SciFinder®

The choice for chemistry research.™

SciFinder Web使用介绍

刘盈盈

SciFinder客户顾问

2014.9

提纲

- 介绍
  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
- **SciFinder Web使用常见问题**

美国化学文摘社—Chemical Abstracts Service

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

SciFinder的覆盖内容

CAS REGISTRY℠
- >8300万有机无机物质
- >6400万生物序列
- >4亿条实验和预测数据
- 物质报道文献，回溯到1802年
- 每天更新

References from CAplus℠
- >3800万期刊，专利，学位论文记录.
- >1万种科技期刊的覆盖
- 63家专利发行机构的专利
- 1997年以来的3.65亿条引文记录
- 回溯到1800年
- 每天更新

References from MEDLINE®
- > 1900万条生命科学相关文献
- > 5600 期刊
- 回溯到1946年
- 每天更新

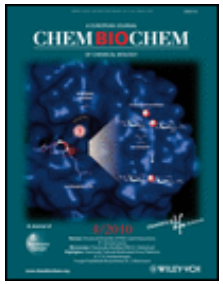
Markush Structures
- >100万专利中的Markush结构
- 回溯到1961年
- 每天更新

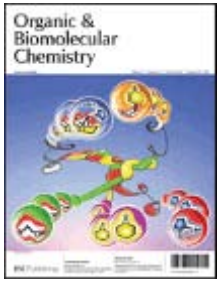
CASREACT®
- CAS提供的反应信息包含:
  - 反应中的结构信息
  - 反应中所有物质的CAS No
  - 详细的反应条件
  - 实验过程
- >5760万单步多不反应
- >1350万物质合成制备信息
- 反应回溯到 1840
- 反应条件起始于 2003
- 每天更新

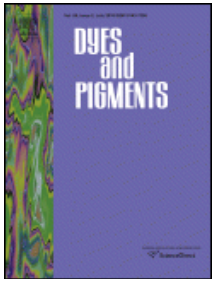
CHEMLIST®
- 全球范围内的法规信息
- >30.8万的化合物
- 1980至今的数据
- 每周更新

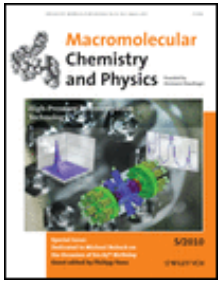
CHEMCATS®
- CHEMCATS 提供物质的供应商信息
- >7500万商业信息
- >2600万不同种类物质
- >880 个全球范围内的供应机构
- >1,005 商品目录的覆盖
- 每周更新

