SciFinder®

The choice for chemistry research.™

SciFinder Web使用介绍

刘衍兰

SciFinder培训专员

2014.10

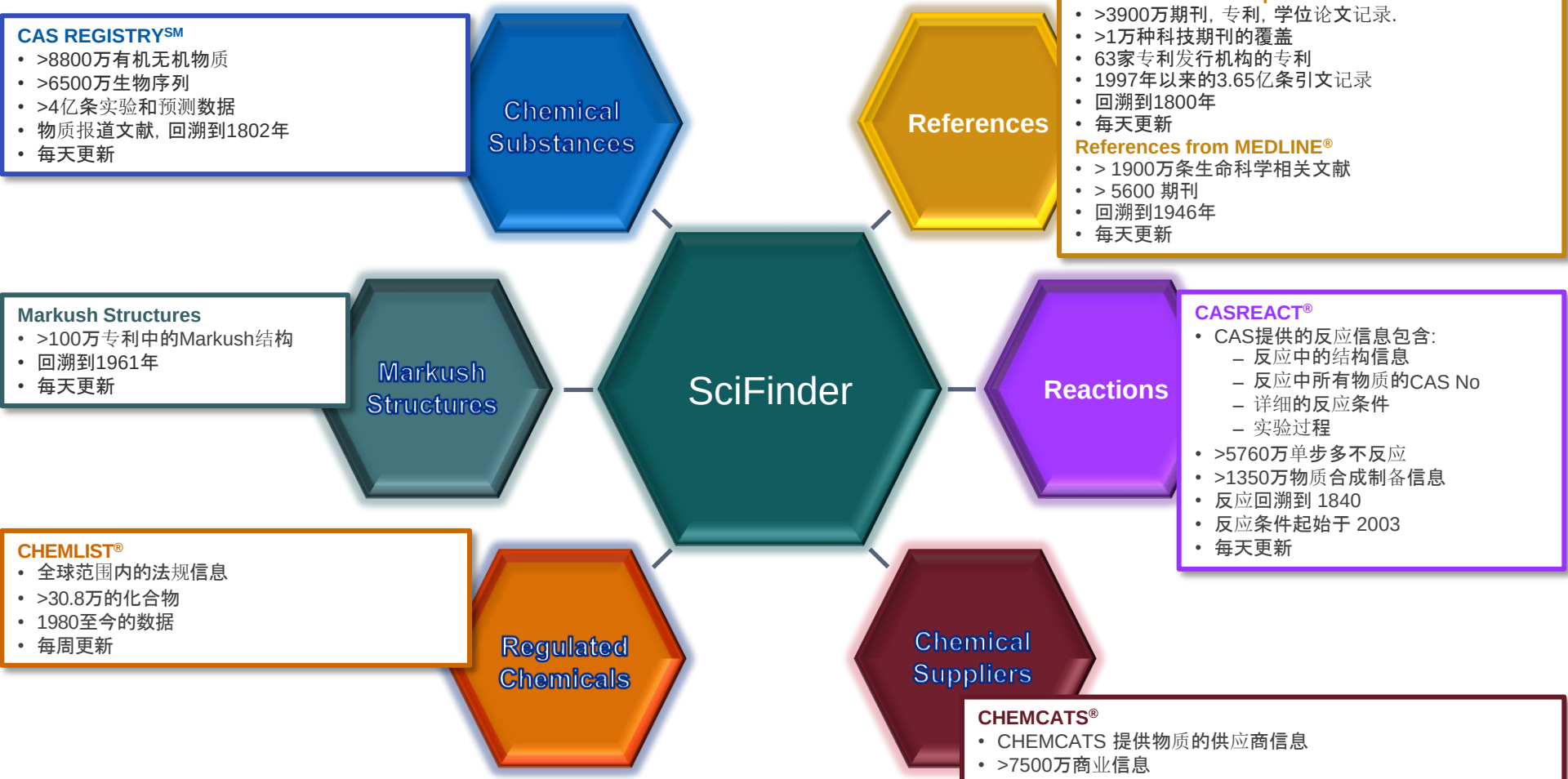
提纲

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

美国化学文摘社—Chemical Abstract Service

- 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



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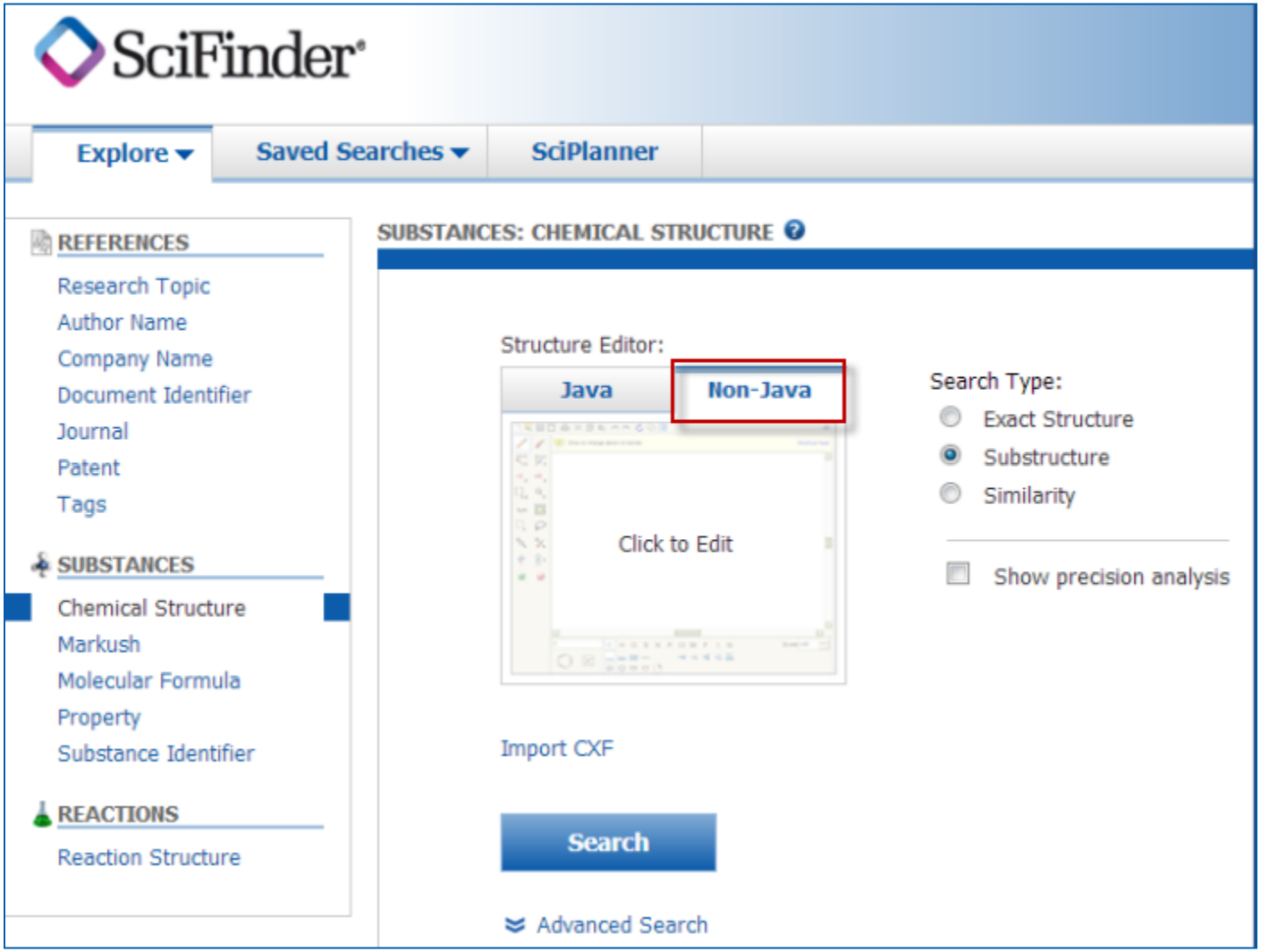
Non-Java结构面板



美国专利全文PDF链接

SciFinder®
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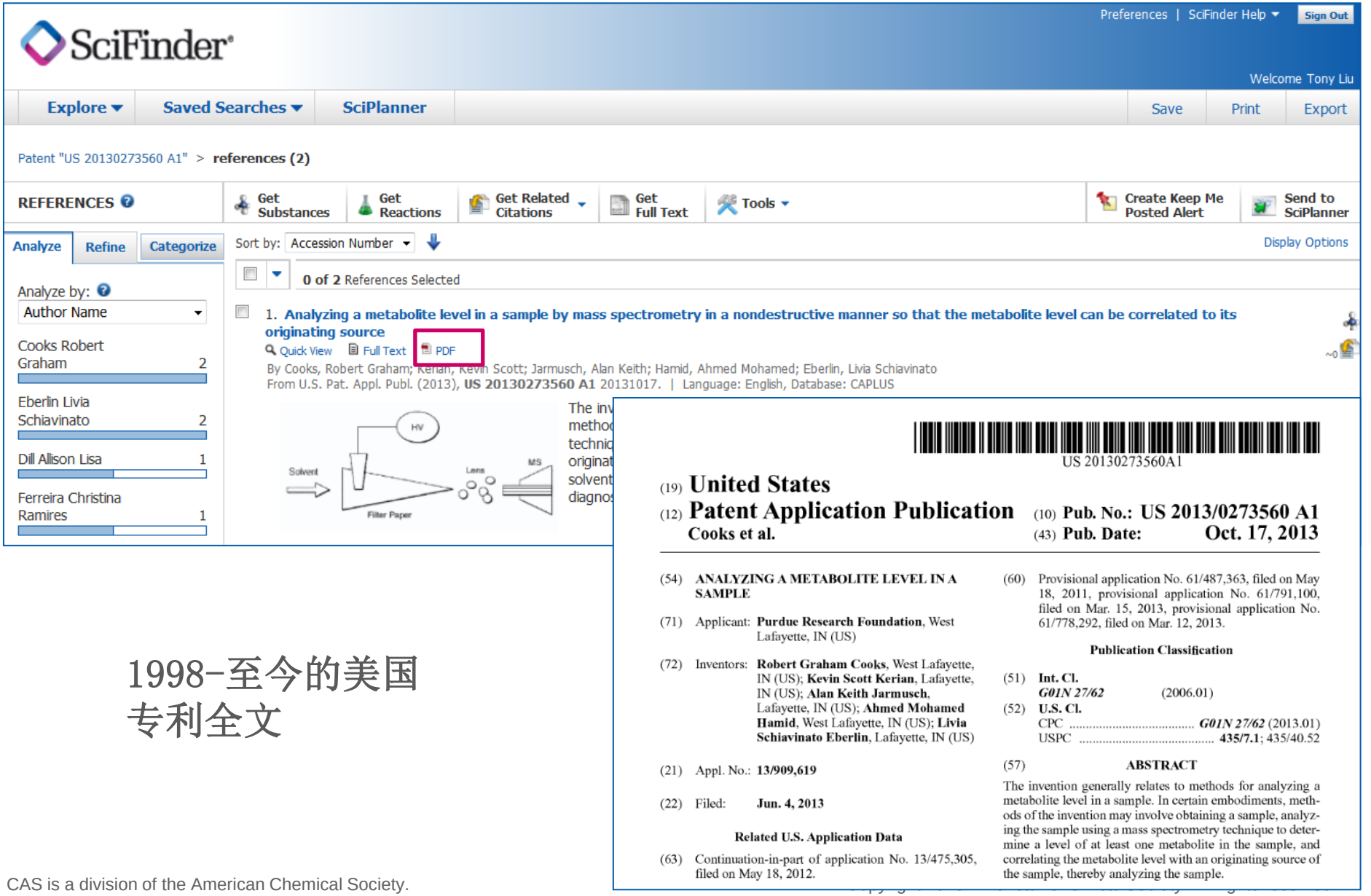
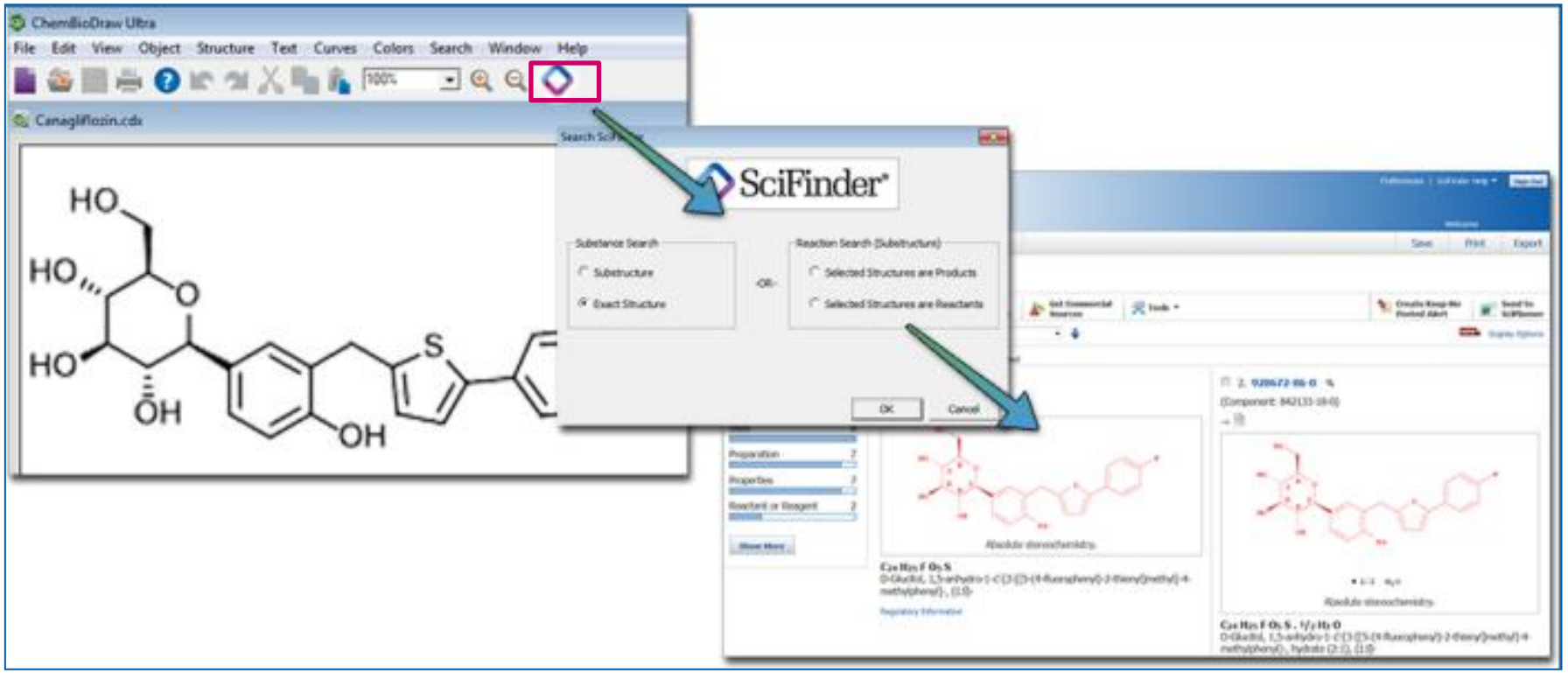


1998-至今的美国专利全文

SciFinder和ChemDraw整合



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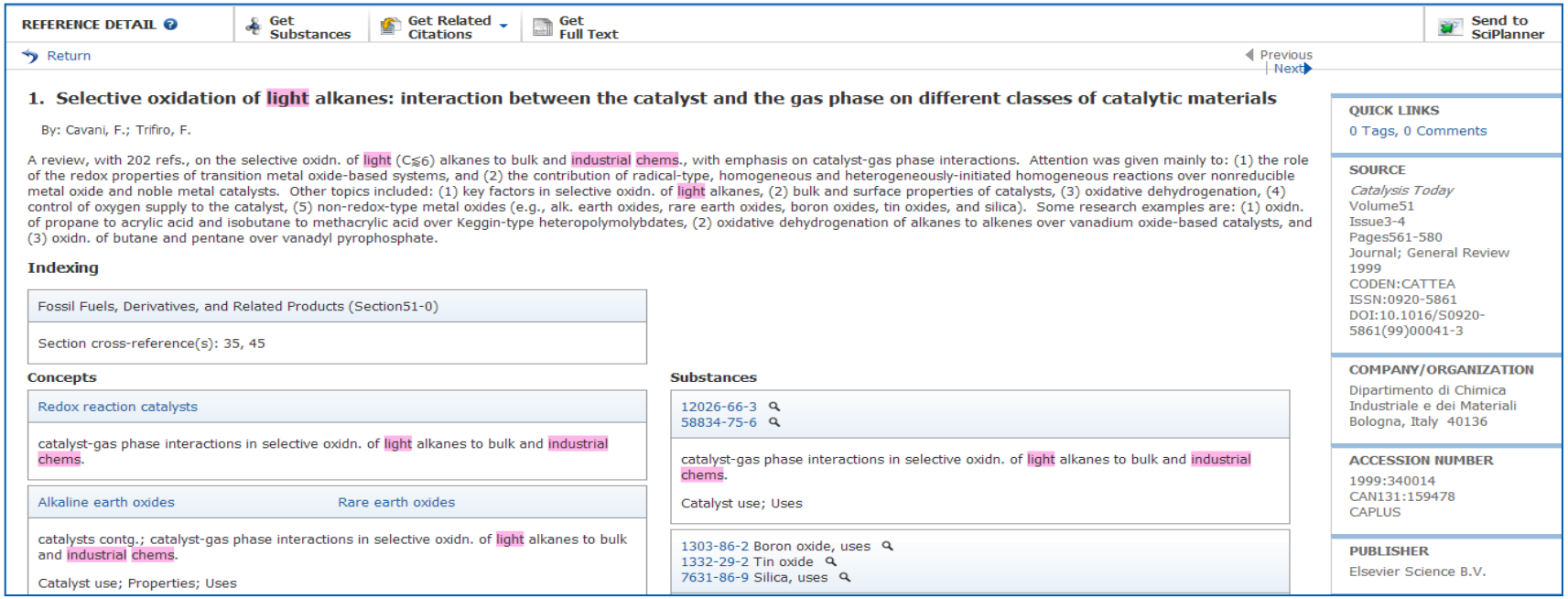
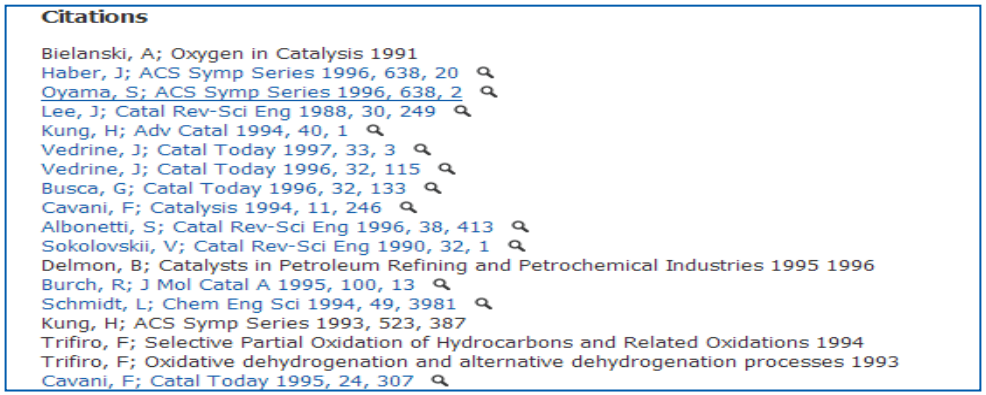
SciFinder中的文献记录





