





SciFinder Scholar 使用简介

—, SciFinder® ScholarTM Content

SciFinder Scholar 收集由 CAS 出版的数据库的内容以及 MEDLINE[®]数据库(by the National Library of Medicine ,NLM),所有的记录都为英文(但如果 MEDLINE 没有英文标题的则以出版的文字显示)。

数据库	内容		
Reference Databases (文献数据库)			
<u>CAplus</u> SM	包含来自 150 多个国家、9000 多种期刊的文献,覆盖 1907 年到现在的所有文献以及部分 1907 年以前的文献,包括有期刊、专利、会议录、论文、技术报告、书等,涵盖化学、生化、化学工程以及相关学科,还有尚未完全编目收录的最新文献。(目前 > 2,430 万条参考书目记录,每天更新 3000 条以上)		
MEDLINE®	包含来自 70 多个国家、3900 多种期刊的生物医学文献,覆盖 1951 到现在的所有文献,以及尚未完全编目收录的最新文献。(目前 > 1300 万参考书目记录,每周更新 4 次)		
Structure Database (结构数据库)			
REGISTRY	涵盖从 1957 年到现在的特定的化学物质 ,包括有机化合物、生物序列、配位化合物、聚合物、合金、片状无机物。REGISTRY 包括了在 CA SM 中引用的物质以及特定的注册。例如:管制化学品列表如 TSCA 和EINECS 中的注册。(目前 > 7400 万条物质记录 ,每天更新约 7 万条 ,每种化学物质有唯一对应的 CAS 注册号)		
Reaction Date	tabase (反应数据库)		
CASREACT®	包括从 1907 年到现在的单步或多步反应信息。CASREACT 中的反应包括 CAS 编目的反应以及下列来源 ZIC/VINITI 数据库(1974—1991, by InfoChem GmbH), INPI(Institut National de la Propriete Insutrielle, 法国)1986 年以前的数据,以及由教授 Klaus Kieslich 博士指导编辑的生物转化数据库。(目前 > 800 万条反应记录和 403,000 条文献记录,每周更新约 700-1300 条)		
Commercial	Sources Database(商业来源数据库)		
CHEMCATS ®	化学品的来源信息,包括化学品目录手册以及图书馆等内的供应商的地址、价格等信息。(目前 > 740 万条商业化学物质记录,来自 655 家供应商的 793 种目录)		
Regulatory L	Regulatory Database (管制数据库)		
CHEMLIST ®	1979 年到现在的管制化学品的信息,包括物质的特征、详细目录、来源以及许可信息等。(>22.8 万种化合物的详细清单,来自 13 个国家和国际性组织,每周更新>50 条新记录)		





□, What You Can Find with SciFinder Scholar

通过 SciFinder Scholar 您可以得到以下信息:

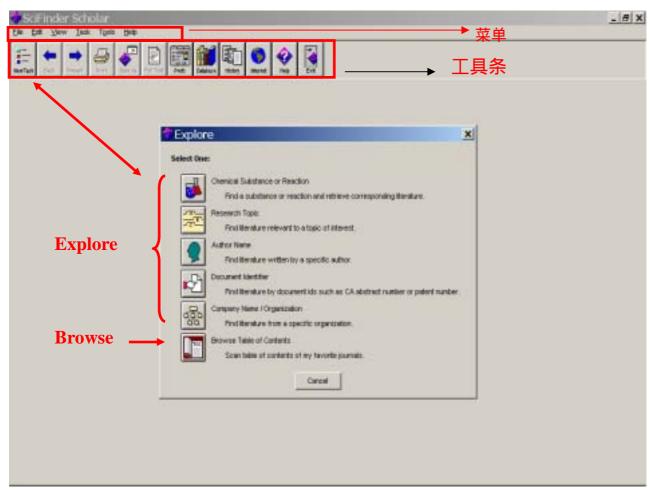
Area	Information Available in SciFinder Scholar
Document	• Title
Information	Author/inventor
	 Company name/corporate source/patent assignee
(文献信息)	Publication year
	 Source, publication, date, publisher, volume, issue, pagination, CODEN, ISSN
	 Patent identification, including patent, application, priority, and
	patent family information
	Abstract of the article or patent
	Indexing
	Supplementary terms
	• Citations
	Substances, sequences, and reactions discussed within the document
Substance	Chemical name
Information	CAS Registry Number®
	Molecular formula
(物质信息)	Structure diagram
	 Sequence information, including GenBank[®] and patent annotations Property data
	Commercial source information from chemical supplier catalogs
	Regulatory information
	Editor notes
	 Documents in which the substance is referenced
	 Reactions in which the substance participates
	A list of other databases available from STN, for related information
Reaction	Reaction diagrams, including reactants, products, reagents, catalysts,
Information	solvents, and step notes
, <u></u>	Citation hyperlinked to the reference record
(反应信息)	Additional reactions, references, substance details, commercial
	sources, and regulatory information for all reaction participantsNotes

注意:检索结果可以打印、保存,但如要保存需注意文件名和文件所在的文件 夹(包括上层目录)名都必须是英文,否则可能会出现无法保存,试用期内也 不能保存。





三、SciFinder® Scholar™ 使用的简单介绍:



主要分为 Explore 和 Browse:

3.1, Explore

Explore Tool 可获取化学相关的所有信息及结构等,有如下方式:(如上图所示)

- <u>Chemical Substance or Reaction</u> Retrieve the corresponding literature
 - ✓ By chemical structure
 - ✓ By substance identifier
 - ✓ By molecular formula
- Research Topic to find literature relevant to a topic of interest.
- Author Name to locate literature written by a specific author.
- <u>Document Identifier</u> to find literature for a specific CA Accession Number or Patent Number.
- <u>Company Name / Organization</u> to locate literature for a specific company, university, governmental agency, or other organization.