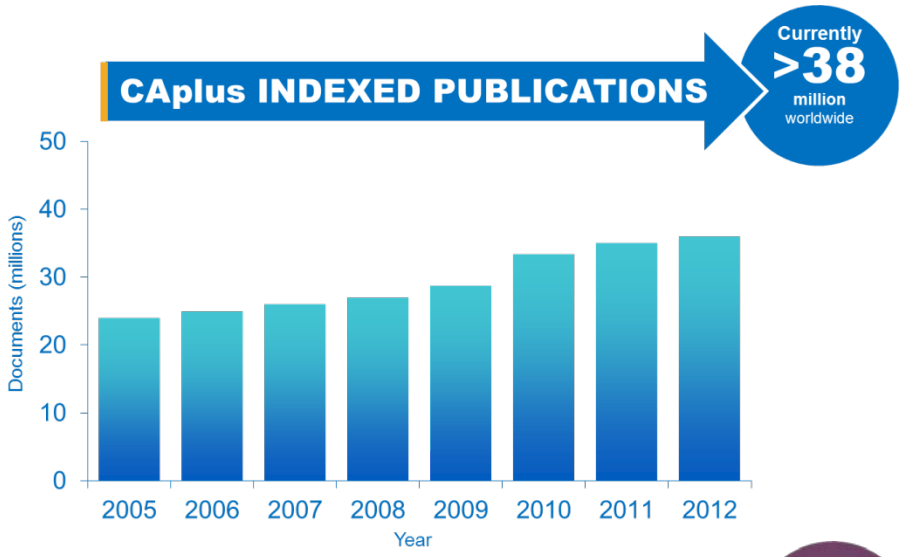
CAplus℠ 涵盖上万种期刊及63个专利发行机构专利

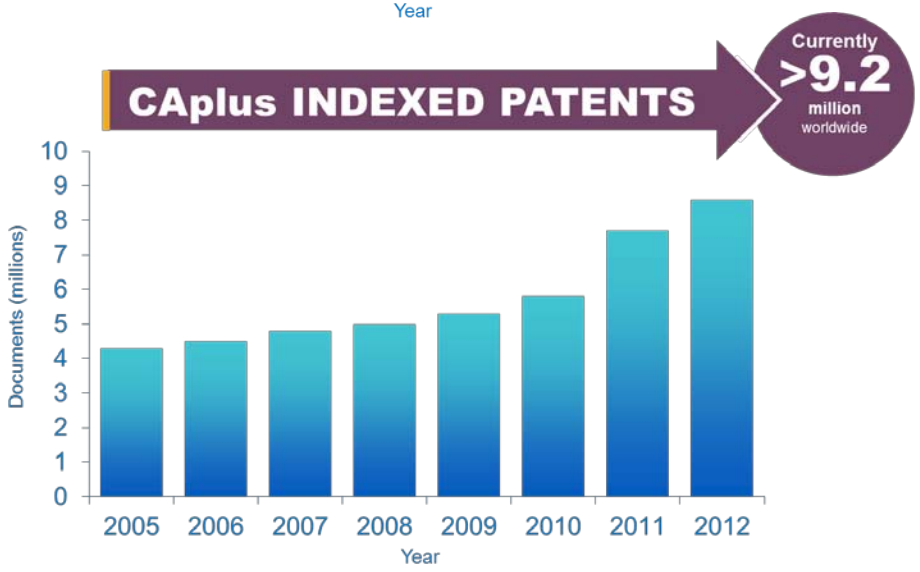




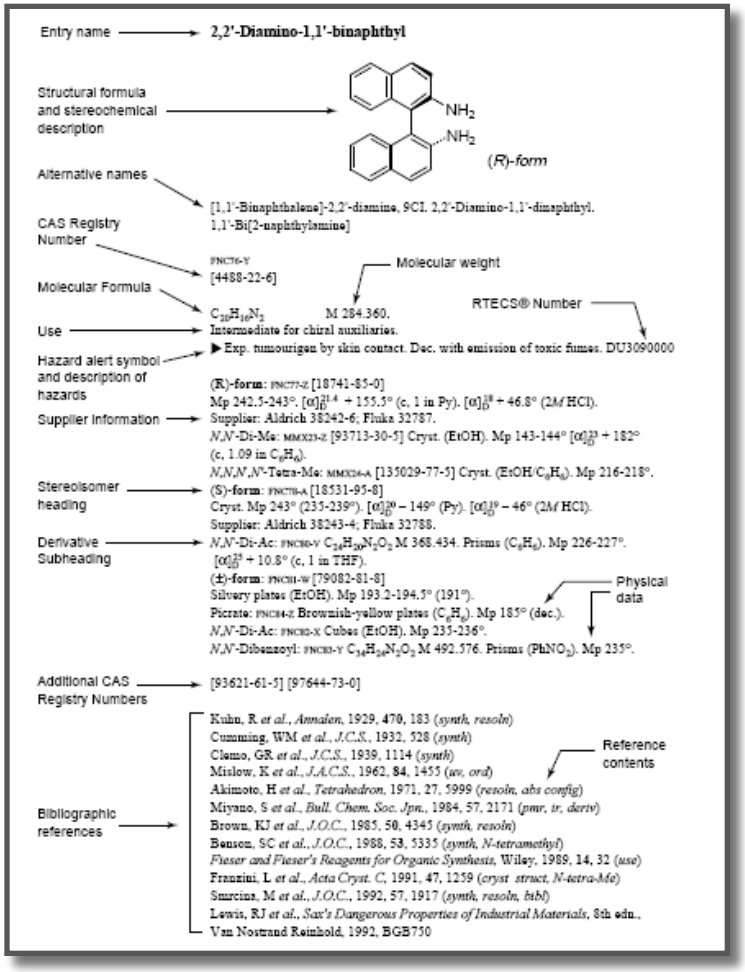


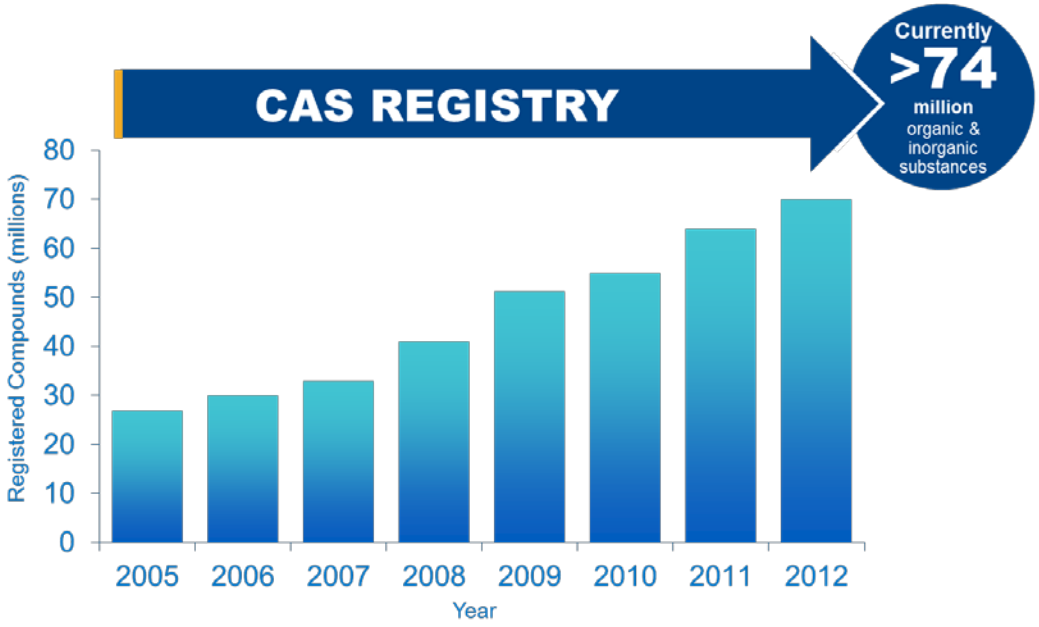




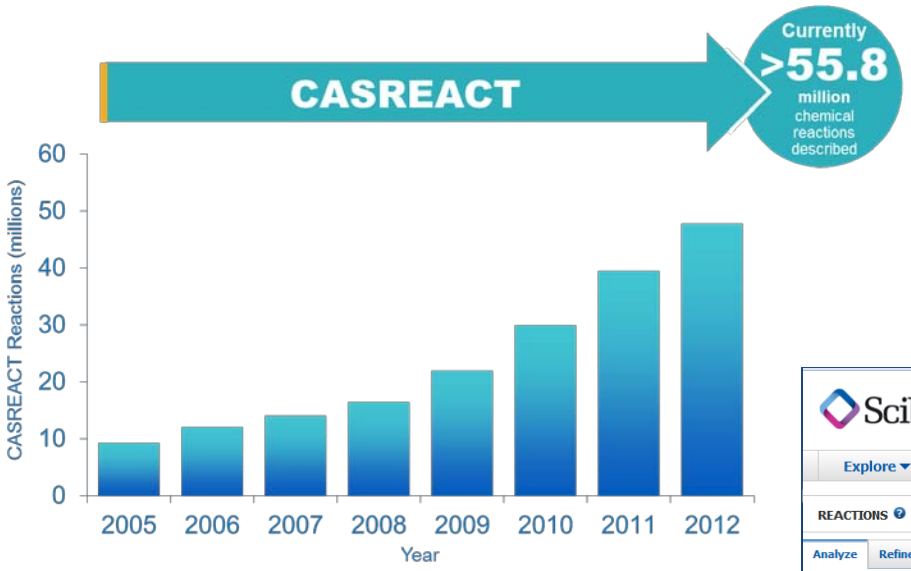


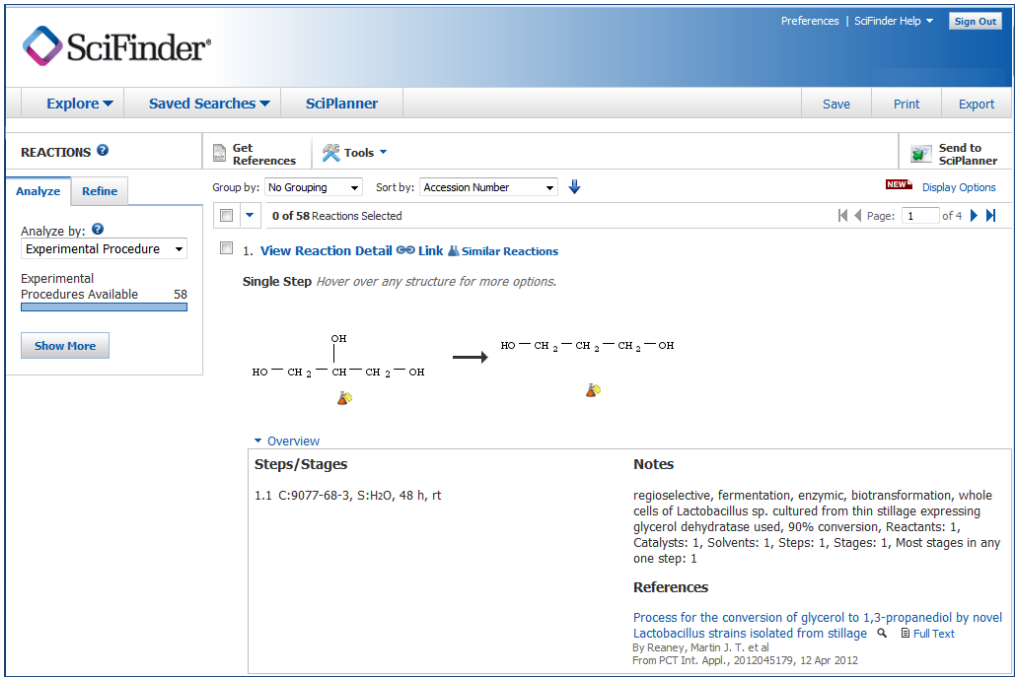
CAS REGISTRY℠ 是化学物质信息的“黄金标准”





