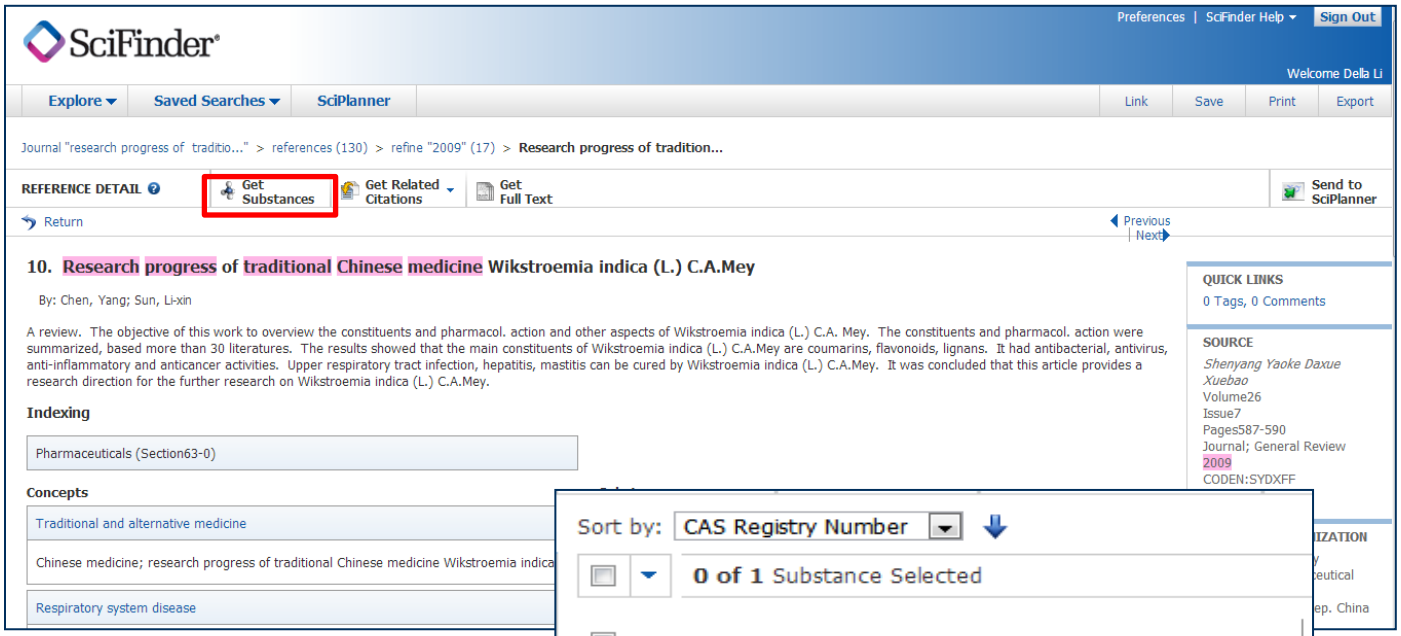
Refine-主题词限定



Refine-文献类型限定

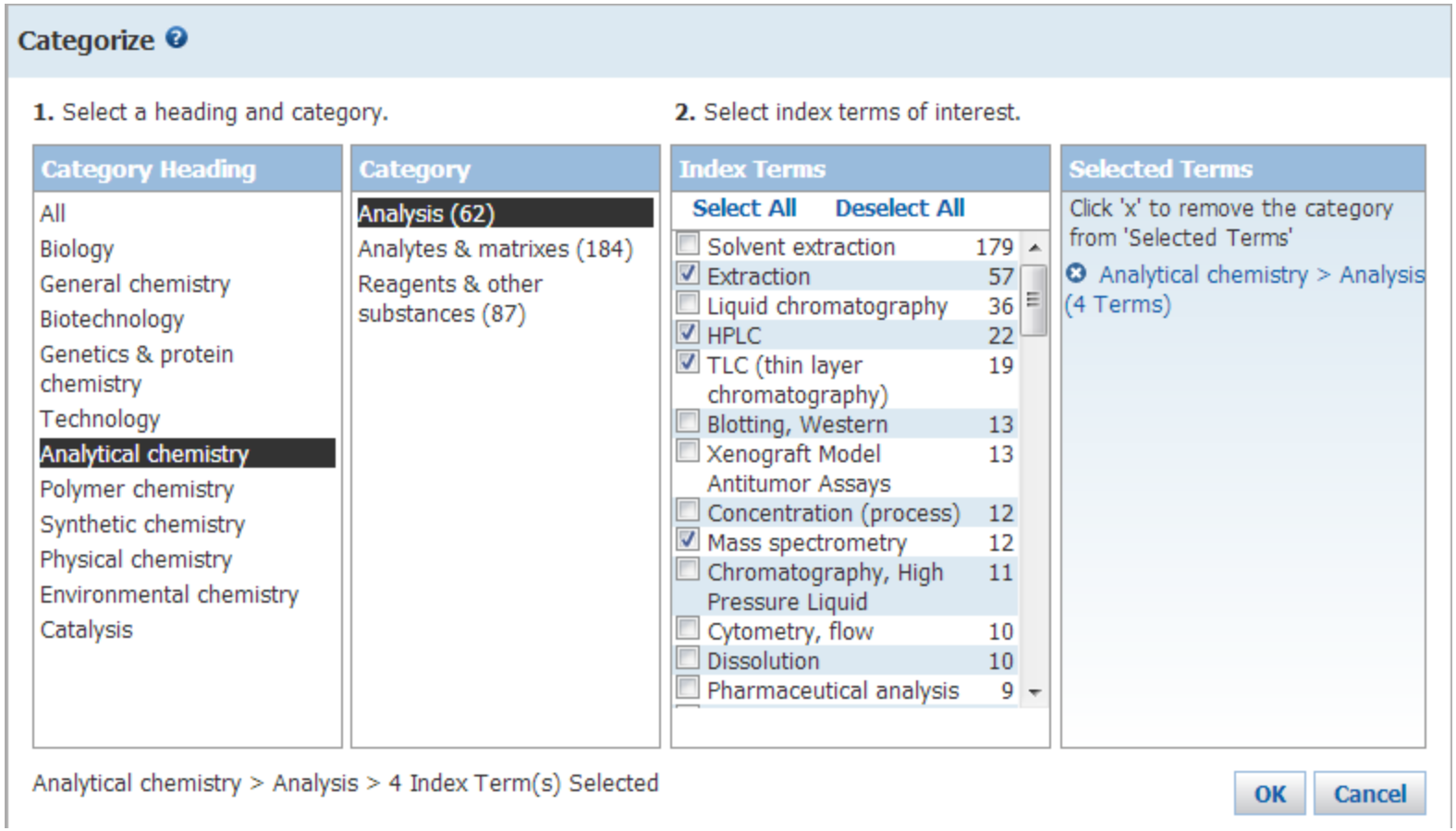


从文献获得物质



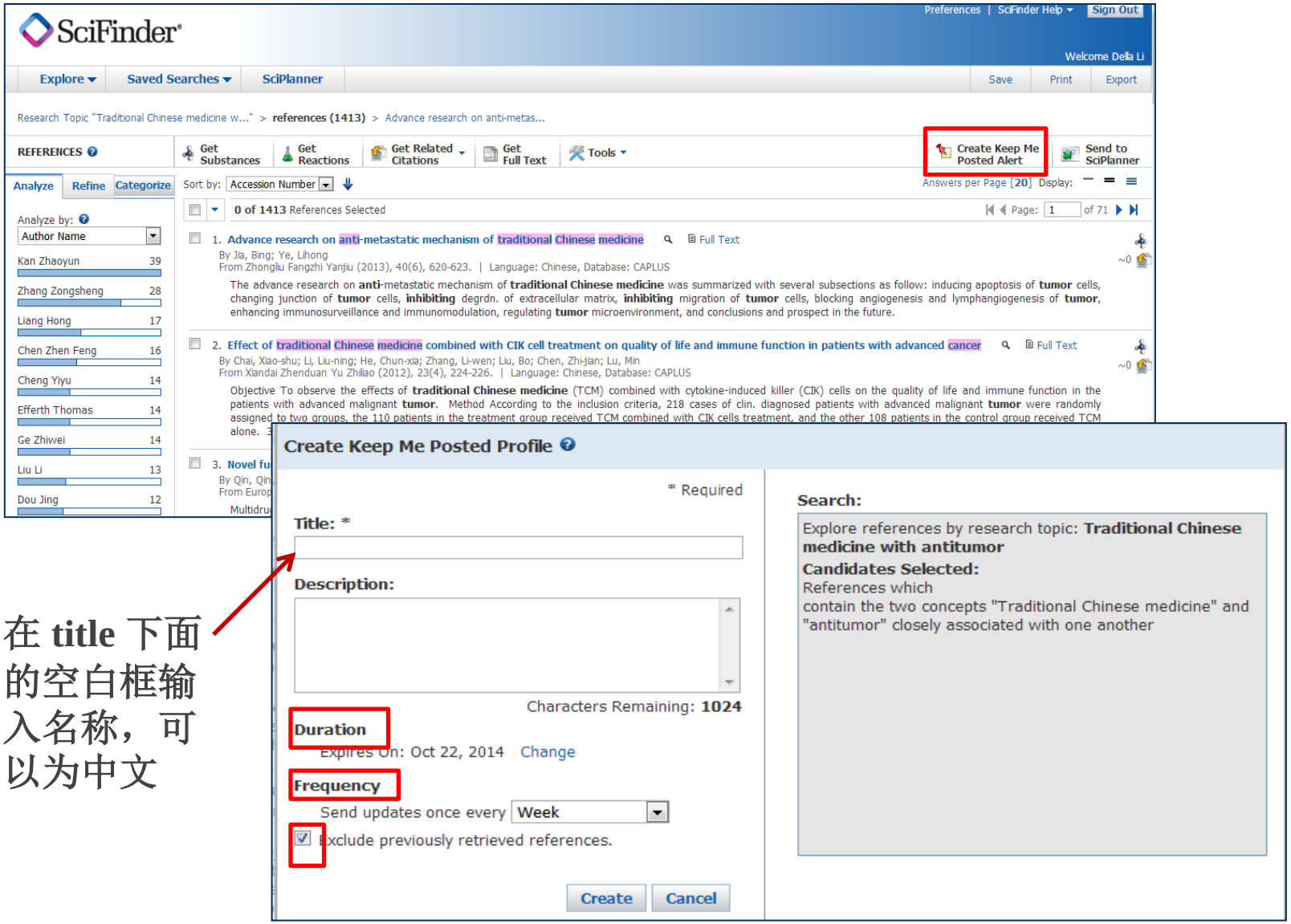
从文献可以直接获得文献中的物质，反应，引用等信息

系统分类功能



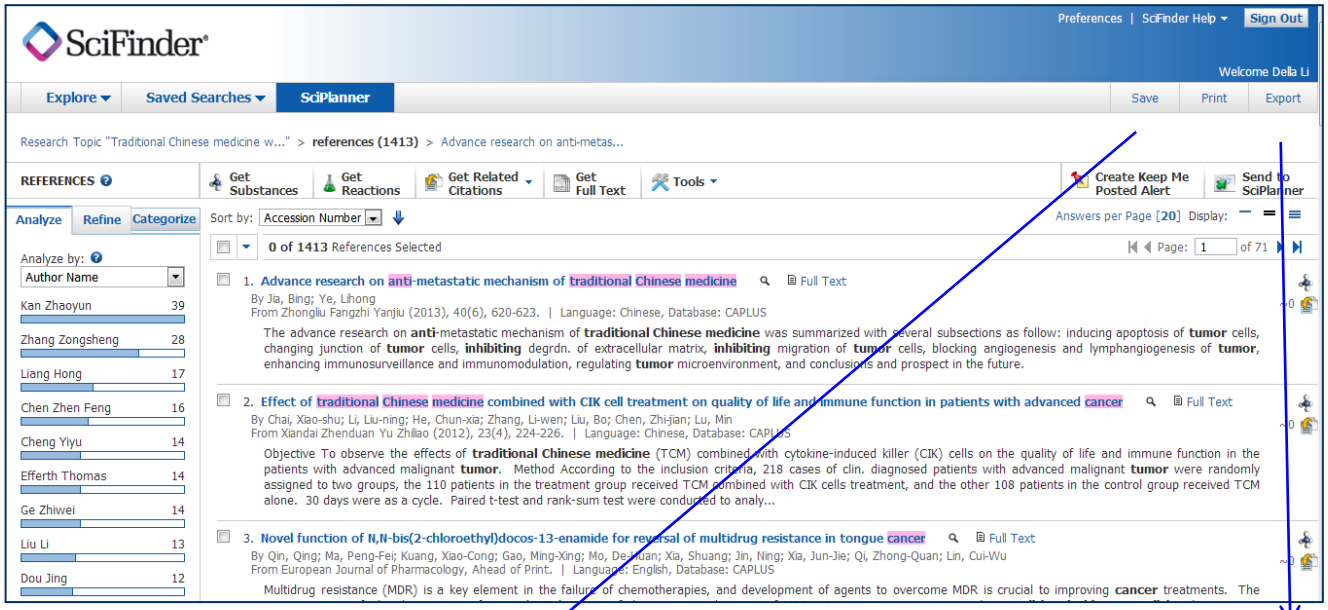
Categorize—基于CAS索引获得更多详细的信息

定题服务功能

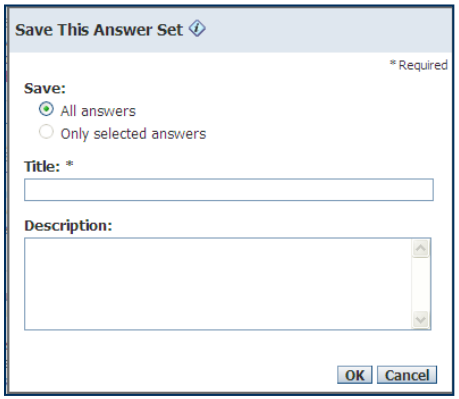


在 **title** 下面的空白框输入名称，可以为中文

保存,打印,导出



导出：
将结果保存到本地电脑



保存：
检索结果保存到CAS 的服务器上

ris 格式保存，可以导入到Endnote 中

提纲

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  - SciFinder中的结构面板使用技巧
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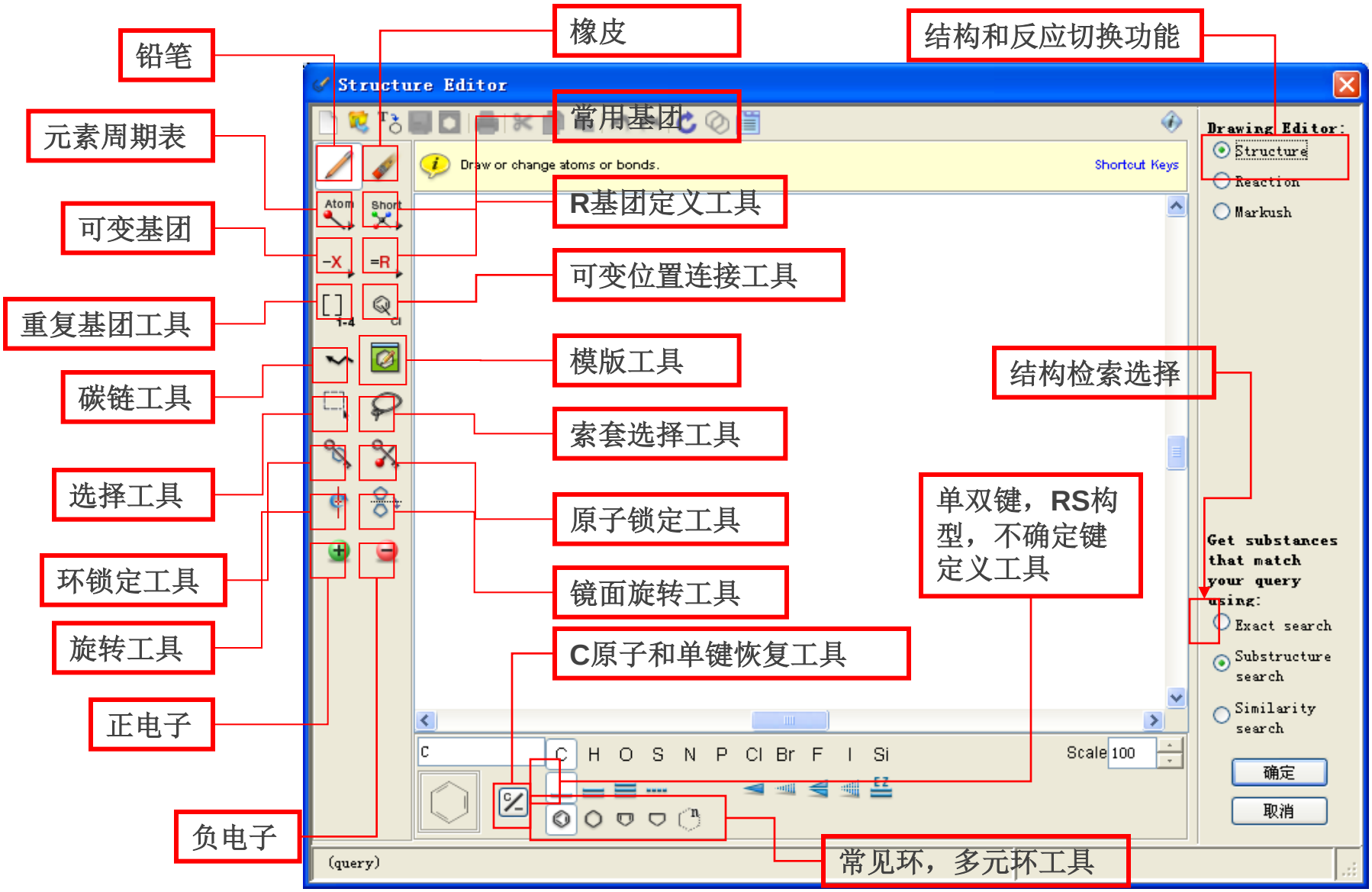
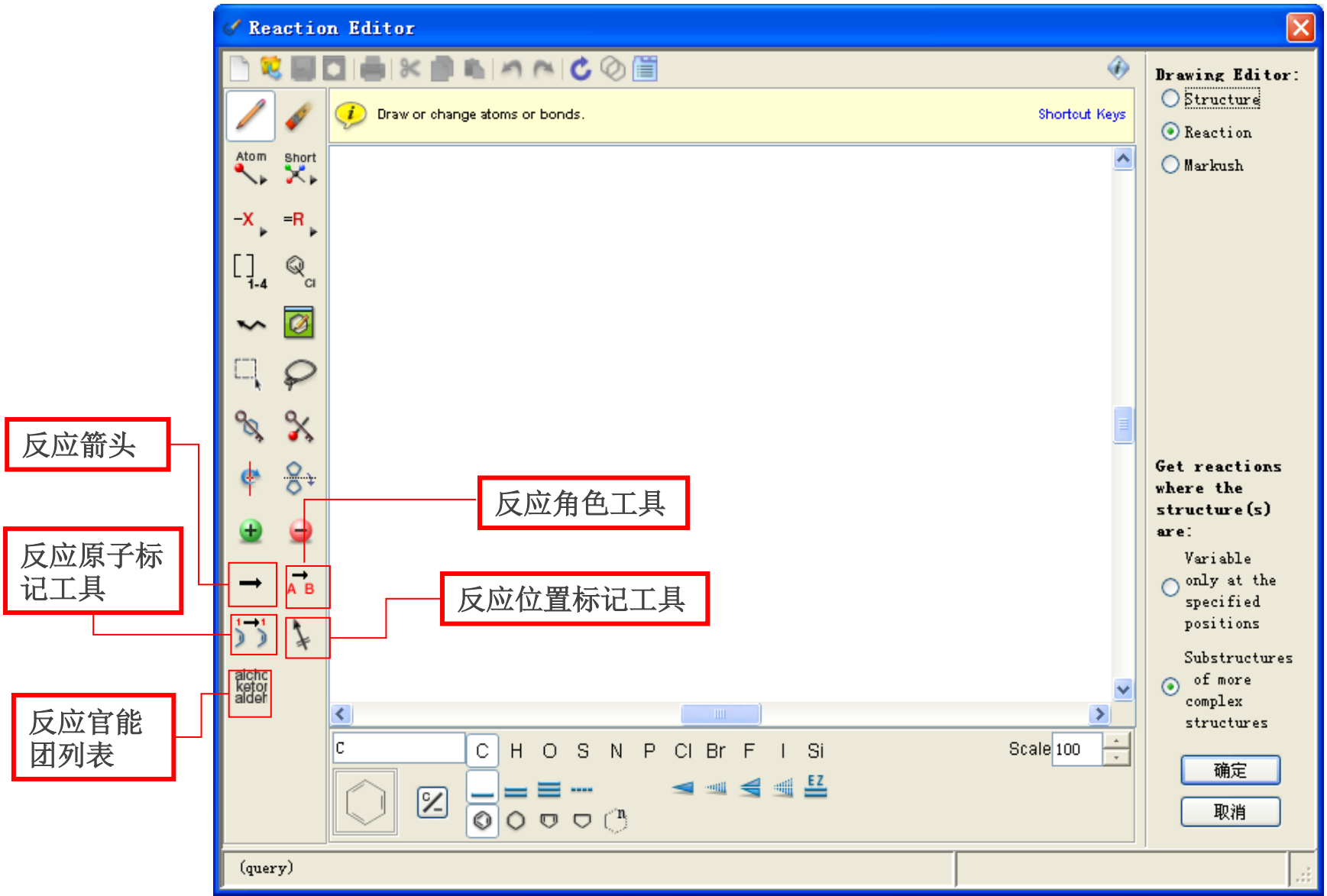
  - SciFinder中的反应检索技巧
- **SciFinder Web的注册和常见问题**

SciFinder结构绘制工具



SciFinder中的反应定义工具



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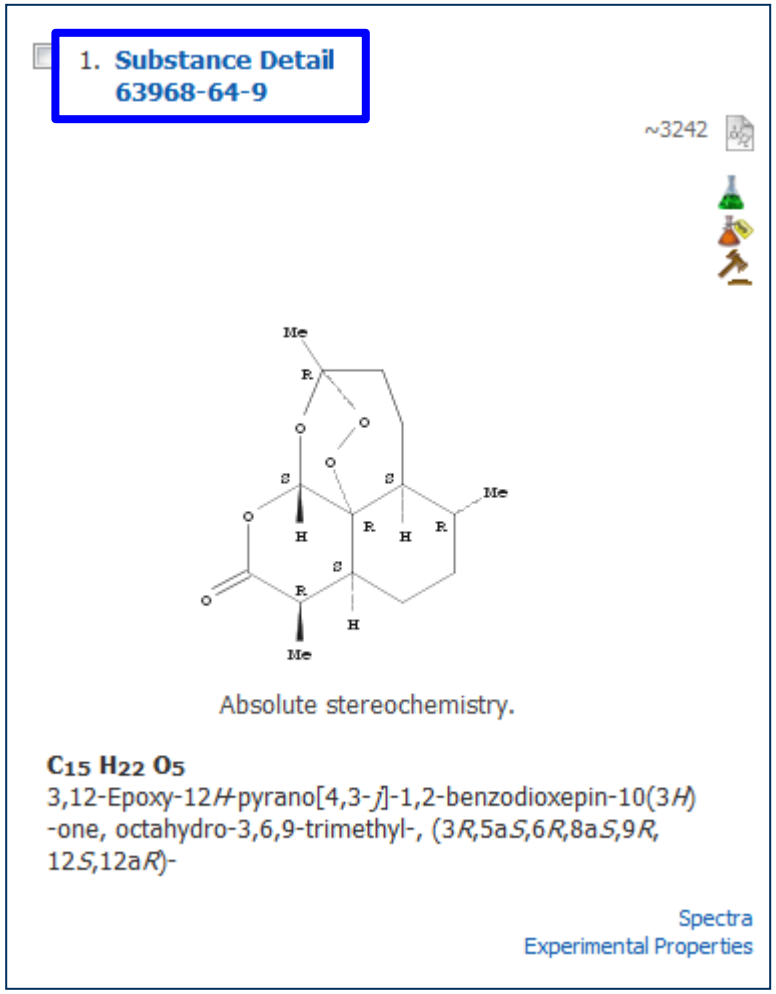
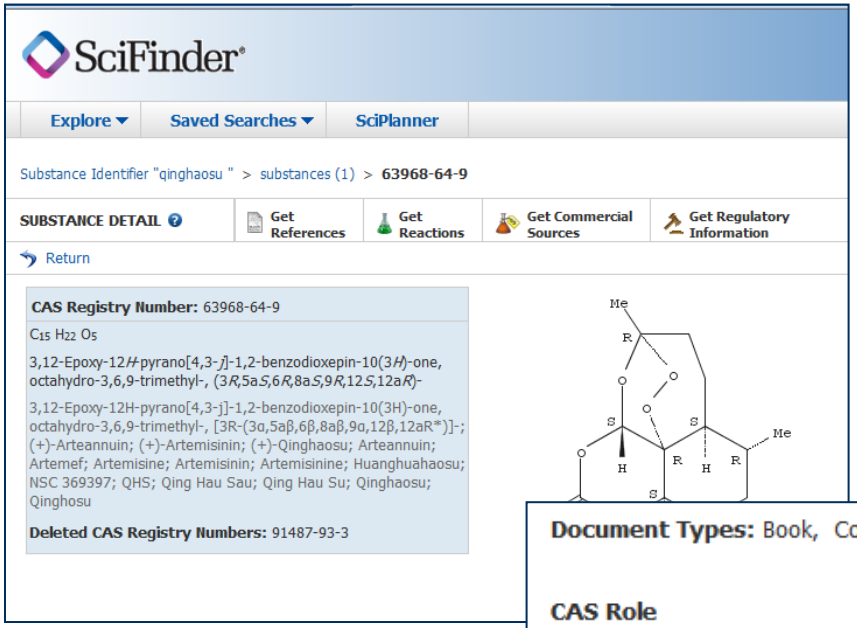
SciFinder中的物质结果界面



一个完整的物质结果界面包含：

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

Substance Detail—查看物质详细信息



物质的的**CAS**号、分子式、结构式、化学名、别名

Document Types: Book, Conference, Dissertation, Journal, Patent, Report

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

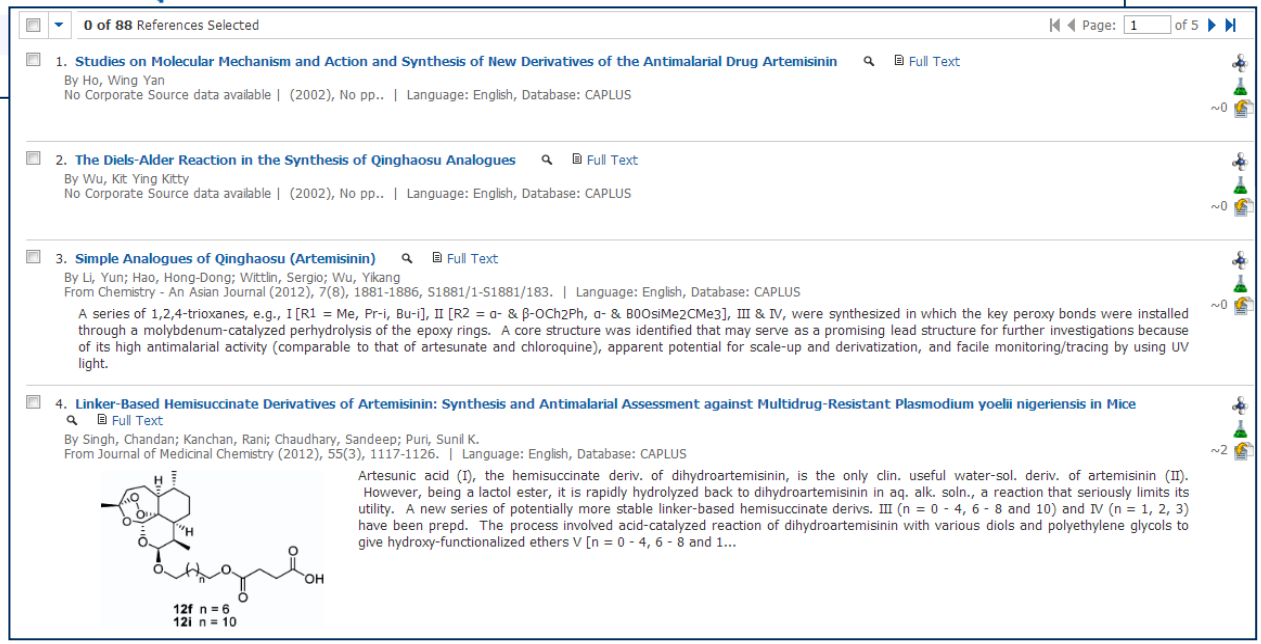
按照**CAS Role**分类的专利、非专利文献列表。对某类文献感兴趣，仅需点击交叉处的　即可方便快捷地获取。

查看物质的衍生物信息

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

勾选自己感兴趣的文献

关于青蒿素衍生物的非专利文献有88篇



0 of 88 References Selected Page: 1 of 5

1. **Studies on Molecular Mechanism and Action and Synthesis of New Derivatives of the Antimalarial Drug Artemisinin** Full Text
By Ho, Wing Yan
No Corporate Source data available | (2002), No pp.. | Language: English, Database: CAPLUS

2. **The Diels-Alder Reaction in the Synthesis of Qinghaosu Analogues** Full Text
By Wu, Kit Ying Kitty