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

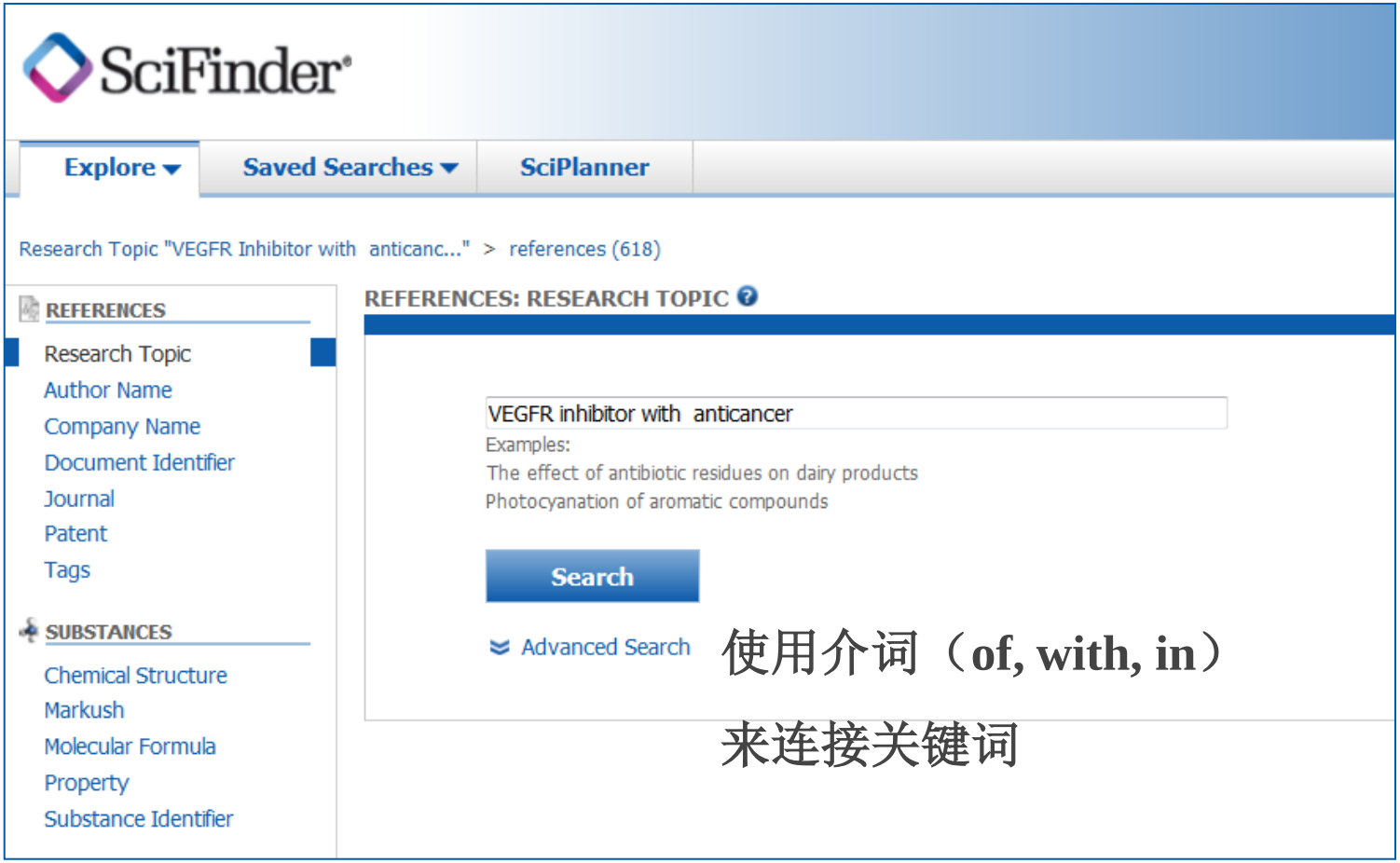
SciFinder中的文献检索方法

- **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

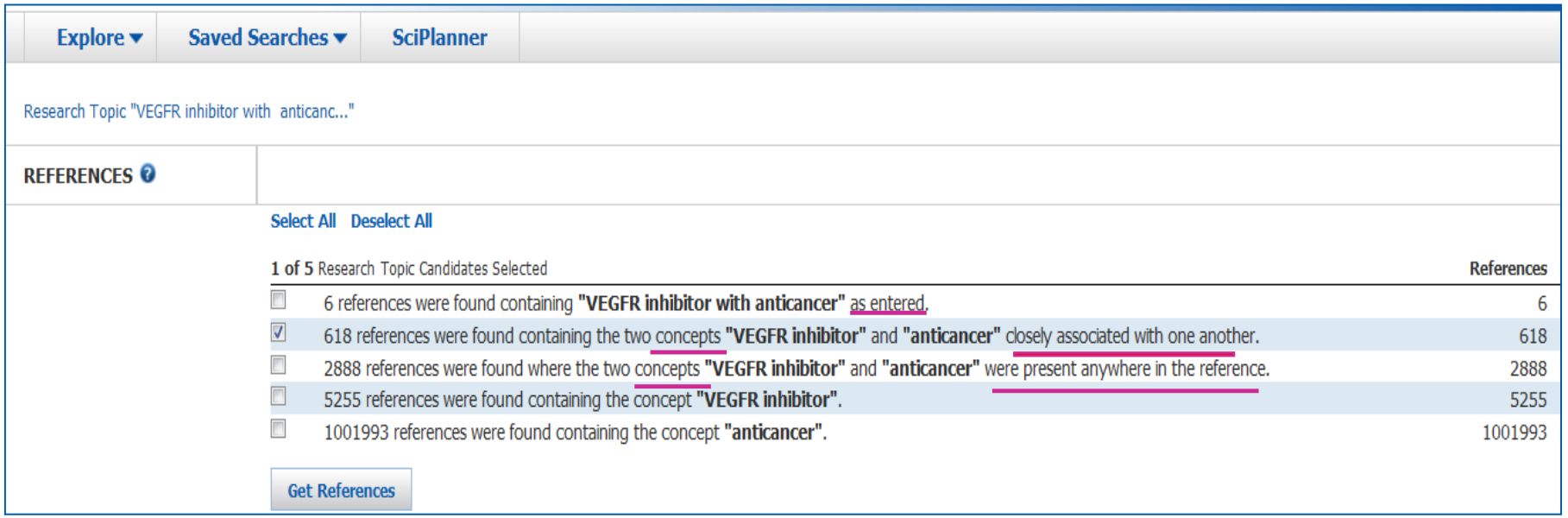
- **检索方法推荐**
  - 关注某特定领域的文献——-主题检索
  - 关注物质有关的文献———-先获得物质，再获得文献
  - 关注某科研人员的文献——-作者名检索

SciFinder Web中的主题检索

主题： **VEGFR inhibitor with anticancer**(VEGFR抑制剂在抗肿瘤方面的研究进展）



主题检索的候选项



- “as entered” 表示完全匹配
- “concept”表示做了同意词的扩展
- “closely associated with one another”表示同时出现在一个句子中
- “present anywhere in the reference” 表示同时出现在一段话中

SciFinder 中的文献检索结果及后处理

文献分析、
限定工具　系统分类工具

SciFinder提供强大的文献处理工具，帮助处理文献

SciFinder提供的引文排序— Citing Reference

REFERENCES

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

Analyze | Refine | Categorize

Sort by: Citing References

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

Display Options

Page: 1 of 31

Analyze by: Author Name

Ciardiello Fortunato	15
Troiani Teresa	11
Myers Jeffrey N	9
Fontanini Gabriella	8
Jiang Yuyang	8
Tan Chunyan	8
Tan Yuting	8
Tortora Giampaolo	8
Zhang Shixi	8
Bhide Rajeev S	7

1. ...apy elicits malignant progression of tumors to increased local invasion and distant metastasis

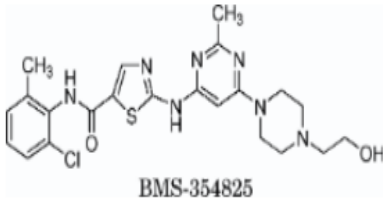
By Paez-Ribes, Marta; Allen, Elizabeth; Hudock, James; Takeda, Takaaki; Okuyama, Hiroaki; Vinals, Francesc; Inoue, Masahiro; Bergers, Gabriele; Hanahan, Douglas; Casanovas, Oriol
From Cancer Cell (2009), 15(3), 220-231. | Language: English, Database: CAPLUS

Multiple angiogenesis **inhibitors** have been therapeutically validated in preclin. **cancer** models, and several in clin. trials. Here we report that angiogenesis **inhibitors** targeting the VEGF pathway demonstrate **anti-tumor** effects in mouse models of pancreatic neuroendocrine **carcinoma** and glioblastoma but concomitantly elicit **tumor** adaptation and progression to stages of greater malignancy, with heightened invasiveness and in some cases increased lymphatic and distant metastasis. Increased invasiveness is also seen by genetic ablation of the Vegf-A gene in both models, substantiating the results...

2. **Discovery of N-(2-Chloro-6-methyl-phenyl)-2-(6-(4-(2-hydroxyethyl)-piperazin-1-yl)-2-methylpyrimidin-4-ylamino)thiazole-5-carboxamide (BMS-354825), a Dual Src/Abl Kinase Inhibitor with Potent Antitumor Activity in Preclinical Assays**

Quick View | Full Text

By Lombardo, Louis J.; Lee, Francis Y.; Chen, Ping; Norris, Derek; Barrish, Joel C.; Behnia, Kamelia; Castaneda, Stephen; Cornelius, Lyndon A. M.; Das, Jagabandhu; Doweyko, Arthur M.; et al
From Journal of Medicinal Chemistry (2004), 47(27), 6658-6661. | Language: English, Database: CAPLUS

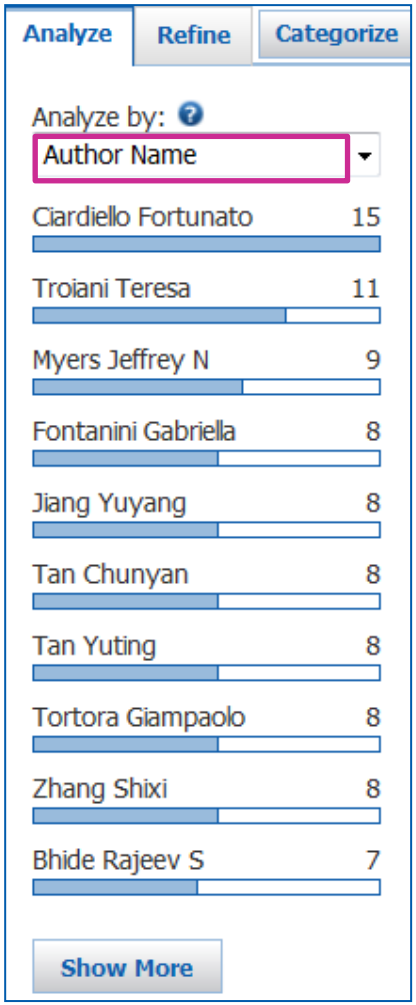


BMS-354825

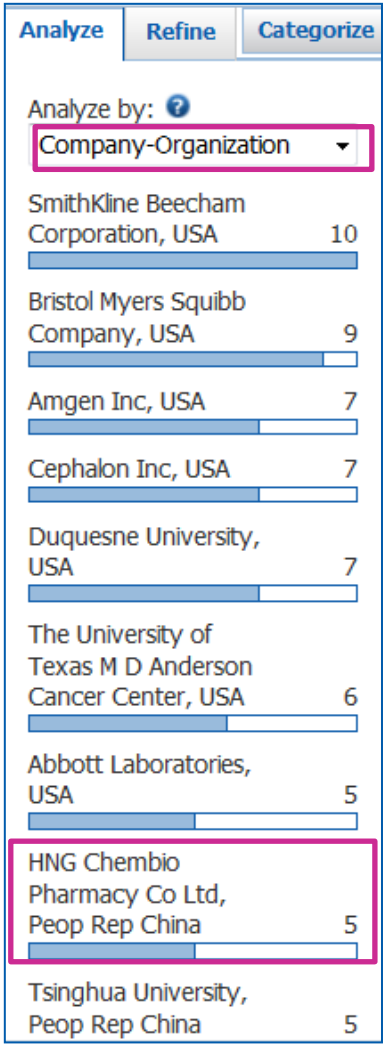
A series of substituted 2-(aminopyridyl)- and 2-(aminopyrimidinyl)thiazole-5-carboxamides was identified as potent Src/Abl kinase **inhibitors** with excellent antiproliferative activity against hematol. and solid **tumor** cell lines. Compd. I was orally active in a K562 xenograft model of chronic myelogenous leukemia (CML), demonstrating complete **tumor** regressions and low toxicity at multiple dose levels. On the basis of its robust in vivo activity and favorable pharmacokinetic profile, I was selected for addnl. characterization for oncol. indications.