CASREACT® 是检索化学反应最权威的来源





CASREACT是世界上最大的，更新速度最快的反应数据库

提纲

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  - SciFinder Web中的内容
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索方法
  - SciFinder Web中的反应记录及反应检索
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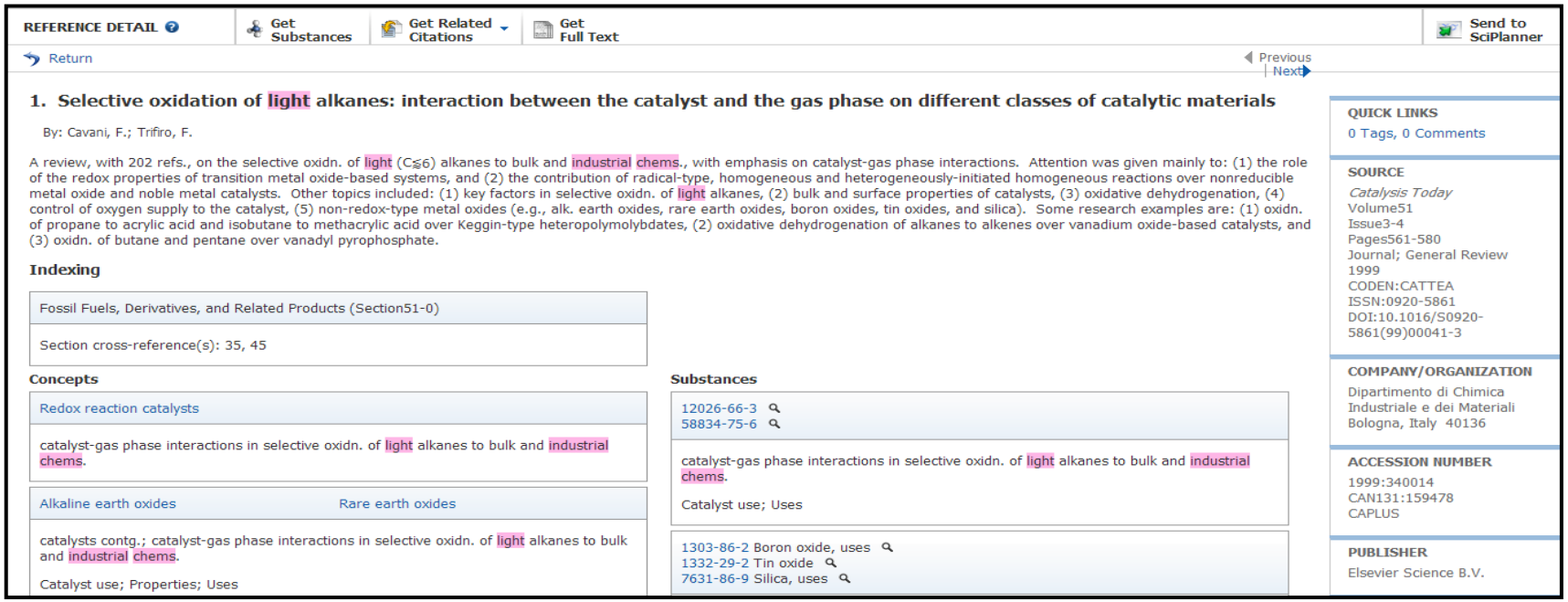
SciFinder中的文献记录