3.2, Browse Journal Table of Contents

可直接浏览 1800 多核心期刊的摘要及其引文等编目内容,如果带有 型 则可直接点击,就会通过 ChemPort[®] Connection. SM 获取全文 (in-house)





3.3 工具条按钮简述:

Toolbar Button		Function
New Task	——————————————————————————————————————	开始一个新任务;
Back	Back	显示上一屏;
Forward	Forward	显示下一屏;
Print	Print	依据打印设定进行打印;
Save As	Seve As	按不同格式进行保存; Example: Rich Text Format
Full Text	Full Text	通过 <u>ChemPort</u> [®] <u>Connection</u> SM 索取全文;
Prefs	Prefs	打开 Preference Editor, 个性化设置使用 SciFinder Scholar;
Database	Database	打开 Preference Editor 中的 Databases 栏 对执行任务时需要检索的数据库进行选择;
History	History	显示您当前进程所执行过的操作;
Internet	Internet	显示 <u>SciFinder Scholar</u> 的网上资源;
Help	Help	帮助;
Exit	Exit	退出;

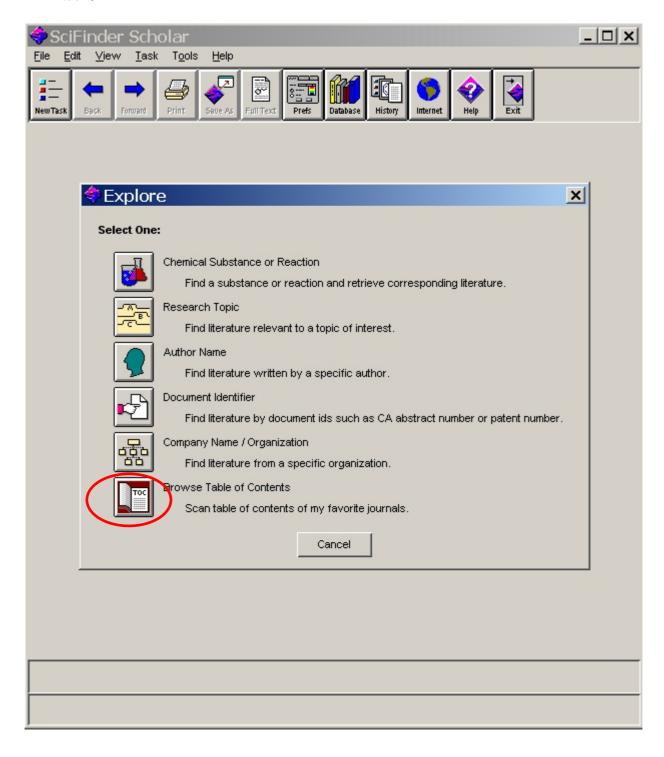




四、Browse Journal Table of Contents

示例:查看 Journal of the American Chemical Society 的目录并链接全文;

4.1 点击 Browse Table of Contents.

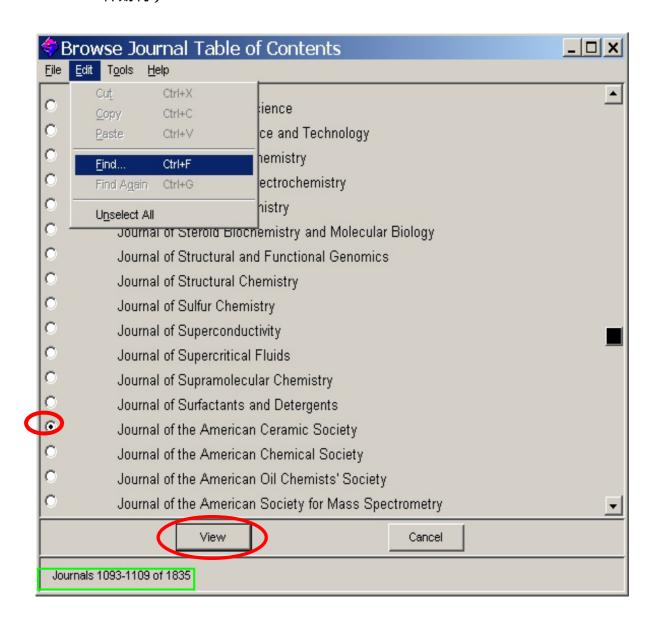






4.2 选择您想查阅的期刊,点击 View;

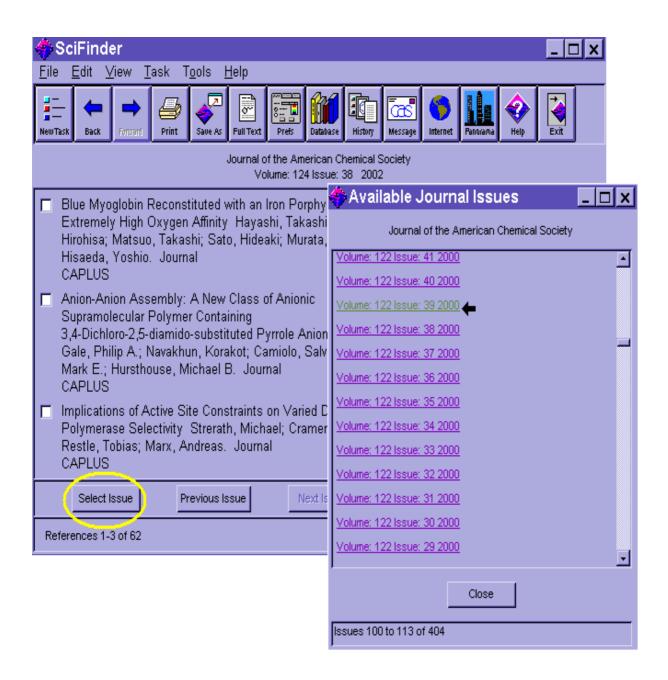
(也可通过 Edit 菜单 Find, 查找所需期刊,注意名称必须完全匹配,一次只能查看一种期刊)