SciFinder中的Analyze

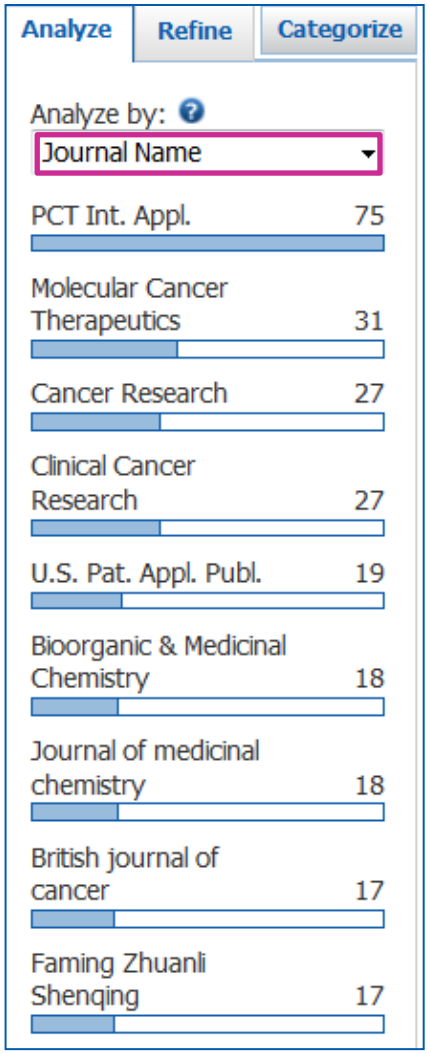
领域内主要研究人员，专家



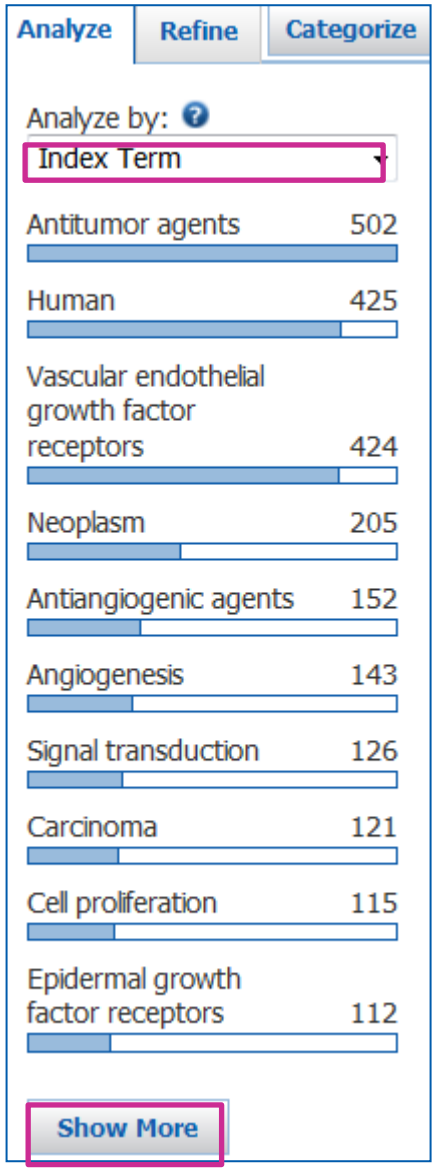
主要研究机构，合作伙伴，竞争对手



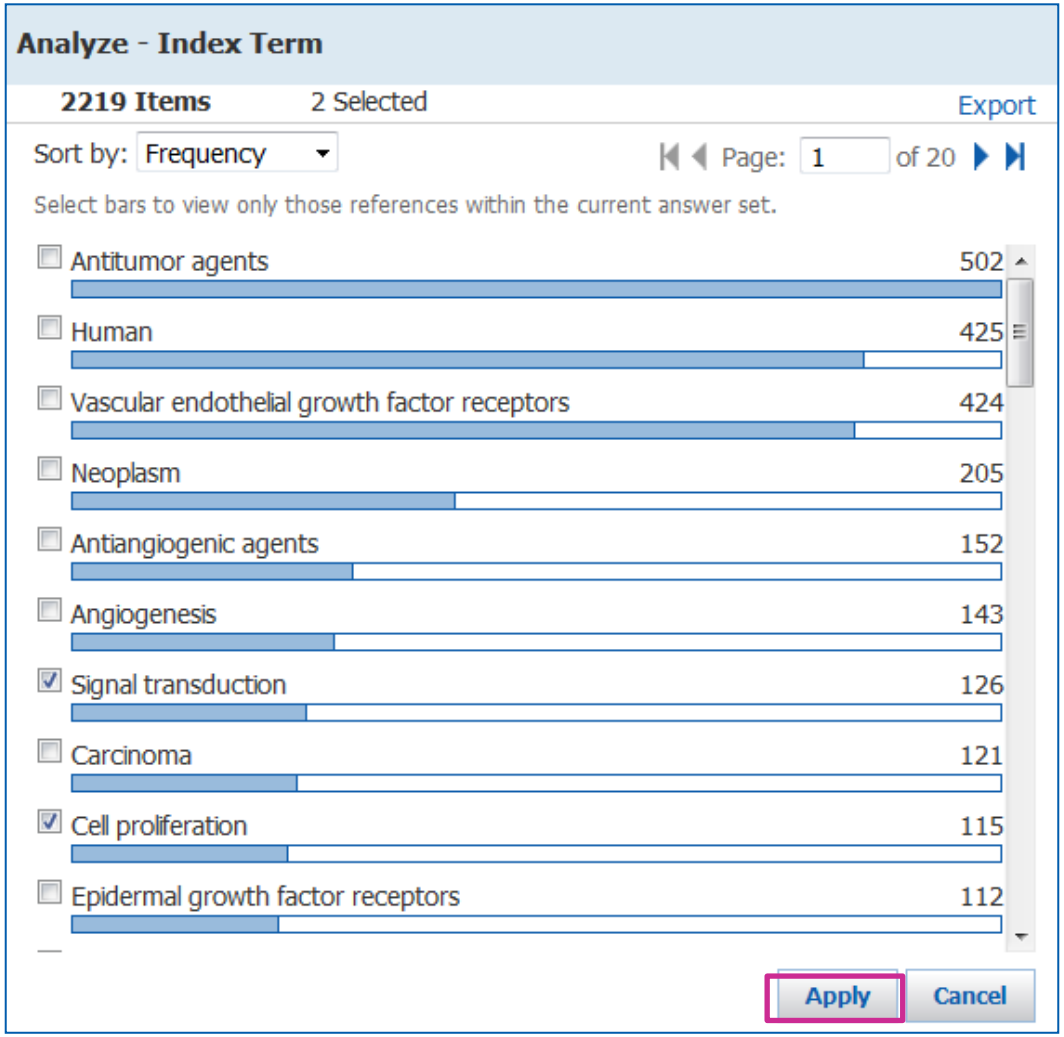
主要出版杂志，机构，潜在投稿期刊



SciFinder中的Analyze- Index Term

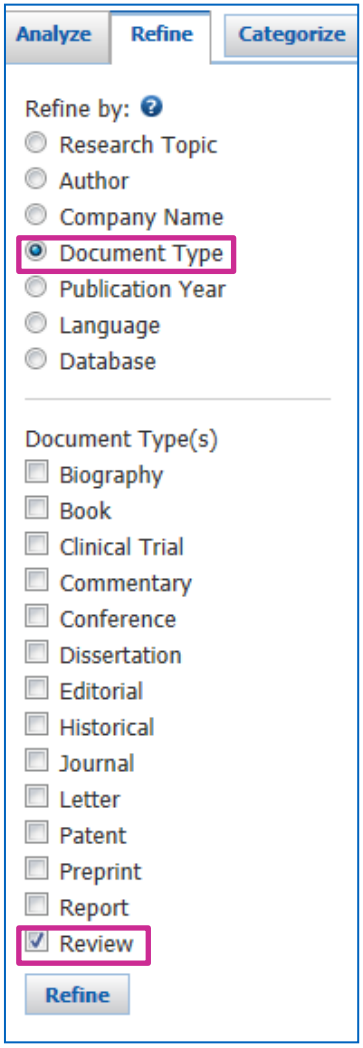


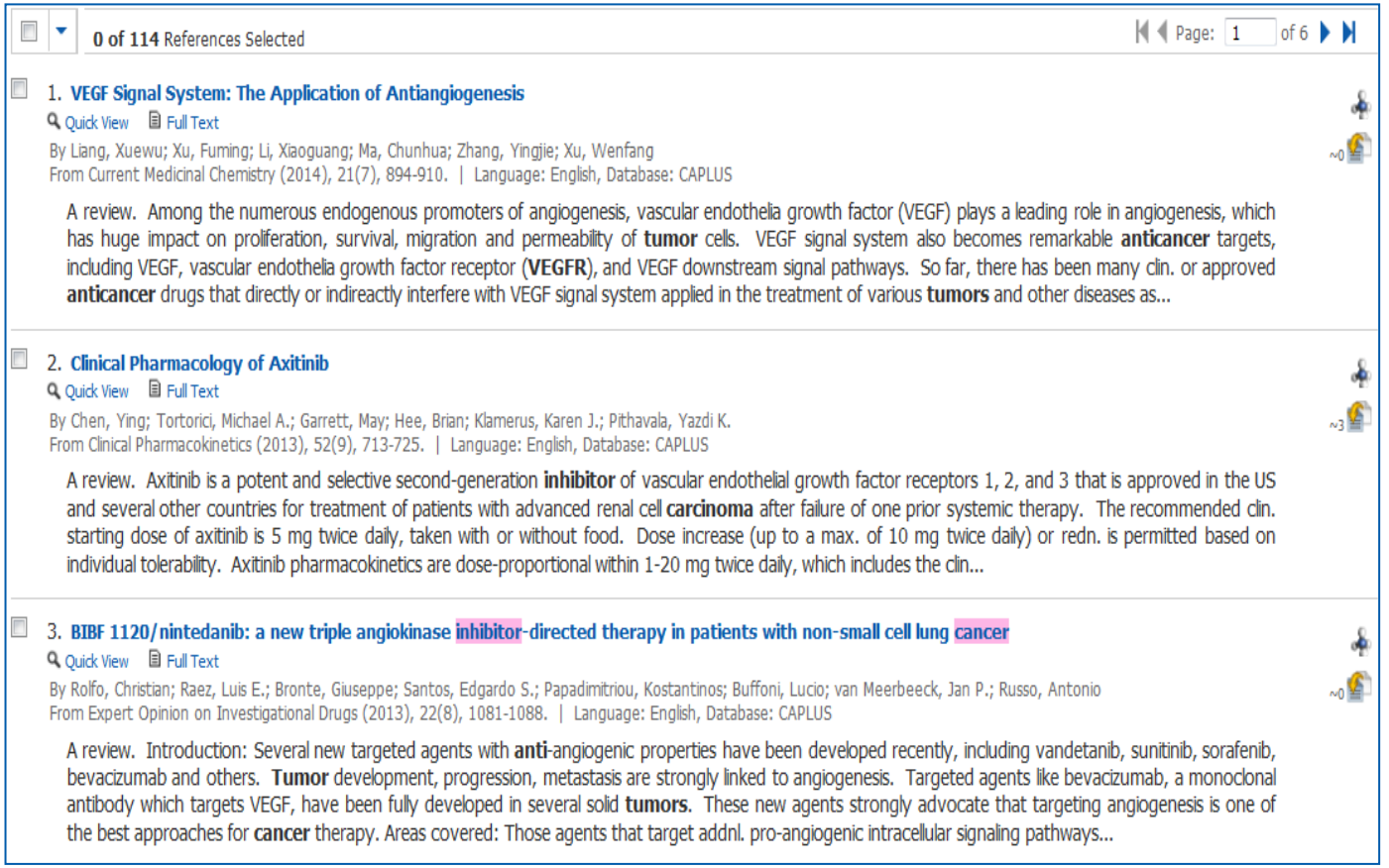
索引词（Index Term）：可以帮助我们对文献的内容进行大致的了解



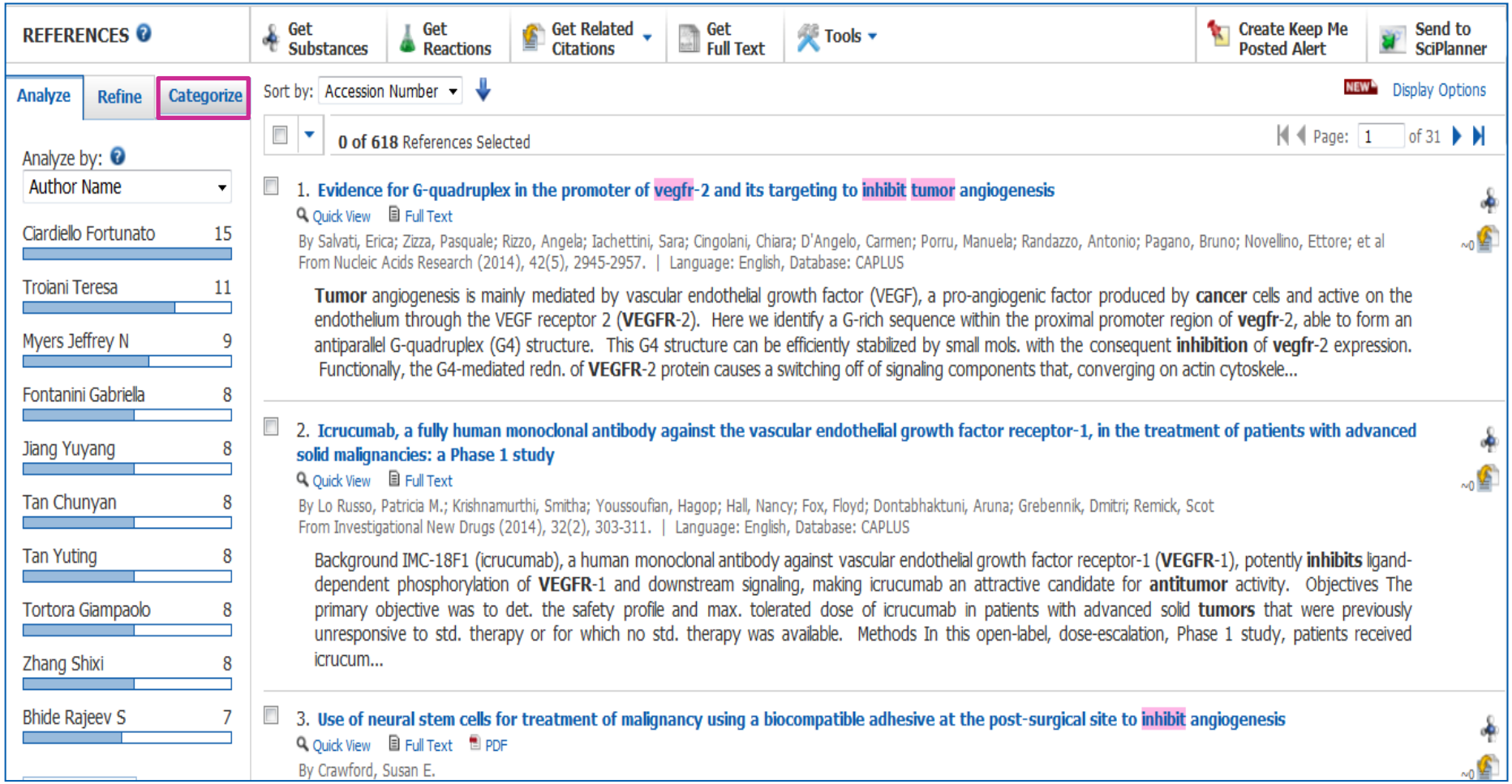
SciFinder中的Refine

文献类型限定：获得最新综述类文献



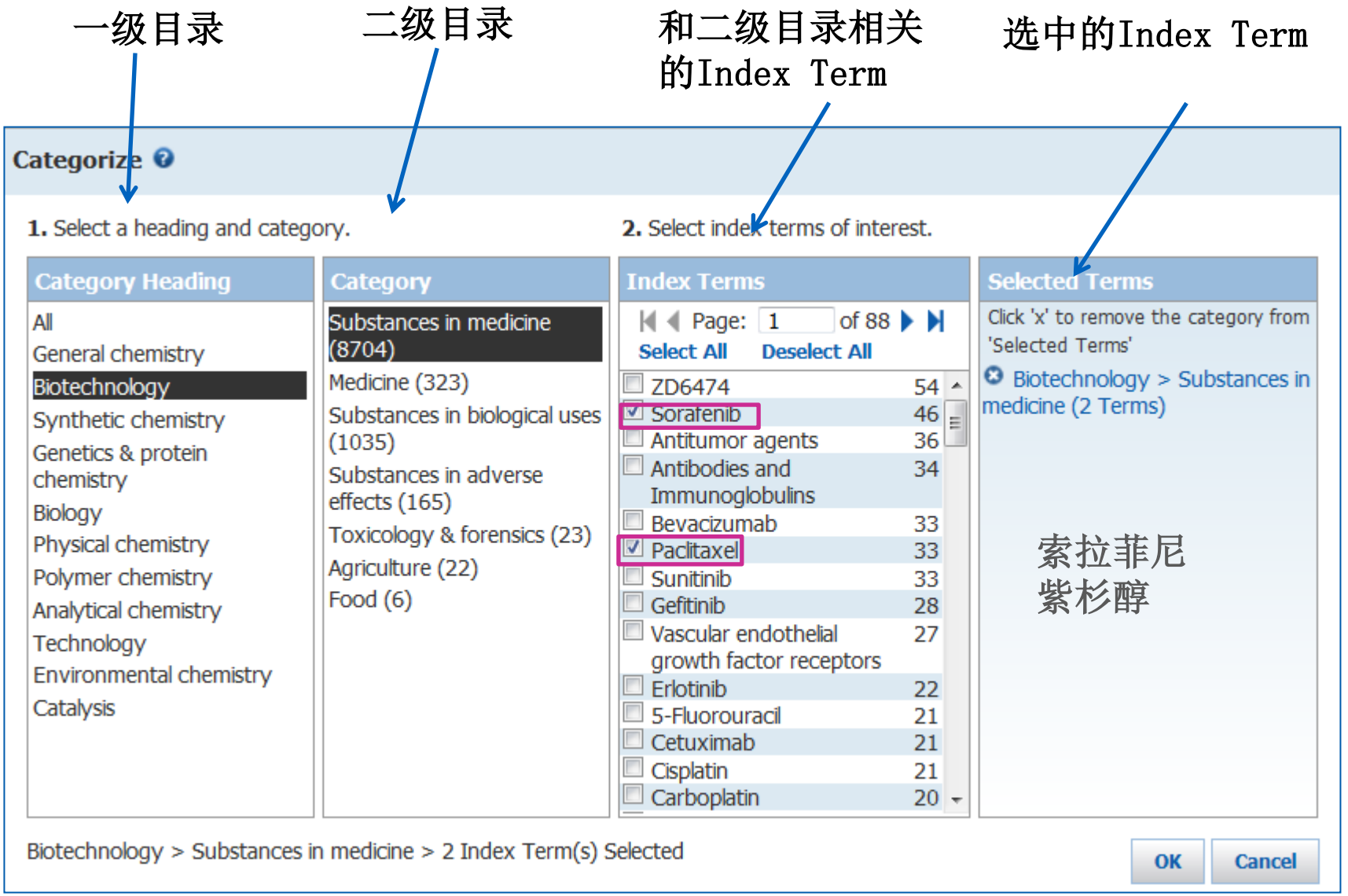


SciFinder 中的Categorize



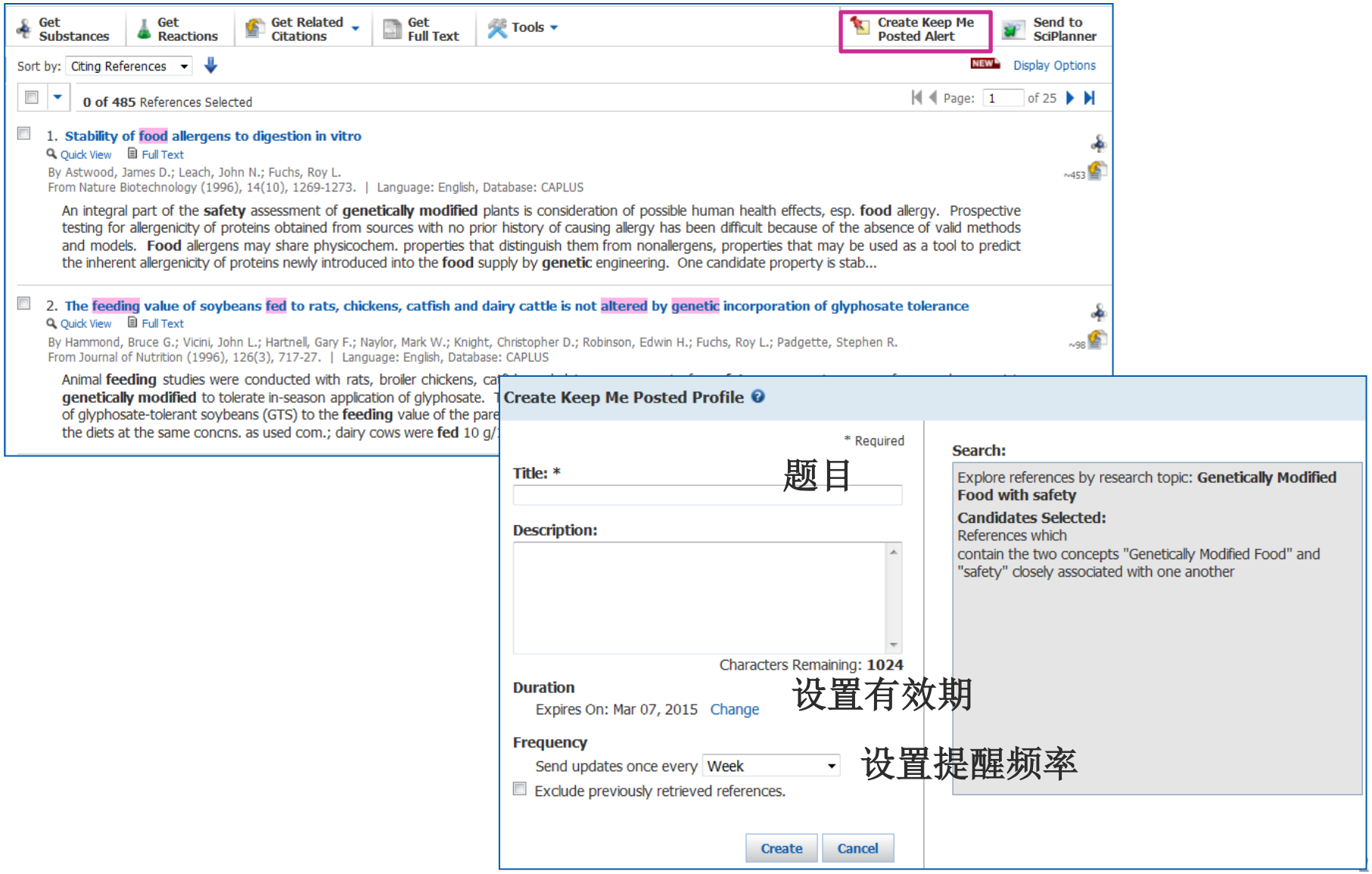
Categorize系统分类功能，基于Index Term，对文献依学科方向进行分类

SciFinder中的Categorize

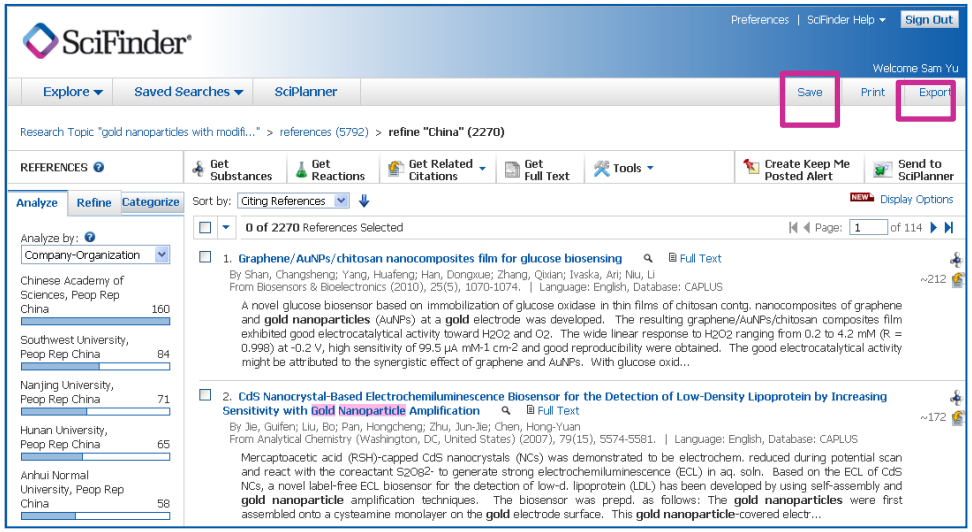


SciFinder中的KMP

随时跟踪科研最新进展



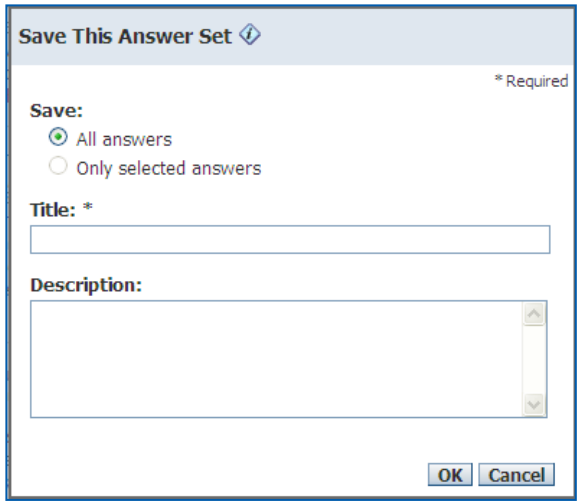
结果集的保存

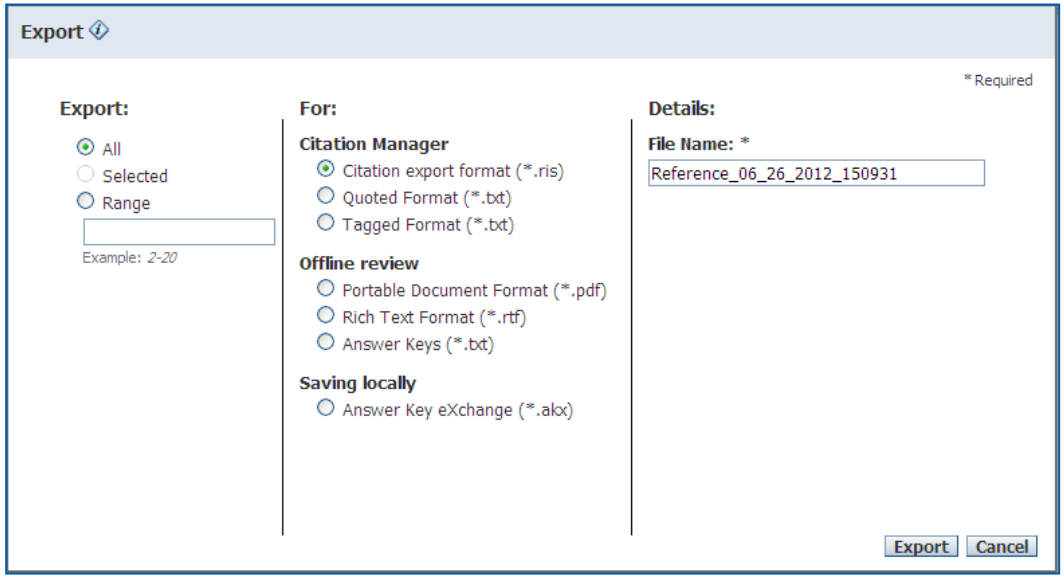


Export：

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

Offline Review:保存过成PDF，RTF格式，用于脱机浏览





Save：

保存在服务器上，可登陆后查看

SciFinder主题检索小结

- 关键词的选择以及关键词用介词连接
- 候选项选择含有concept和closed associated with 的选项
- 使用citing reference排序可以获得被引用次数最多的文献
- 使用KMP功能跟踪科研进展
- 使用Analyze, Refine和categorize进行后处理
- 结果集的保存

提纲

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  - SciFinder Web中的内容
  - SciFinder Web中的新功能
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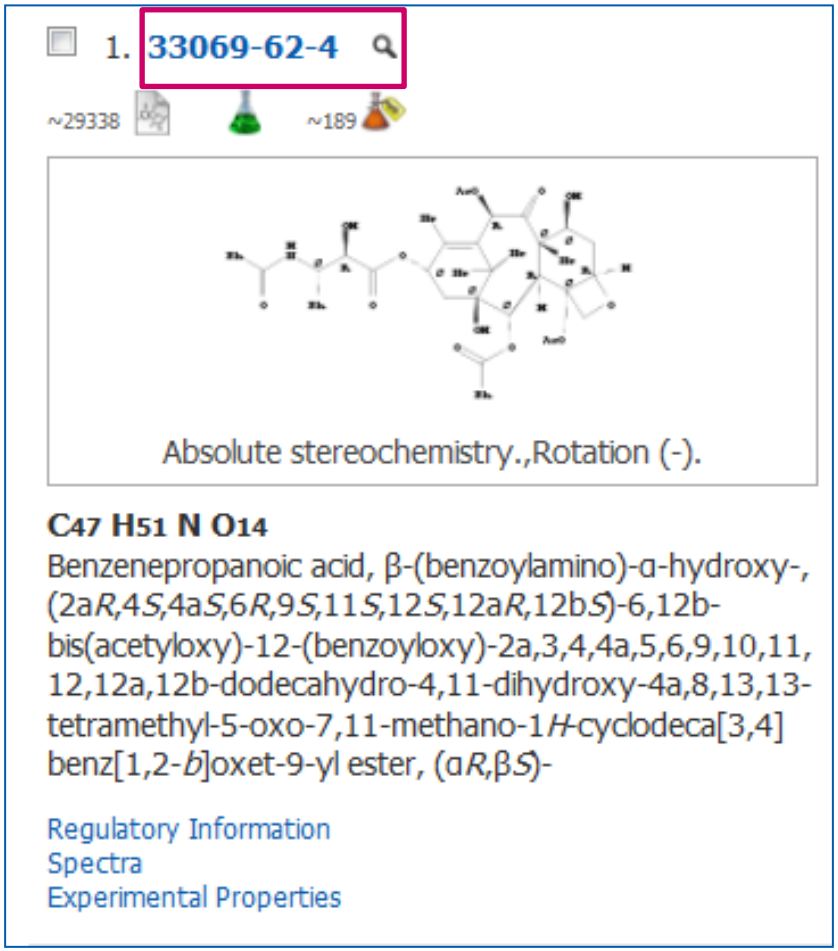
- **SciFinder Web的注册和常见问题**