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

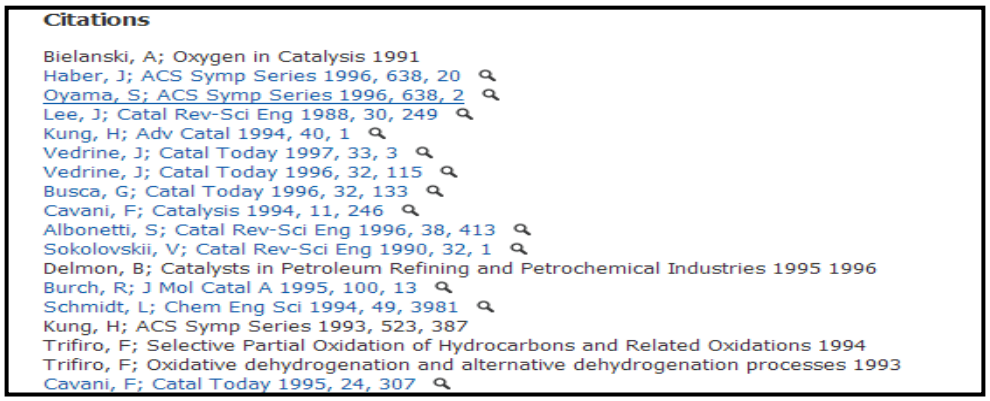
QUICK LINKS
0 Tags, 0 Comments

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

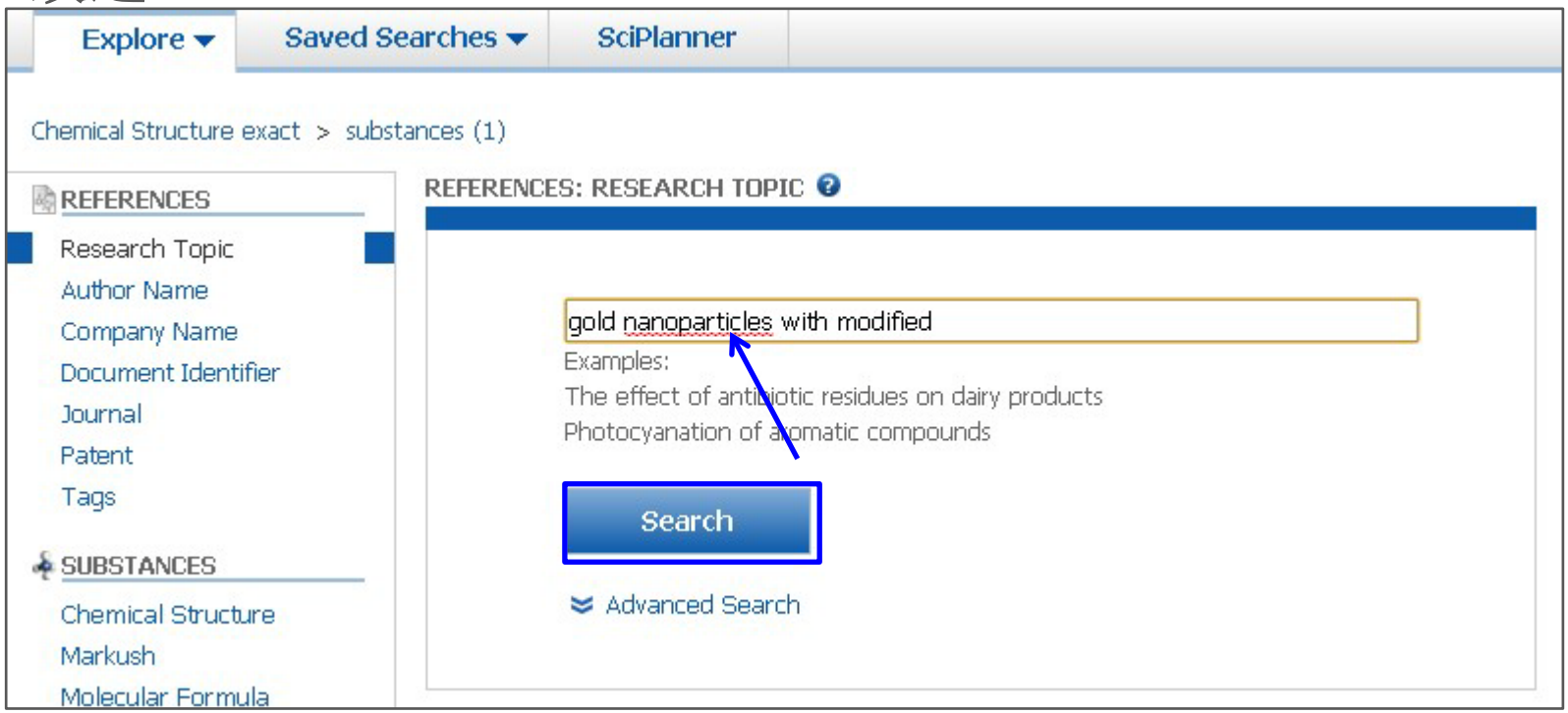
SciFinder中的文献检索方法

- **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

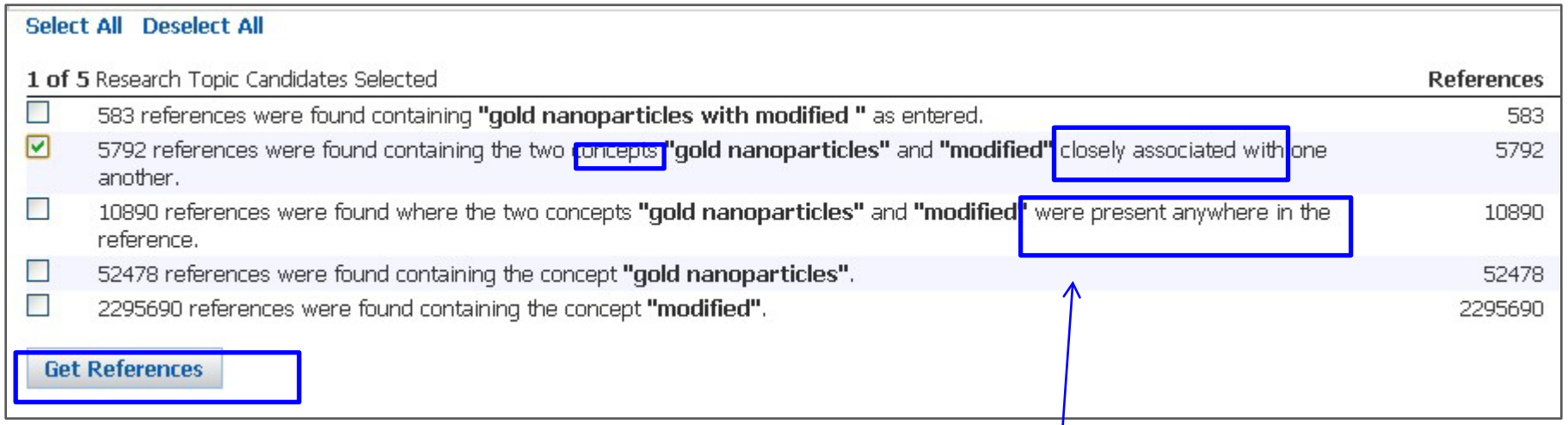
- **检索方法推荐**
  - 关注某特定领域的文献——-主题检索
  - 关注物质有关的文献————-先获得物质，再获得文献
  - 关注某科研人员的文献——-作者名检索

