SciFinder检索工具介绍

SciFinder®

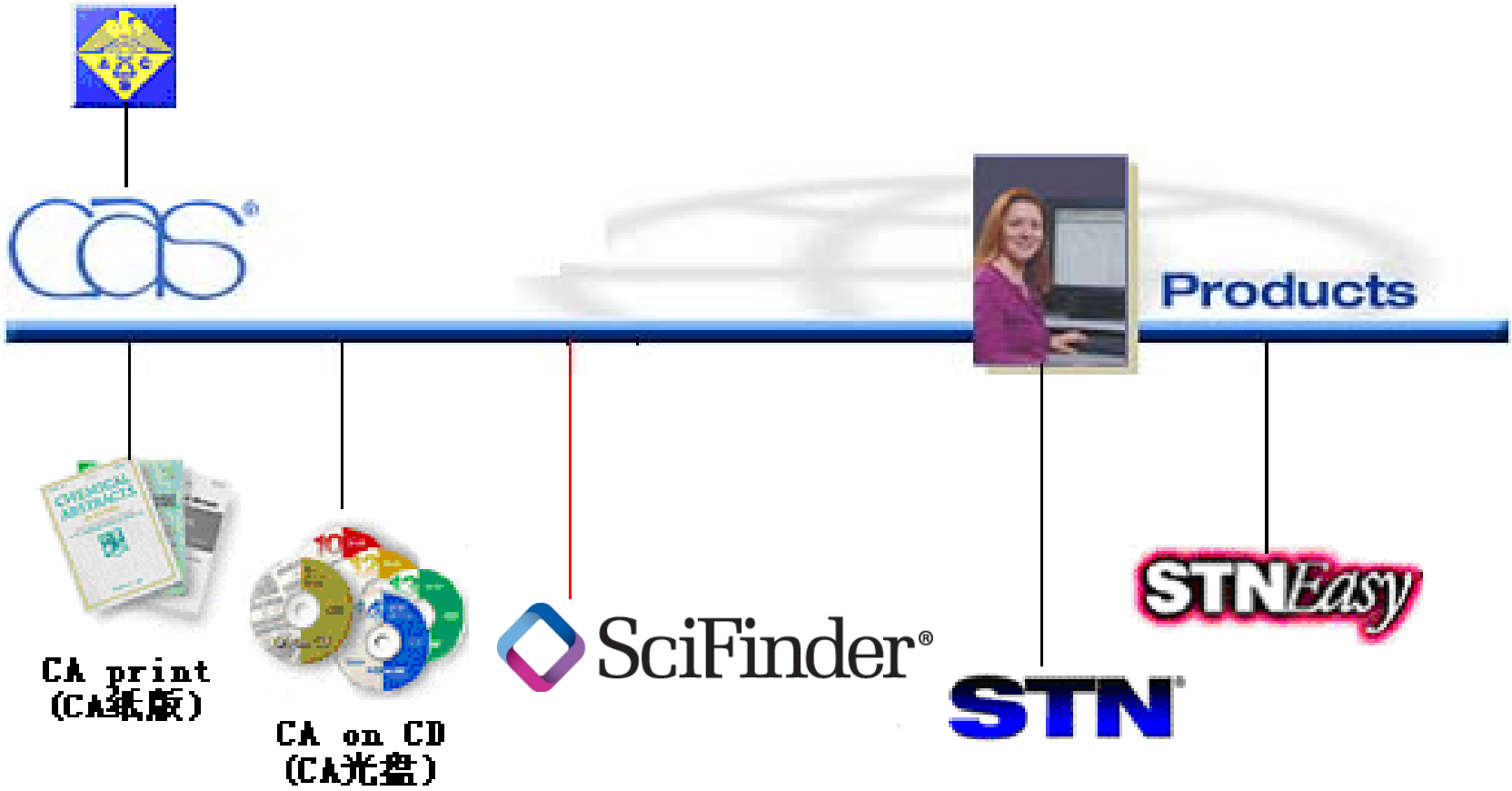
美国化学文摘社　中国代表处
陈东亮
15989176146
joe@igroup.com.cn