SciFinder中的物质结果界面



紫杉醇的物质检索结果

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

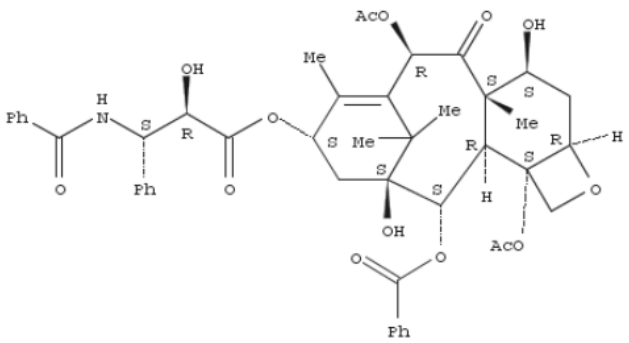
Substance Detail—查看物质详细信息

CAS Registry Number: 33069-62-4

C47 H51 N O14

Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2a*R*,4*S*,4a*S*,6*R*,9*S*,11*S*,12*S*,12a*R*,12b*S*)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, (α*R*,β*S*)-

Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αR*,βS*),11α,12α,12aα,12bα]]-; Tax-11-en-9-one, 5β,20-epoxy-1,2α,4,7β,10β,13α-hexahydroxy-, 4,10-diacetate 2-benzoate 13-ester with (2R,3S)-N-benzoyl-3-phenylisoserine (8CI); 7,11-Methano-1H-cyclodeca[3,4]benz[1,2-b]oxete, benzenepropanoic acid deriv.; (-)-Paclitaxel; 5β,20-



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。

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

生物活性和靶点信息

Bioactivity Indicators

	References
Antidiabetic agents	143
Antifibrotic agents	67
Anti-infective agents (all) >>> Antibacterial agents	155
Anti-infective agents (all) >> Antibiotics	862
Anti-infective agents (all) >>> Anti-HIV agents	94
Anti-infective agents (all) > Anti-infective agents	94
Anti-infective agents (all) >> Antimicrobial agents	122
Anti-infective agents (all) >>> Antiviral agents	367
Anti-infective agents (all) >> Fungicides	193
Anti-inflammatory agents (all) > Antiarthritics	148
Anti-inflammatory agents (all) > Anti-inflammatory agents	830
Anti-inflammatory agents (all) > Antirheumatic agents	200
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory drugs	133
Antiproliferative agents (all) > Antimitotic agents	164
Antiproliferative agents (all) > Antiproliferative agents	501
Antitumor agents (all) > Alkylating agents, biological	644
Antitumor agents (all) > Antiangiogenic agents	1027
Antitumor agents (all) > Antitumor agents	15182

Target Indicators

	References
Agglutinins and Lectins (all) > Galectins	10
Albuminoids (all) > Fibrins	36
Apoptosis-regulating proteins (all) > Apoptosis-inducing factors	13
Apoptosis-regulating proteins (all) > Apoptosis-regulating proteins	52
Apoptosis-regulating proteins (all) > Bad proteins	41
Apoptosis-regulating proteins (all) > Bak proteins	27
Apoptosis-regulating proteins (all) > Bax proteins	280
Apoptosis-regulating proteins (all) > Bcl-2 proteins	548
Apoptosis-regulating proteins (all) > Bcl-x proteins	180
Apoptosis-regulating proteins (all) >> Inhibitor of apoptosis proteins	108
Basigins	12
Bid proteins	35
Bim proteins	28
Blood-coagulation factors (all) > Blood-coagulation factor III	12
Blood-coagulation factors (all) > Fibrinogens	21

Substance Detail—查看物质详细信息

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

Top

Biological Properties	Value	Condition	Note
Bioconcentration Factor	591	pH 1 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 2 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 3 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 4 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 5 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 6 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 7 Temp: 25 °C	(34)
Bioconcentration Factor	591	pH 8 Temp: 25 °C	(34)
Bioconcentration Factor	590	pH 9 Temp: 25 °C	(34)
Bioconcentration Factor	582	pH 10 Temp: 25 °C	(34)

Top

Chemical Properties	Value	Condition	Note
Koc	3350	pH 1 Temp: 25 °C	(34)
Koc	3350	pH 2 Temp: 25 °C	(34)
Koc	3350	pH 3 Temp: 25 °C	(34)
Koc	3350	pH 4 Temp: 25 °C	(34)

Density Properties	Value	Condition	Note
Density	1.39±0.1 g/cm3	Temp: 20 °C Press: 760 Torr	(34)
Molar Volume	610.5±5.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(34)

Lipinski and Related Properties	Value	Condition	Note
Freely Rotatable Bonds	17		(34)
H Acceptors	15		(34)
H Donors	4		(34)
H Donor/Acceptor Sum	19		(34)
logP	3.950±0.808	Temp: 25 °C	(34)
Molecular Weight	853.91		(34)

Substance Detail—查看物质详细信息

Experimental Properties: Biological Chemical 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 of 72	(1)CAS
Half-Life (Biological)	See full text	1 of 37	(7)CAS
LC50	See full text	1 of 2	(8)CAS
LD50	See full text		(9)CAS
Median Lethal Dose(LD50)	8.3 mg/kg	Organism: rat Route: intravenous	(14)CAS

Top

Chemical Properties	Value	Condition	Note
logD	See full text		(10)CAS
logP	See full text	1 of 3	(11)CAS
Potential of Electrode Reaction	See full text		(28)CAS
Solubility	See full text	1 of 18	(30)CAS

Top

Lipinski and Related Properties	Value	Condition	Note
logP	See full text	1 of 3	(11)CAS

Top

Optical and Scattering Properties	Value	Condition	Note
Optical Rotatory Power	-48.4 °	Conc: 0.5 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm	(26)CAS
Optical Rotatory Power	-49 °	Solv: methanol (67-56-1); Wavlen: 589.3 nm; Temp: 20 °C	(20)APC
Optical Rotatory Power	-49 °	Solv: methanol (67-56-1); Wavlen: 589.3 nm; Temp: 20 °C	(21)NLM
Optical Rotatory Power	-50 °	Conc: 1.0 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3	(23)CAS

Top

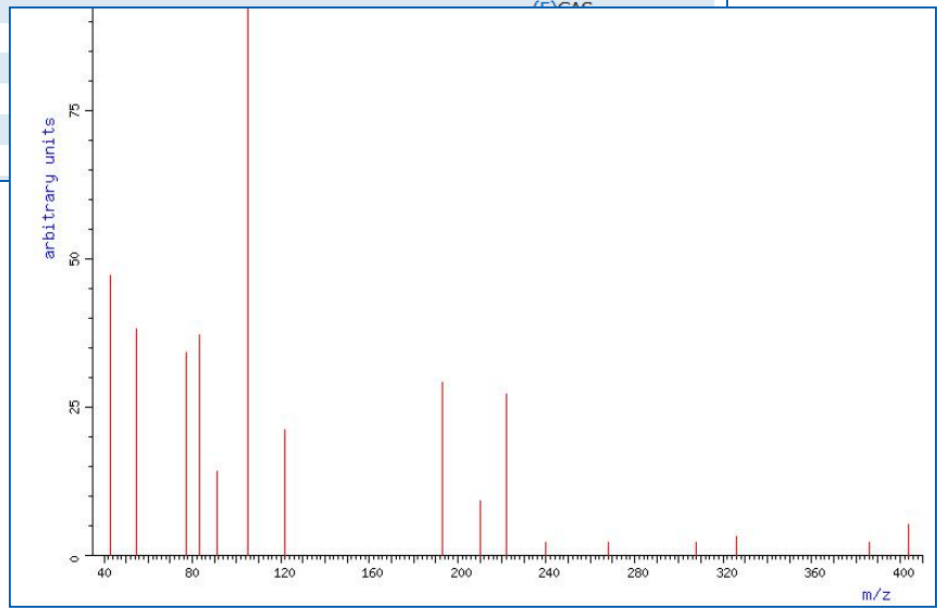
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See full text	1 of 5	(3)CAS
IR Absorption Spectrum	See full text	1 of 6	(3)CAS
Mass Spectrum	See spectrum		(12)WSS
Mass Spectrum	See full text	1 of 20	(13)CAS
Phosphorus-31 NMR Spectrum	See full text		(27)CAS
Proton NMR Spectrum	See full text	1 of 12	(17)CAS
Raman Spectrum	See full text	1 of 2	(29)CAS
Two-Dimensional NMR Spectrum	See full text		(31)CAS
UV and Visible Absorption Spectrum	See full text	1 of 3	(32)CAS

Top

Structure-related Properties	Value	Condition	Note
Bond Length	See full text		(2)CAS
X-Ray Diffraction Pattern	See full text	1 of 4	(33)CAS

Top

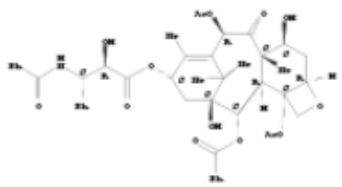
Thermal Properties	Value	Condition	Note
Enthalpy	See full text		(4)CAS
Entropy	See full text		(4)CAS
Gibbs Free Energy	See full text	1 of 2	
Glass Transition Temperature	151 °C		
Melting Point	228.6 °C		
Melting Point	223 °C		
Melting Point	216 °C		
Melting Point	213-217 °C		



物质有关的文献信息

1. 33069-62-4

~29338 ~189



Absolute stereochemistry.,Rotation (-).

C47 H51 N O14

Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2a*R*,4*S*,4a*S*,6*R*,9*S*,11*S*,12*S*,12a*R*,12b*S*)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester, (α*R*,β*S*)-

Regulatory Information
Spectra
Experimental Properties

一键获得文献，可以获得全部，也可以勾选特别感兴趣的内容，不勾选，默认获得全部

Get References

Limit results to:

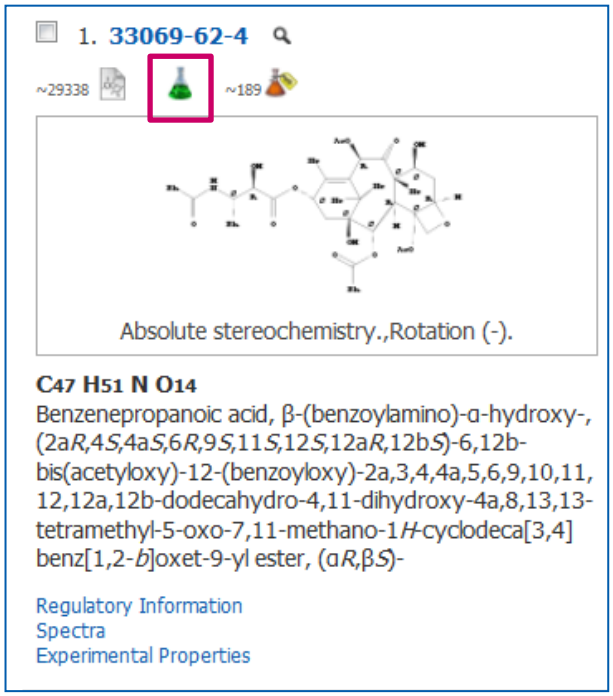
- ☐ Adverse Effect, including toxicity
- ☐ Analytical Study
- ☐ Biological Study
- ☐ Combinatorial Study
- ☐ Crystal Structure
- ☐ Formation, nonpreparative
- ☐ Miscellaneous
- ☐ Occurrence
- ☐ Prophetics in Patents
- ☐ Preparation
- ☐ Process
- ☐ Properties
- ☐ Reactant or Reagent
- ☐ Spectral Properties
- ☐ Uses

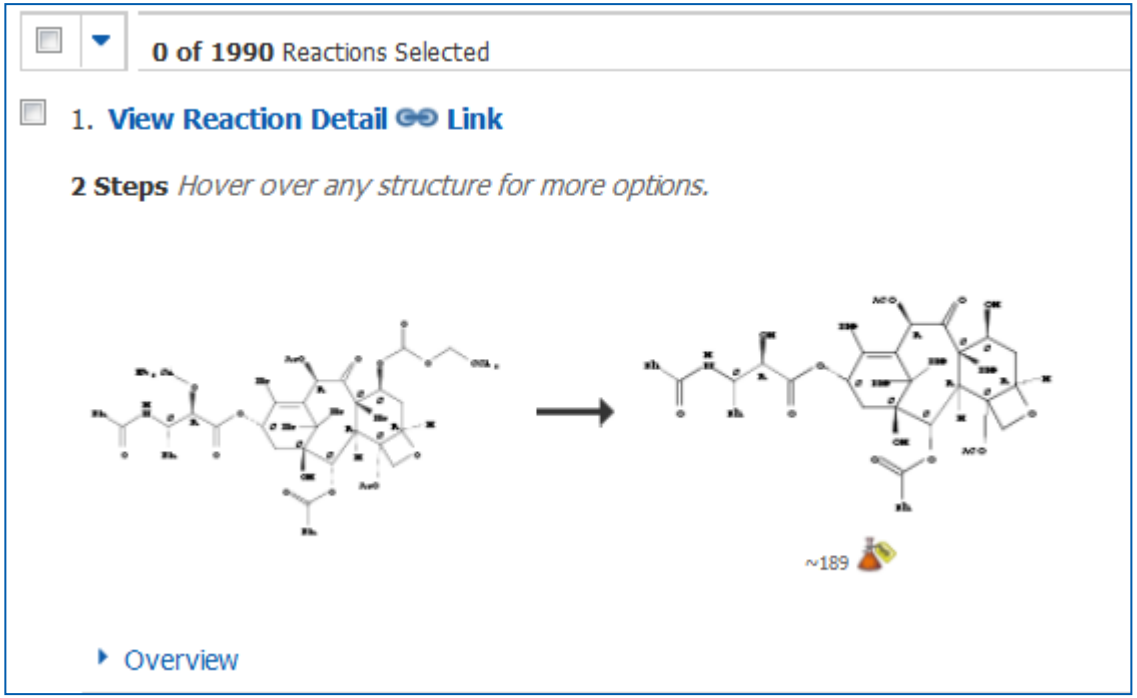
For each sequence, retrieve:

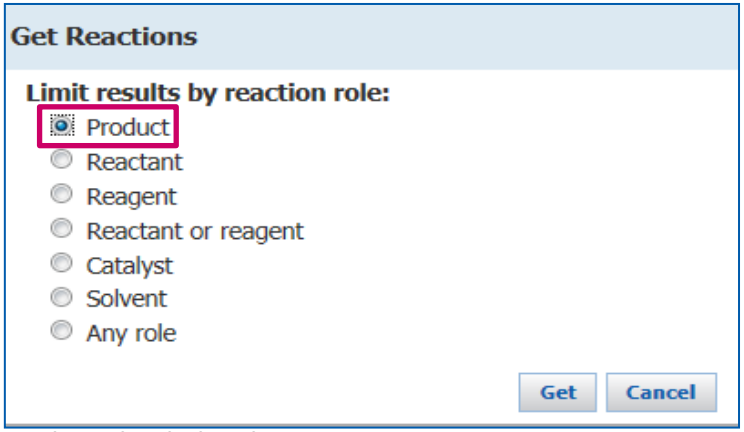
- ☐ Additional related references, e.g., activity studies, disease studies.