SciFinder Web中的主题检索

主题： gold nanoparticles with modified（金纳米颗粒的改进）



主题检索的候选项

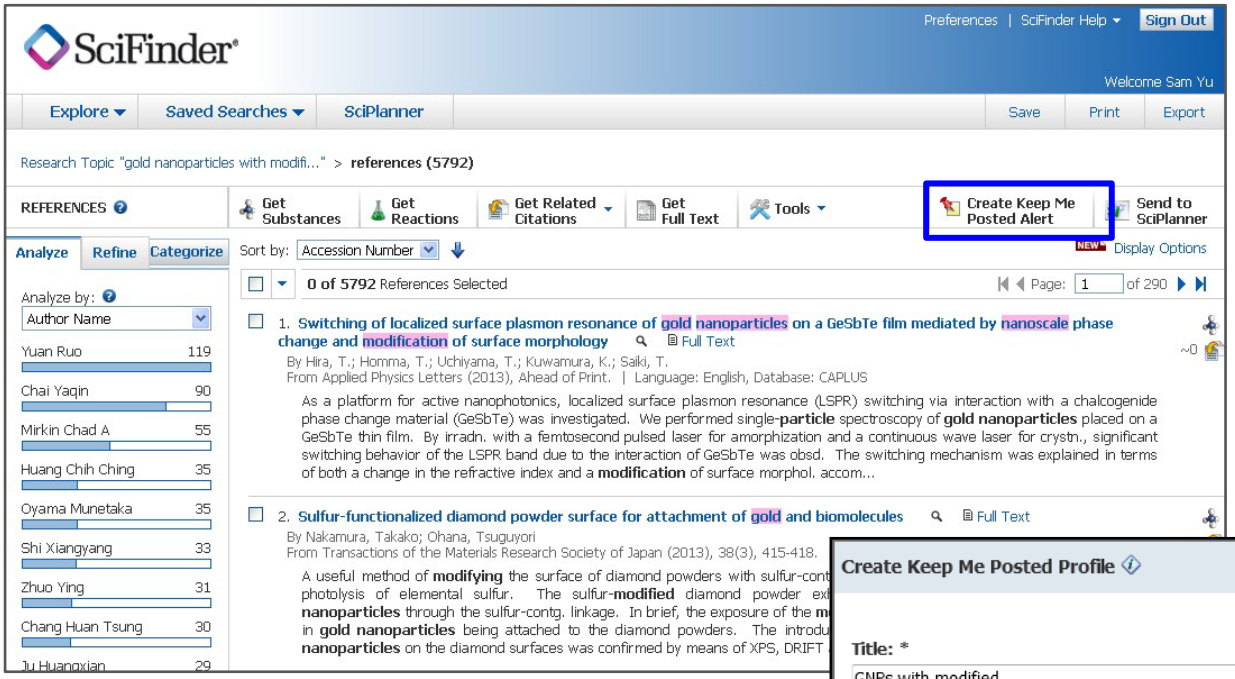


“Concept”表示做了同意词的扩展

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

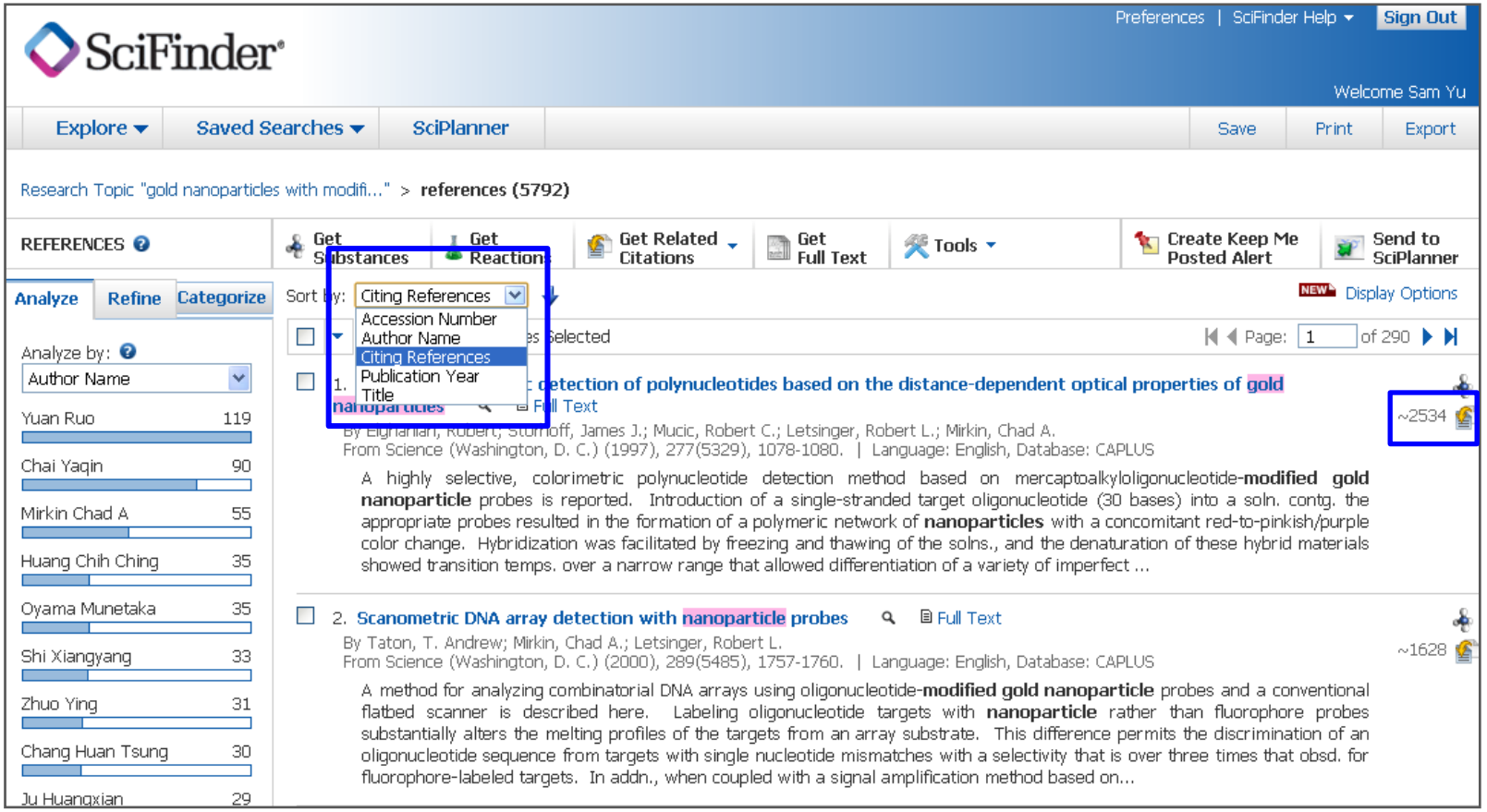
“present anywhere in the reference” 表示同时出现在一段话中

SciFinder中的KMP



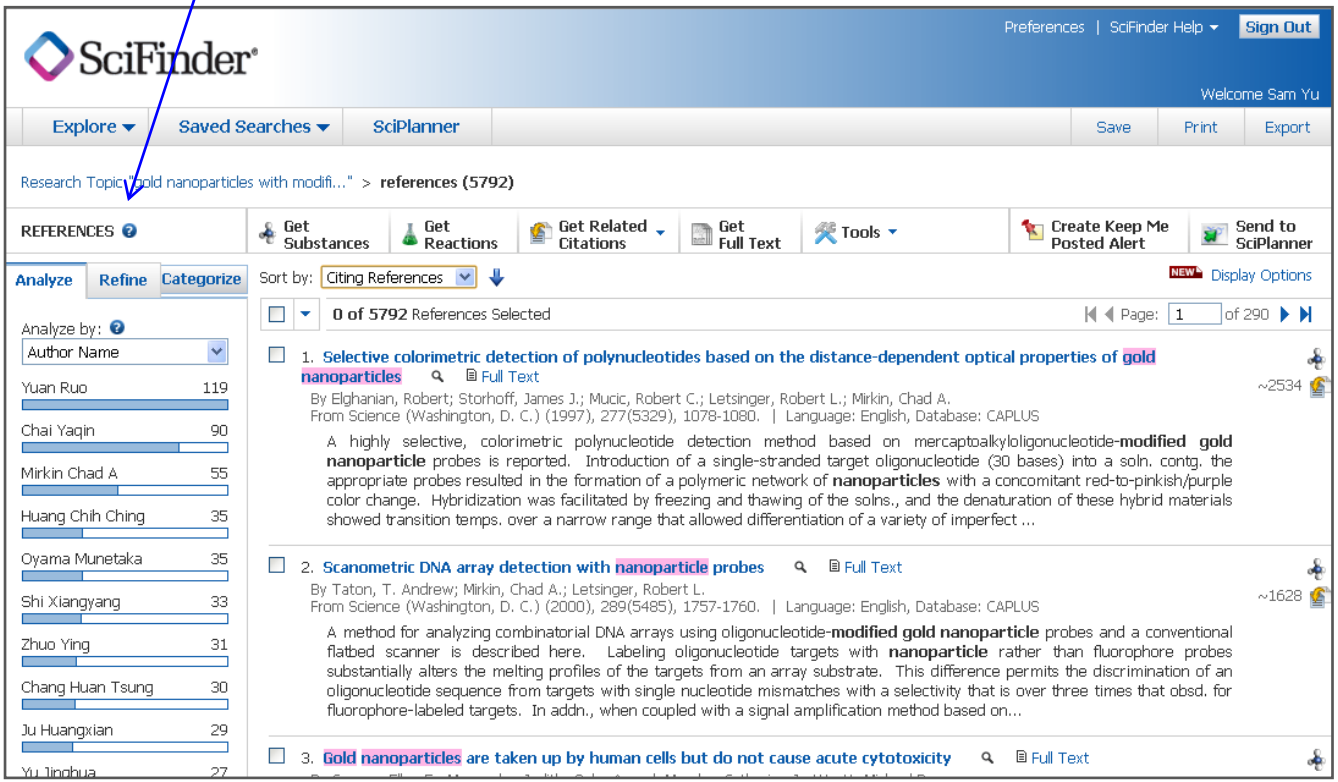
KMP是SciFinder提供的自动提醒功能，能及时将最新资讯，推送到用户的邮箱中