CAS | SciFinder®
CAS is a division of the American Chemical Society

- 美国化学文摘服务社（CAS）

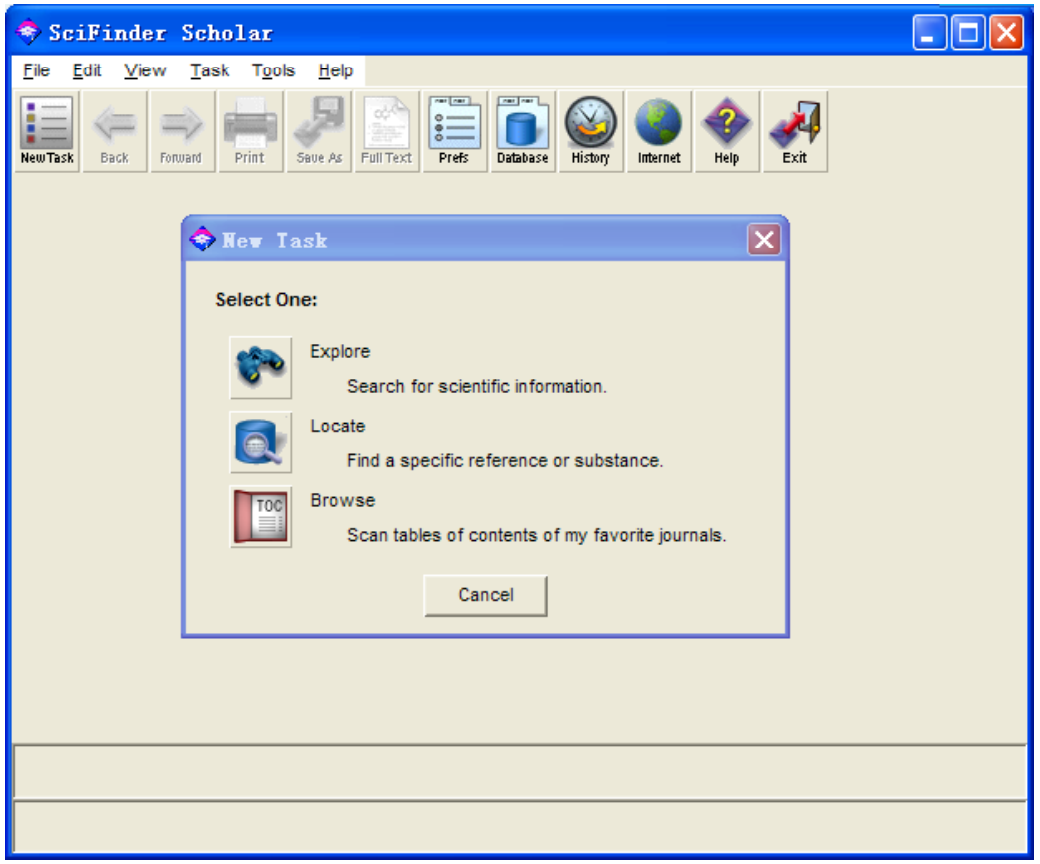
- 1907年 美国化学学会（ACS）分支机构
- 全球最大的科学协会组织
- 非盈利组织
- >1000 PHD从事文献编辑工作