Get Cancel

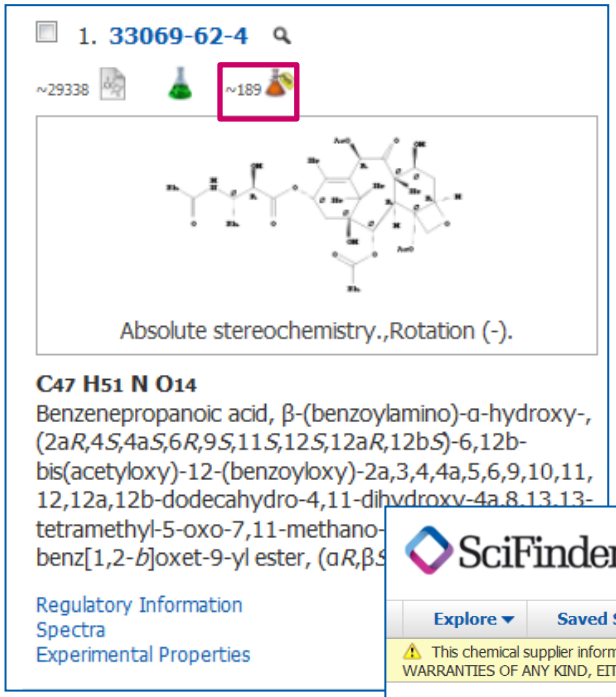
物质有关的反应



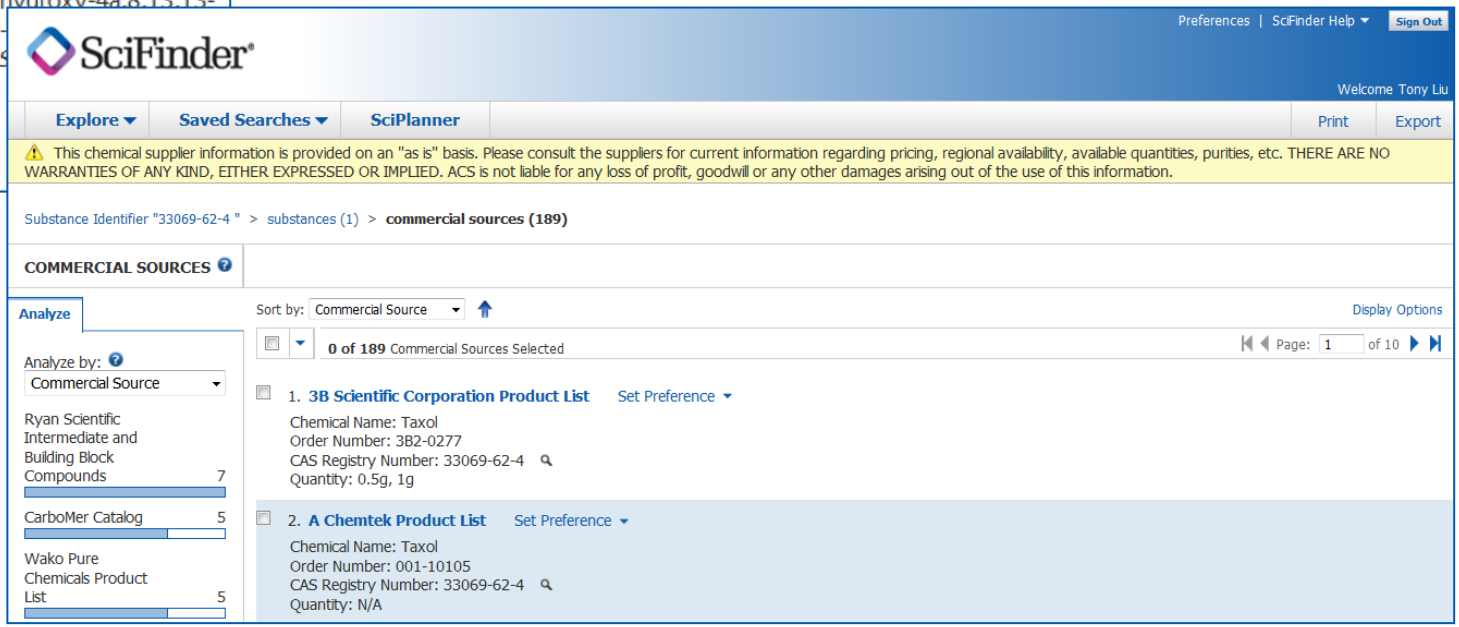




物质有关的商品信息



可以直接Export到Excel中，又或者使用分析工具，对商业信息进行处理

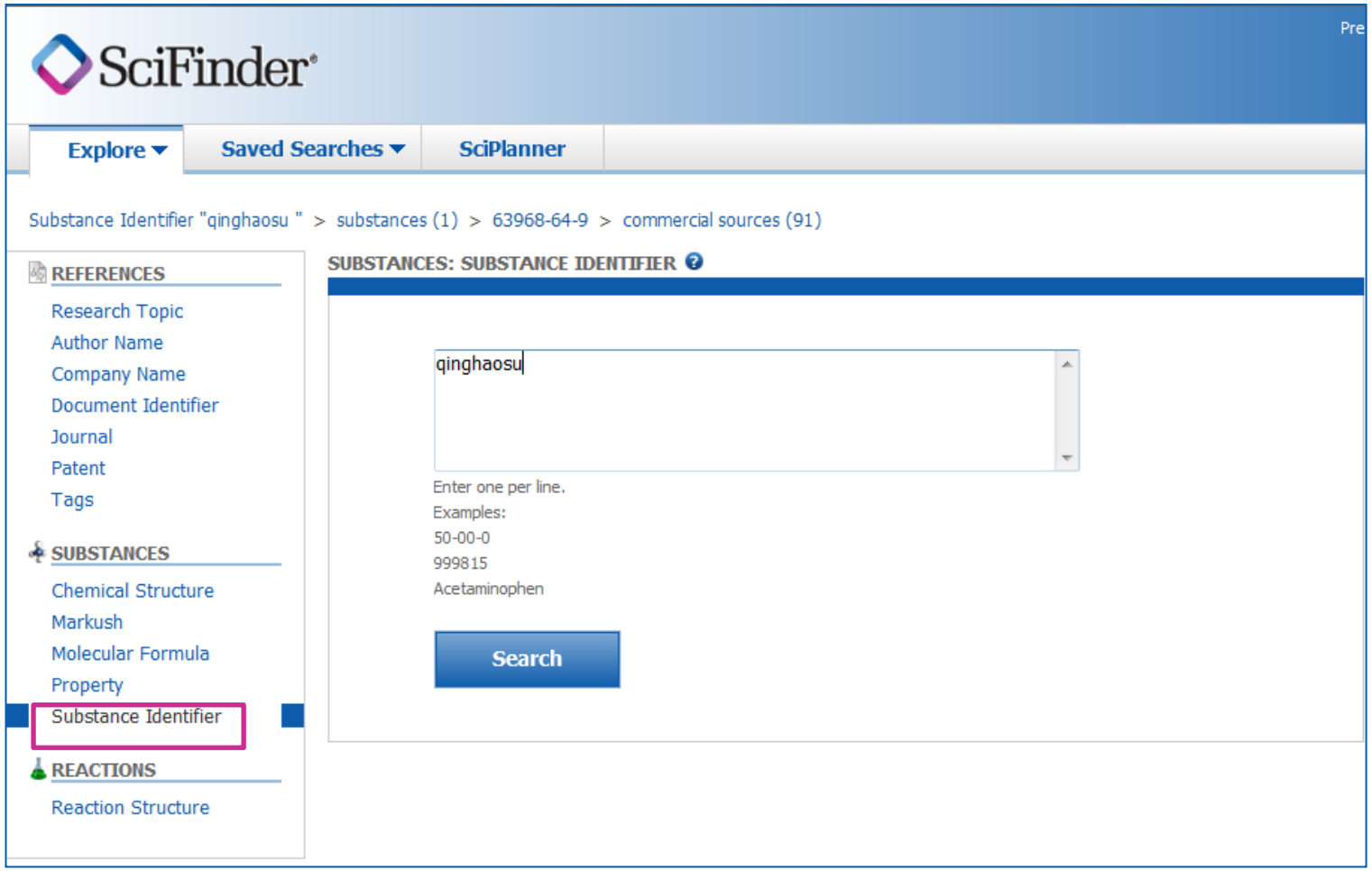


SciFinder中的物质检索方法

- **功能方面**
  - 物质名称，CAS No
  - 分子式
  - 结构式
  - 理化性质

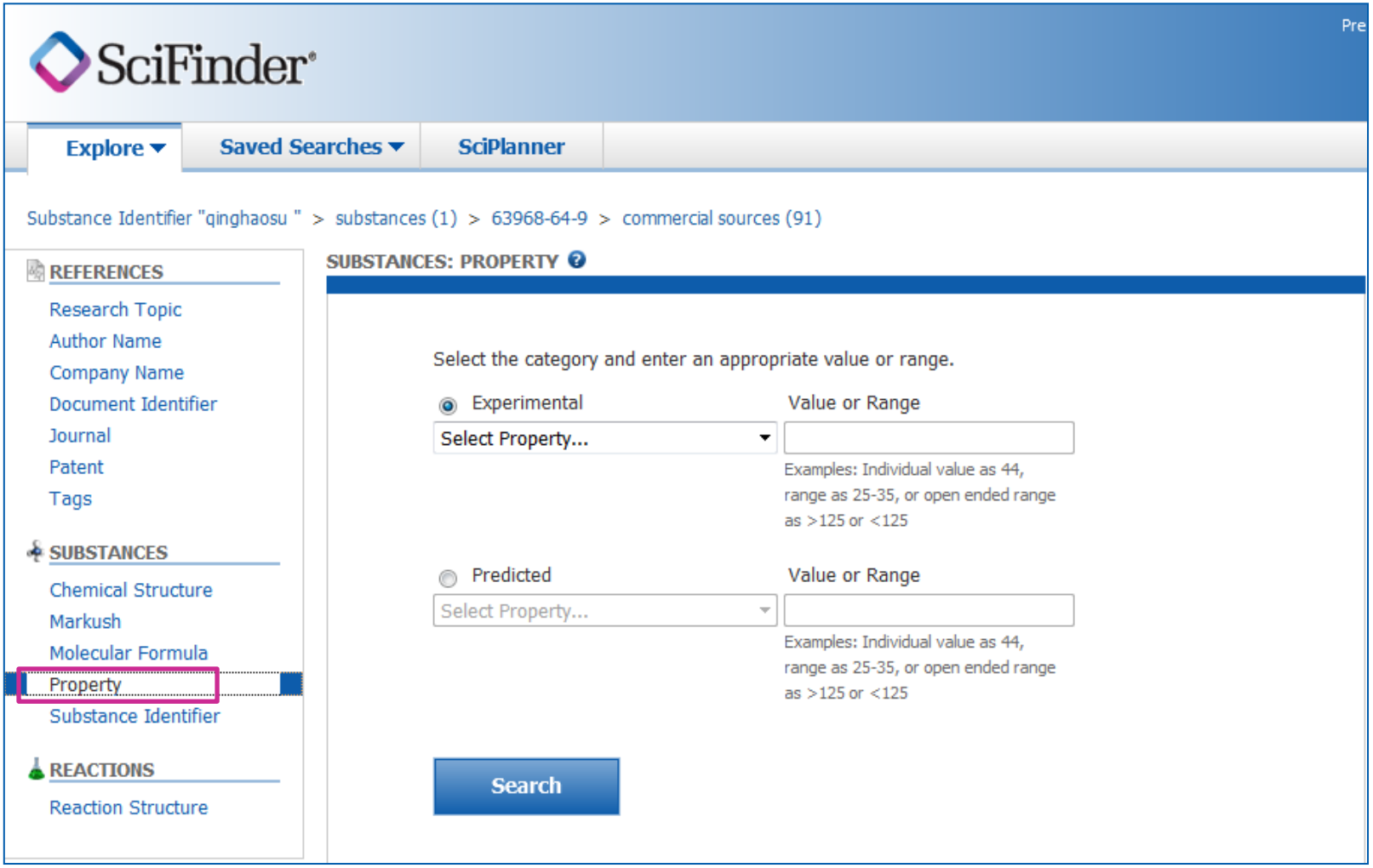
- **推荐的物质检索功能**
  - 有机物，天然产物及衍生物　---结构比较方便
  - 无机物　---分子式比较方便
  - 高分子化合物　---首先分子式，其次结构