No Corporate Source data available | (2002), No pp.. | Language: English, Database: CAPLUS

3. **Simple Analogues of Qinghaosu (Artemisinin)** Full Text
By Li, Yun; Hao, Hong-Dong; Wittlin, Sergio; Wu, Yikang
From Chemistry - An Asian Journal (2012), 7(8), 1881-1886, S1881/1-S1881/183. | Language: English, Database: CAPLUS
A series of 1,2,4-trioxanes, e.g., I [R1 = Me, Pr-i, Bu-i], II [R2 = α- & β-OCH2Ph, α- & BOOSiMe2CMe3], III & IV, were synthesized in which the key peroxy bonds were installed through a molybdenum-catalyzed perhydrolysis of the epoxy rings. A core structure was identified that may serve as a promising lead structure for further investigations because of its high antimalarial activity (comparable to that of artesunate and chloroquine), apparent potential for scale-up and derivatization, and facile monitoring/tracing by using UV light.

4. **Linker-Based Hemisuccinate Derivatives of Artemisinin: Synthesis and Antimalarial Assessment against Multidrug-Resistant Plasmodium yoelii nigeriensis in Mice** Full Text
By Singh, Chandan; Kanchan, Rani; Chaudhary, Sandeep; Puri, Sunil K.
From Journal of Medicinal Chemistry (2012), 55(3), 1117-1126. | Language: English, Database: CAPLUS
Artesunic acid (I), the hemisuccinate deriv. of dihydroartemisinin, is the only clin. useful water-sol. deriv. of artemisinin (II). However, being a lactol ester, it is rapidly hydrolyzed back to dihydroartemisinin in aq. alk. soln., a reaction that seriously limits its utility. A new series of potentially more stable linker-based hemisuccinate derivs. III (n = 0 - 4, 6 - 8 and 10) and IV (n = 1, 2, 3) have been prepd. The process involved acid-catalyzed reaction of dihydroartemisinin with various diols and polyethylene glycols to give hydroxy-functionalized ethers V [n = 0 - 4, 6 - 8 and 1...