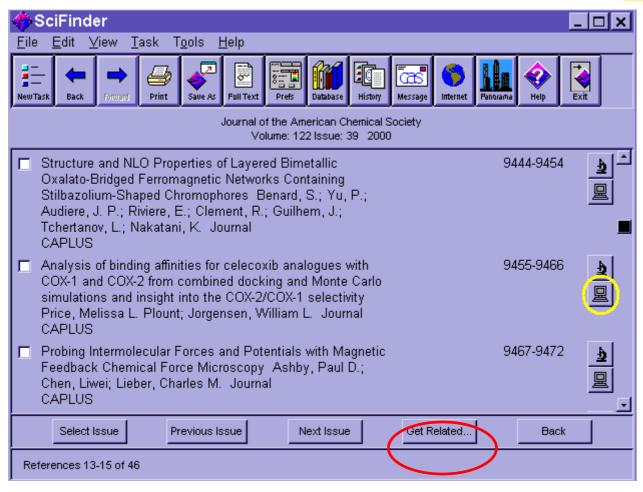
4.3 默认结果显示的是最新一期的目录, Previouse、Next、Select 可以浏览其他期的目录内容;

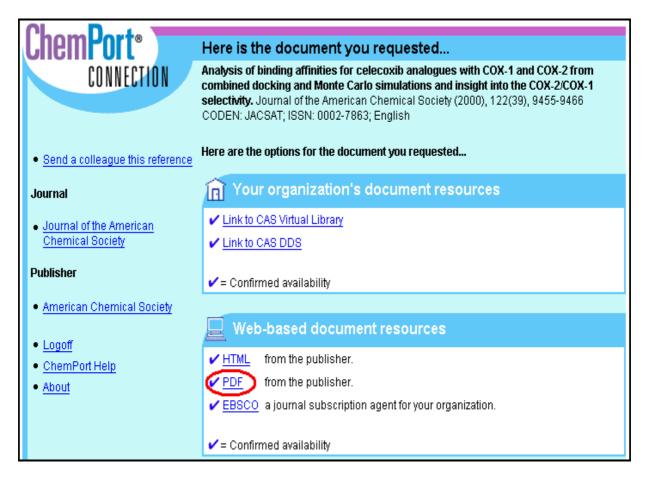


4.4 如果有电脑图标,点击就可以启动 ChemPort® ConnectionSM 获取全文:













The full text is displayed. (如果是已经订阅或开放的电子文献,就可以直接查看全文,当然也有可能出现要求付费才能查看的页面)

J. Am. Chem. Soc. 2000, 122, 9455-9466

9455

Analysis of Binding Affinities for Celecoxib Analogues with COX-1 and COX-2 from Combined Docking and Monte Carlo Simulations and Insight into the COX-2/COX-1 Selectivity

Melissa L. Plount Price and William L. Jorgensen*

Contribution from the Department of Chemistry, Yale University, New Haven, Connecticut 06520-8107 Received March 22, 2000. Revised Manuscript Received July 21, 2000

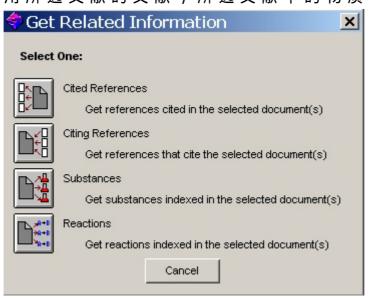
Abstract: The origins of binding affinity and COX-2/COX-1 selectivity for analogues of celecoxib have been explored using an approach that combines docking with Monte Carlo (MC) simulations. These inhibitors are COX-2-selective nonsteroidal antiinflammatory drugs (NSAIDs) that are of current interest because the gastrointestinal irritation they cause is reduced compared to that caused by traditional NSAIDs. We report a novel docking method, based on a combined Tabu and Monte Carlo protocol, that determines starting conformations for MC simulations. Using the docking-predicted starting conformations, relative changes in binding free energies were computed for methyl, ethyl, hydroxymethyl, hydroxyl, thiomethyl, methoxy, trifluoromethyl, chloro, fluoro, and unsubstituted derivatives with the MC free energy perturbation (FEP) method. The computed free energies are in good accord with IC50 values, and the structural information from the simulations can be used to explain the experimentally observed binding trends. In addition, the docking and FEP results have provided clarification of the binding conformation of the phenylsulfonamide moiety and the origin of COX-2/COX-1 selectivity. Namely, the COX-2 Val \rightarrow COX-1 lle subtitution is accompanied by an unfavorable conformational shift of the phenylsulfonamide ring.

Introduction

Nonsteroidal antiinflammatory drugs (NSAIDs) inhibit prostaglandin synthesis by blocking the cyclooxygenation of arachiRecently, a second generation of NSAIDs has been developed for the treatment of rheumatoid arthritis and osteoarthritis. These drugs selectively inhibit the COX-2 isozyme and differ clinically from traditional NSAIDs by having a reduced incidence of

4.5 Get Related 功能

可以查看关联信息;选中某一文献或整期查找;(分别有:所选文献引用的文献,引用 所 选 文 献 的 文 献 , 所 选 文 献 中 的 物 质 , 所 选 文 献 中 的 反 应



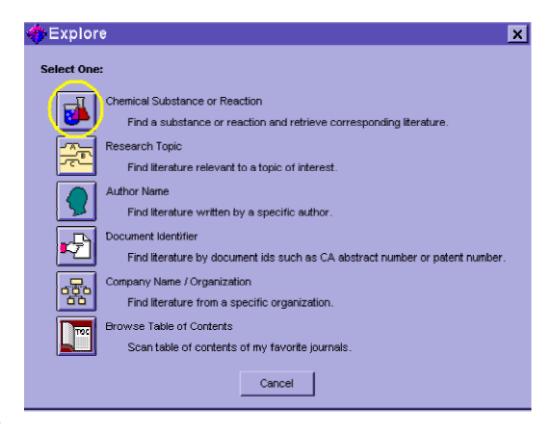




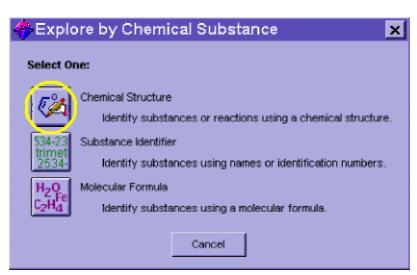
五、Explore

5.1 Explore by Chemical Substance or Reaction:

点击 Chemical Substance Or Reaction 开始,见下图:



弹出:

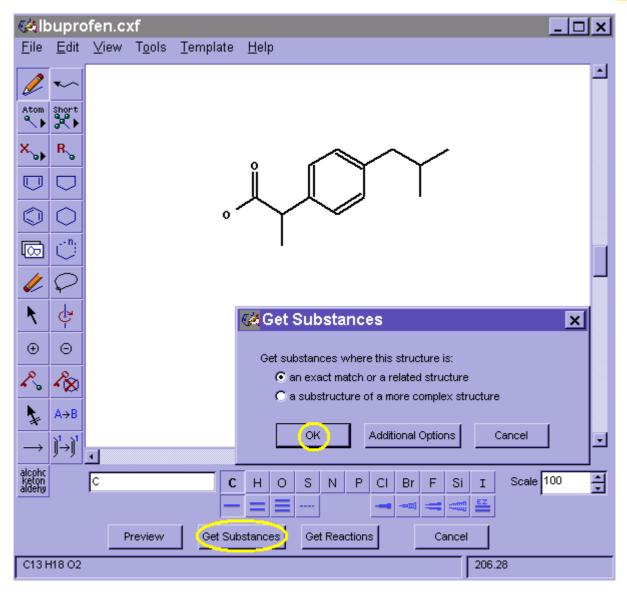


5.1.1 Explore by Chemical Structure,如上图

则进入 Scholar 的结构绘制窗口,画出 Ibuprofen 的结构;点击 Get Substances, 弹出窗口,再点击 OK 即可,







Additional Options 可以进一步提出检索条件;

进入检索结果界面:

图中的图标说明:

References for the substance (物质的引文)

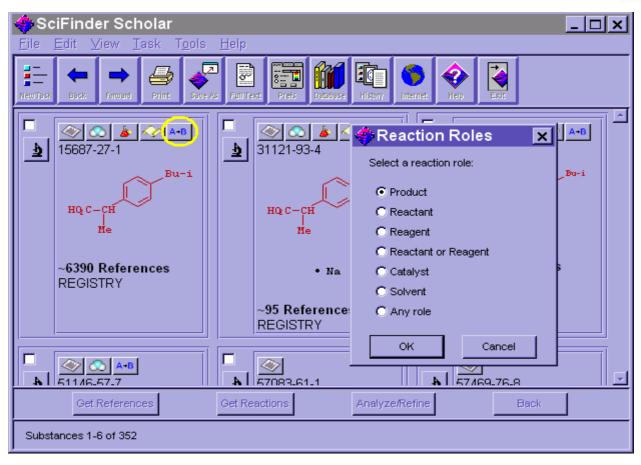
上 Commercial source information (商业来源信息)

Regulated chemicals listing (管制化学品列表)

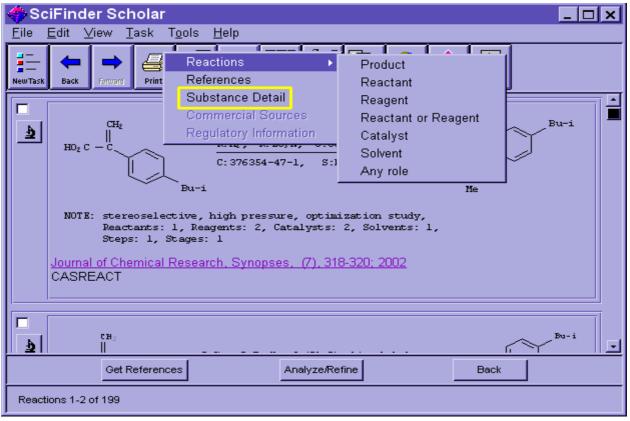
A-B Reactions that involve the substance (获取反应)







点击 A B 图标,弹出窗口,选择该物质在反应中的位置,如选择 Product,则将 Ibuprofen作为产物的反应都检索出来。

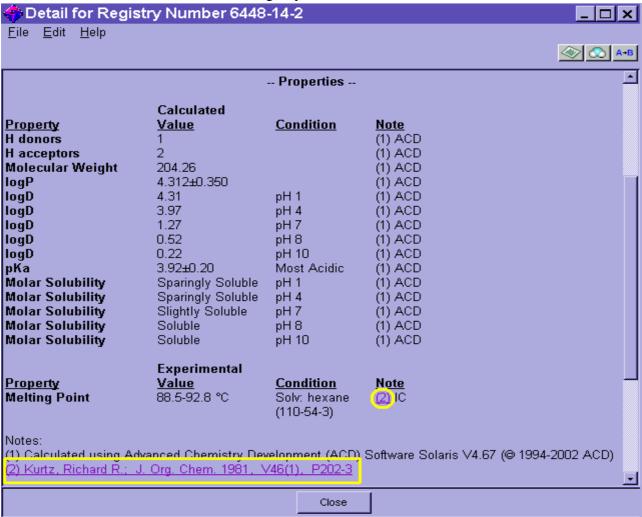


Get References 可以获取相关文献, Analyze/Refine 可以对结果进行分析或二次检索;

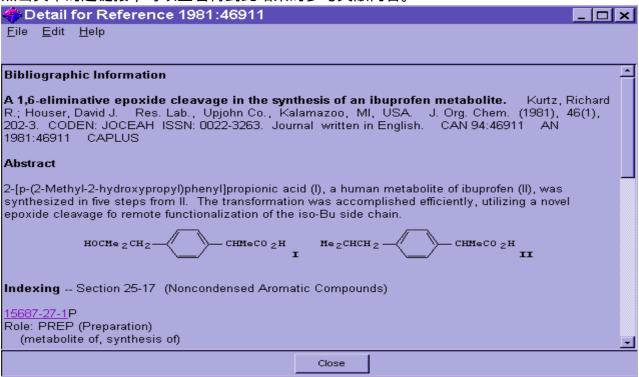




也可以点击反应式中的任何物质获取更多信息,如果点击 Reactions,则弹出选项,这里我们选择了 Substance Detail,提供 CAS Registry 记录,