SciFinder提供的引文排序— Citing Reference



SciFinder 中的文献检索结果

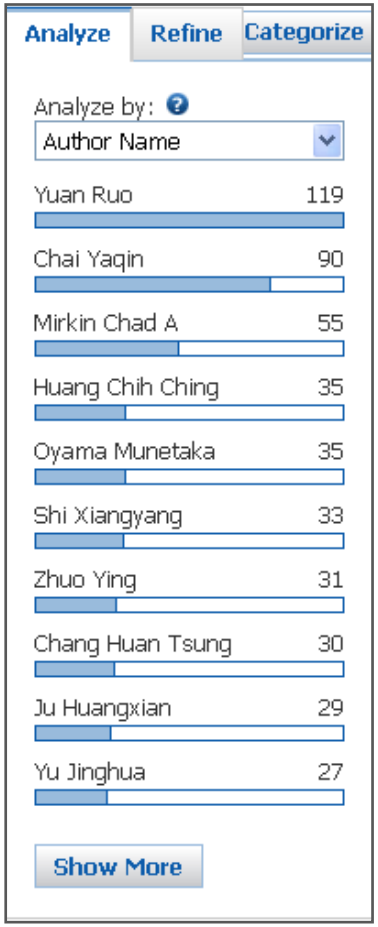
文献分析工具



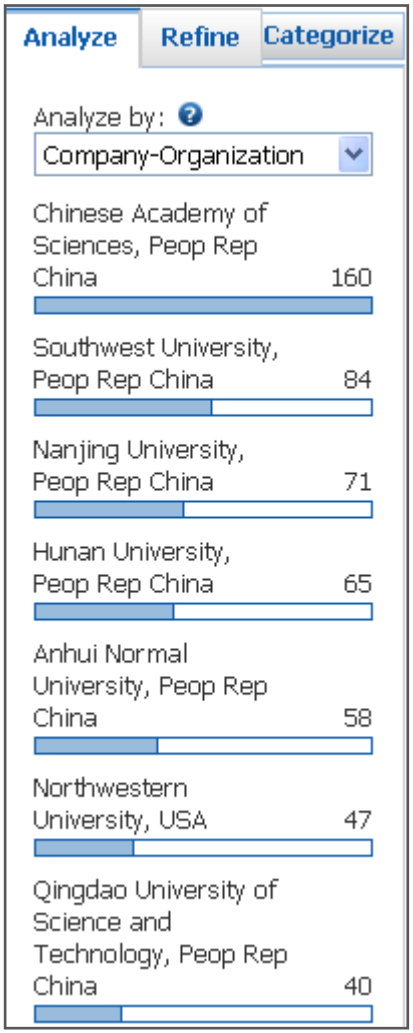
SciFinder提供强大的文献处理工具，帮助处理文献

SciFinder中的Analysis

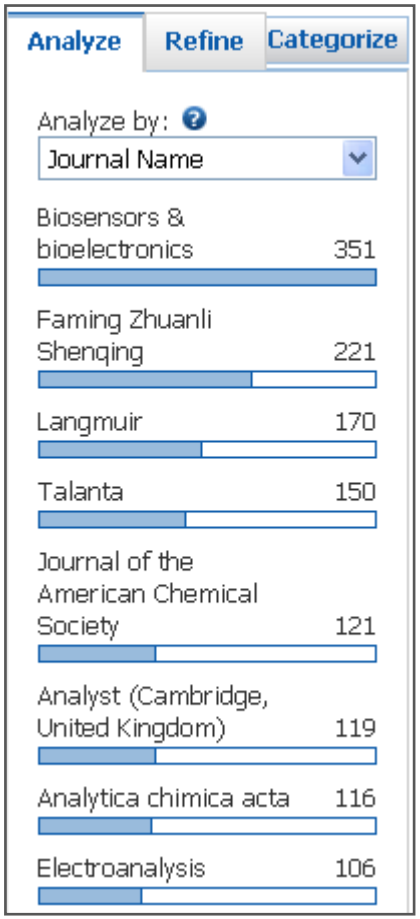
领域内主要研究人员，专家



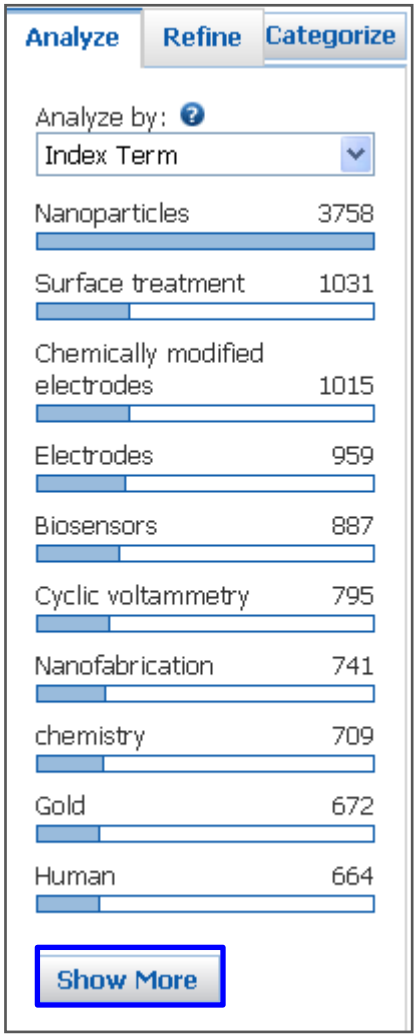
主要研究机构，合作伙伴，竞争对手



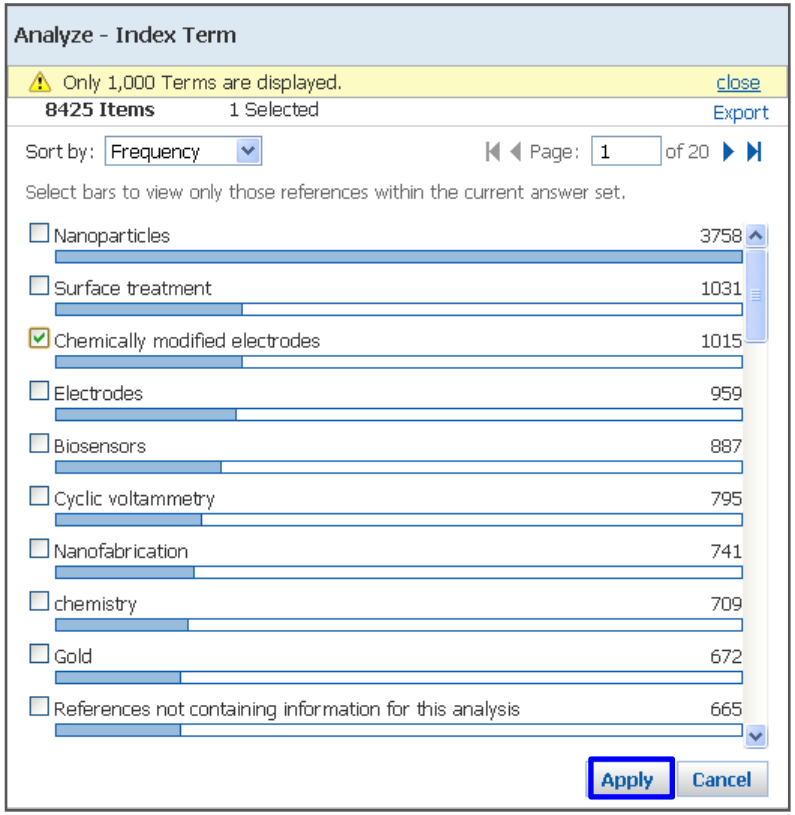
主要出版杂志，机构，潜在投稿期刊



SciFinder中的Analysis By Index Term



索引词（Index Term）：可以帮助我们对文献的内容进行大致的了解

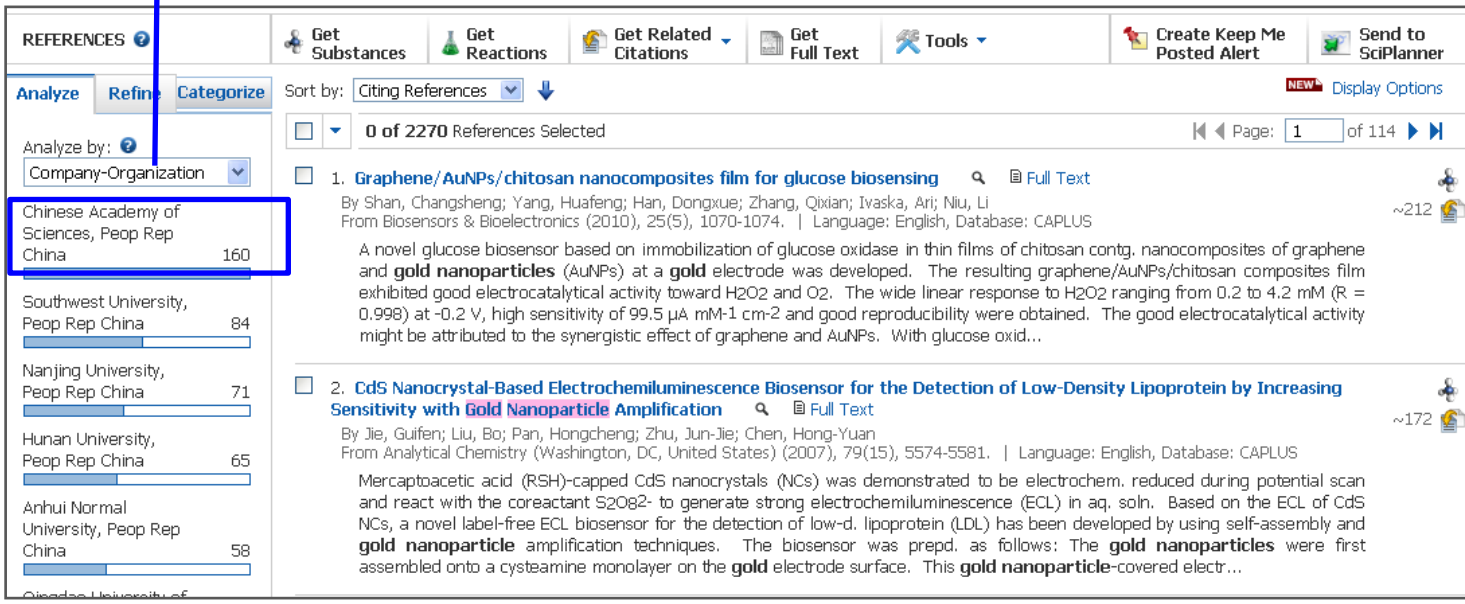


选择感兴趣的内容，点击Apply

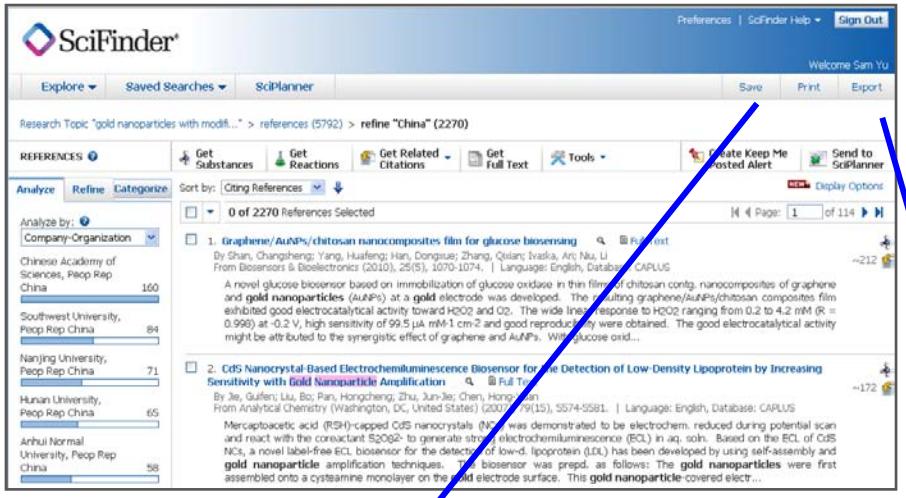
SciFinder中的Refine

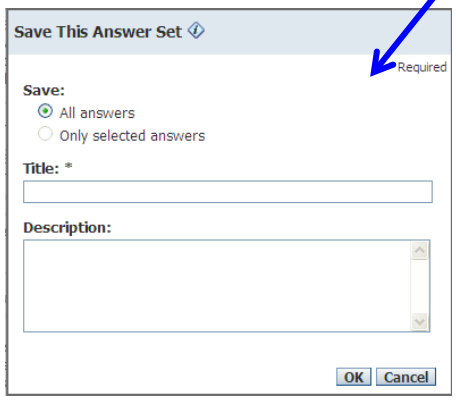