12f n = 6
12i n = 10

Substance Detail—查看生物活性信息

Bioactivity Indicators NEW

	References
Anti-infective agents (all) >>> Antimalarials	805
Anti-infective agents (all) >>> Antiviral agents	34
Anti-infective agents (all) >> Parasiticides	43
Anti-inflammatory agents (all) > Anti-inflammatory agents	41
Antitumor agents (all) > Antitumor agents	169
Natural products MD pharmaceutical	108

Target Indicators NEW

	References
Cytokines (all) >> Chemokines	13
Cytokines (all) >> Tumor necrosis factors	11
DNA-binding proteins (all) >>> Transcription factor NF-κB	21
Enzymes (all) >>>> Adenosine triphosphatase	15
Enzymes (all) >>> 26S proteasome	15
Enzymes (all) >>>>>>> Src kinase	13
Glycoproteins (all) >> P-glycoproteins	15
Hemoproteins (all) >>> Cytochrome P 450	12
Hemoproteins (all) >>> Cytochrome P 450 3A4	12
Phosphoproteins (all) >> P-glycoproteins	15
Proteins	19
Receptors (all) > Toll-like receptors	13
RNA formation factors (all) >>> Transcription factor NF-κB	21
Transport proteins (all) >> P-glycoproteins	15
Transport pro… endoplasmic …	

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Substance Identifier "qinghaosu " > substances (1) > 63968-64-9 > get references (24)

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Hyde Roderick A 13

Malaska Stephen L 13

Sweeney Elizabeth A 13

Wood Lowell L Jr 12

Paris Daniel 3

Bakshi Pancham 2

Mullan Michael J 2

Ait Ghezala Ghania 1

1. **Enhanced IL-12p40 production in LPS-stimulated macrophages by inhibiting JNK activation by artemisinin** Full Text

By Cho, Young-Chang; Lee, Sung Ho; Lee, Mina; Kim, Hyun Jung; Oak, Min-ho; Lee, Ik-Soo; Kang, Bok Yun

From Archives of Pharmacal Research (2012), 35(11), 1961-1968. | Language: English, Database: CAPLUS

Artemisinin can be isolated from Artemisia annua L. In addn. to its well-known anti-malarial activity, artemisinin has antitumor and anti-microbial effects. In this study, we investigated the effect of artemisinin on the prodn. of IL-12p40, which is important in the generation of T helper 1 responses. Artemisinin significantly induced IL-12p40 prodn. in LPS-stimulated RAW264.7 macrophage cells. To elucidate the signaling mols. regulated by artemisinin in induced IL-12p40 prodn., the DNA-binding activity of several transcription factors and activation of mitogen-activated protein kinase (MA...

2. **Artemisinin attenuates post-infarct myocardial remodelling by down-regulating the NF-κB pathway** Full Text

By Gu, Yongwei; Wang, Xi; Wang, Xin; Yuan, Mingjie; Wu, Gang; Hu, Juan; Tang, Yanhong; Huang, Congxin

From Tohoku Journal of Experimental Medicine (2012), 227(3), 161-170. | Language: English, Database: CAPLUS

Myocardial infarction (MI) leads to progressive left ventricular (LV) dilatation and is assocd. with interstitial fibrosis in the non-infarcted myocardium. The NF-κB signaling pathway plays an important role in ventricular remodeling after MI. Recent studies have indicated that the anti-malarial agent artemisinin can inhibit NF-κB activation, which may attenuate post-infarct myocardial remodeling. In this study, we investigated the effect of artemisinin on post-infarct myocardial remodeling using a rat model of MI. Adult male Sprague Dawley rats were divided into a sham group (n = 10) and ...

Substance Detail—物质预测性质信息

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

Top

Biological Properties	Value	Condition	Note
Bioconcentration Factor	38.6	pH 1 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 2 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 3 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 4 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 5 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 6 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 7 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 8 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 9 Temp: 25 °C	(27)
Bioconcentration Factor	38.6	pH 10 Temp: 25 °C	(27)

Top

Chemical Properties	Value	Condition	Note
Koc	476	pH 1 Temp: 25 °C	(27)
Koc	476	pH 2 Temp: 25 °C	(27)
Koc	476	pH 3 Temp: 25 °C	(27)
Koc	476	pH 4 Temp: 25 °C	(27)
Koc	476	pH 5 Temp: 25 °C	(27)
Koc	476	pH 6 Temp: 25 °C	(27)
Koc	476	pH 7 Temp: 25 °C	(27)
Koc	476	pH 8 Temp: 25 °C	(27)
Koc	476	pH 9 Temp: 25 °C	(27)
Koc	476	pH 10 Temp: 25 °C	(27)
logD	2.39	pH 1 Temp: 25 °C	(27)
logD	2.39	pH 2 Temp: 25 °C	(27)
logD	2.39	pH 3 Temp: 25 °C	(27)
logD	2.39	pH 4 Temp: 25 °C	(27)
logD	2.39	pH 5 Temp: 25 °C	(27)
logD	2.39	pH 6 Temp: 25 °C	(27)
logD	2.39	pH 7 Temp: 25 °C	(27)
logD	2.39	pH 8 Temp: 25 °C	(27)
logD	2.39	pH 9 Temp: 25 °C	(27)
logD	2.39	pH 10 Temp: 25 °C	(27)
logP	2.391±0.772	Temp: 25 °C	(27)
Mass Intrinsic Solubility	Sparingly Soluble (0.16 g/L)	Temp: 25 °C	(27)
Mass Solubility	Sparingly Soluble (0.16 g/L)	pH 1 Temp: 25 °C	(27)
Mass Solubility	Sparingly Soluble (0.16 g/L)	pH 2 Temp: 25 °C	(27)
Mass Solubility	Sparingly Soluble (0.16 g/L)	pH 3 Temp: 25 °C	(27)
Mass Solubility	Sparingly Soluble (0.16 g/L)	pH 4 Temp: 25 °C	(27)

Molar Solubility	Sparingly Soluble (5.7E-4 mol/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(27)
Molecular Weight	282.33		(27)
Vapor Pressure	2.76E-6 Torr	Temp: 25 °C	(27)

Top

Density Properties	Value	Condition	Note
Density	1.24±0.1 g/cm3	Temp: 20 °C Press: 760 Torr	(27)
Molar Volume	226.4±5.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(27)

Top

Lipinski and Related Properties	Value	Condition	Note
Freely Rotatable Bonds	0		(27)
H Acceptors	5		(27)
H Donors	0		(27)
H Donor/Acceptor Sum	5		(27)
logP	2.391±0.772	Temp: 25 °C	(27)
Molecular Weight	282.33		(27)

Top

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(28)
Proton NMR Spectrum	See spectrum		(28)

Top

Structure-related Properties	Value	Condition	Note
Polar Surface Area	54.0 A2		(27)

Top

Thermal Properties	Value	Condition	Note
Boiling Point	389.9±42.0 °C	Press: 760 Torr	(27)
Enthalpy of Vaporization	63.93±3.0 kJ/mol	Press: 760 Torr	(27)
Flash Point	172.0±27.9 °C		(27)

Substance Detail—物质实验性质信息

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

Top

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1)CAS
Half-Life (Biological)	See full text	1 of 2	(1)CAS
Median Lethal Dose(LD50)	5576 mg/kg	Organism: rat Route: oral	(15)APC
Median Lethal Dose(LD50)	5105 mg/kg	Organism: mouse Route: oral	(15)APC
Median Lethal Dose(LD50)	2800 mg/kg	Organism: mouse Route: intramuscular	(15)APC
Median Lethal Dose(LD50)	2571 mg/kg	Organism: rat Route: intramuscular	(15)APC
Median Lethal Dose(LD50)	1558 mg/kg	Organism: mouse Route: intraperitoneal	(15)APC
Minimum Inhibitory Concentration	See full text	1 of 2	(20)CAS

Top

Chemical Properties	Value	Condition	Note
Ionization Potential	See full text		(2)CAS
logP	See full text	1 of 2	(12)CAS
Molecular Electric Dipole Moment	See full text		(21)CAS
Solubility	See full text	1 of 9	(7)CAS

Top

Density Properties	Value	Condition	Note
Density	1.300 g/cm3		(7)CAS

Top

Flow and Diffusion Properties	Value	Condition	Note
Diffusion Coefficient	See full text		(8)CAS

Density Properties	Value	Condition	Note
Density	1.300 g/cm3		(7)CAS

Top

Flow and Diffusion Properties	Value	Condition	Note
Diffusion Coefficient	See full text		(8)CAS

Top

Lipinski and Related Properties	Value	Condition	Note
logP	See full text	1 of 2	(12)CAS

Top

Optical and Scattering Properties	Value	Condition	Note
Optical Rotatory Power	+87.9 °	Solv: 1,4-dioxane (123-91-1); Wavlen: 589.3 nm	(22)CAS
Optical Rotatory Power	+75-+78 °	Conc: 1.0 g/100mL; Solv: ethanol (64-17-5); Wavlen: 589.3 nm; Temp: 20 °C	(16)CAS
Optical Rotatory Power	+68.2 °	Conc: 0.97 g/100mL; Solv: chloroform (67-66-3); Temp: 25 °C	(18)IC
Optical Rotatory Power	+67.6 °	Conc: 1.75 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 25 °C	(17)CAS
Optical Rotatory Power	+66.6 °	Conc: 1.57 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 24 °C	(17)CAS
Optical Rotatory Power	+66.3 °	Conc: 1.64 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 17 °C	(15)APC
Optical Rotatory Power	+61 °	Conc: 0.2 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 24 °C; Len: 1 dm	(5)CAS

Substance Detail—查看实验谱图信息

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS
Circular Dichroism Spectrum	See full text	1 of 2	(6)CAS
IR Absorption Spectrum	See full text	1 of 11	(2)CAS
Mass Spectrum	See spectrum		(13)WSS
Mass Spectrum	See spectrum		(13)WSS
Mass Spectrum	See full text	1 of 10	(14)CAS
Proton NMR Spectrum	See full text	1 of 10	(17)CAS
Raman Spectrum	See full text	1 of 2	(24)CAS
Two-Dimensional NMR Spectrum	See full text	1 of 2	(8)CAS
UV and Visible Absorption Spectrum	See full text		(6)CAS
UV and Visible Emission/Luminescence Spectrum	See full text		(26)CAS

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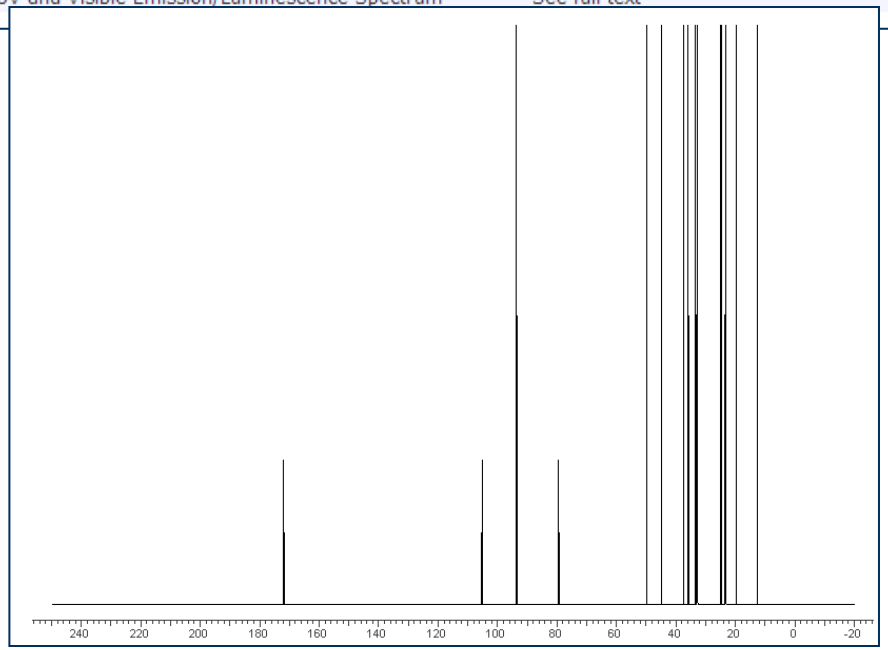
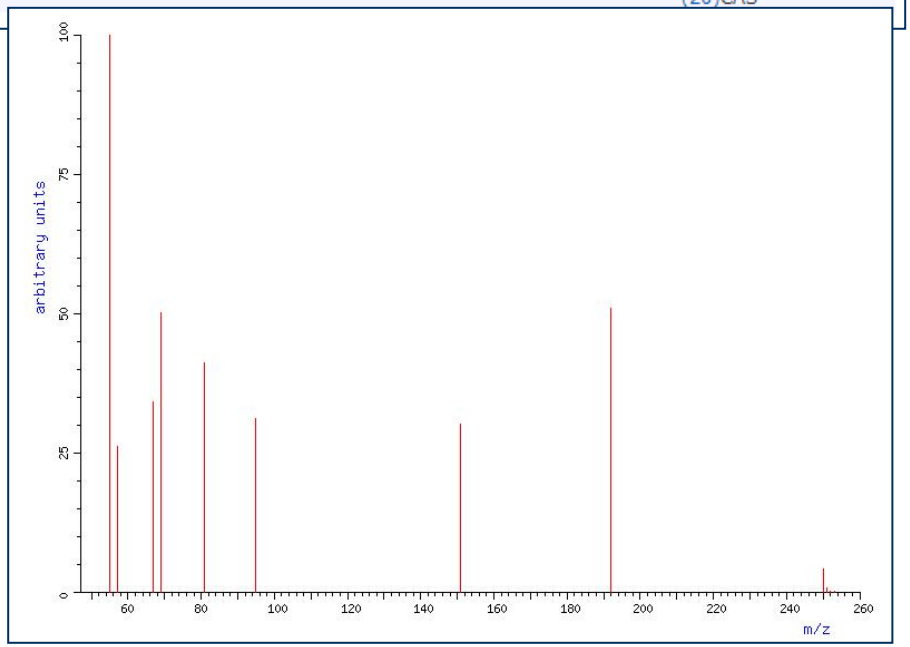
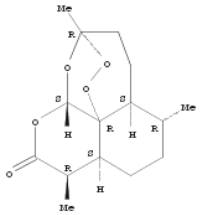




物质有关的反应

1. **Substance Detail**
63968-64-9

~3242



Absolute stereochemistry.