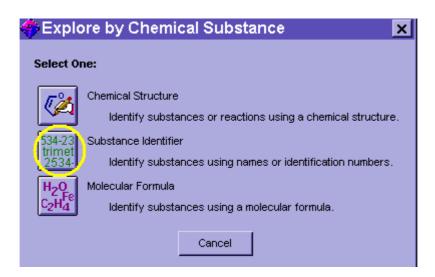
点击其中的超链接,可以查看得到此结果的参考文献内容。



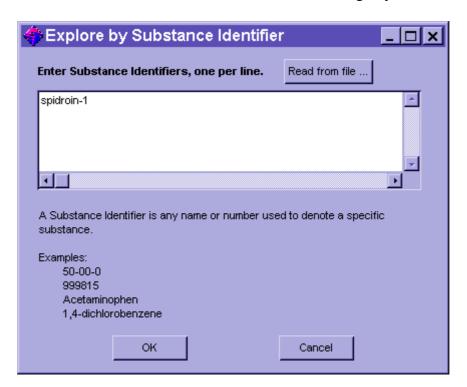




5.1.2 Explore by Substance Identifier,如下:



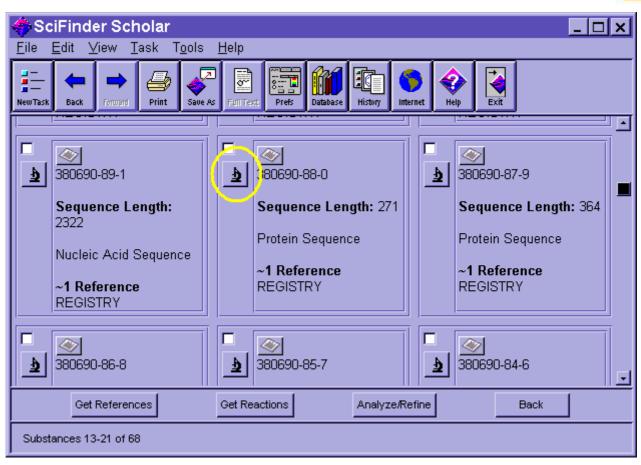
输入感兴趣的物质的名称,每行一个,也可输入 CAS Registry,再点击 OK:

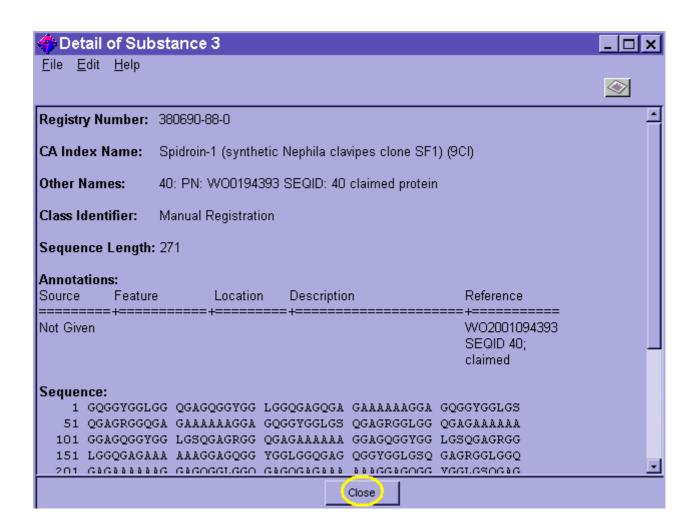


则搜索出相关的蛋白质或核酸序列 —— 每个都有各自的 CAS Registry Number,点击显微镜图标,可以查看每个物质的详细信息;





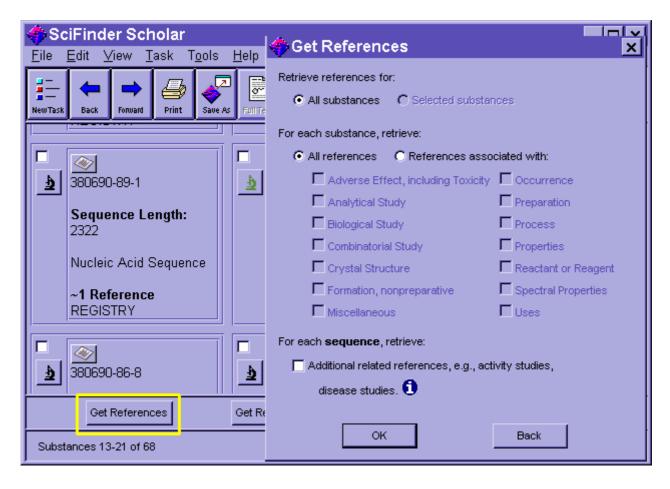


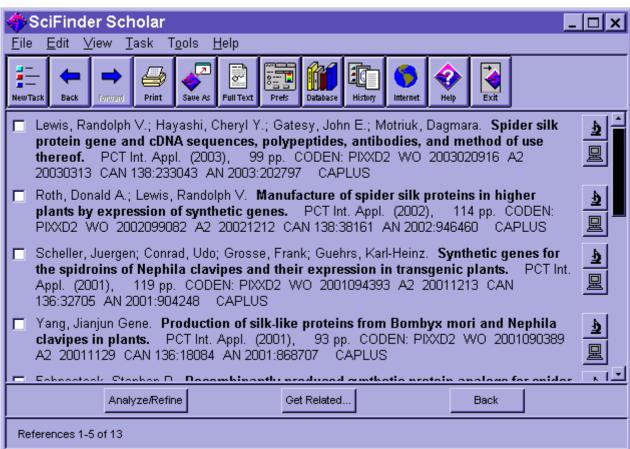






点击 Get References.可以查看与该物质相关的文献,也可选择该物质在该文献中的地位;

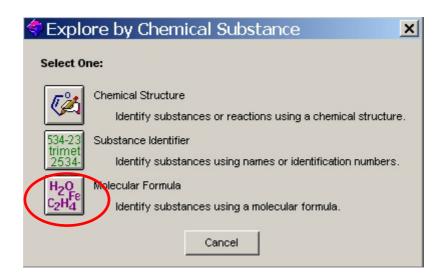


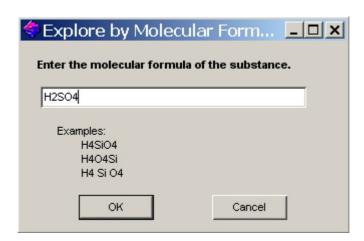






5.1.3 Explore by Molecular Formula





通过分子式进行检索: SciFinder Scholar 会分析您所输入的分子式,并重新编排原子,使之成为能被计算机识别的 Hill System Order,搜索 CAS Registry 数据库,并显示匹配结果;