物质名称检索

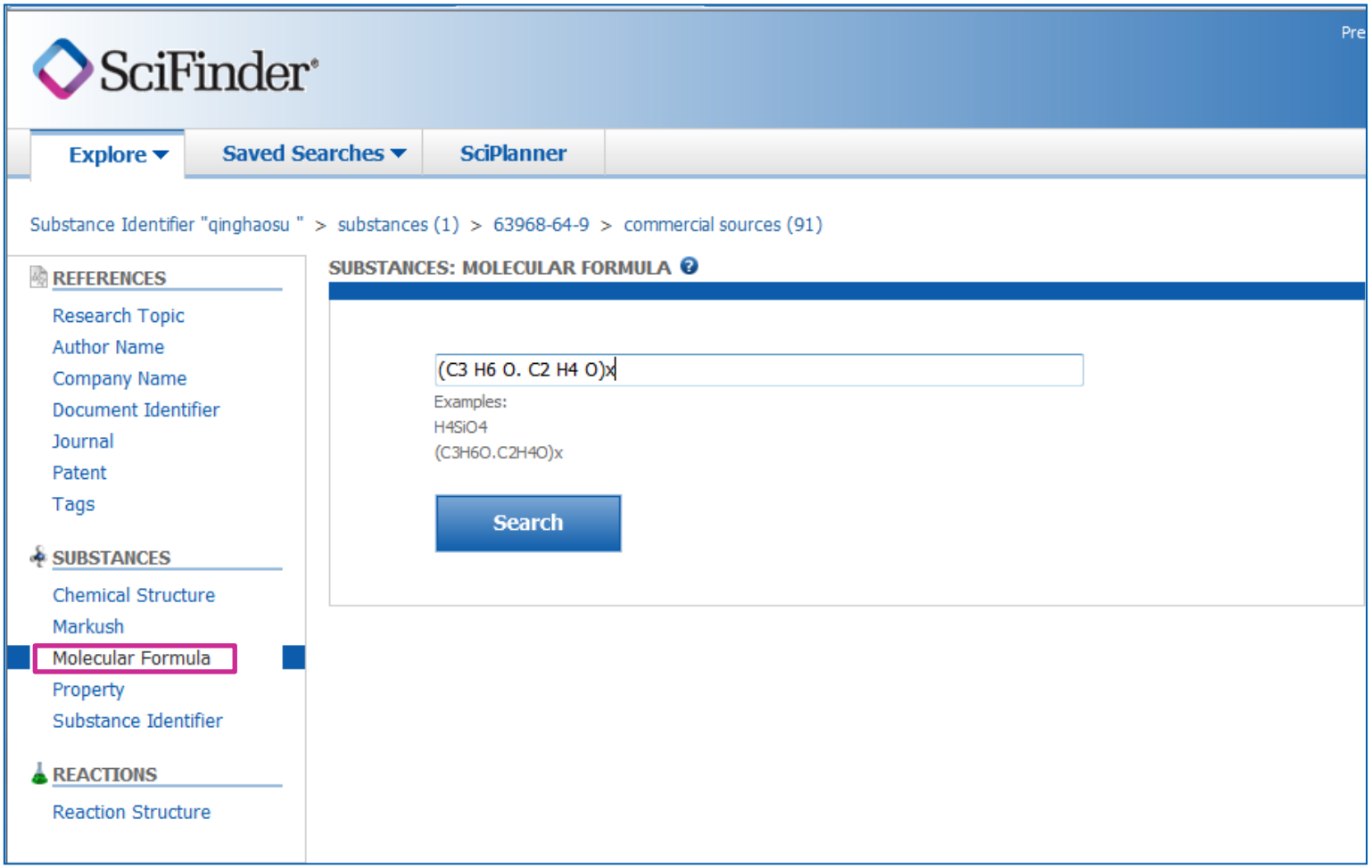


直接输入物质的名称，CAS No，俗名，都能检索，一次最多检索25个物质，用换行换开

理化性质检索

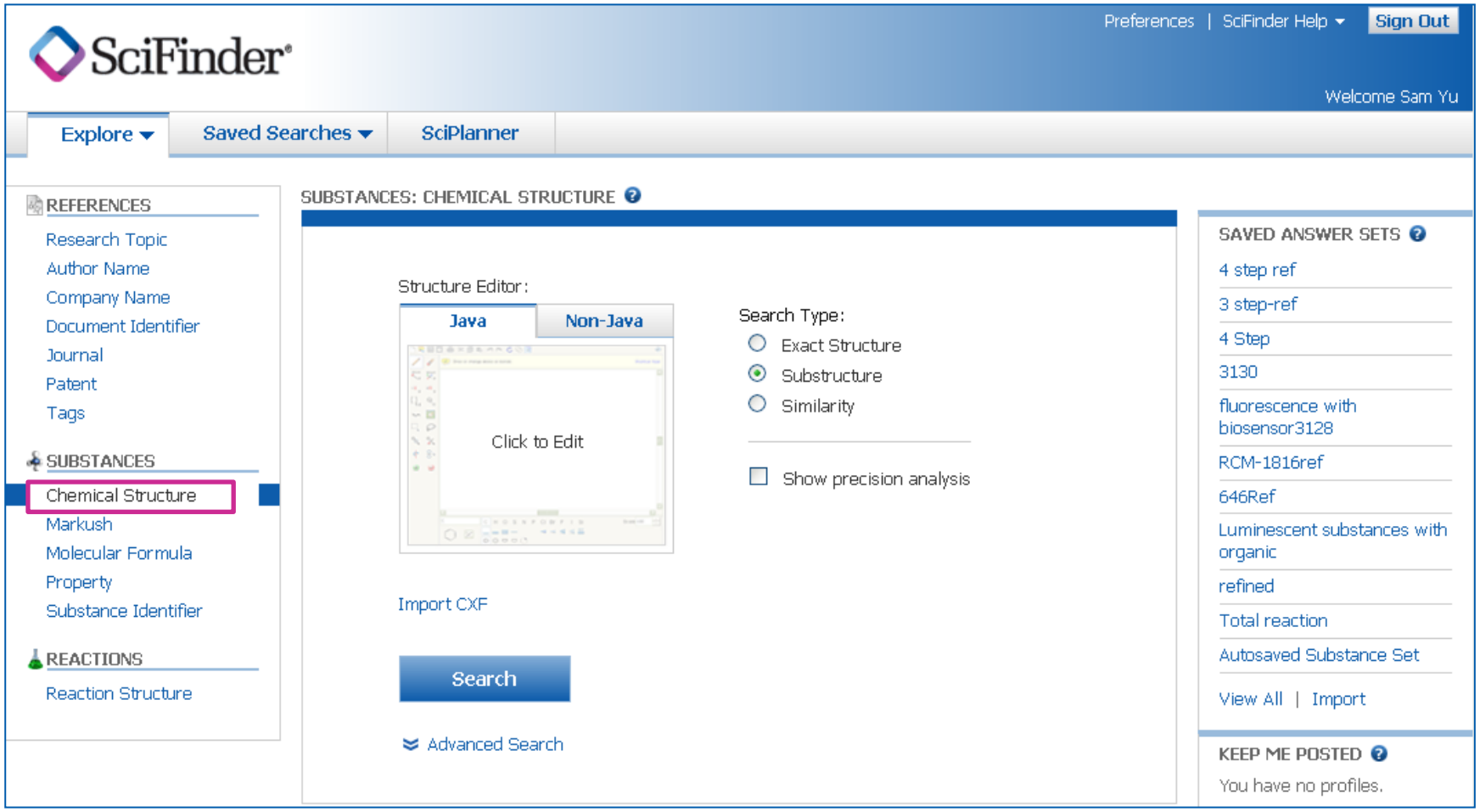


分子式检索

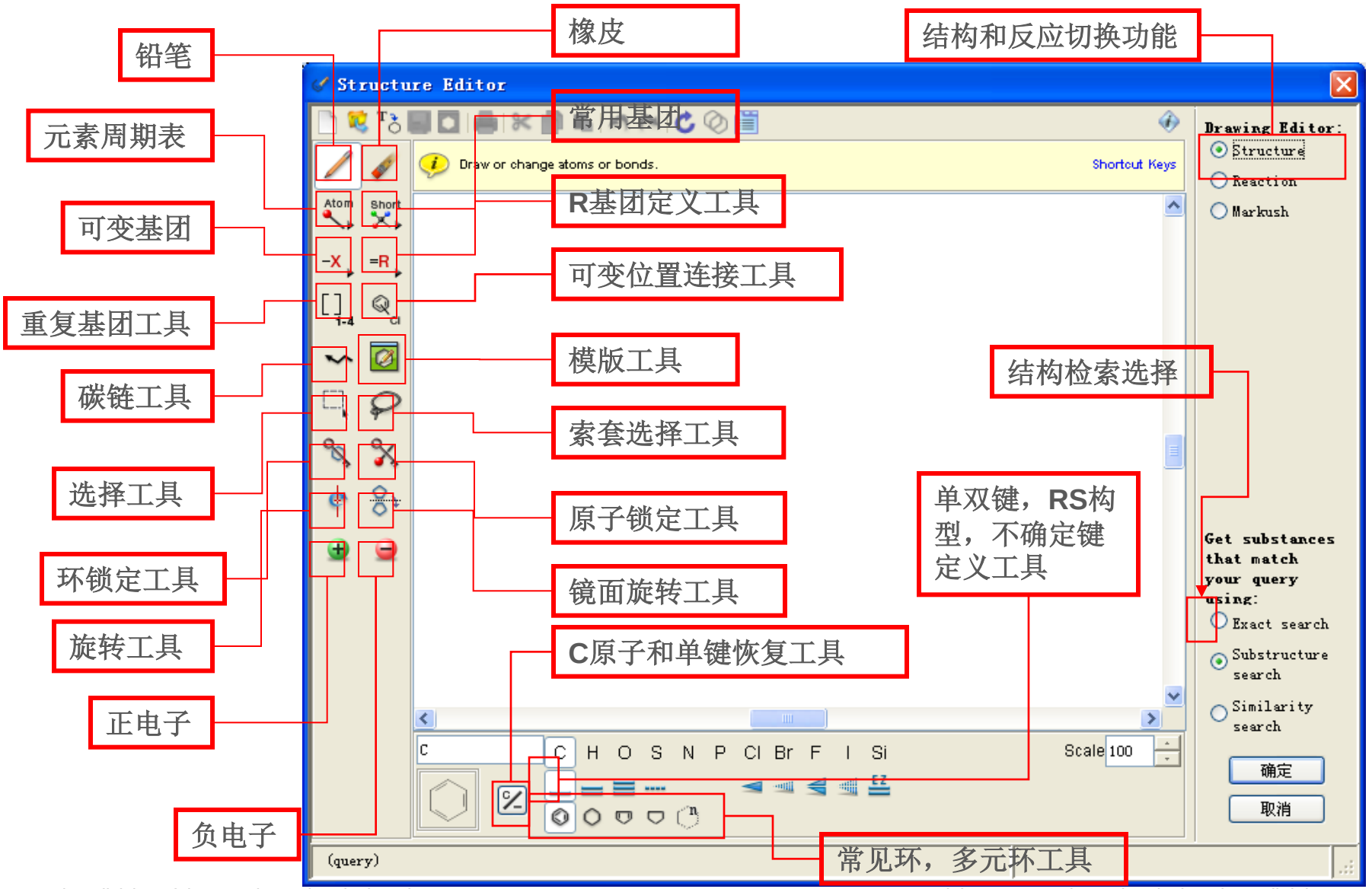


SciFinder中的分子式的检索，需要按照HILL排序方式输入，简单来说，CH写前面，其他的按照字母顺序写

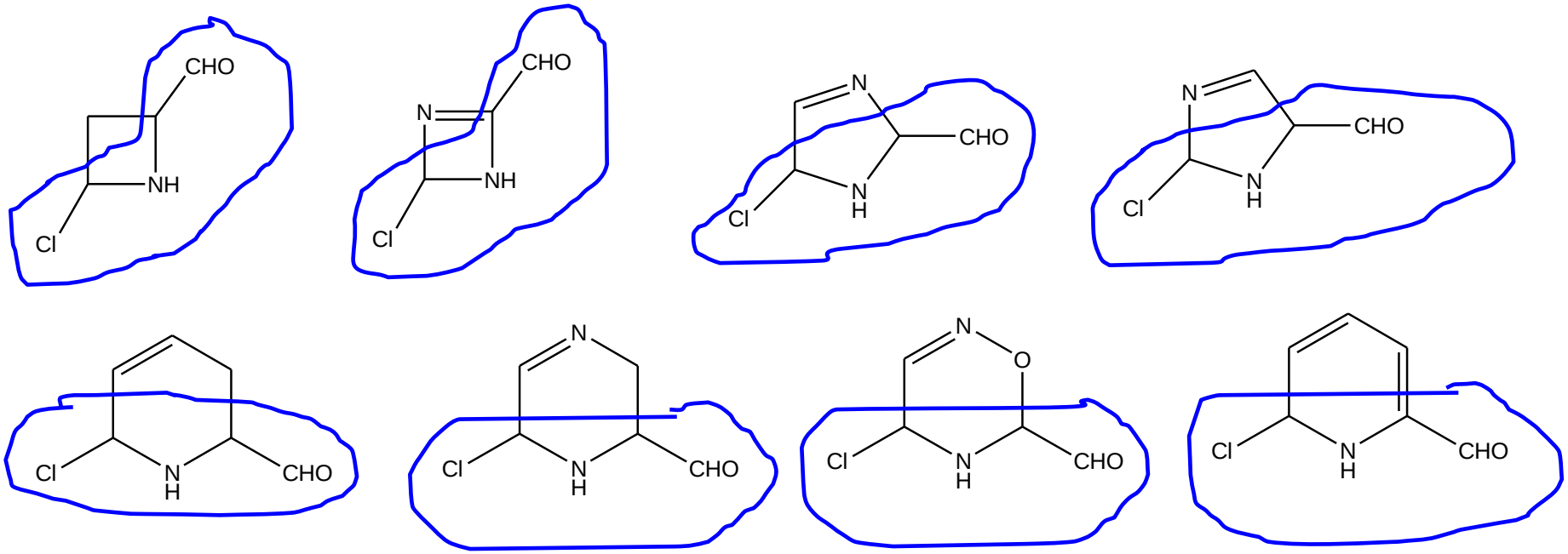
结构式检索



SciFinder结构绘制工具

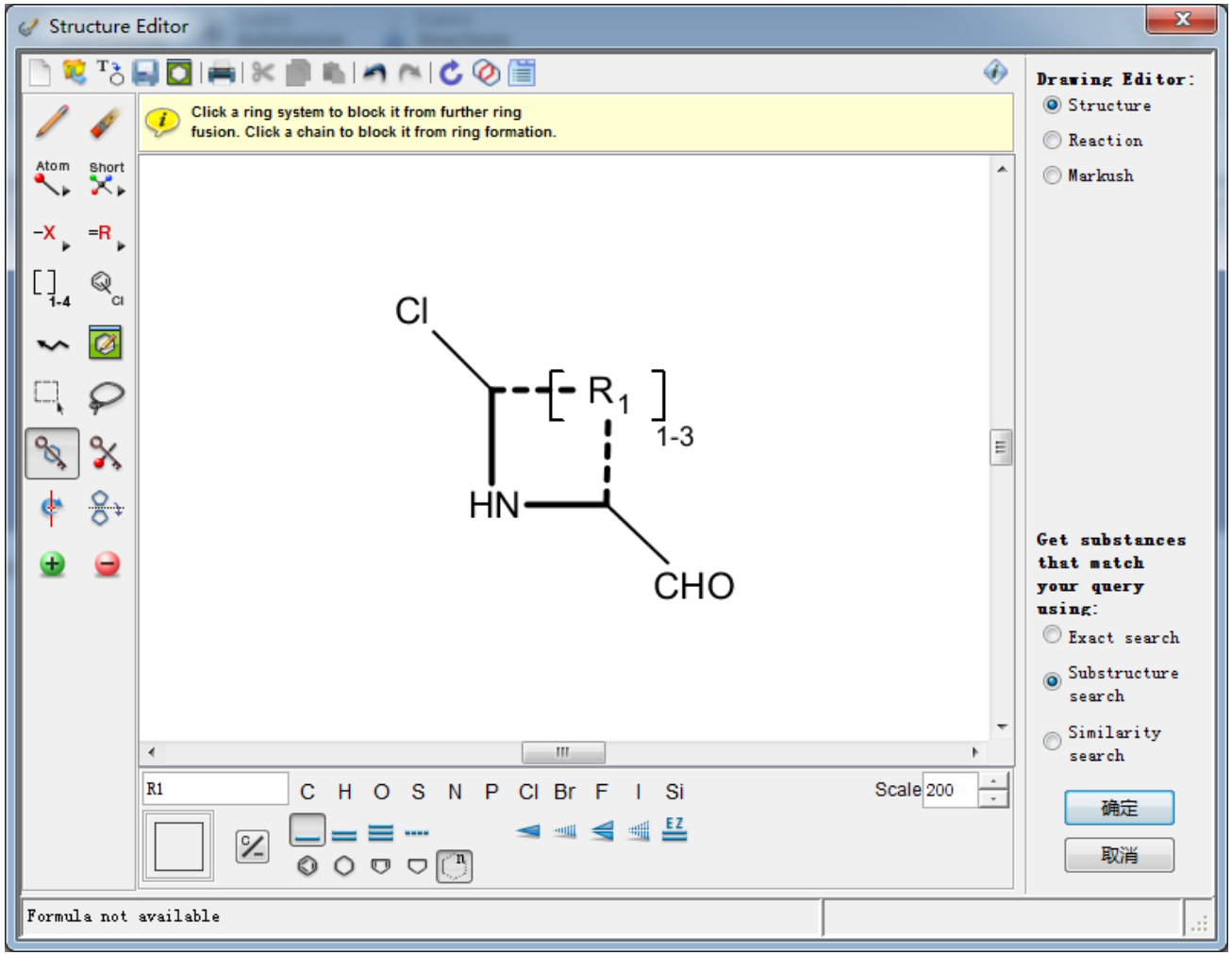


想获得以下的一系列物质



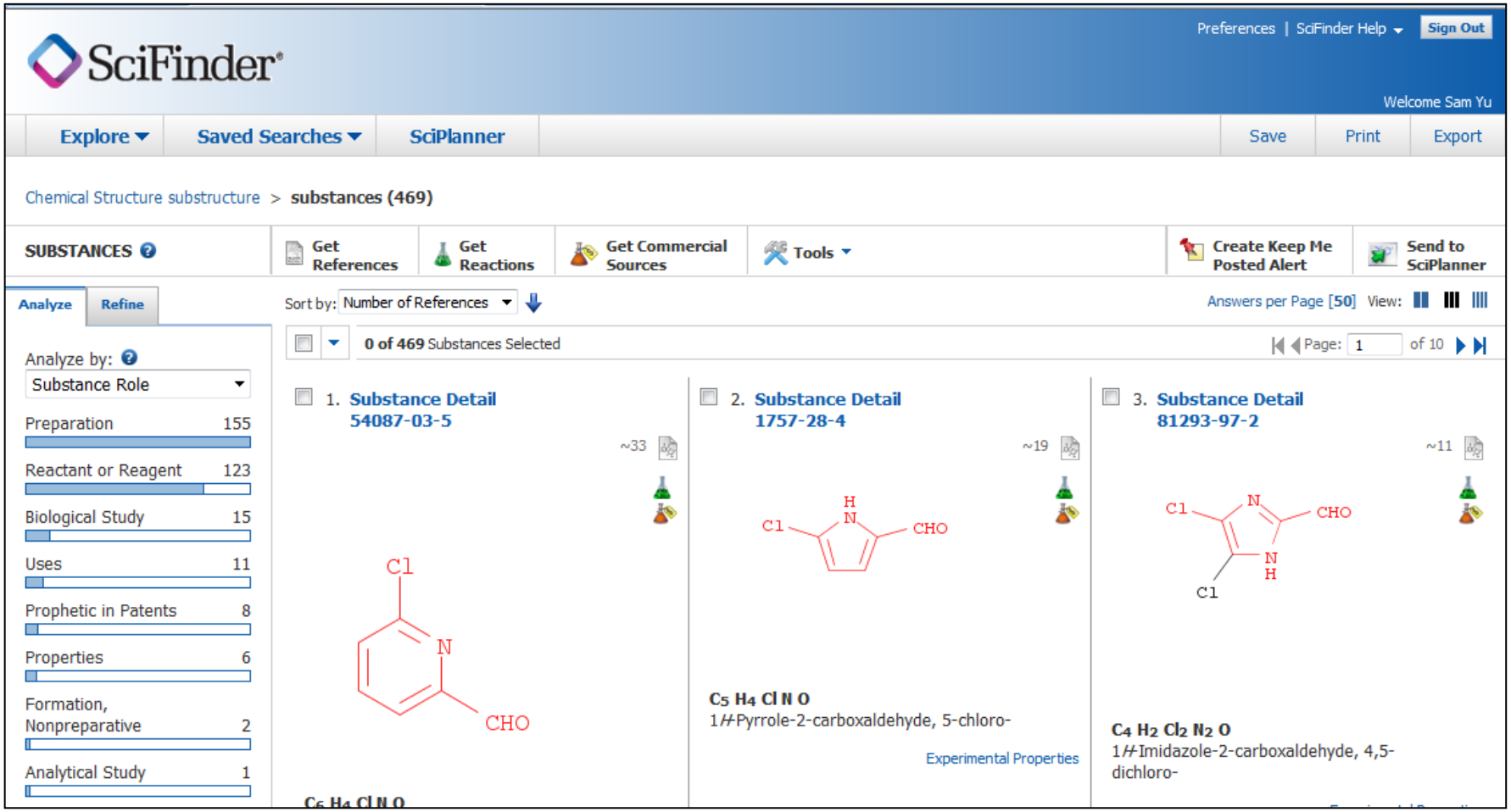
° ° ° ° ° °

结构定义



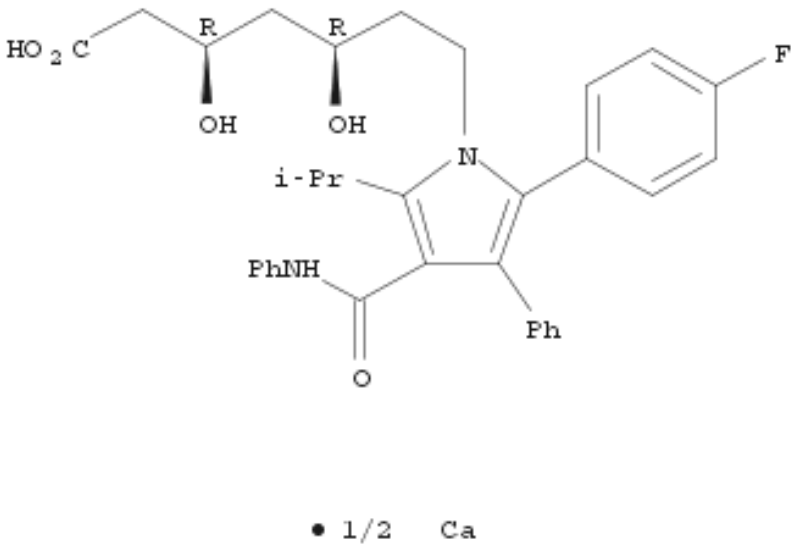
用亚结构检索获得所有的物质

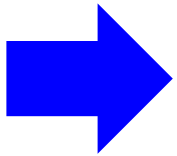
亚结构检索结果



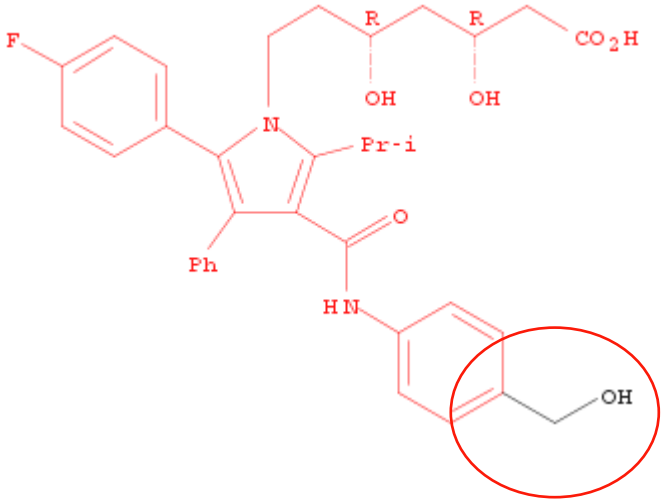
案例研究

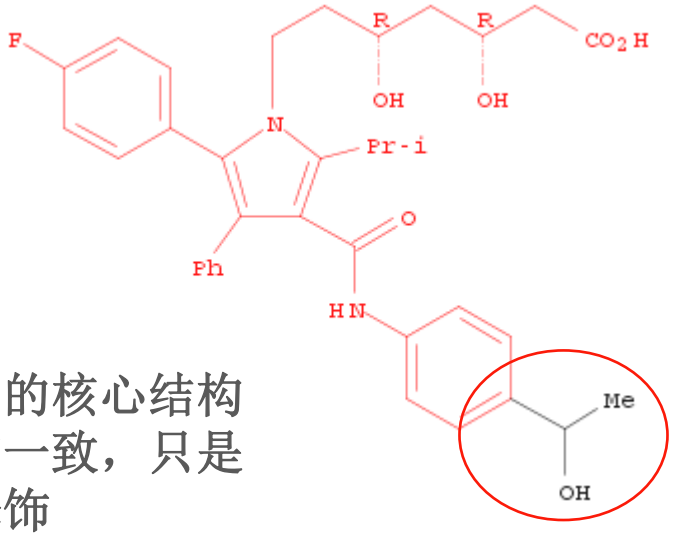
对某一结构进行改造，看是否有更好的新结构



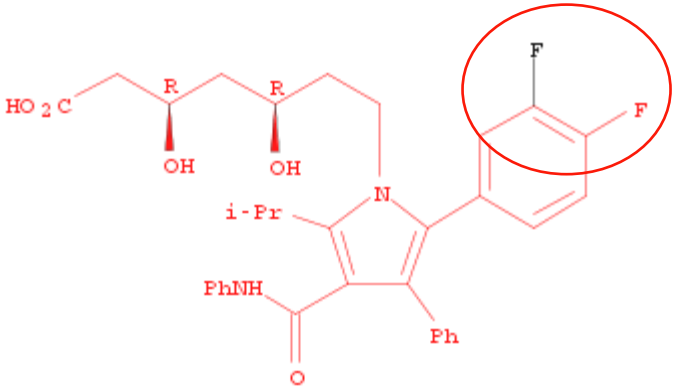


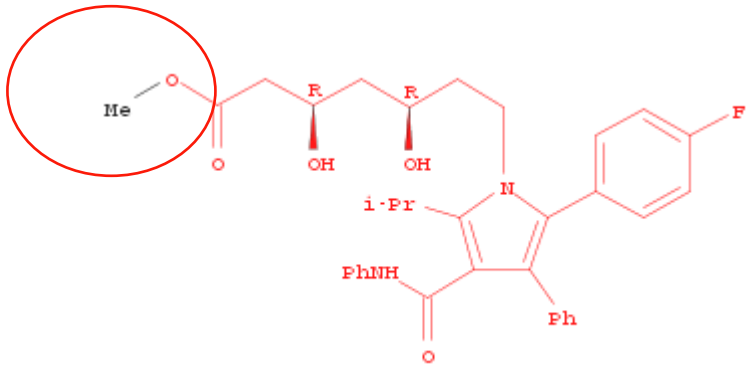
Substructure Search—用于检索结构的修饰物



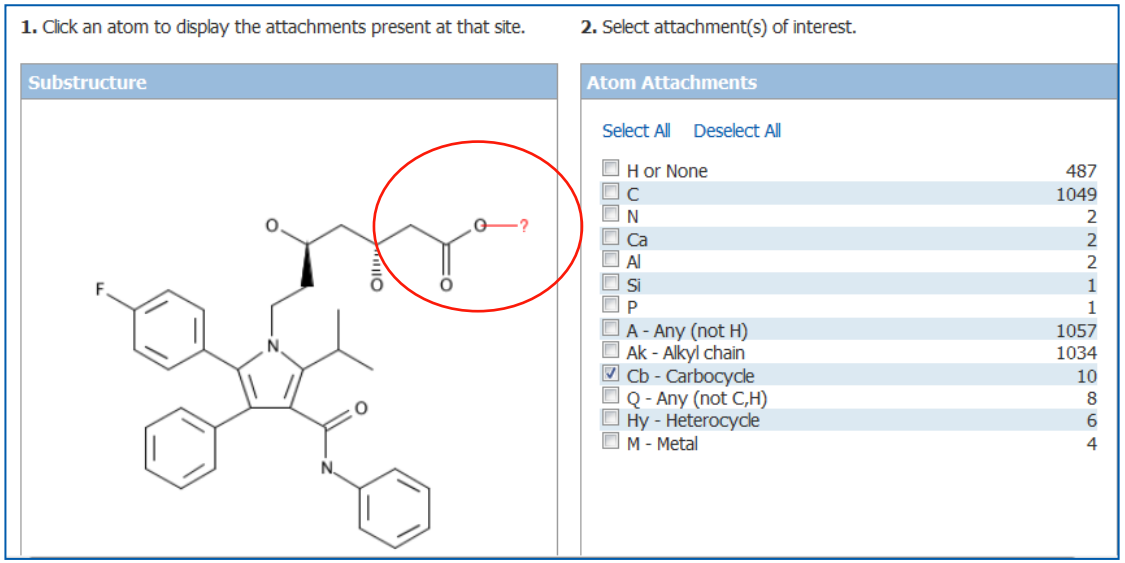


这些物质的核心结构都和母核一致，只是多了些修饰





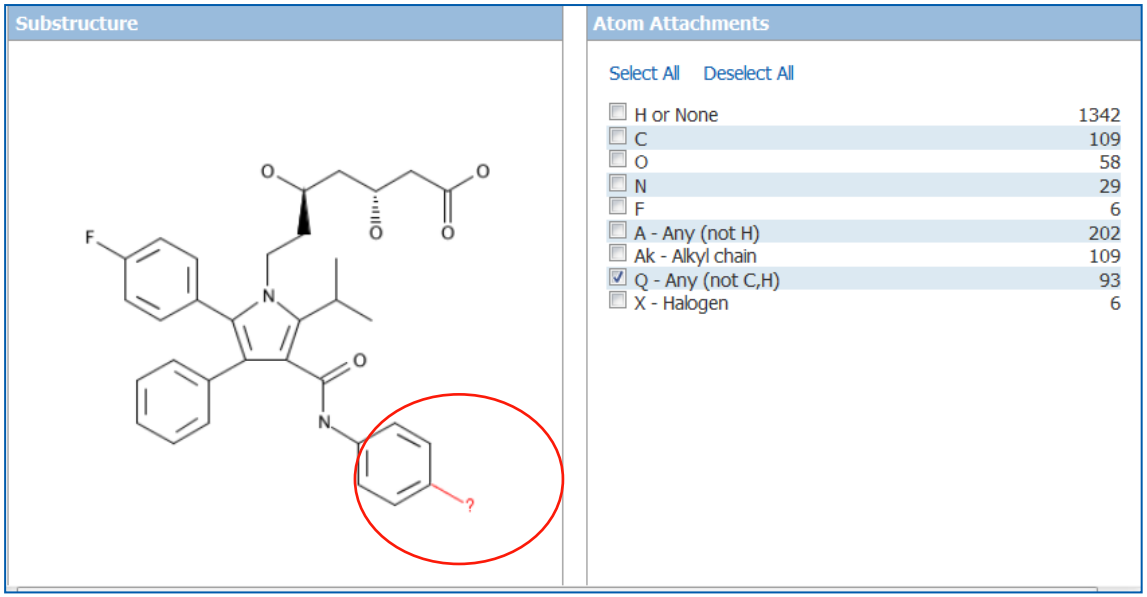
Atom Attachment直接限定感兴趣的修饰位点



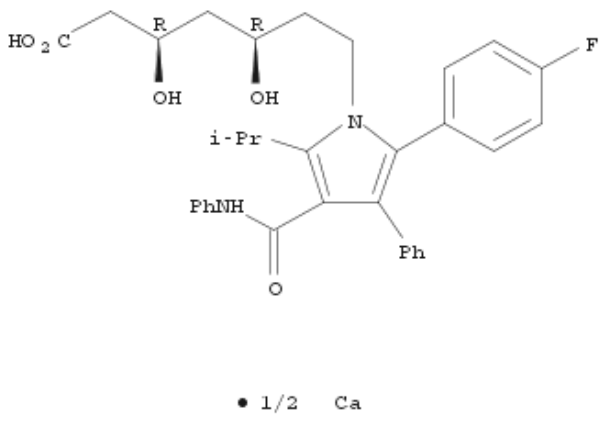
对支链O的修饰研究

对苯环对位修饰研究

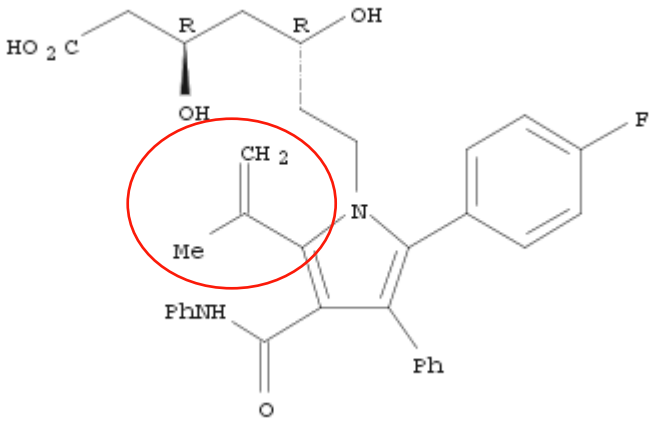
对特定位点的修饰了解，帮助了解该位点都已经有了什么类型的修饰研究，便于开创新的修饰结构，也可配合文献调研，获得与构效关系有关的判断。