$C_{15}H_{22}O_5$
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-

Get Reactions

Limit results by reaction role:

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- ( ) Reactant
- ( ) Reagent
- ( ) Reactant or reagent
- ( ) Catalyst
- ( ) Solvent
- ( ) Any role

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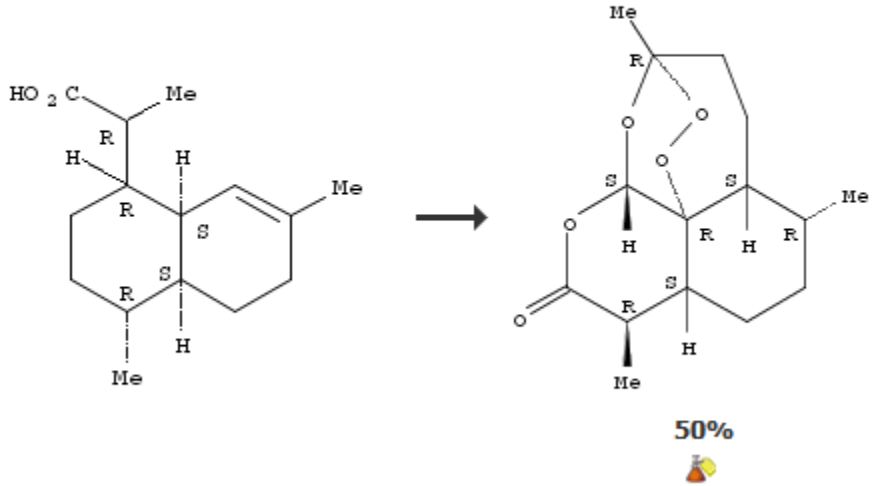
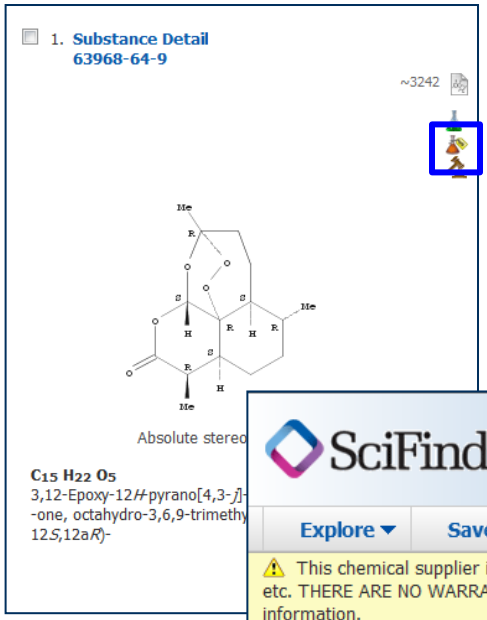


Overview

物质有关的商业来源



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

COMMERCIAL SOURCES

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Accel Pharmtech Product List 2

AK Scientific Product Catalog 2

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ChemPacific Product

Sort by: Catalog Name

Answers per Page [20]

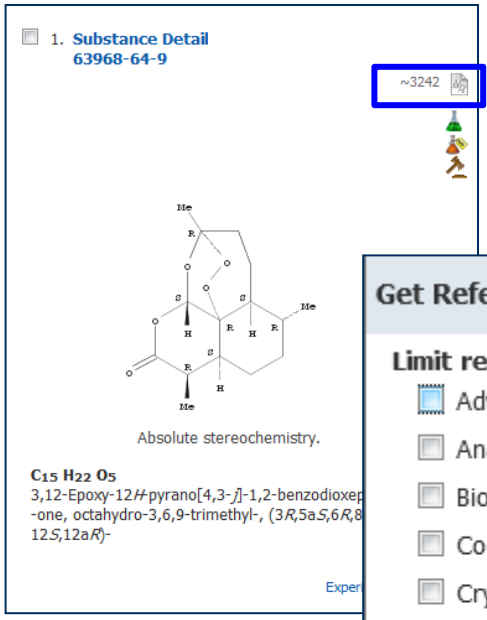
0 of 91 Commercial Sources Selected

Page: 1 of 5

1. **3B Scientific Corporation Product List**
Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 12 Jul 2012
Order Number: 3B2-3802
Quantity: 1g
63968-64-9 Astemisinin
Link

2. **A Chemtek Product List**
Supplier Name: A Chemtek, Catalog Publication Date: 13 Mar 2013
Order Number: 031-18967
Quantity: N/A
63968-64-9 Artemisnini

物质有关的文献信息



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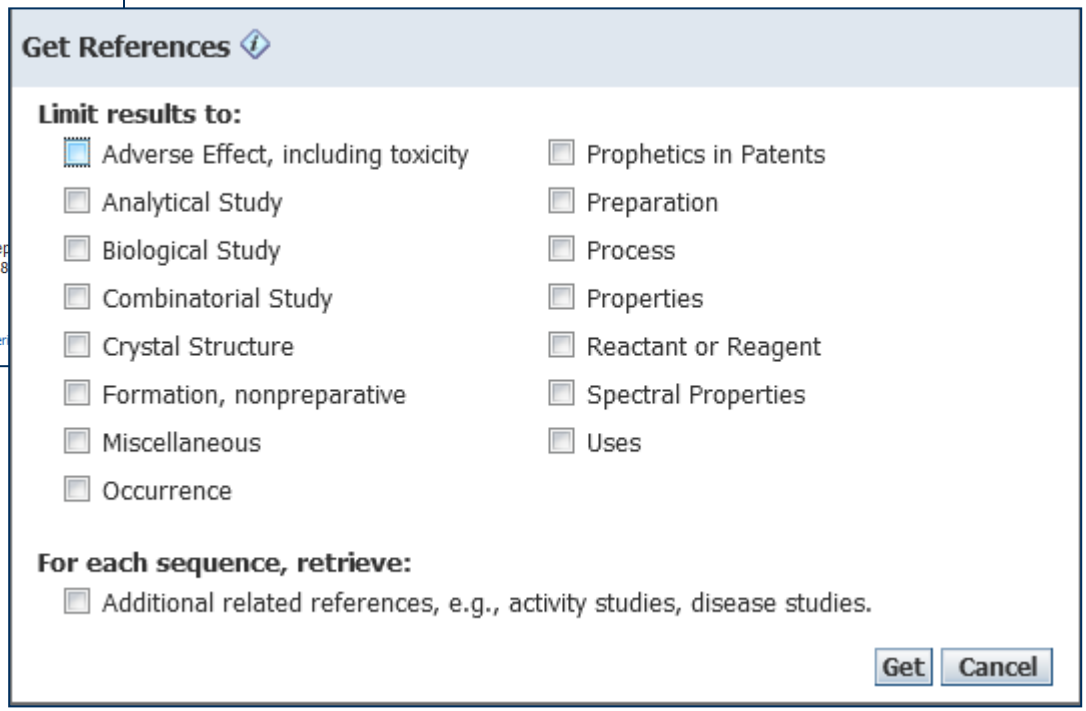

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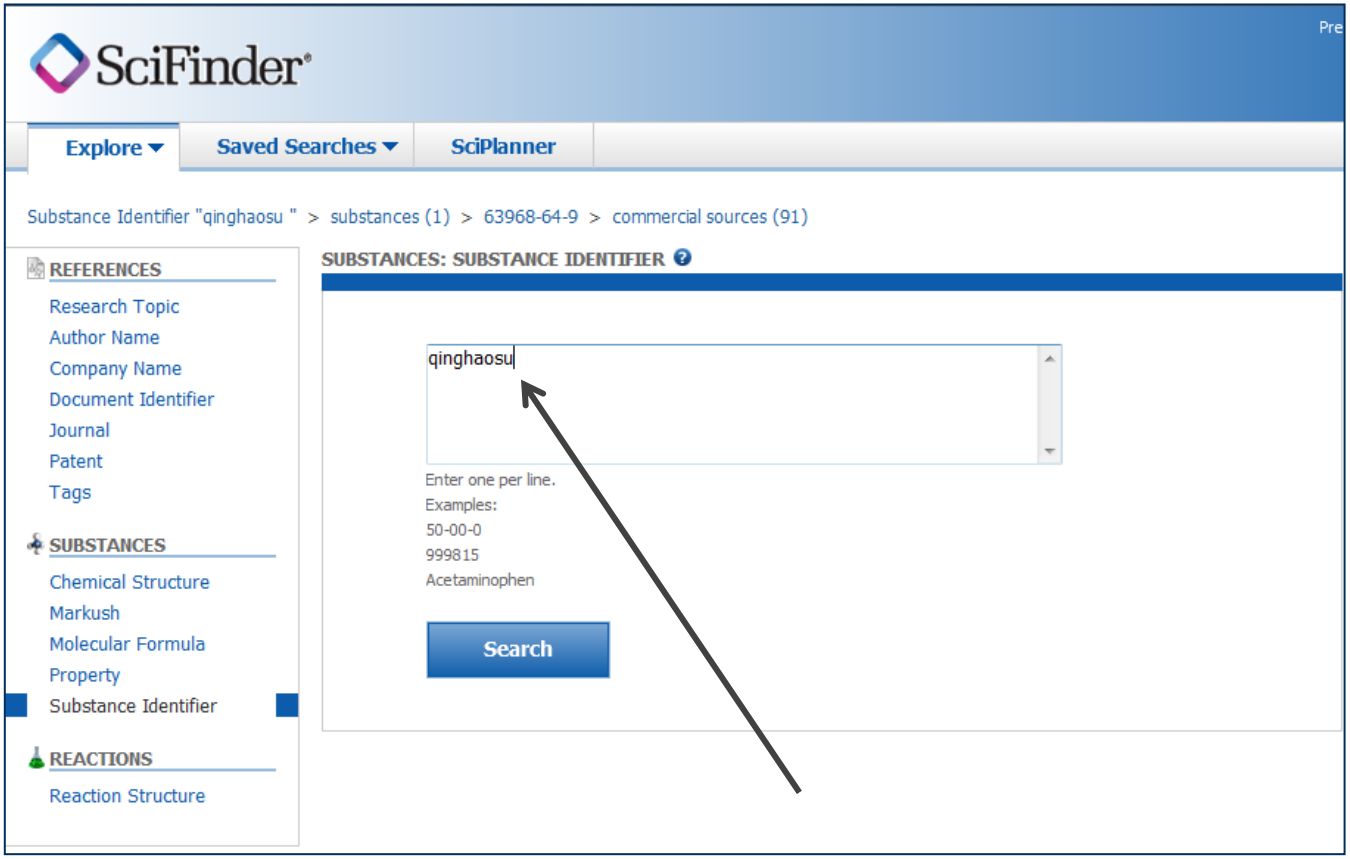
- 功能方面
  - 物质名称，CAS No
  - 分子式
  - 结构式
  - 理化性质
- 推荐的物质检索功能
  - 有机物，天然产物及衍生物 ---结构比较方便
  - 无机物 ---分子式比较方便
  - 高分子化合物 ---首先分子式，其次结构

物质名称检索



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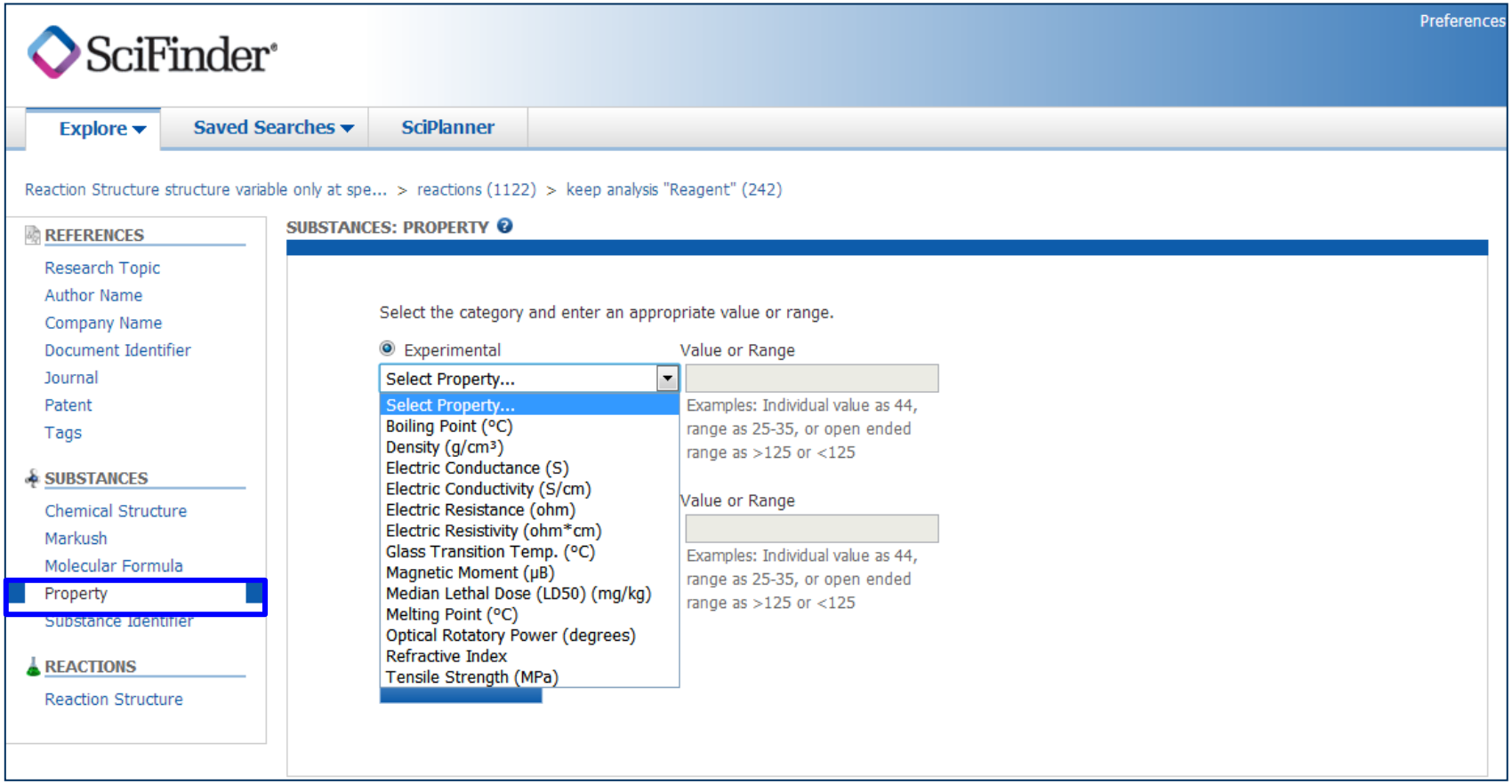
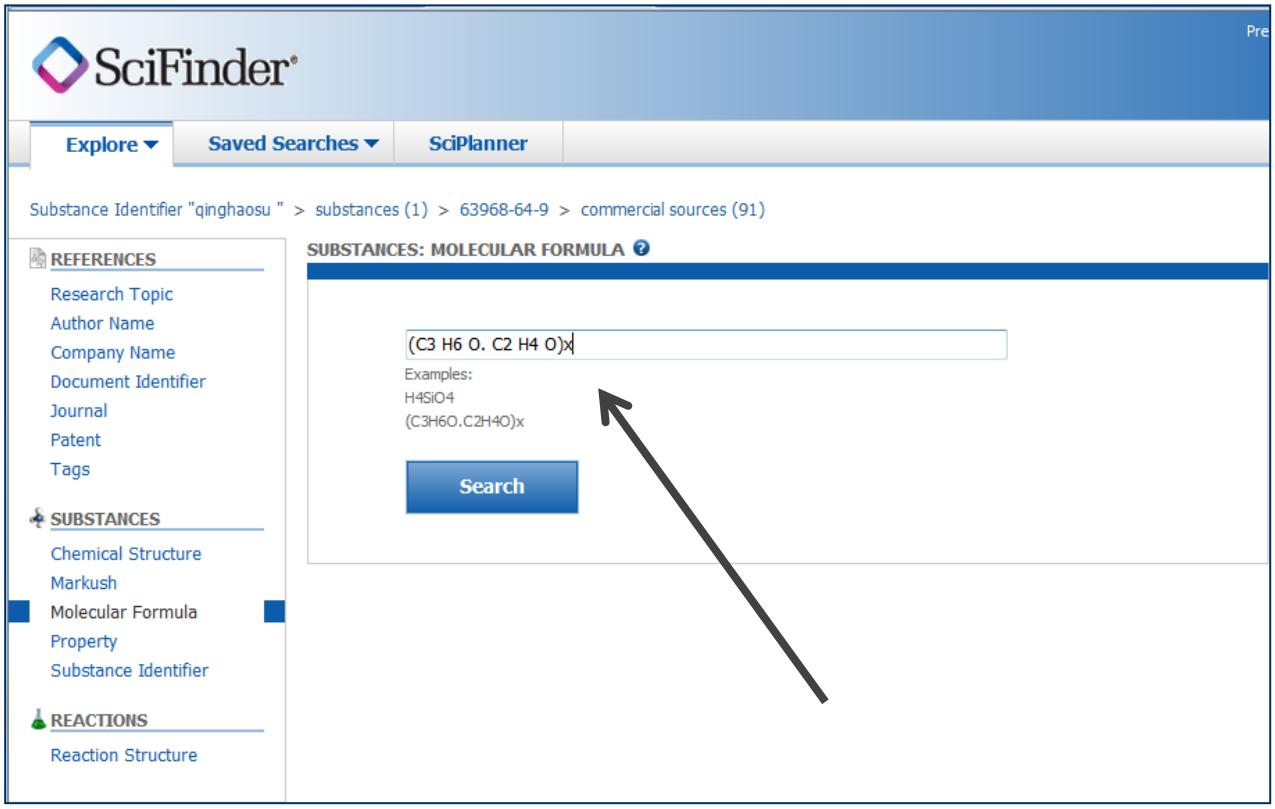