如果输入的原子是模糊的,则弹出窗口提示修改,如元素符号的上标、下表,元素符号之间以空格隔开等(多数情况下会自动修正);如果是多组分的物质如聚合物,盐类等,则各个组分之间以英文的句号.隔开。如 Component1.Component2

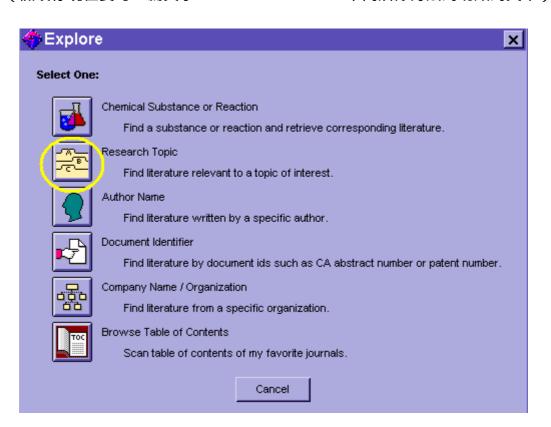


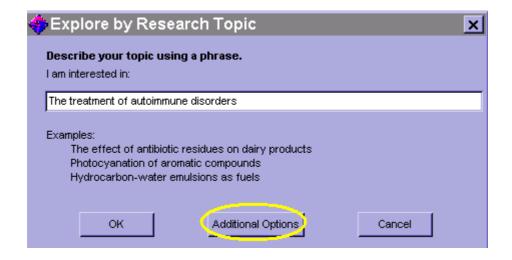


5.2 Explore by Research Topic

通过研究主题来检索;

(假设你现在要写一篇关于 autoimmune disorders 不同治疗方法的功效的文章)









Explore by Rese	arch Topic - Addit	tional Options 🔀			
Describe your topic using a phrase. I am interested in:					
The treatment of autoimmu	ine disorders				
Examples: The effect of antibiotic residues on dairy products Photocyanation of aromatic compounds Hydrocarbon-water emulsions as fuels You may limit your search by any of the following:					
Limit by Publication Yea	r	_			
☑ Limit by Document Type					
☐ Biography	☐ Dissertation	☐ Patent			
☐ Book	☐ Editorial	☐ Preprint			
Clinical Trial	☐ Historical	 Report			
Commentary	✓ Journal	Review			
Conference	Letter				
Limit by Language					
Limit by Author					
☐ Limit by Company Name					
		V			
ОК	Remove Options	Cancel			

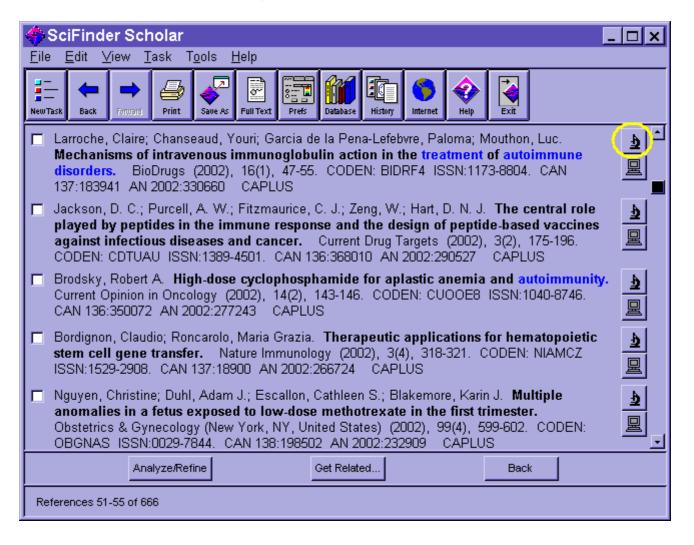
按上述方法输入后,点击 OK:

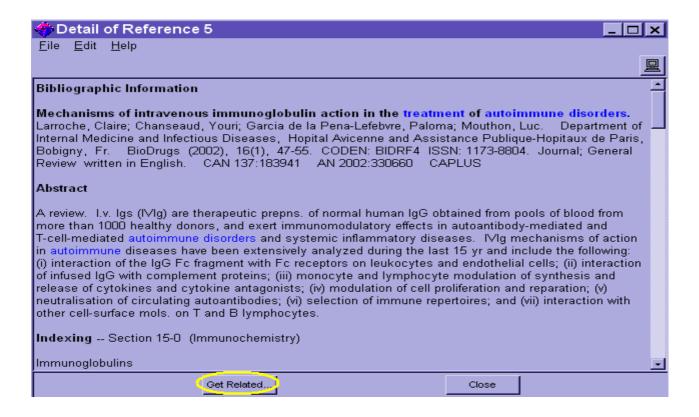
Topic Candidates	_ 🗆 ×			
<u>File Edit Task Tools Help</u>				
Select Candidates of interest (limited by Document Type):				
91 references were found containing "The treatment of autoimmune	_			
disorders" as entered.				
☑ 666 references were found containing the two concepts "treatment" and				
"autoimmune disorders" closely associated with one another.				
2234 references were found where the two concepts "treatment" and				
"autoimmune disorders" were present anywhere in the reference.				
3898540 references were found containing the concept "treatment".				
7697 references were found containing the concept "autoimmune				
disorders".				
Get References Back				
Candidates 1-5 of 5				





再选中您最感兴趣的内容,获取文献:

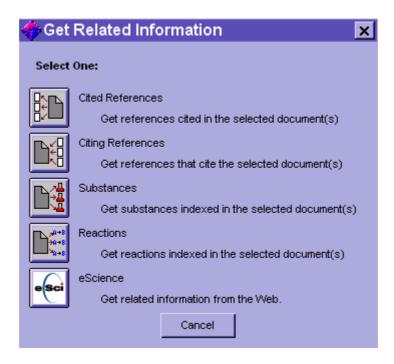




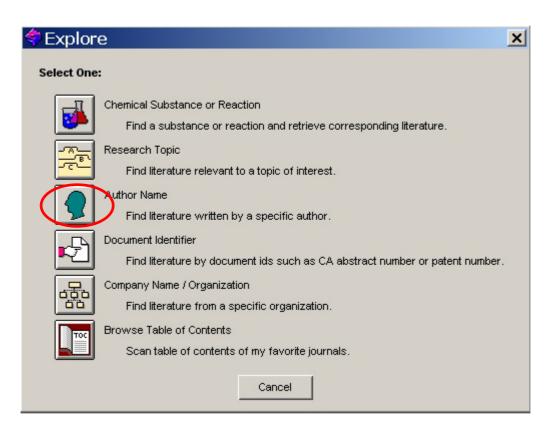




注意: Get Related 功能中多了 eScience —— 可以将您的检索扩展到整个网络;



5.3 Explore by Author Name





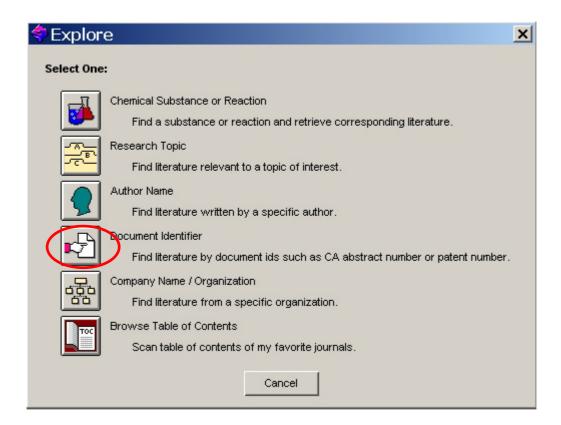


SEXPlore by Author Name		
Enter the author's name.		
Last name (required):		
First name or initial:		
Middle name or initial:		
Look for alternative spellings of the last name.		
OK Cancel		

输入作者的姓名(英文,或拼音),OK。

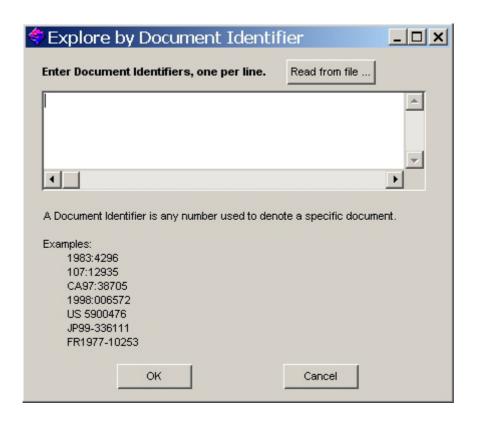
注意:必须填入 Last name (姓),如果不能确认则可选择下面的选项 (alternative spelling);不区分大小写;对于复姓如 O'Sullivan, Chace-Scott, or Johnson Taylor可直接输入;如果带有元音变音的,输入字母即可,或在后面接一个e,会同时搜索名、姓以及姓、名;对于不确认的名,可以输入首字母;

5.4 Explore by Document Identifier









Document Identifier (文件标识)

Number	Examples
CA Accession Number	120: 15297 1994: 15297
Patent number	CA 2107100
Patent application number	JP 1992-502228
Priority application number	IT 1998-BO661
PubMed ID (National Library of Medicine)	2004123

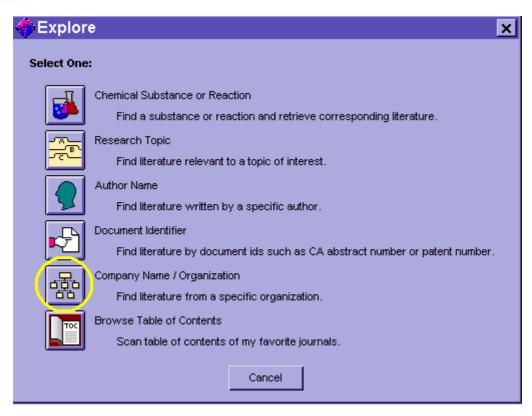
5.5 Explore by Company Name / Organization

假定您现在正在制造一种纤维能够比拟蜘蛛网生物聚合物的天然特性;并且您已获悉 Wyoming 大学的科学家已经研究合成蛛丝很多年;

Click Company Name/Organization.







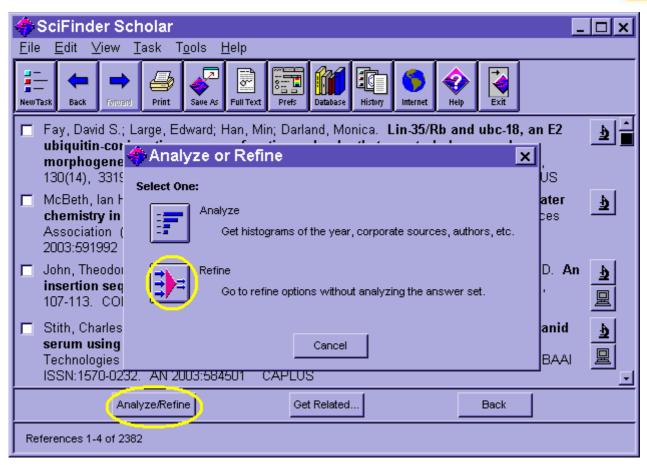
Type University of Wyoming and click **OK**.