Refine ：帮助用户迅速获得需要的文献

中科院



结果集的保存

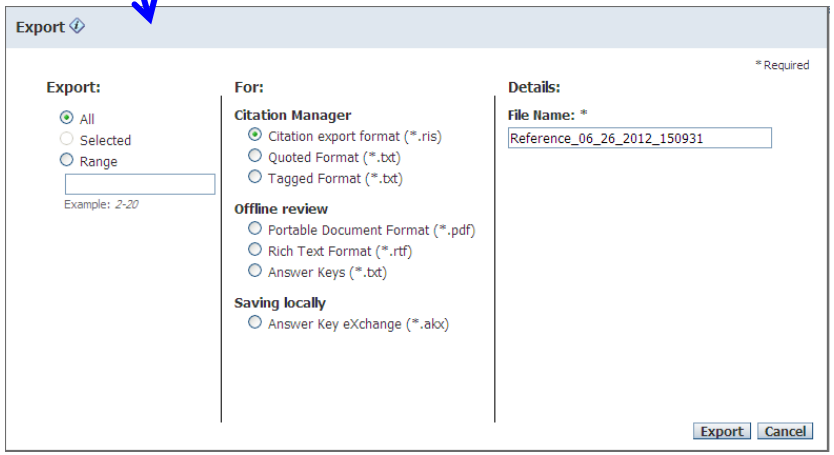




Save：
保存在服务器上，可登陆后查看

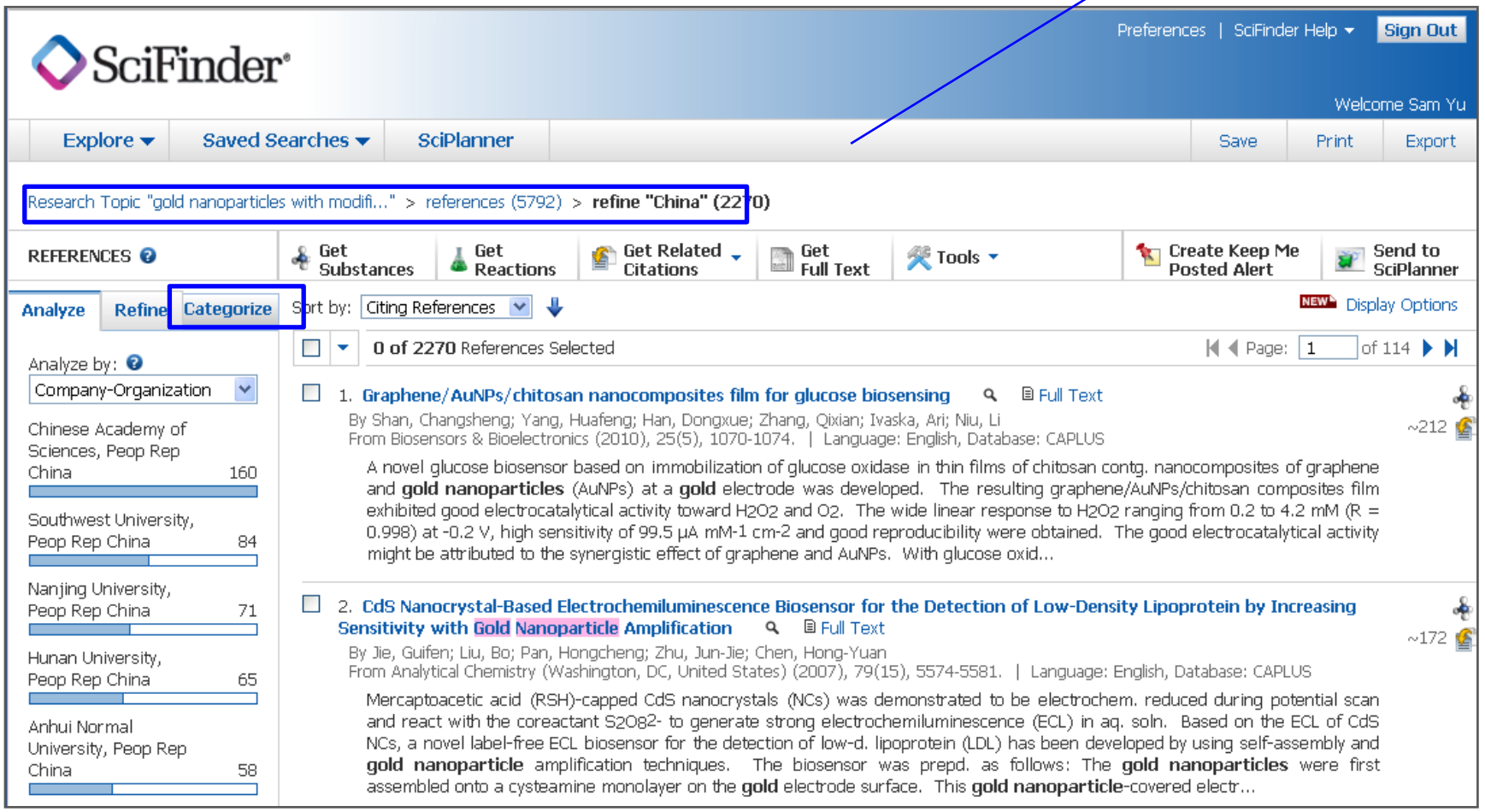
Export：
Citation manager: 保存成RIS格式，用于导入EndNote等文献管理工具

Offline Review:保存过成PDF，RTF格式，用于脱机浏览



SciFinder 中的Categorize

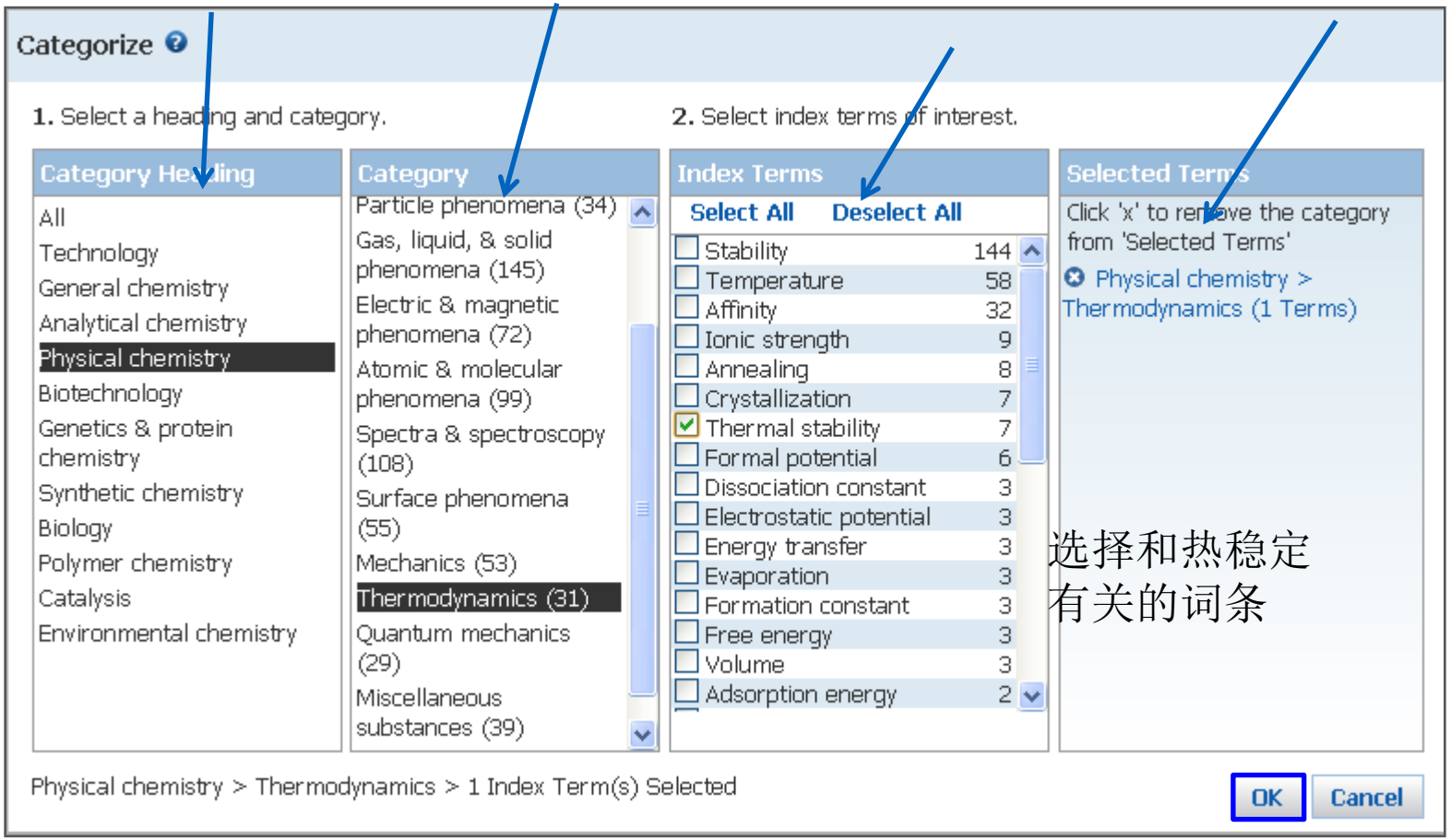
通过历史导航条回到任一检索界面



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

SciFinder中的Categorize

一级目录　　二级目录　　和二级目录相关的Index Term　　选中的Index Term



练习

- 检索和转基因食品安全评估的文献，获得近5年的综述文献

- 检索策略：
  - Topic Search：Genetically Modified Food with safety
  - Refine publish year: 2008-
  - Refine document type: Review