分子式检索

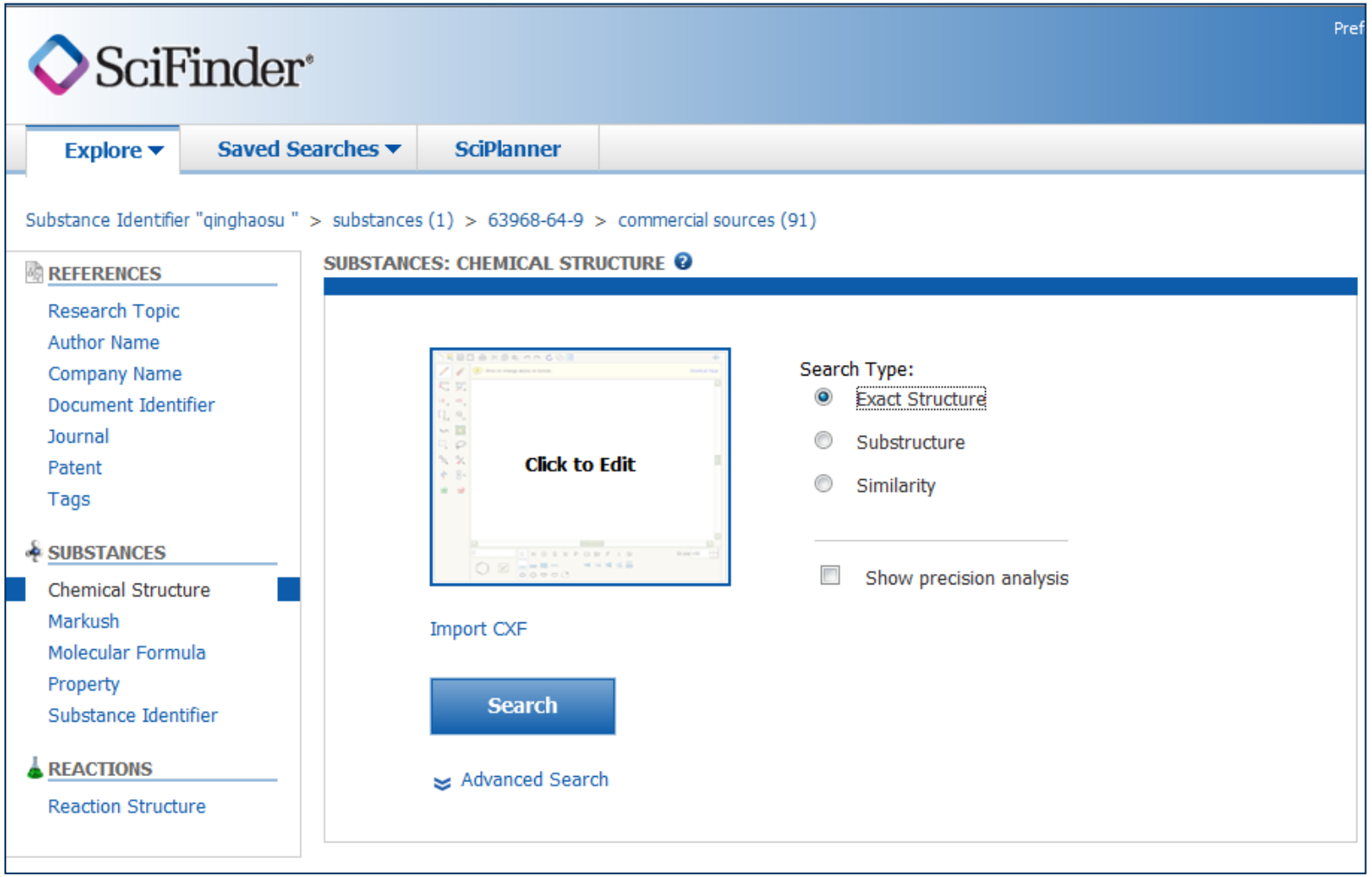


分子式的检索，根据hill排序规则书写，C,H写在前面，其他元素按照字母顺序写

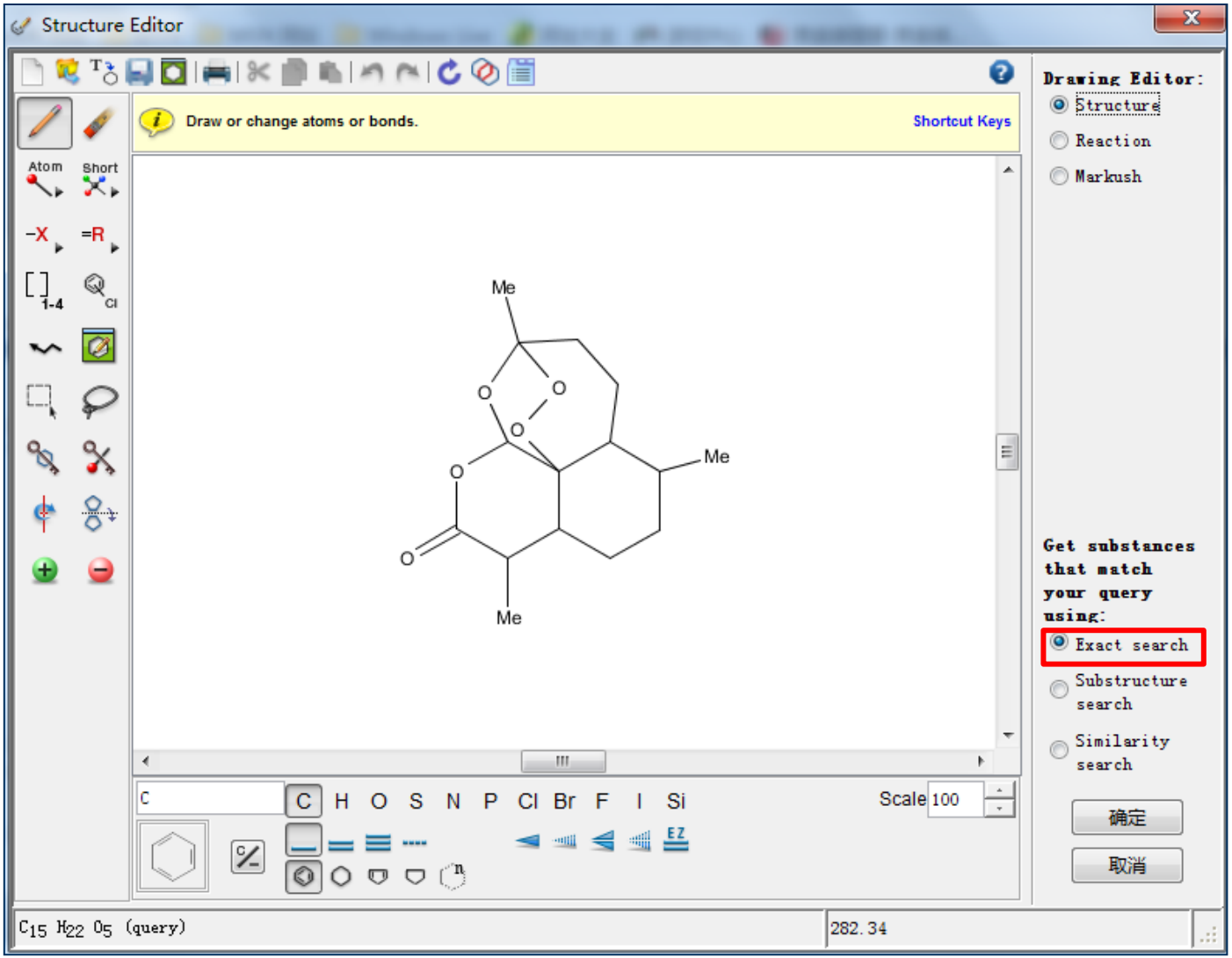
分子式检索

- 多组分物质
  - 包含盐，水合物，合金，混合物等
  - 用“.”将不同组分点开
- Hill排序
  - 单一组分物质
    - 对于不含C的物质，按照字母顺序排序
    - 对于含C的物质，CH写在前面，其他的按照字母顺序排列
    - 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
    - 区分大小写
  - 多组分物质
    - 每一组分必须遵照单一组分物质的分子式来书写。
    - 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。
    - 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