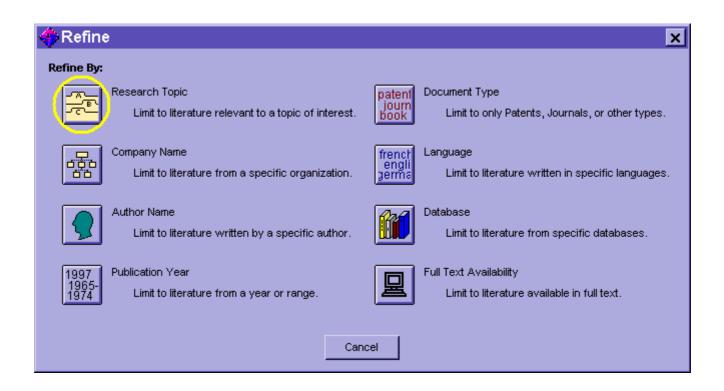


SciFinder Scholar 检索道 2382 篇相关文献,可以进行二次检索或分析 Analyze/Refine, 点击 Refine 进行二次检索.



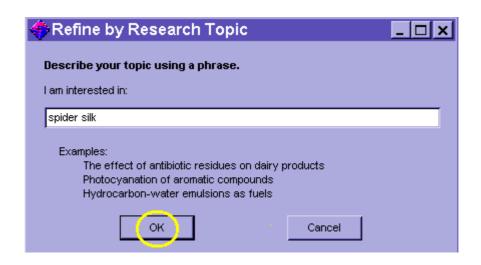




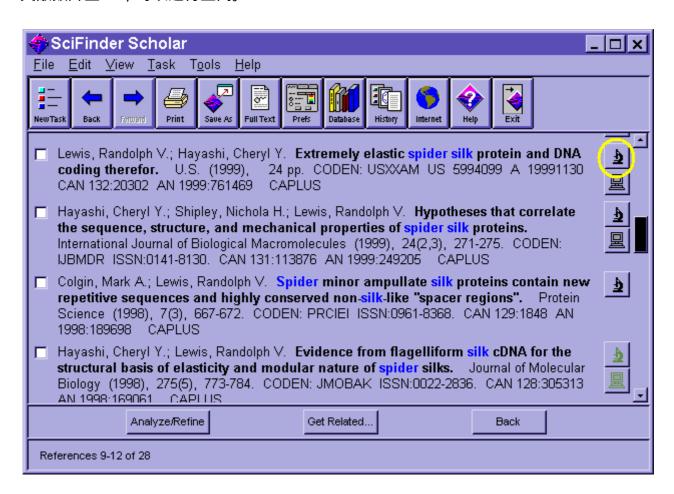






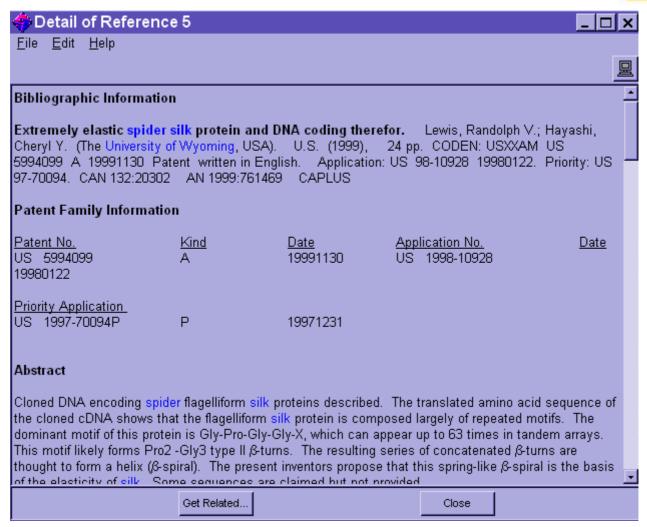


文献数降至28,可以进行查阅。

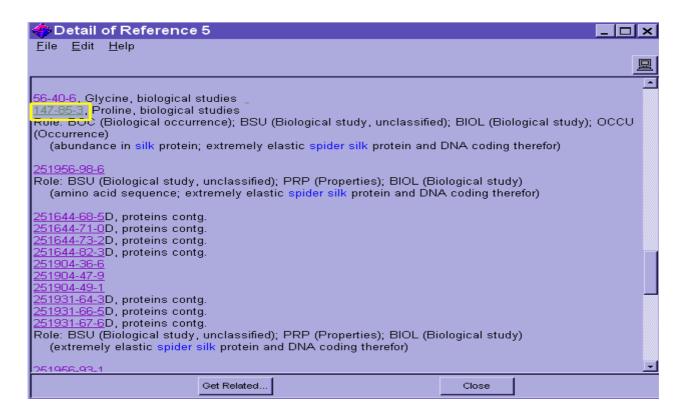








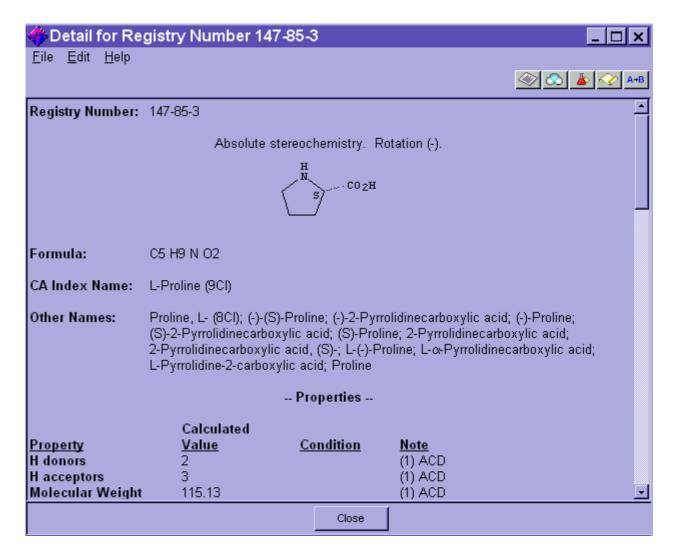
往下拖动,可以看到 CAS Registry Numbers® , Click a hyperlinked CAS Registry Number.







The detail for this Registry Number is displayed.



这里只是对 SciFinder Scholar 的使用作一个简单介绍,更多的内容可以参见 SciFinder Scholar 的帮助文件,菜单中的 Help,或 F1。

如有疑问也可以和我们联系:

iGroup 亚太资讯公司中国办事处

北京:010 - 82015519/20

北京海淀区北太平庄路 25 号豪威大厦 207 室 (100088)

张纬勇





jacky@igorup.com.cn