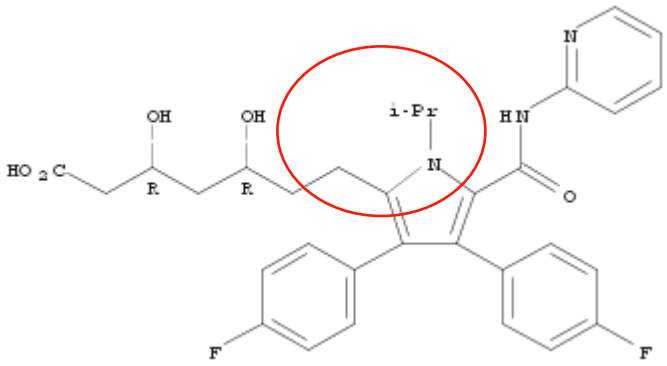


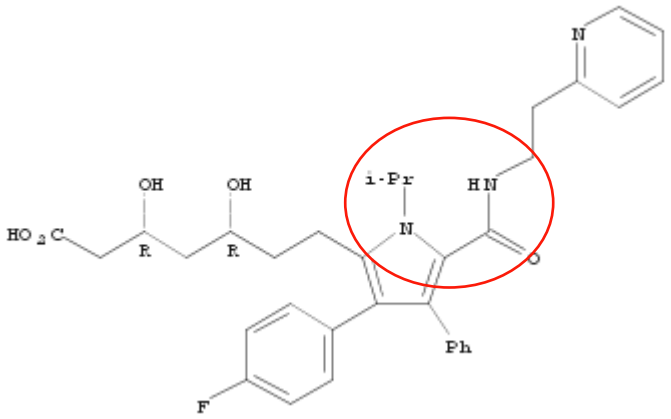
Similarity Search—用于检索结构的类似物



结构都存在相似性，
但是又和原结构有
不同的地方



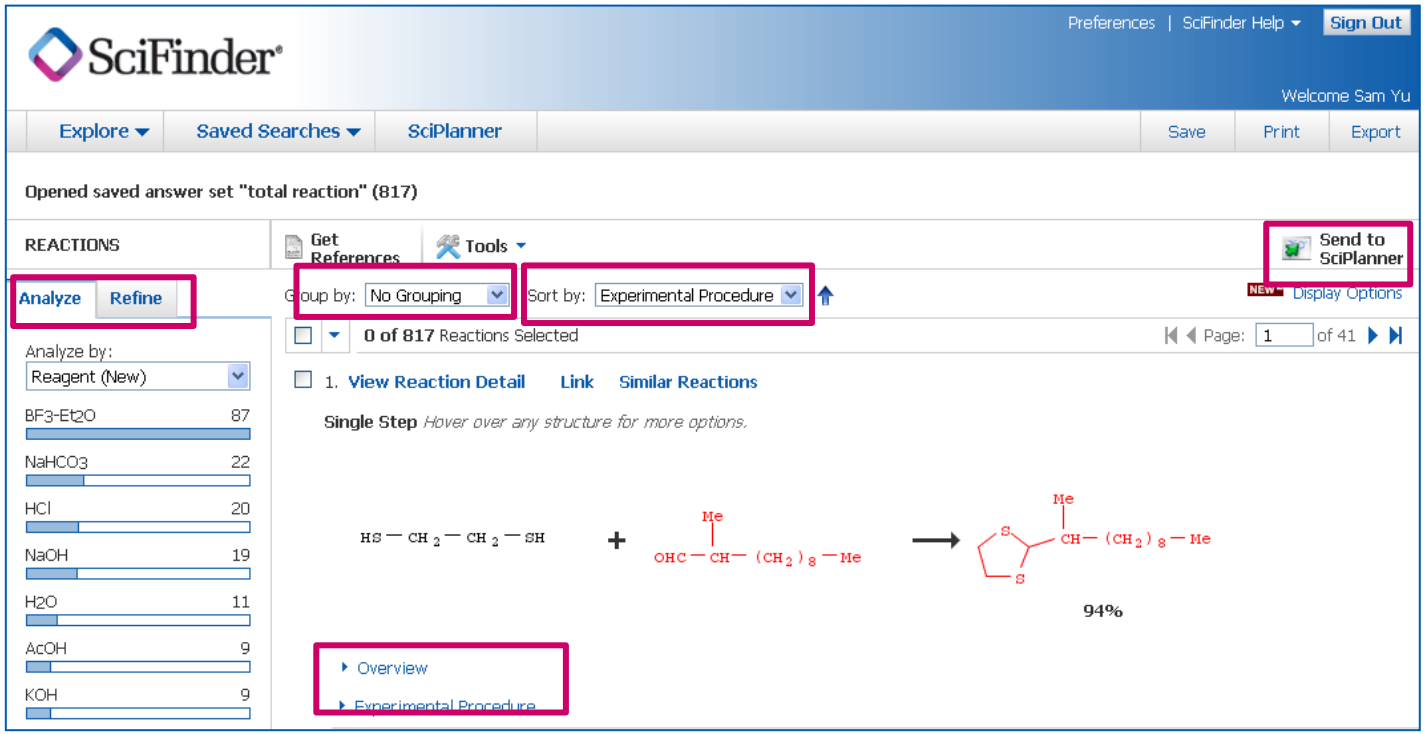




提纲

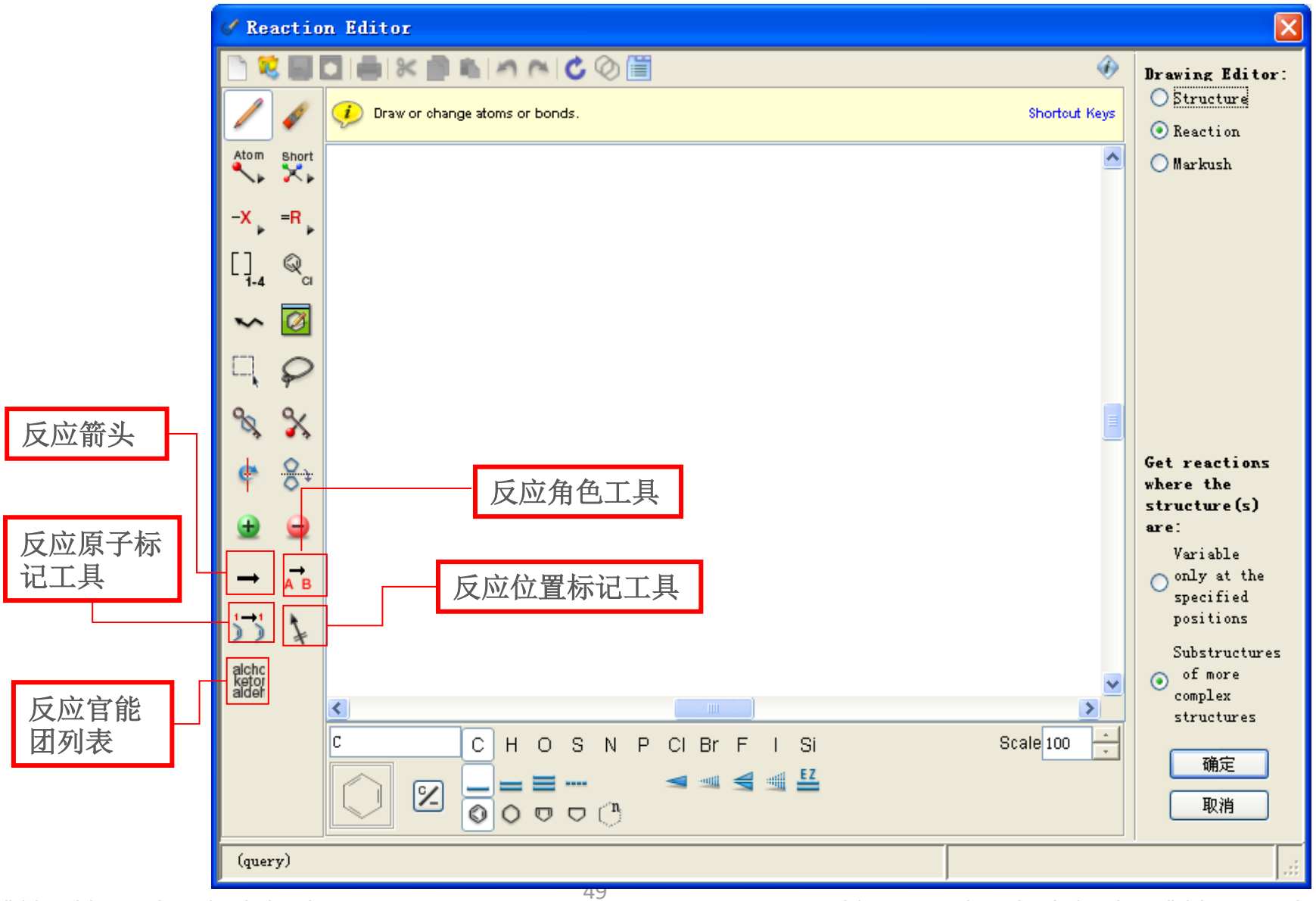
- 介绍
  - SciFinder Web中的内容
  - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索技巧
  - SciFinder Web中的反应记录及反应检索技巧
- **SciFinder Web的注册和常见问题**

SciFinder Web中的反应记录

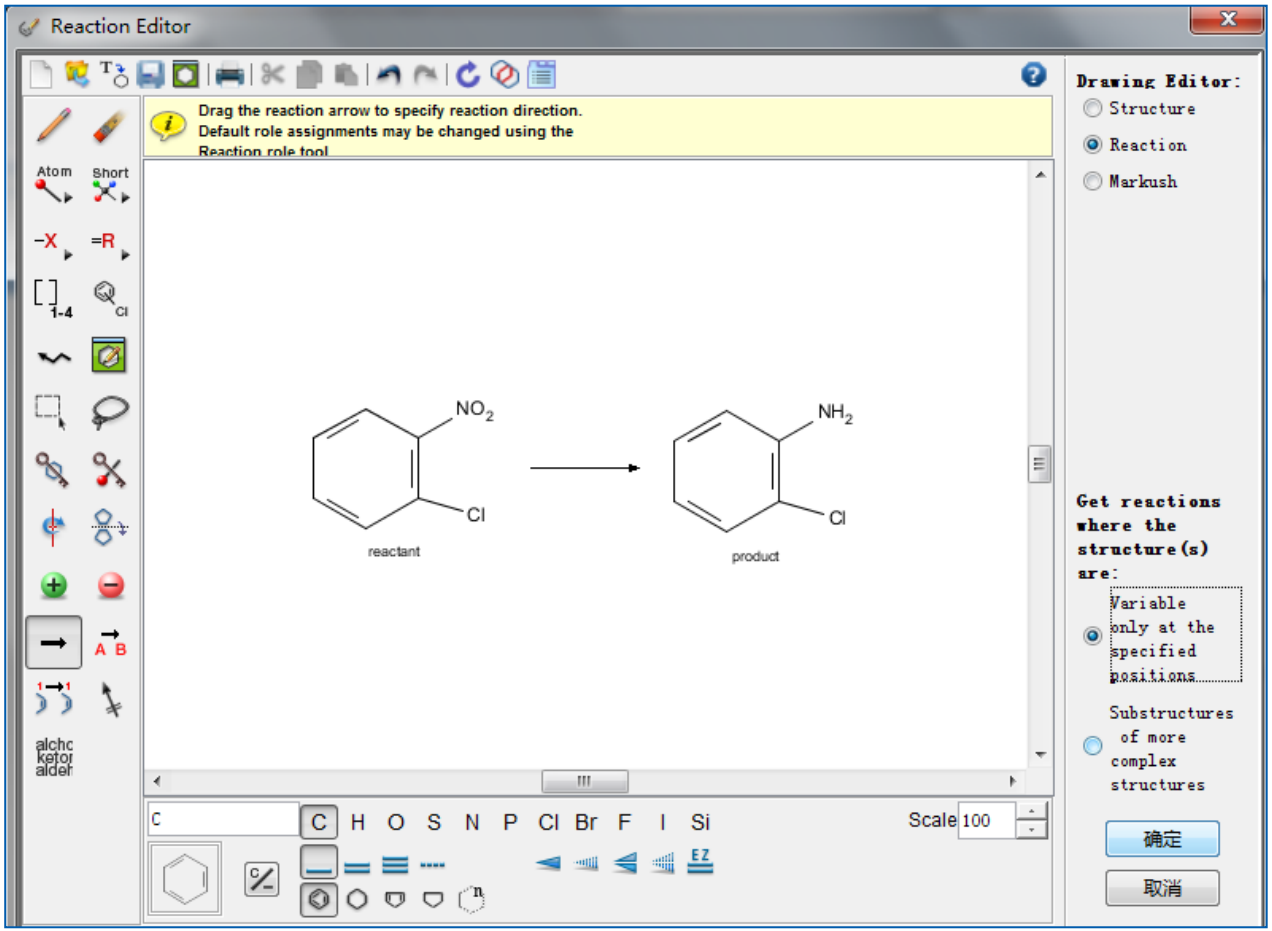


1. 反应分组功能
2. 反应排序功能
3. 反应后处理功能
4. 反应全景及实验过程
5. SciPlanner

SciFinder中的反应定义工具



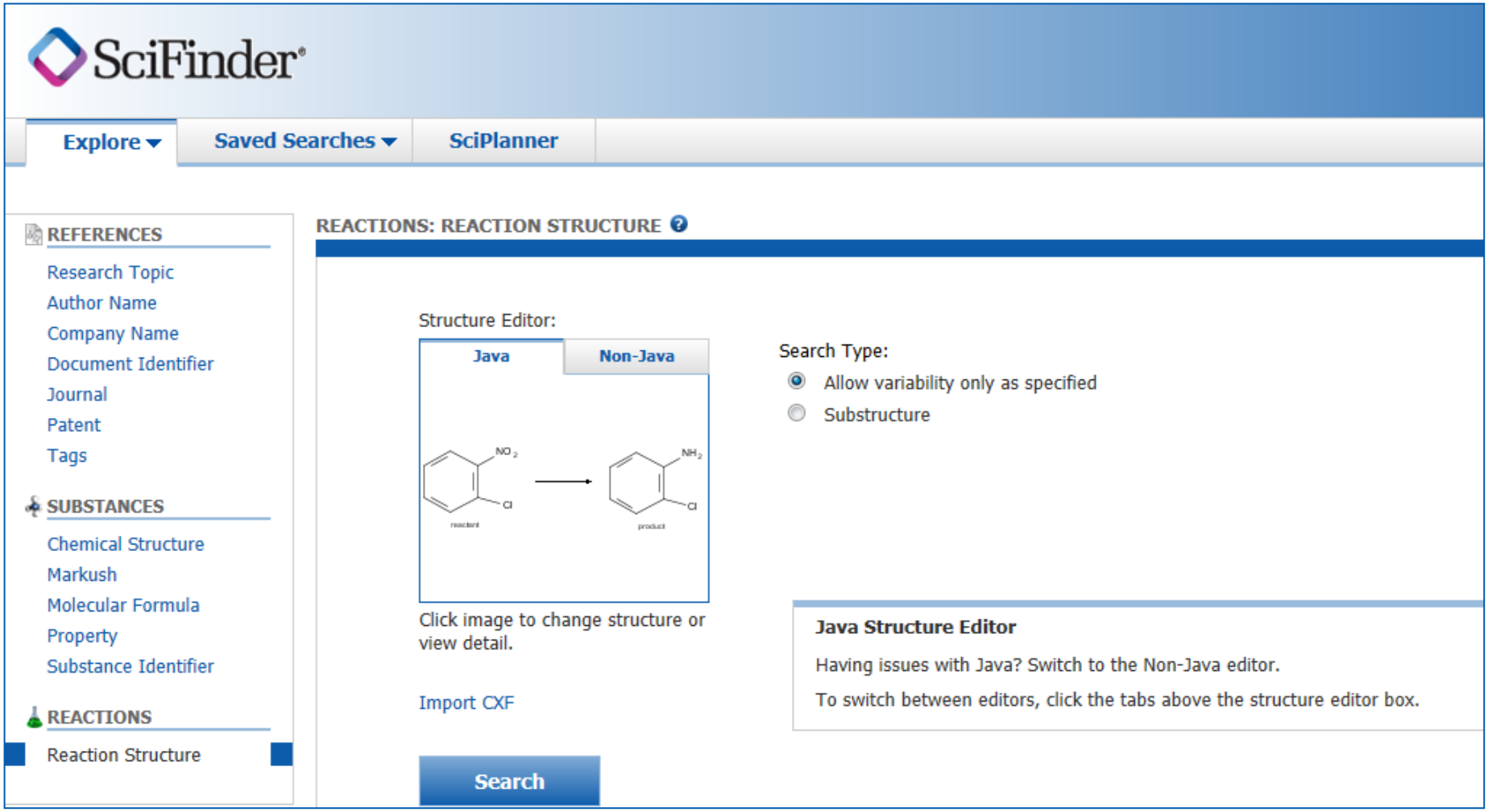
SciFinder反应检索



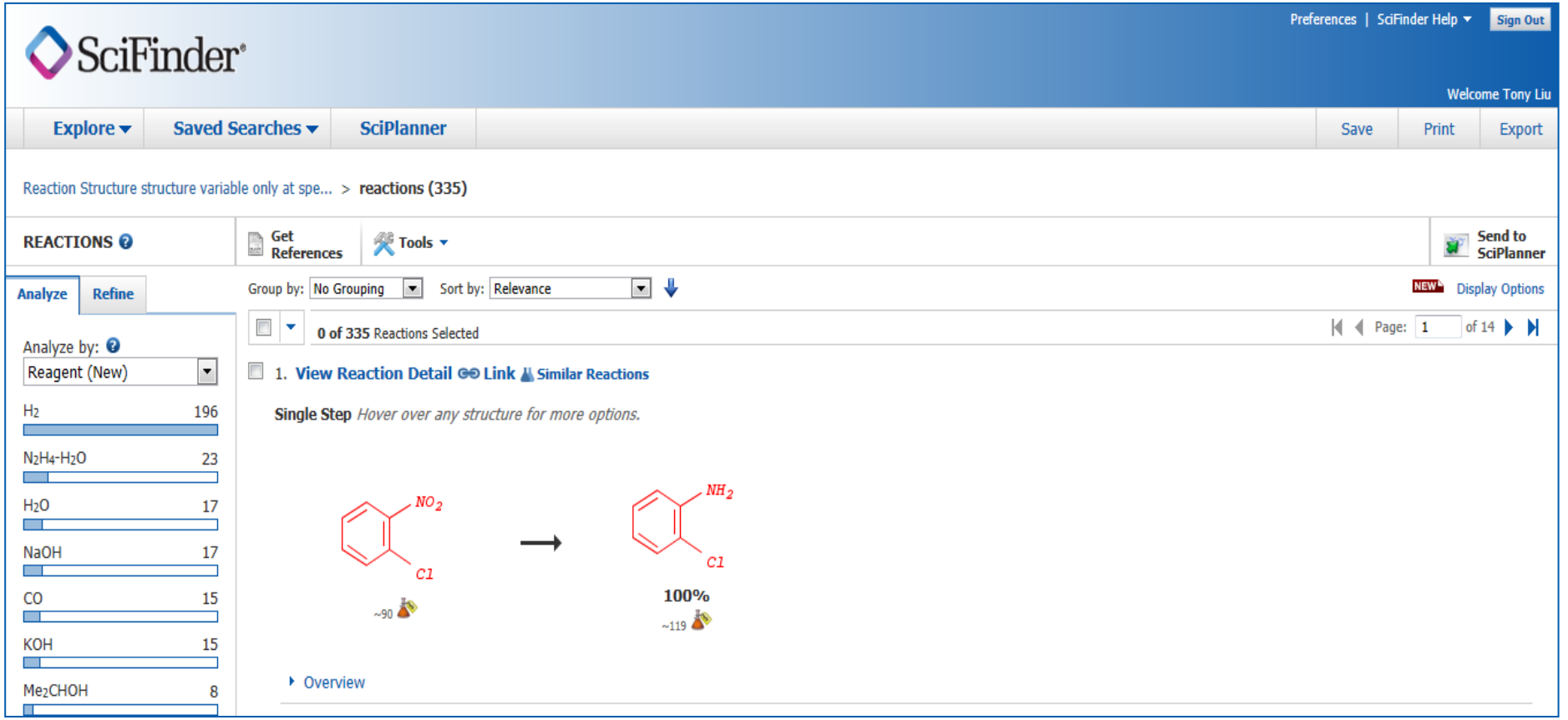
Allow variability only as specified: 仅在特定位点发生变化