结构式检索—精确检索

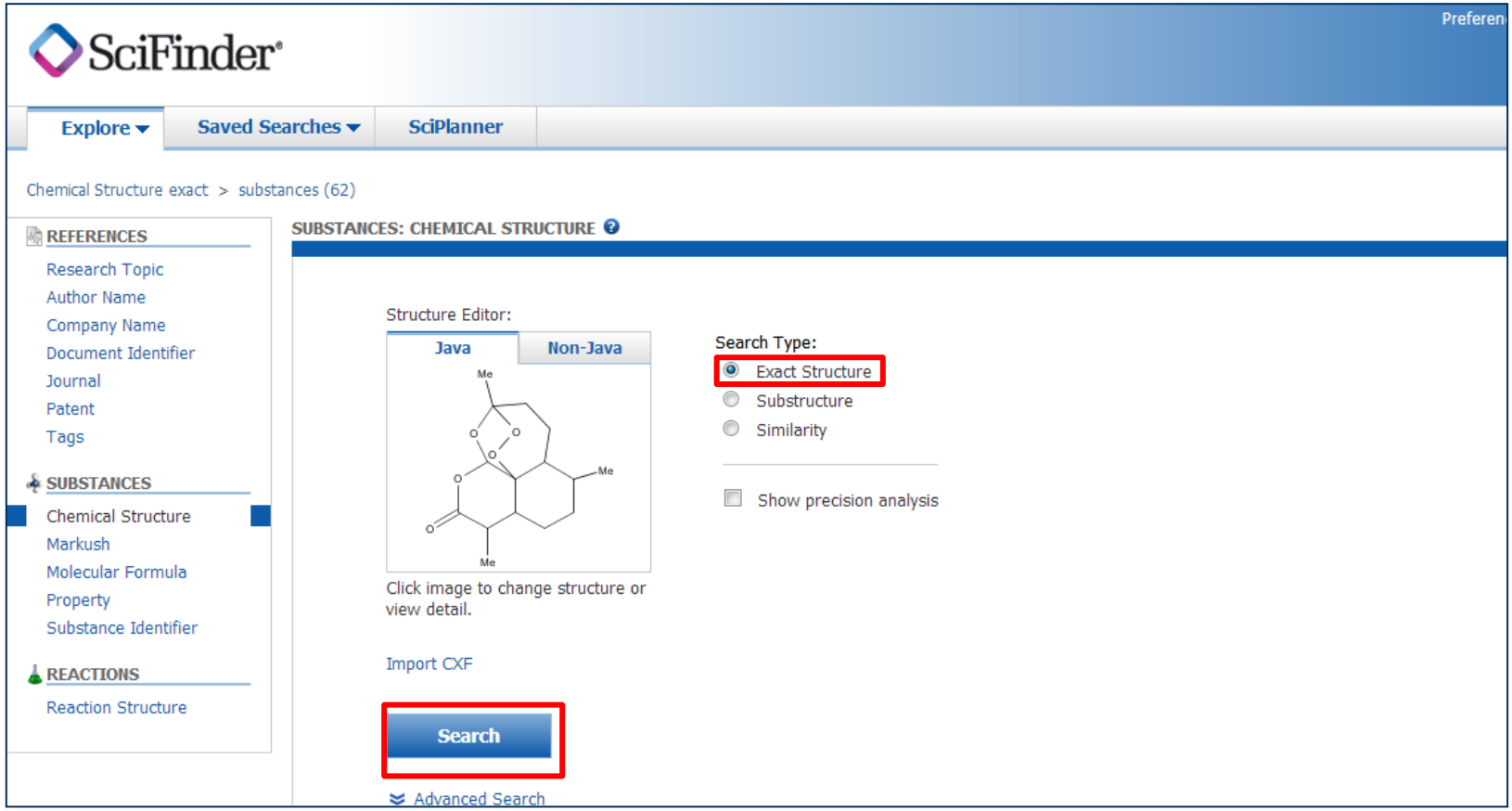


青蒿素结构检索



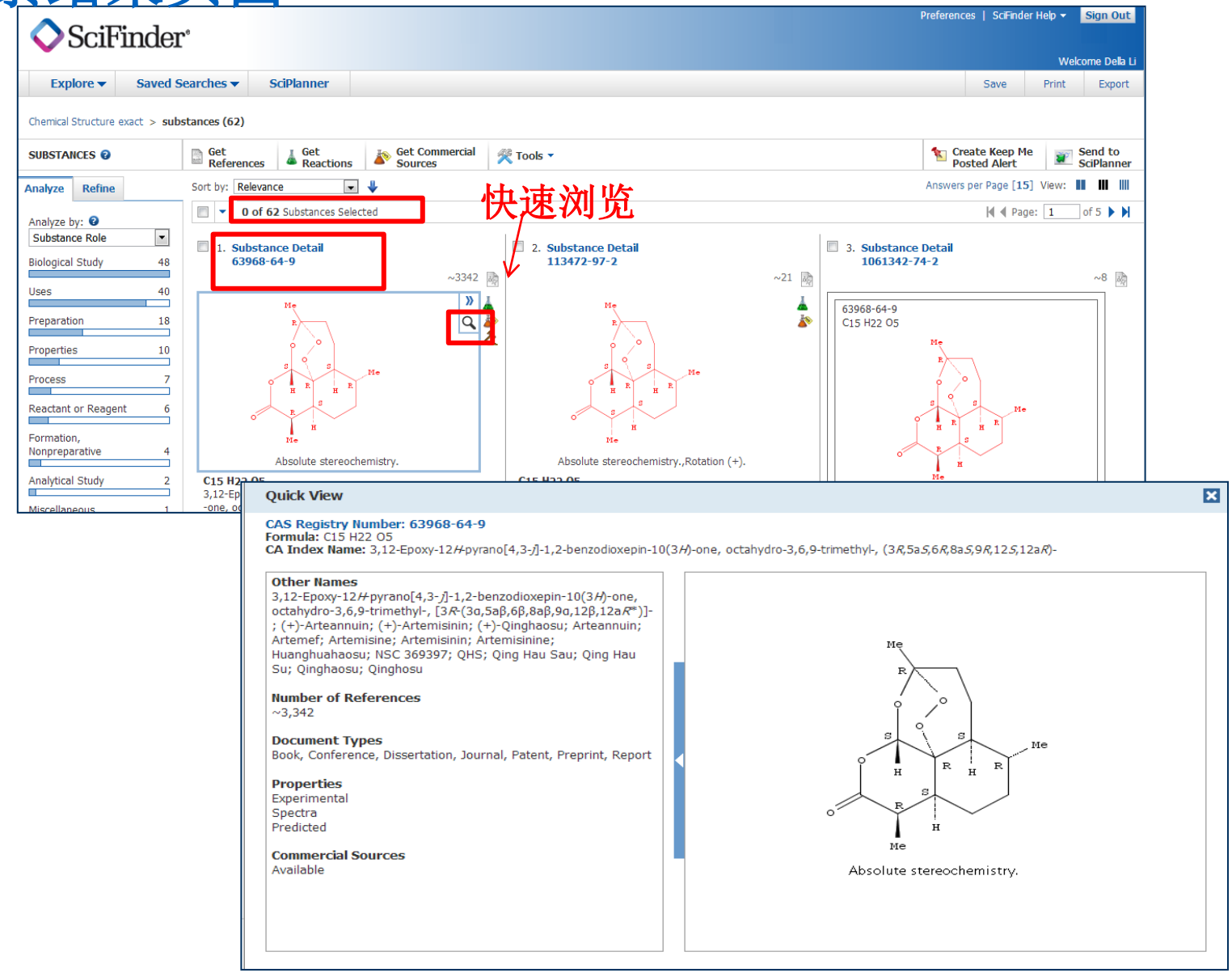
精确结构结构检索

结构检索界面

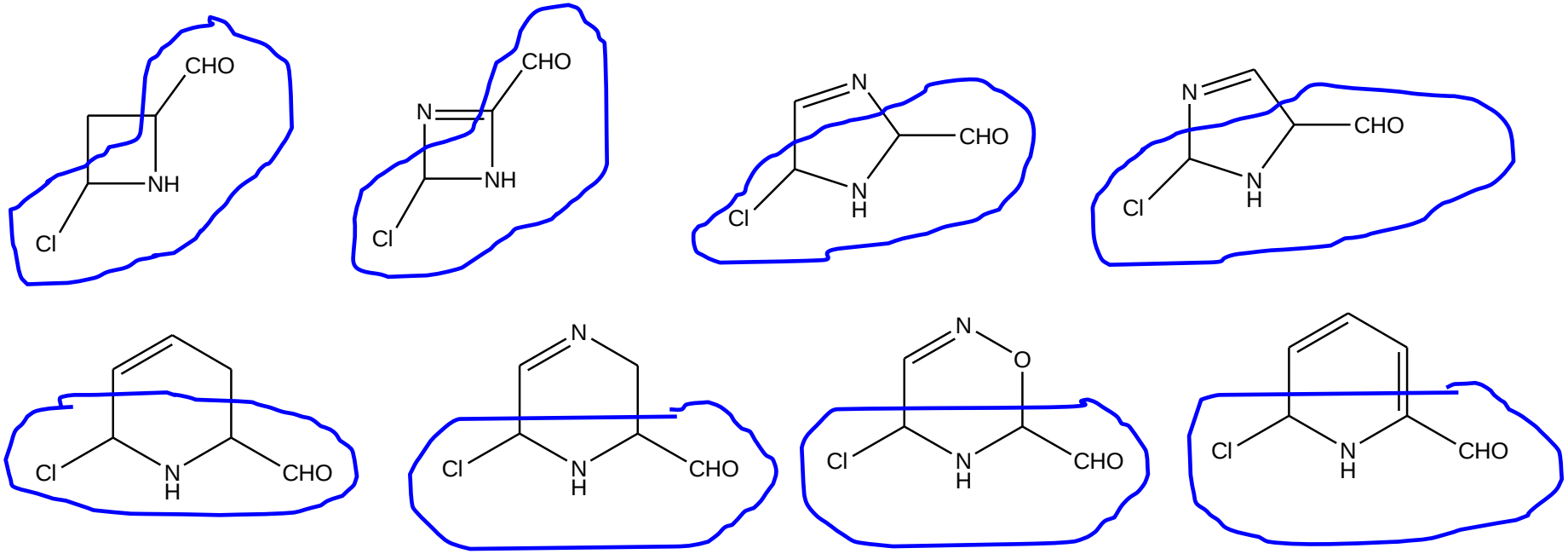


与已绘制的结构完全相同的物质： 同位素化合物， 配位化合物，单体组成的聚合物， 离子化合物，异构体 ， 互变异构体

检索结果页面

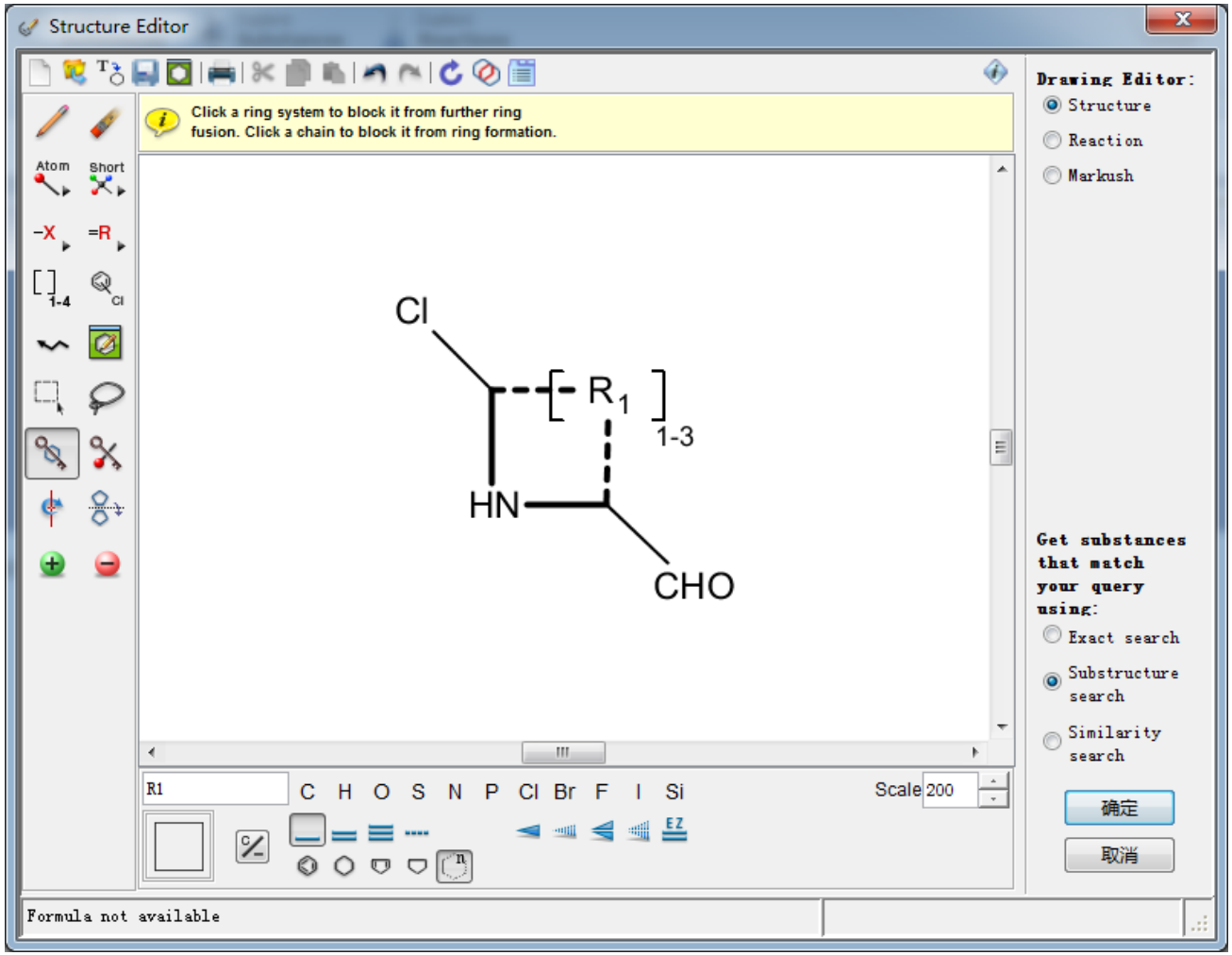


我想获得以下的一系列物质



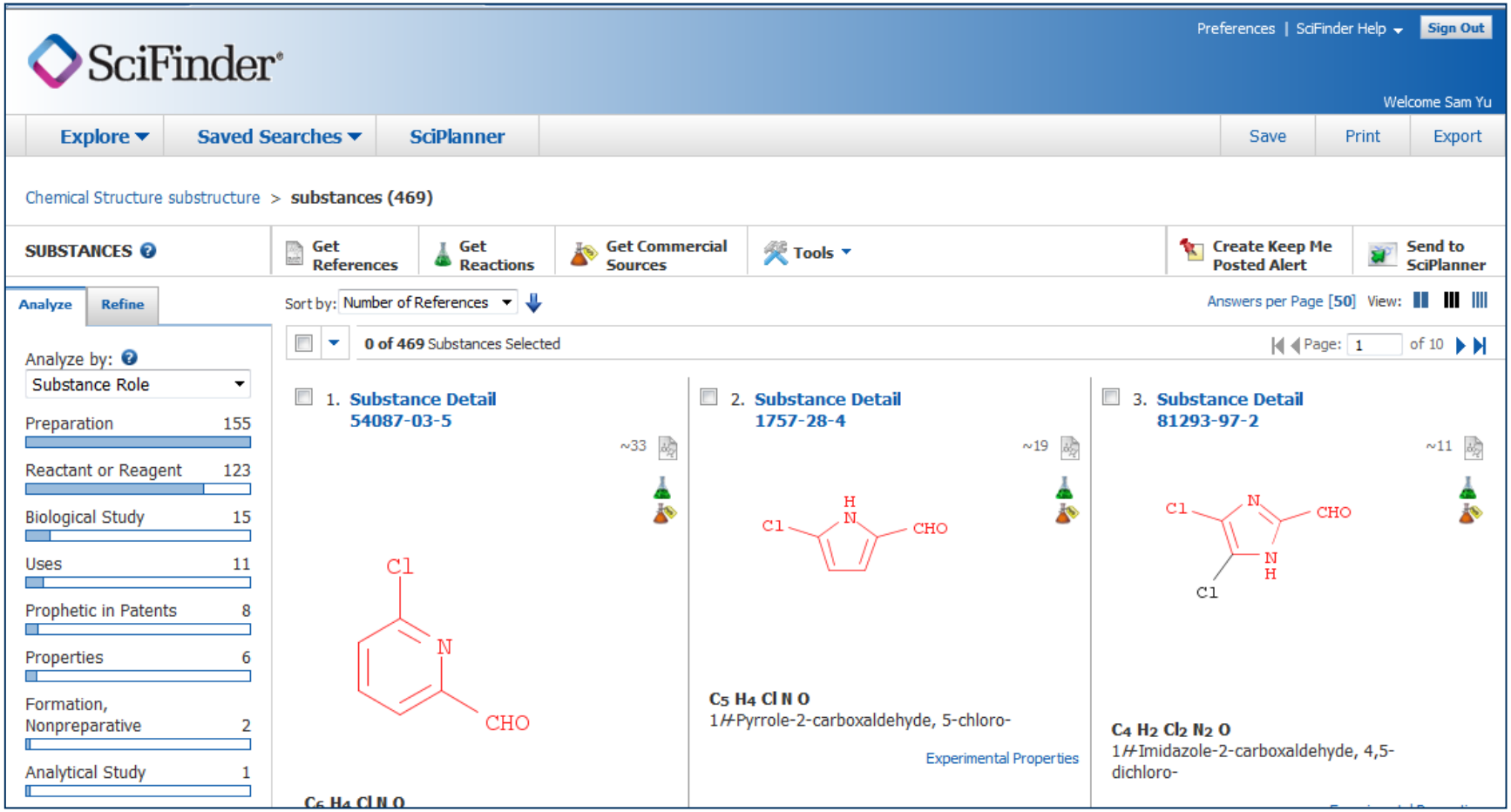
。 。 。 。 。 。

结构定义



用亚结构检索获得所有的物质

亚结构检索结果



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  - SciFinder中的结构面板使用技巧
  - SciFinder中的物质结果及物质检索方法
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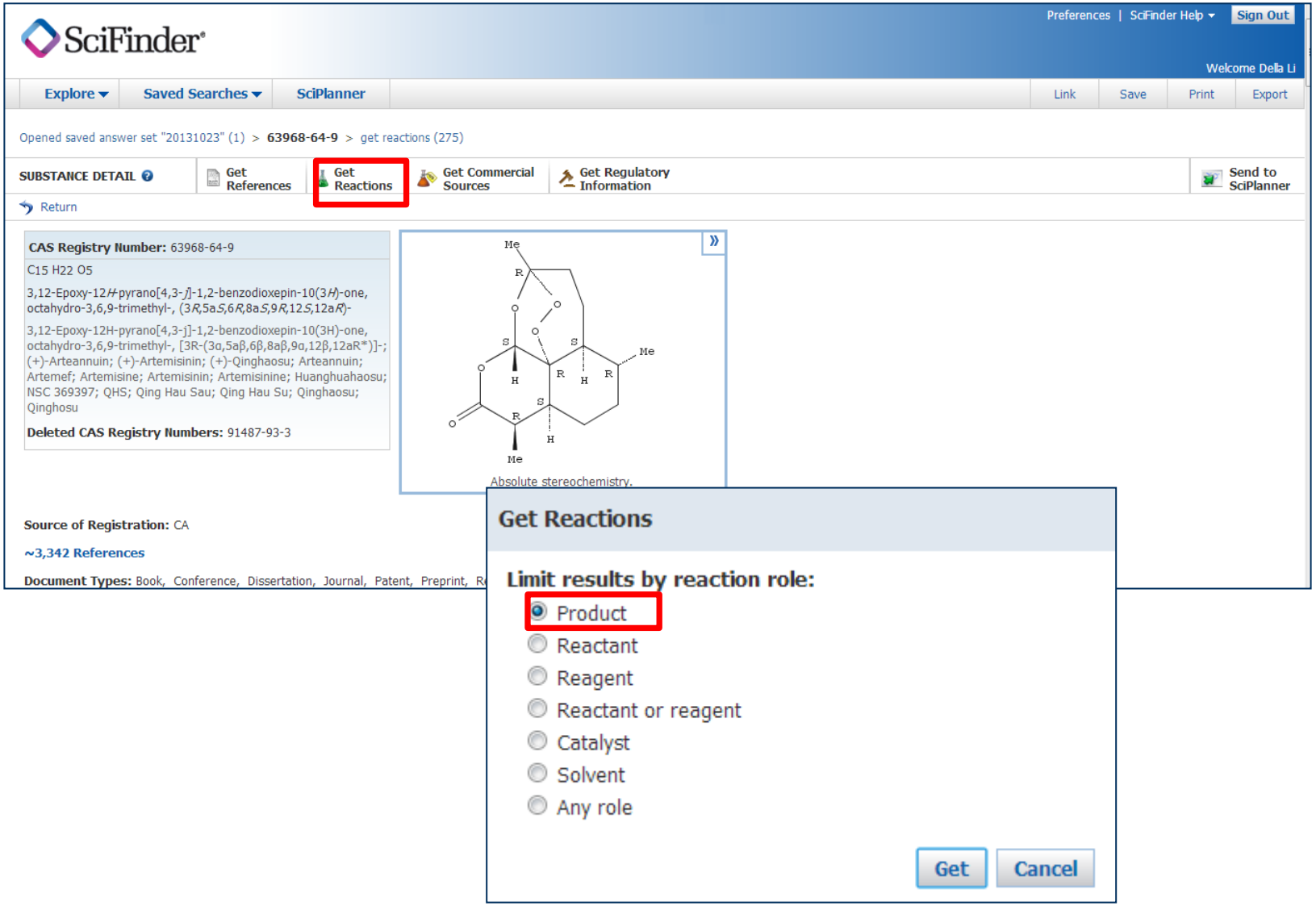
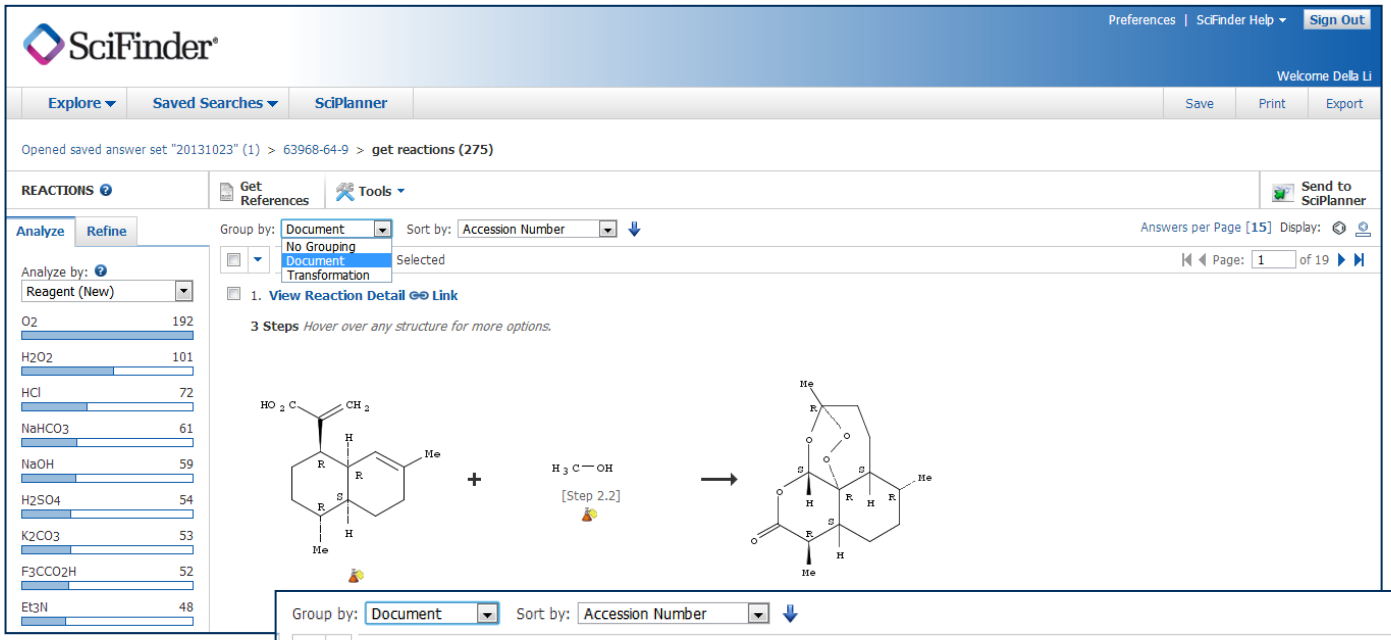
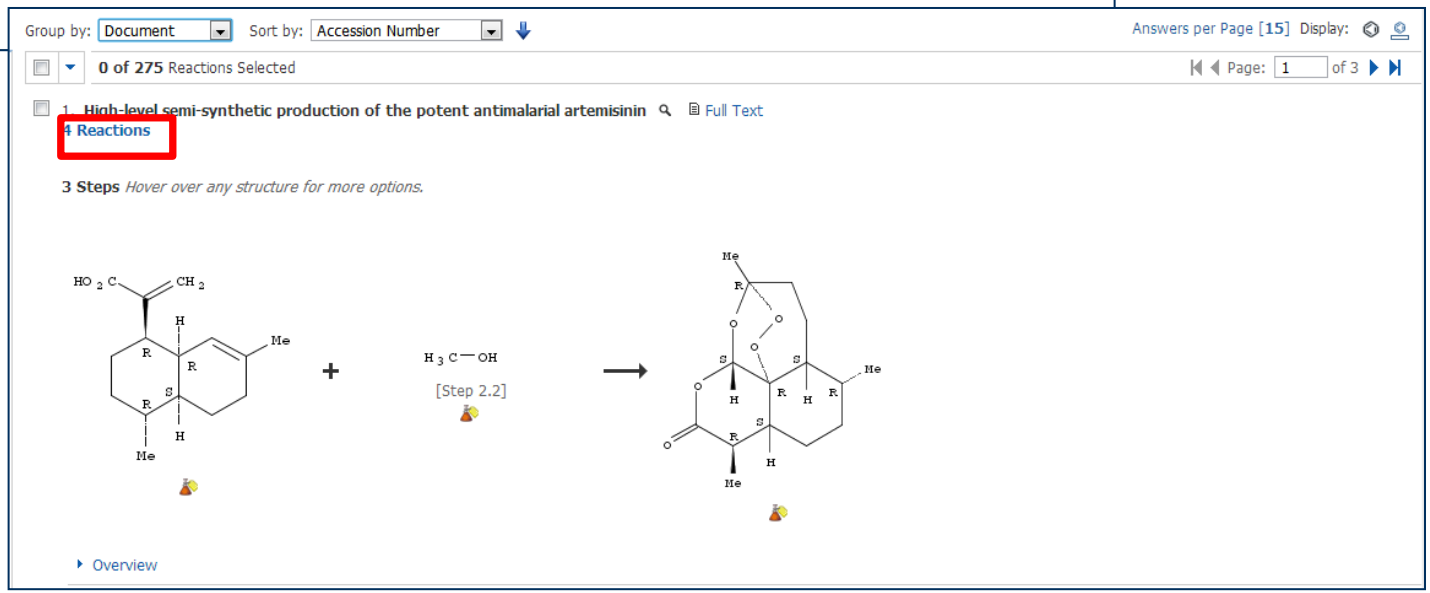
- **SciFinder Web的注册和常见问题**