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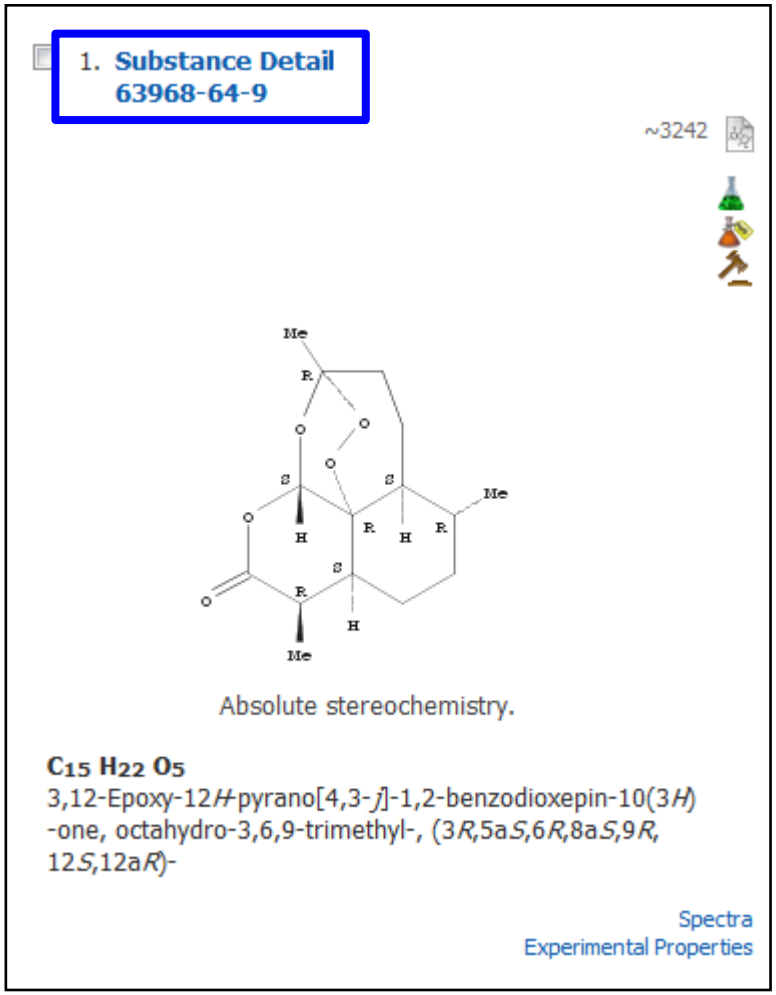
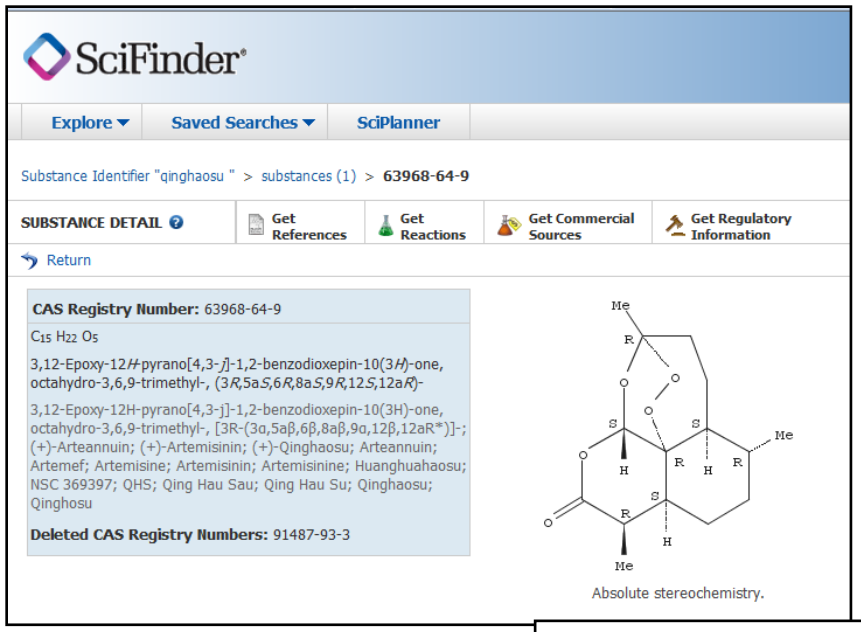
SciFinder中的物质结果界面



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

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。

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	✓	✓	✓	✓

Substance Detail—查看物质详细信息

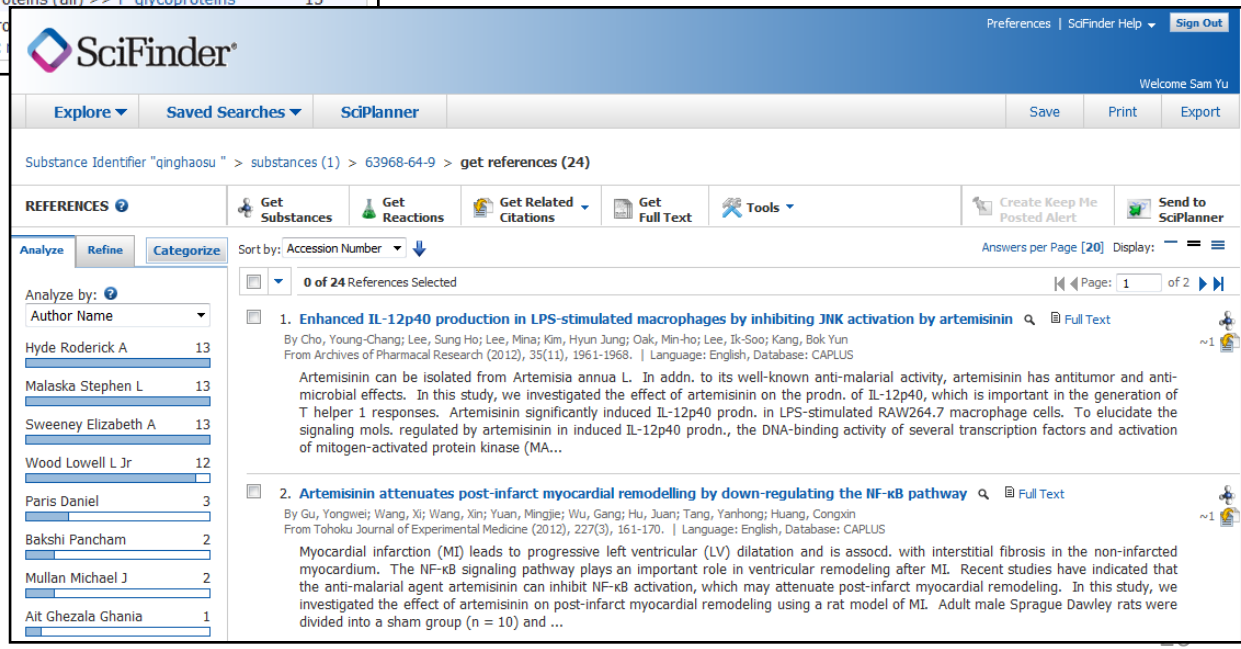
Bioactivity Indicators NEW

	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 …	

物质的生物活性和靶点信息，直接点击，获得相关文献



Substance Detail—查看物质详细信息

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

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	31.2	pH 1 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 2 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 3 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 4 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 5 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 6 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 7 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 8 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 9 Temp: 25 °C	(26)	
Bioconcentration Factor	31.2	pH 10 Temp: 25 °C	(26)	

Lipinski and Related Properties	Value	Condition	Note	Top
Freely Rotatable Bonds	0		(26)	
H Acceptors	5		(26)	
H Donors	0		(26)	
H Donor/Acceptor Sum	5		(26)	
logP	2.269±0.680	Temp: 25 °C	(26)	
Molecular Weight	282.33		(26)	

Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See spectrum		(27)	
Proton NMR Spectrum	See spectrum		(27)	

Substance Detail—查看物质详细信息

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

Biological Properties	Value	Condition	Note	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1)CAS	
Half-Life (Biological)	See full text	1 of 2	(9)CAS	
Median Lethal Dose(LD50)	5576 mg/kg	Organism: rat Route: oral	(14)APC	
Median Lethal Dose(LD50)	5105 mg/kg	Organism: mouse Route: oral	(14)APC	
Median Lethal Dose(LD50)	2800 mg/kg	Organism: mouse Route: intramuscular	(14)APC	
Median Lethal Dose(LD50)	2571 mg/kg	Organism: rat Route: intramuscular	(14)APC	
Median Lethal Dose(LD50)	1558 mg/kg	Organism: mouse Route: intraperitoneal	(14)APC	
Minimum Inhibitory Concentration	See full text	1 of 2	(18)CAS	

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

Optical and Scattering Properties	Value	Condition	Note	Top
Optical Rotatory Power	+87.9 °	Solv: 1,4-dioxane (123-91-1); Wavlen: 589.3 nm	(20)CAS	
Optical Rotatory Power	+75-+78 °	Conc: 1.0 g/100mL; Solv: ethanol (64-17-5); Wavlen: 589.3 nm; Temp: 20 °C	(12)CAS	
Optical Rotatory Power	+68.2 °	Conc: 0.97 g/100mL; Solv: chloroform (67-66-3); Temp: 25 °C	(16)IC	

Substance Detail—查看物质详细信息

Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See full text	1 of 8	(3)CAS	
Circular Dichroism Spectrum	See full text	1 of 2	(4)IC	
IR Absorption Spectrum	See full text	1 of 11	(11)CAS	
Mass Spectrum	See spectrum		(13)WSS	
Mass Spectrum	See spectrum		(13)WSS	
Mass Spectrum	See full text	1 of 10	(1)CAS	
Proton NMR Spectrum	See full text	1 of 10	(15)CAS	
Raman Spectrum	See full text	1 of 2	(5)CAS	
Two-Dimensional NMR Spectrum	See full text	1 of 2	(24)CAS	
UV and Visible Absorption Spectrum	See full text		(22)CAS	
UV and Visible Emission/Luminescence Spectrum	See full text		(25)CAS	

物质的实验谱图