Substructure:亚结构检索，允许有更多取代情况

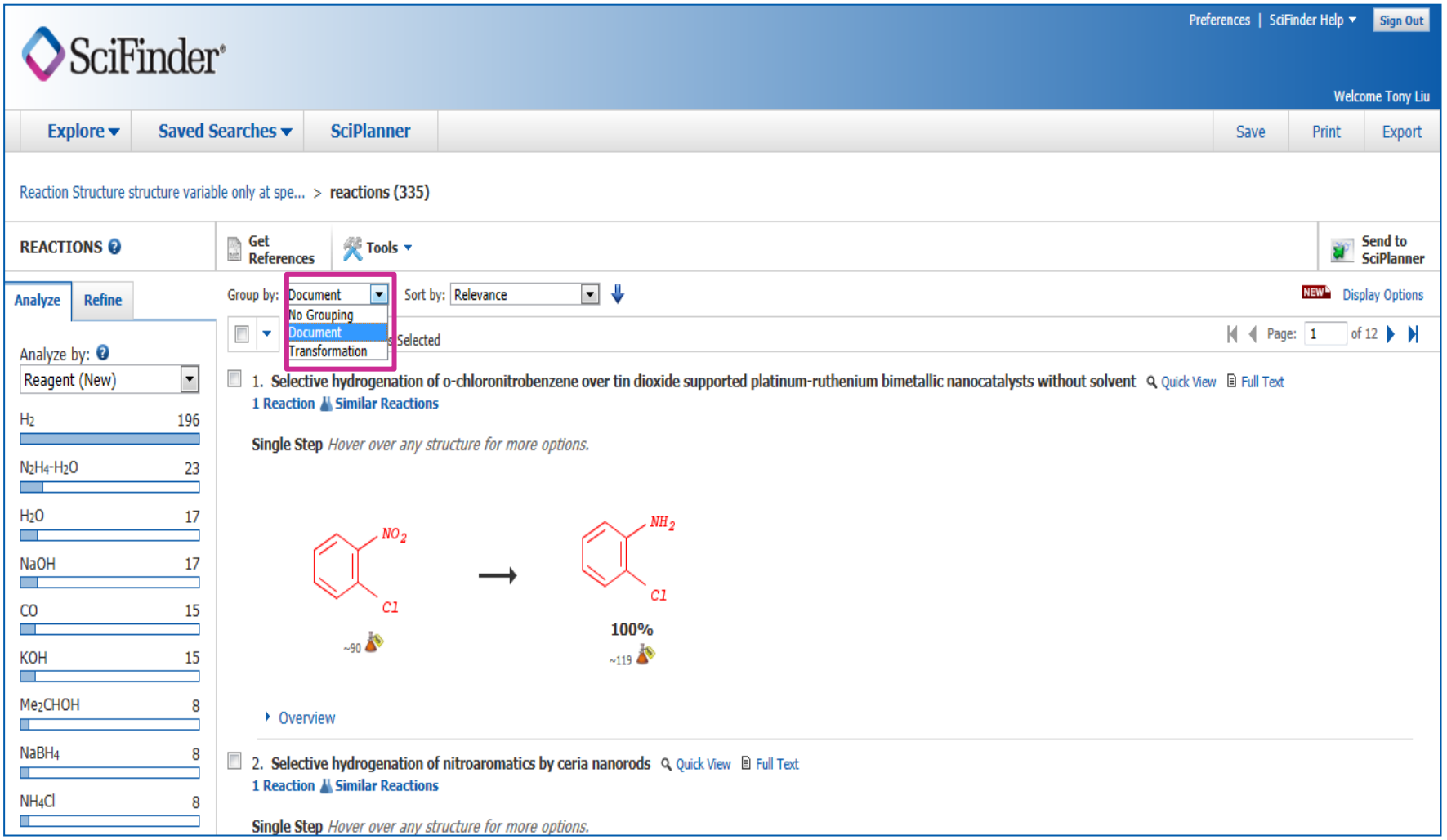
反应检索界面



精确反应检索结果

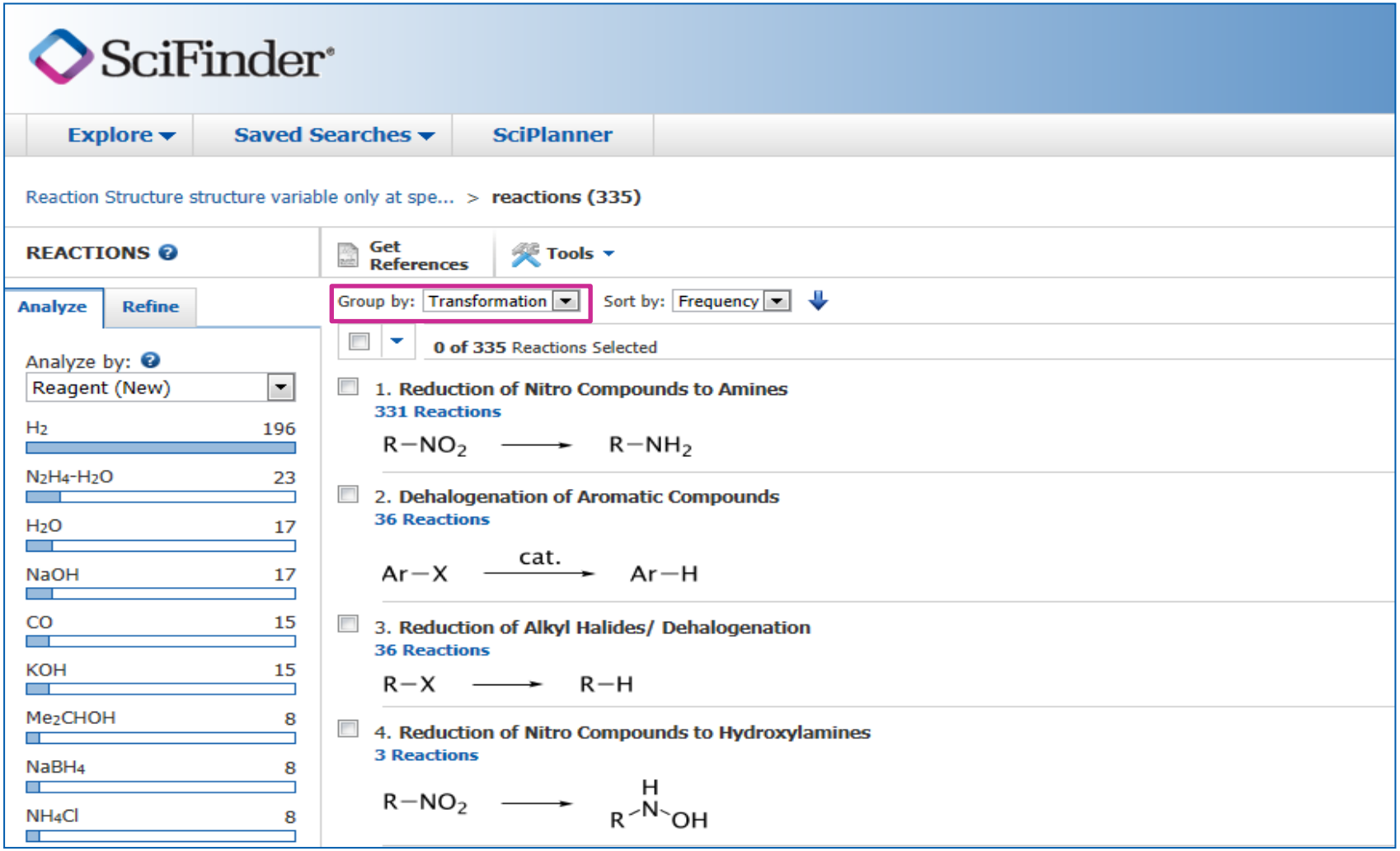


Group by Document 按照出处文献分类显示



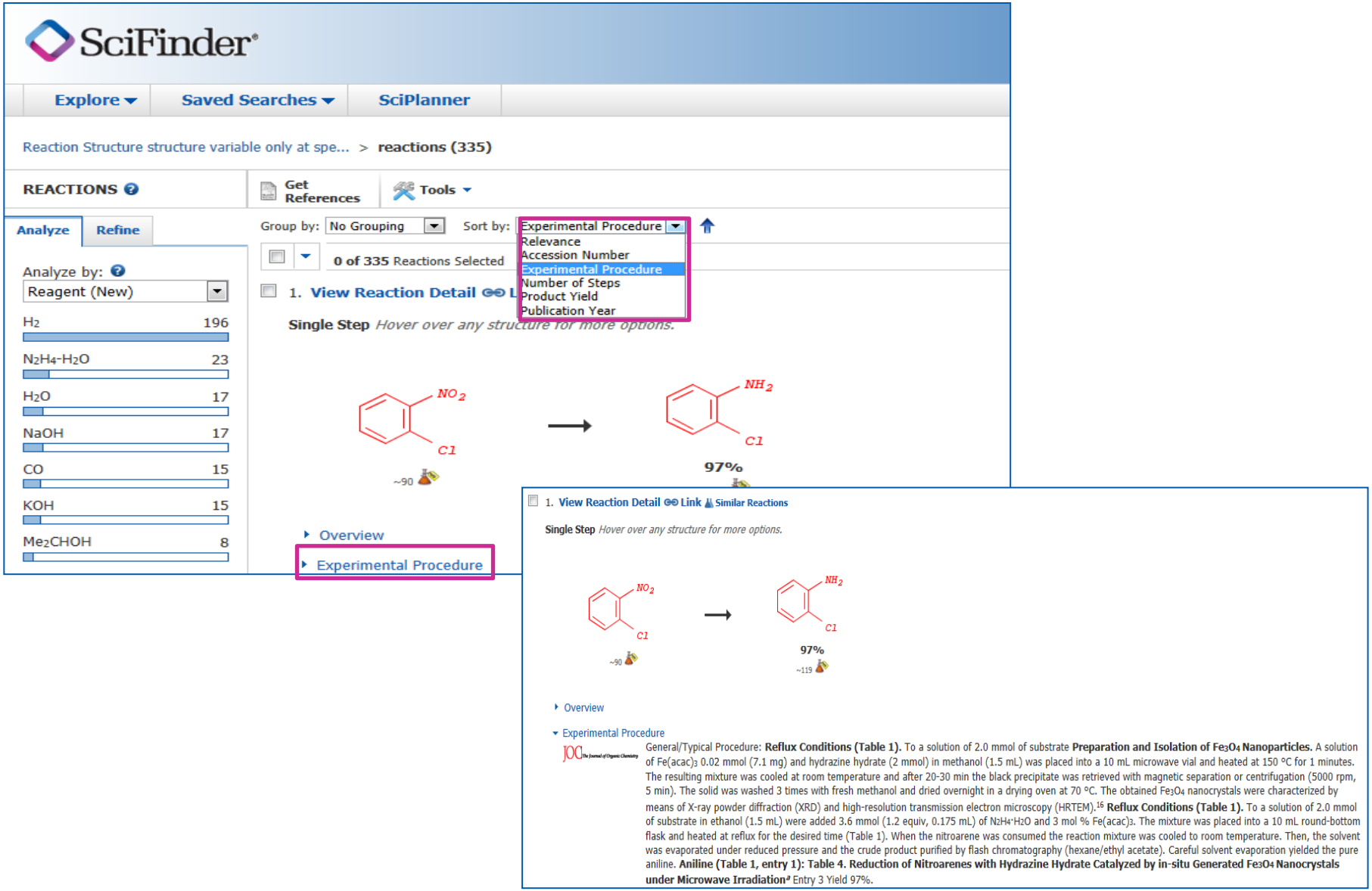
来自同一篇文献的反应都被整合到一起并集中显示

Group by Transformation 按照反应类型分类显示

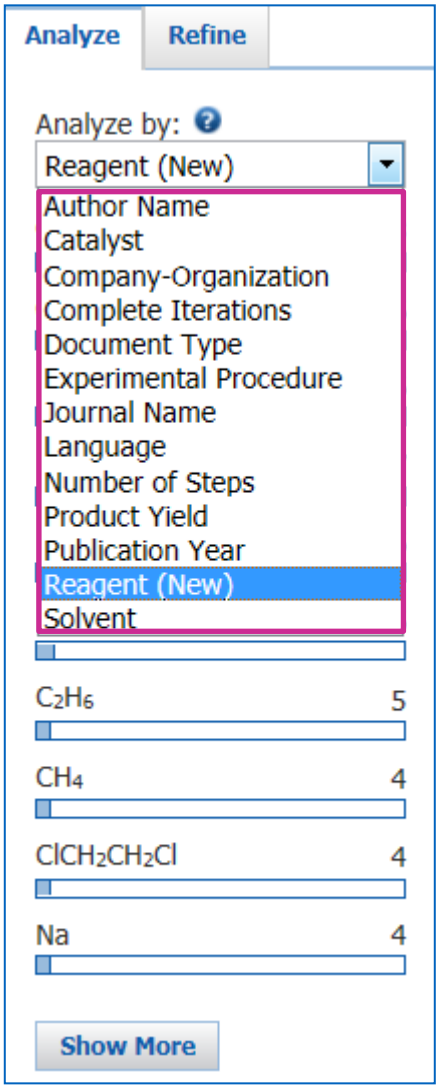


同一类反应被整合到一起并以通式结构集中显示；
仅适用于单步反应，未被分类的反应显示在结果集最后

获得有实验步骤的反应结果集



反应结果集的分析限定工具

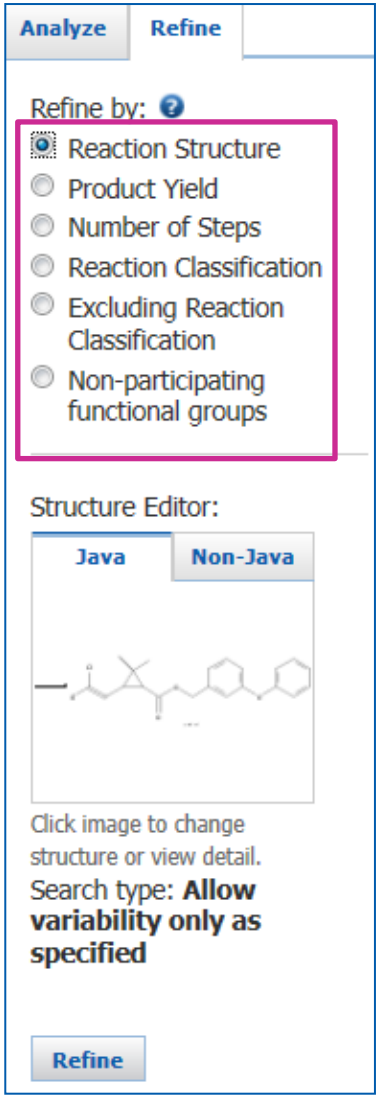


反应分析类型：

作者姓名	出版语言
催化剂	出版年代
机构名称	反应步数
文献类型	产率
期刊名称	试剂
实验步骤	溶剂

反应的限定功能：

反应式
产率
反应步数
反应类型
排除的反应类型
不参与反应的基团



提纲

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  - SciFinder Web中的内容
  - SciFinder Web中的新功能
- **SciFinder Web中的检索和后处理**
  - SciFinder Web中的文献记录及主题检索
  - SciFinder Web中的物质结果及物质检索技巧
  - SciFinder Web中的反应记录及反应检索技巧
- **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 9.x或者FireFox 2.x

Mac 用户支持 Firefox 和 Safari

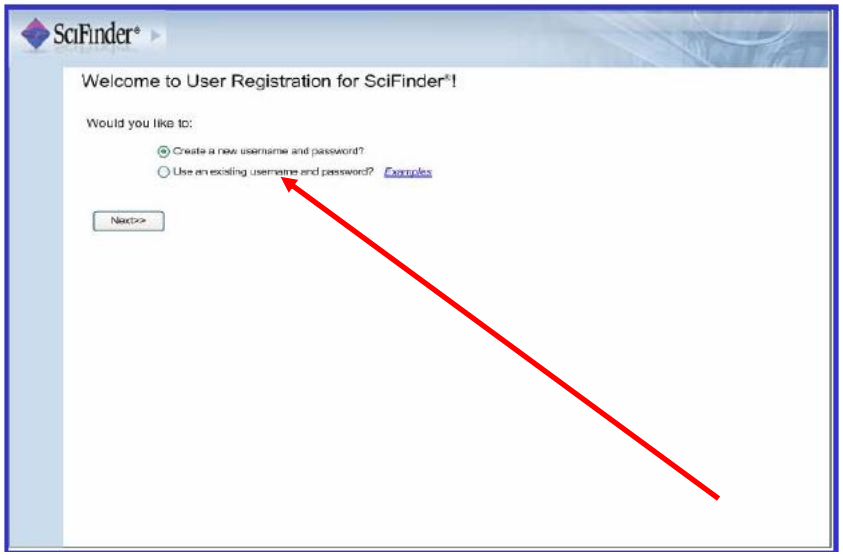
Java 安装（初次使用结构时自动安装，建议安装Java 7）

在图书馆相关页面上找到SciFinder Web注册用的网址

鉴于360浏览器以及360安全卫士会对SciFinder的使用造成一定的影响，建议大家最好不要使用360浏览器。

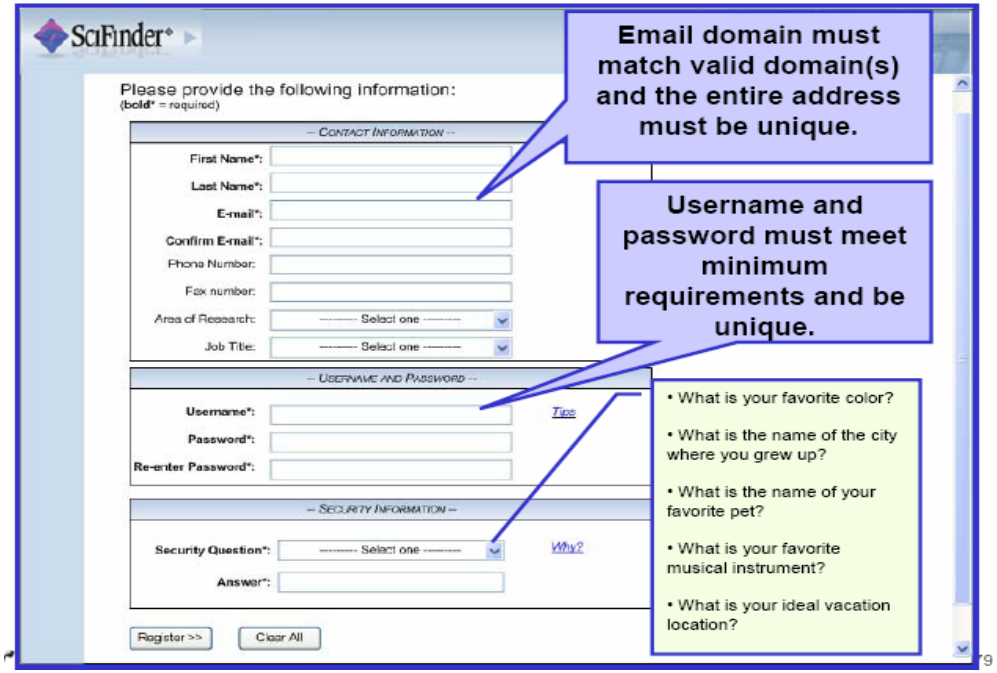
登陆图书馆主页

点击URL创建SciFinder Web账号



开始创建SciFinder Web帐号

请用邮箱注册，一人只能注册一个账号



设置用户名及密码注意事项

用户名：

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

-（破折号）　　_（下划线）

.（句点）　　@（表示“at”的符号）

密码：

必须包含 7-15 个字符，并且至少包含三个以下字符：

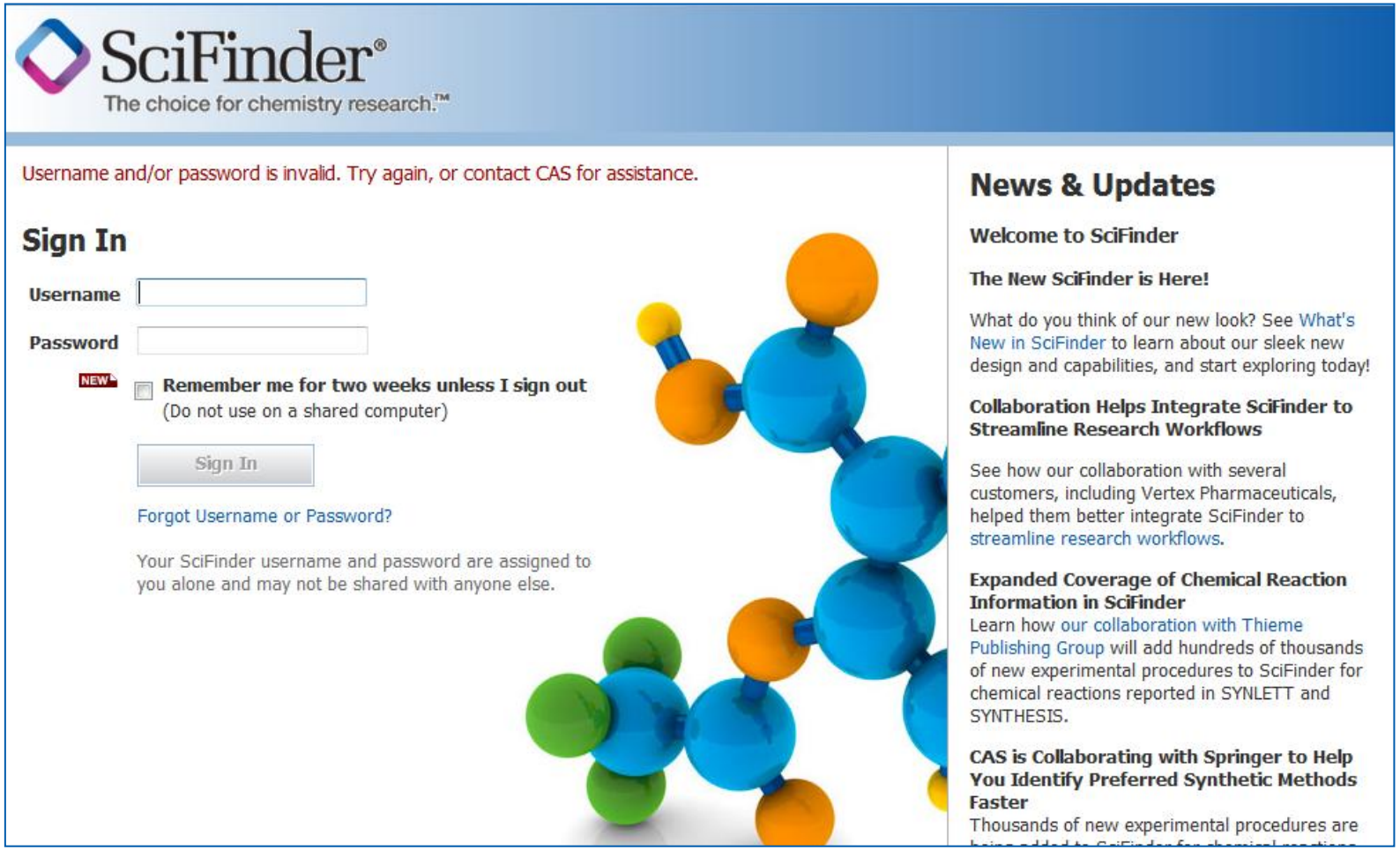
字母	混合的大小写字母
数字	非字母数字的字符（例如 @、#、%、&、*）

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

对新ID的Email确认

48小时内，需要点击邮件中的确认链接

SciFinder Web 常见问题



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

SciFinder Web网络在线资源平台

www.igroup.com.cn/cas

资源下载：**PDF文件**

在线演示：**Flash演示**

网络培训：不定期的网络专题培训

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Thank You

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