从物质获得反应



按照文献出处分类显示

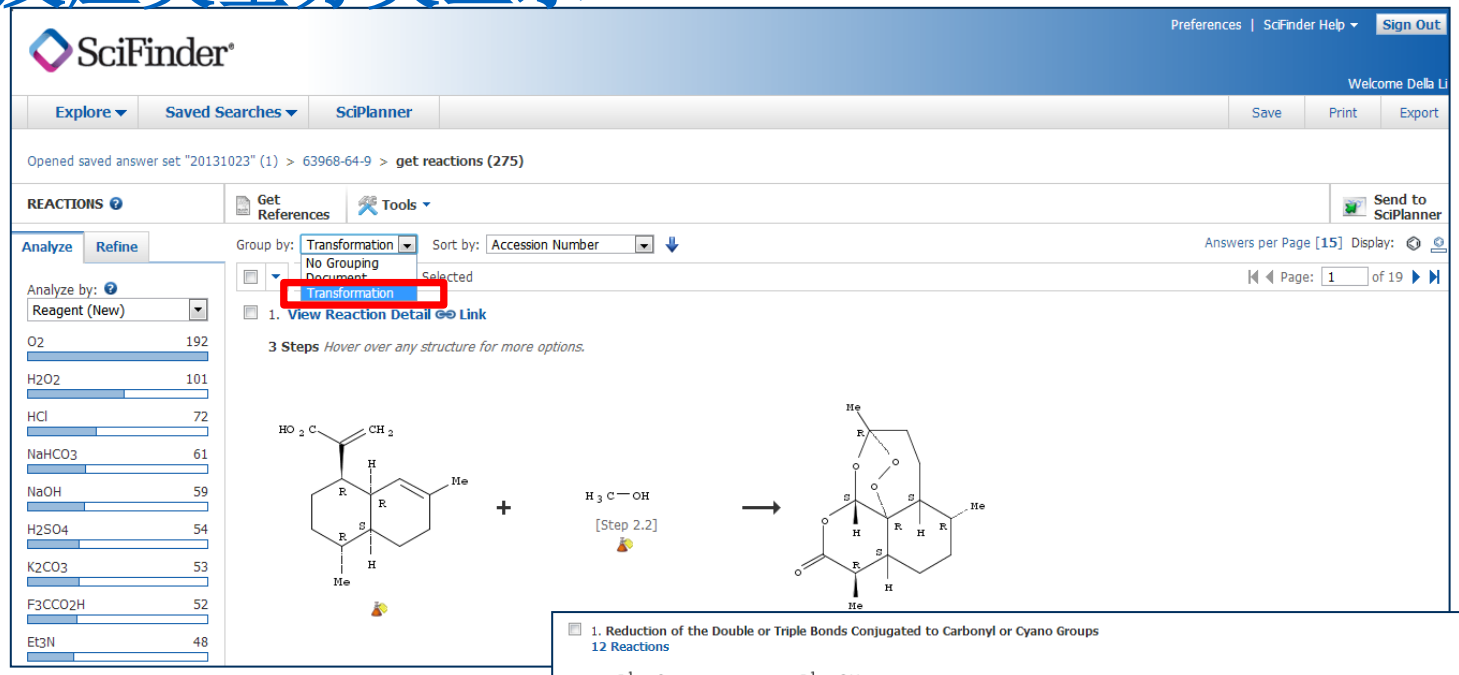


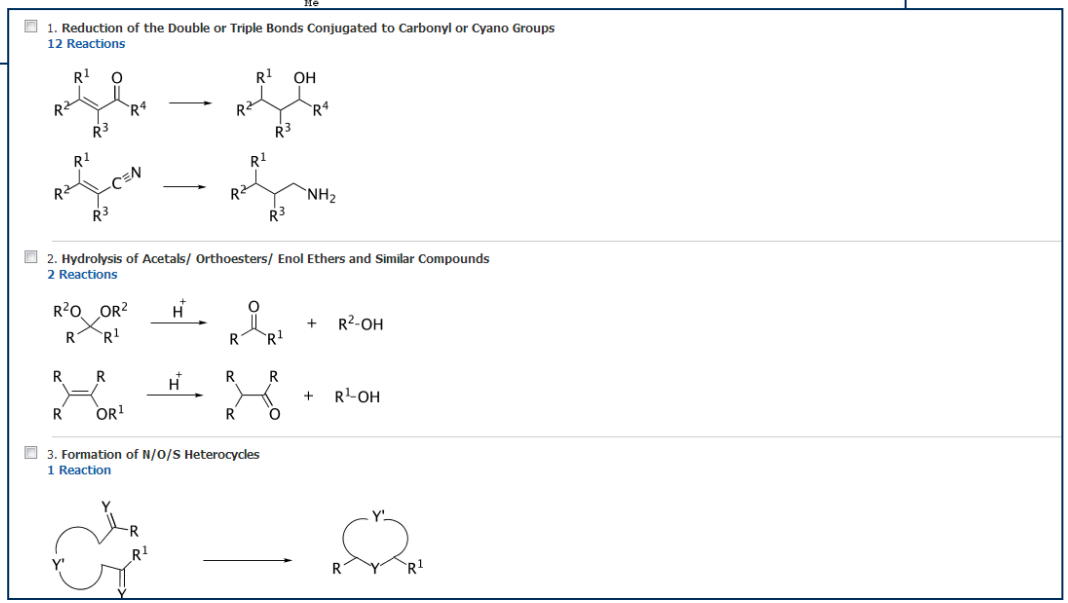


我们获得275条反应

反应筛选的第一步是**Group By Document**，让一篇文献出现一条反应

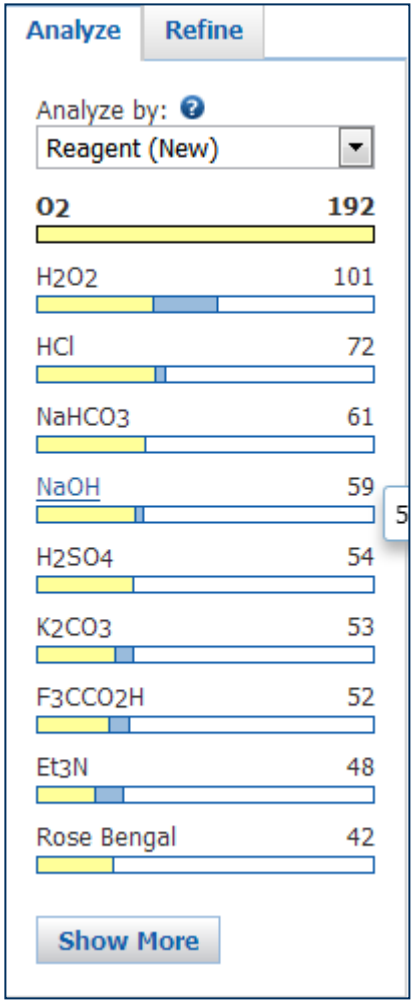
按照反应类型分类显示



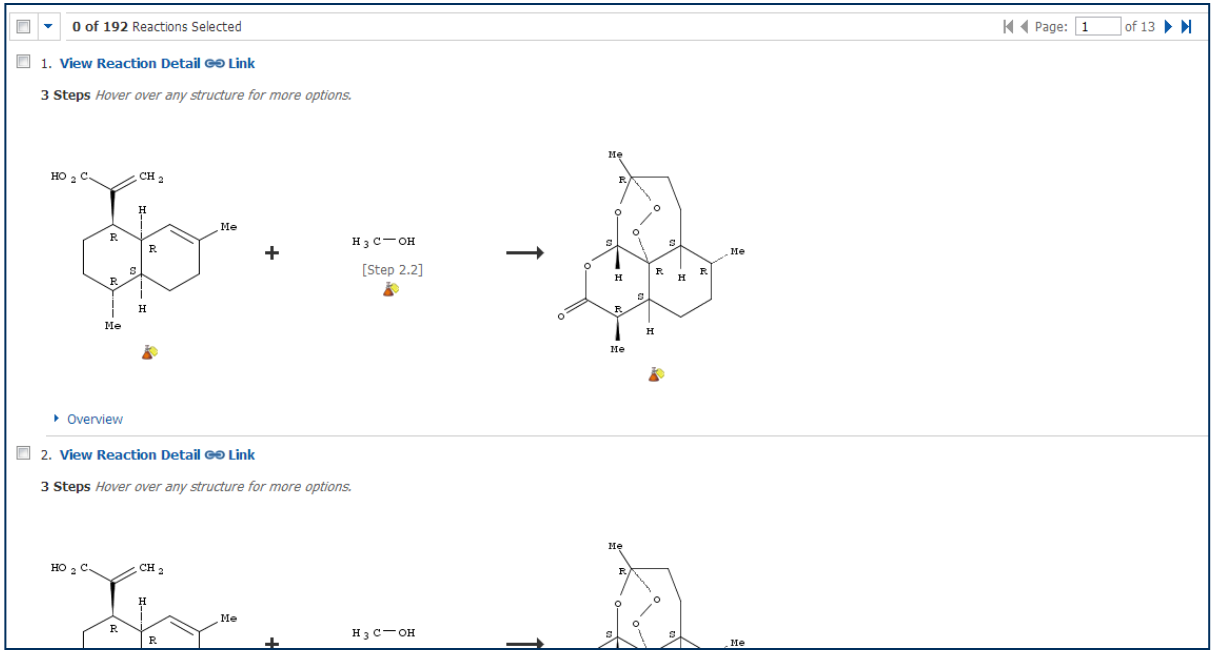


Transformation 帮助我们判断大部分的研究人员采用哪种合成方法

按照试剂进行分析



有192篇文献都用的是0_2这个试剂



按照实验过程进行排序

REACTIONS | Get References | Tools | Send to SciPlanner

Analyze | Refine

Analyze by: Reagent (New)

O2	192
HCl	67
H2O2	66
NaHCO3	61
NaOH	55
H2SO4	54
K2CO3	45
Rose Bengal	42
F3CCO2H	40
HgCl2	39

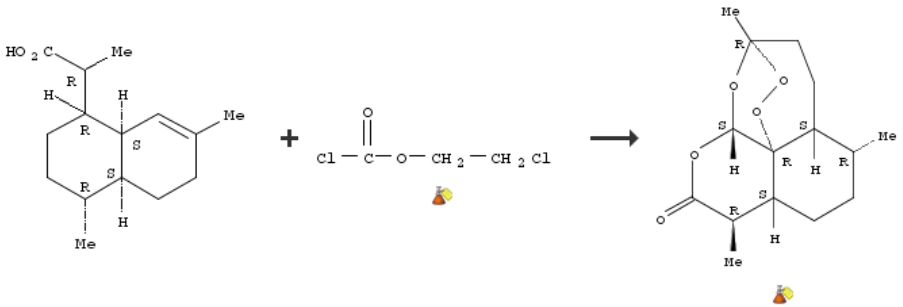
Group by: No Grouping | Sort by: Experimental Procedure | Answers per Page [15] | Display:

Accession Number
Experimental Procedure
Product Yield
Publication Year

0 of 192 Reactions Selected | Page: 1 of 13

1. View Reaction Detail | Link

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



Overview

Experimental Procedure

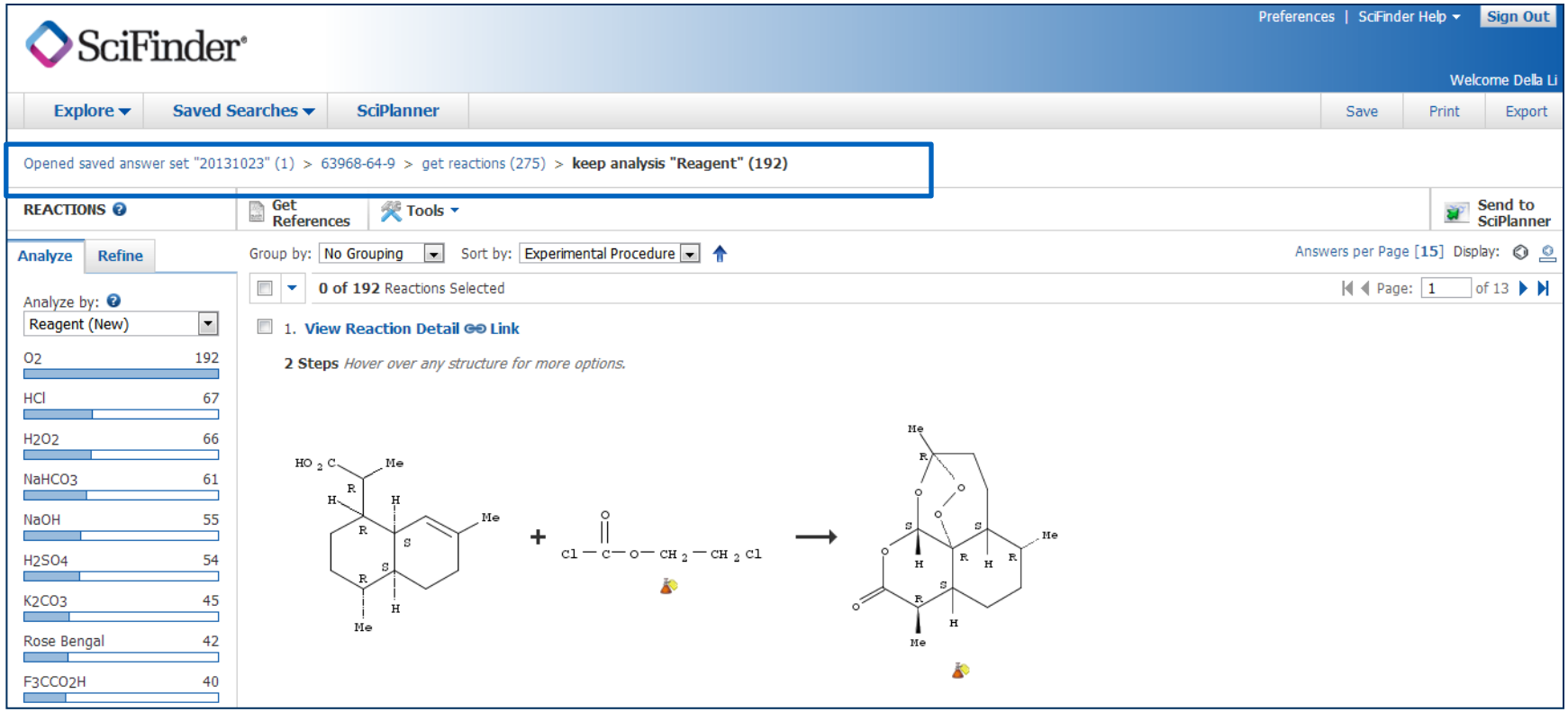
Step 1

Example 10: synthesis of (*3R*)-dihydroarteannuin B acid, 2-chloroethyl mixed carbonate 3.04 g (0.021 mol) of 2-chloroethyl chloroformate are added dropwise within 5 min. to a stirred solution of 5.01 g (0.021 mol) of DHAA and 4.04 g (0.029 mol) of K_2CO_3 in 25 mL of dichloromethane in an ice bath. After addition, stirring is continued for 20-30 min. The mixture is then washed twice with water (2 x 100 mL) and dried over $MgSO_4$. The solution is then concentrated to dryness at reduced pressure and 6.78 g of an oily residue are obtained (crude yield = 93.5 %). The product can be used as such.

Step 2

General/Typical Procedure: **Example 11: synthesis of artemisinin** An amount of 4 g of the dihydroartemisinic acid (DHAA) derivative of formula (I) or (Ia) prepared in examples 1 to 10 above (1 eq.), 0.01 eq. of tetraphenylporphyrin and 80 mL of methylene chloride are introduced at 20°C in a clean 0.2 liter reactor. The mixture is then cooled down to -10°C and air or oxygen is bubbled through the mixture (40-50 mL/min.) under stirring at 300-400 rpm. After 30 min., trifluoroacetic acid (TFA, 0.5 eq.) is added and a halogen lamp is switched on. The mixture is stirred overnight (~19h) at -10°C and then warmed up to 10°C (60 min.) and stirred at 10°C during 60 min. The mixture is then warmed up to 20°C in about 60 min. and then the air introduction is stopped, the lamp switched off and the mixture stirred at 20°C during 2h. Then, the reaction mixture is treated by addition of 20 mL of water then 20 mL of a solution of aqueous saturated $NaHCO_3$. The resulting mixture was then left for decantation and the two layers were separated. The organic layer is then loaded back in the vessel and washed again by addition of 20 mL of water then 20 mL of a solution of aqueous saturated $NaHCO_3$. After decantation and layers separation, the organic layer is washed with 20 ml of water. After decantation, the organic layer is then concentrated under progressive vacuum at 30°C using a rotary evaporator. The dry product crystallizes at room temperature. Then 12 mL of n-heptane are added and the mixture is stirred during 1 h at 20°C. The reaction mixture is then filtrated under Buchner funnel (n°3). The wet solid is then washed first with 8 mL and then with 12 mL of n-heptane. The wet solid is then dried under vacuum at 40°C overnight (~15h). Crude artemisinin is obtained with good titrated yield (62% ti/ti). If desired, an additional recrystallization step in an ethanol/water mixture (70/30) can be performed on the solid product precipitated in n-heptane. Product name: artemisinin Yield: 54.9%

导航条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Save
Print
Export
Opened saved answer set "20131023" (1) > 63968-64-9 > get reactions (275) > keep analysis "Reagent" (192)
REACTIONS
Get References
Tools
Send to SciPlanner
Analyze
Refine
Group by: No Grouping
Sort by: Experimental Procedure
Answers per Page [15] Display:
Analyze by:
Reagent (New)
O2 192
HCl 67
H2O2 66
NaHCO3 61
NaOH 55
H2SO4 54
K2CO3 45
Rose Bengal 42
F3CCO2H 40
0 of 192 Reactions Selected
Page: 1 of 13
1. View Reaction Detail Link
2 Steps Hover over any structure for more options.

提纲

- 介绍
  - SciFinder Web新界面
- **SciFinder Web中的检索**
  - SciFinder中的文献检索
  - SciFinder中的结构面板使用技巧
  - SciFinder中的物质结果及物质检索方法
  - SciFinder中的反应检索技巧
- **SciFinder Web的注册和常见问题**

SciFinder Web的注册和登陆

SciFinder Web的系统要求

Windows用户支持IE 7.x或者FireFox 2.x

Mac 用户支持 Firefox 和 Safari

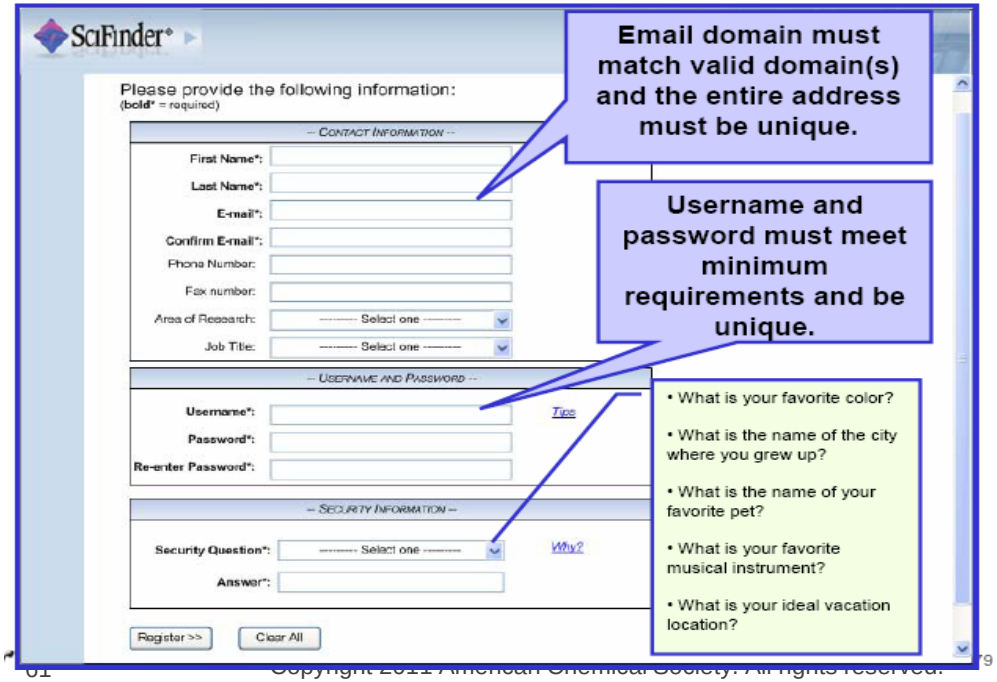
Java 安装（初次使用结构时自动安装，建议安装Java 6）

在图书馆相关页面上找到SciFinder Web注册用的网址

点击URL创建SciFinder Web账号

开始创建SciFinder Web帐号

创建ID所用的IP不能是代理服务器的IP



设置用户名及密码注意事项

用户名：

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

-（破折号）	_（下划线)
.（句点）	@（表示“at”的符号）

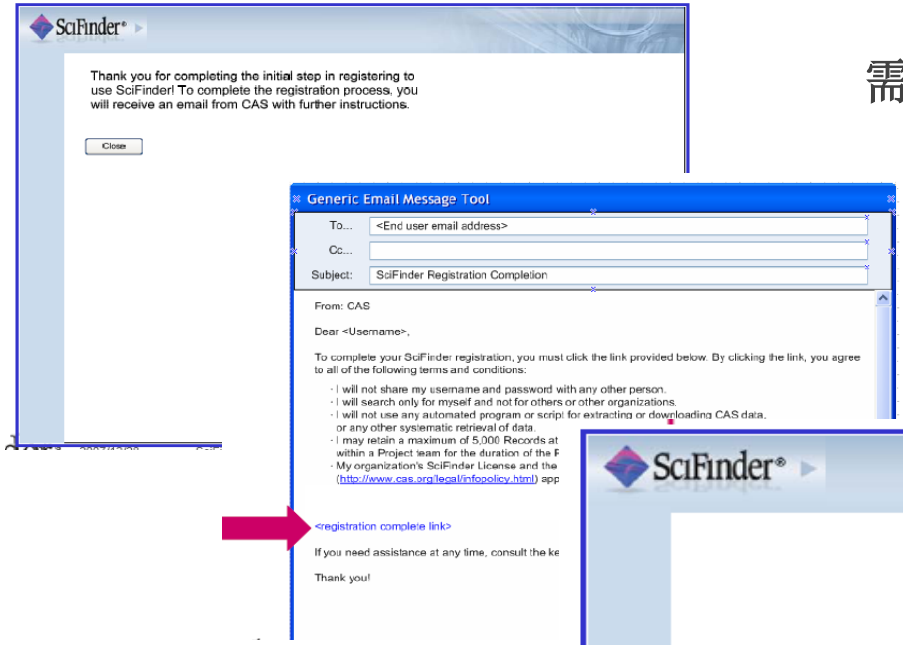
密码：

必须包含 7-15 个字符，并且至少包含三个以下字符：

字母	混合的大小写字母
数字	非字母数字的字符（例如 @、#、%、&、*）

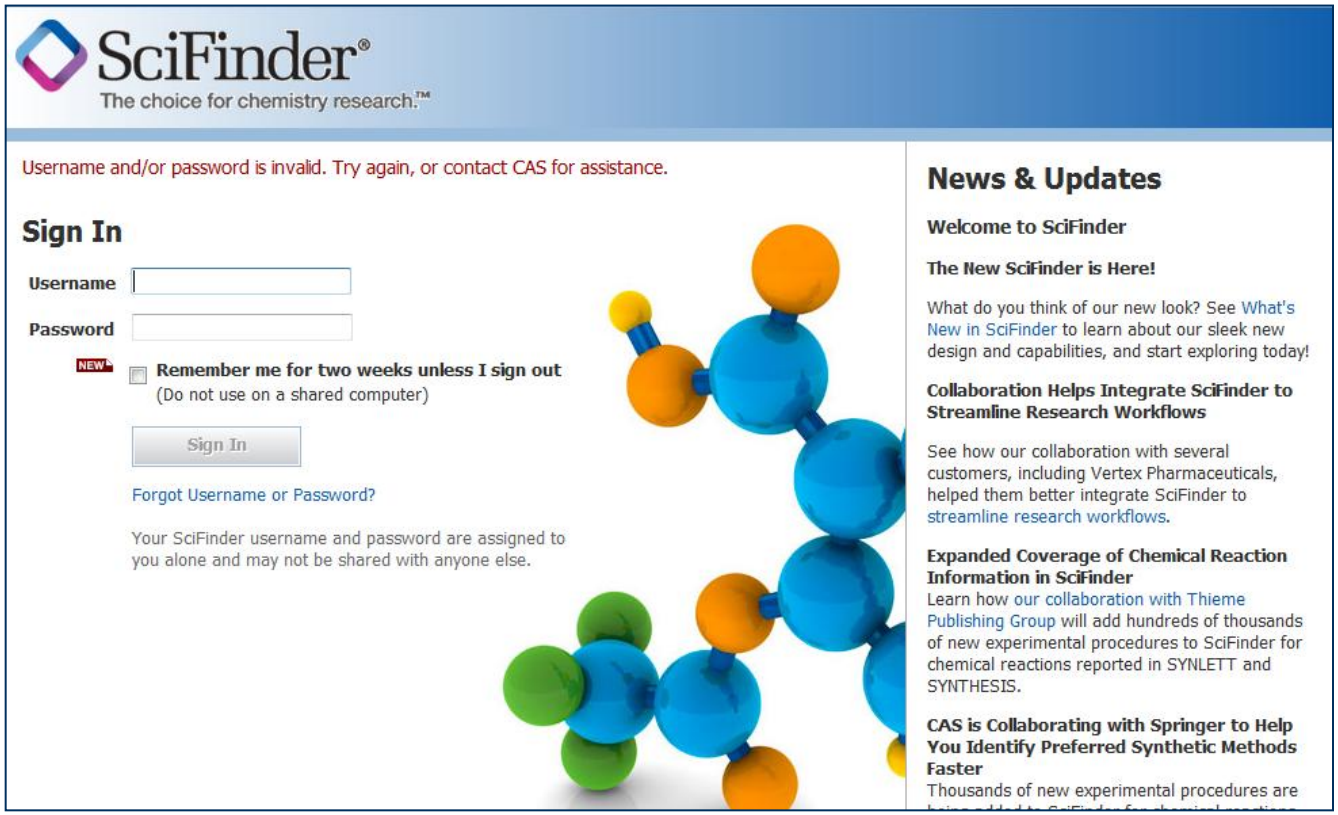
密码设置小技巧：
1：不要和账号中有重复的字符
2：密码格式最好是abc@123

对新ID的Email确认



需要点击邮件中的确认链接

SciFinder Web 常见问题



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

将页面截图下来，一并发给图书馆

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www.igroup.com.cn/cas

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Comprehensive Content

Sophisticated Analysis

Unprecedented Results

Thank You

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