SciFinder的背景---CAS主要产品



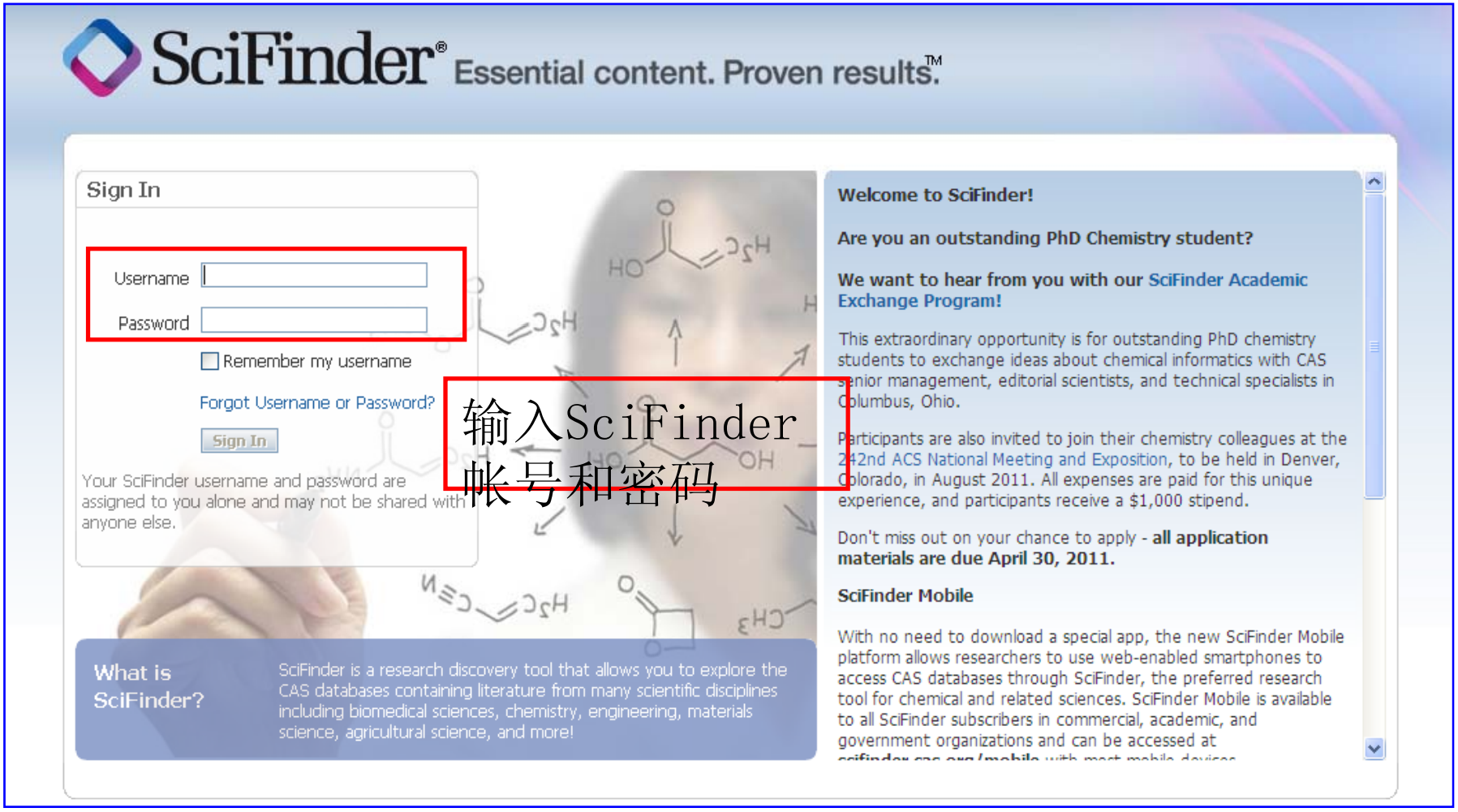
SciFinder scholar VS SciFinder Web

SciFinder® SCHOLAR



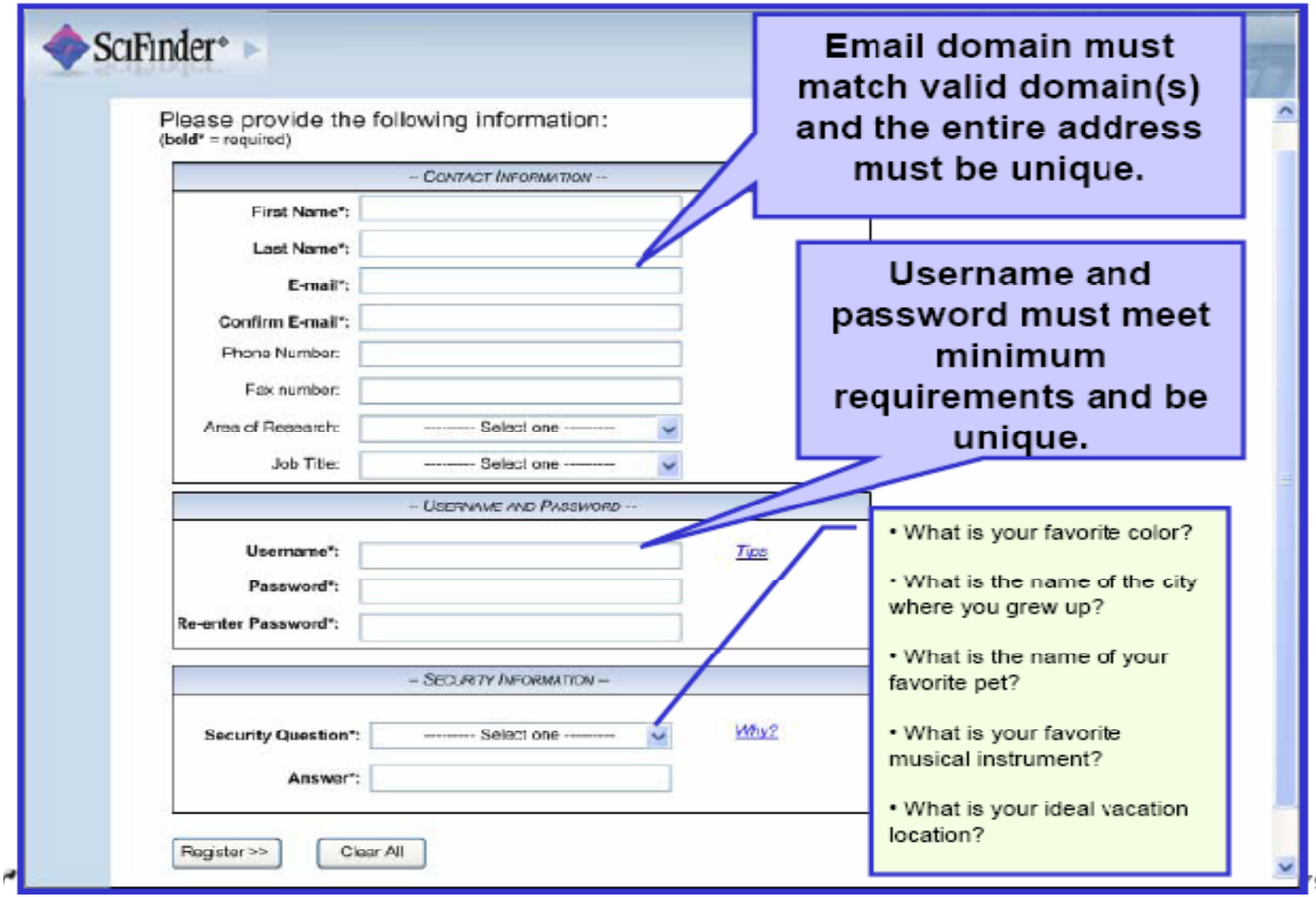
SciFinder登陆界面

Scifinder.cas.org

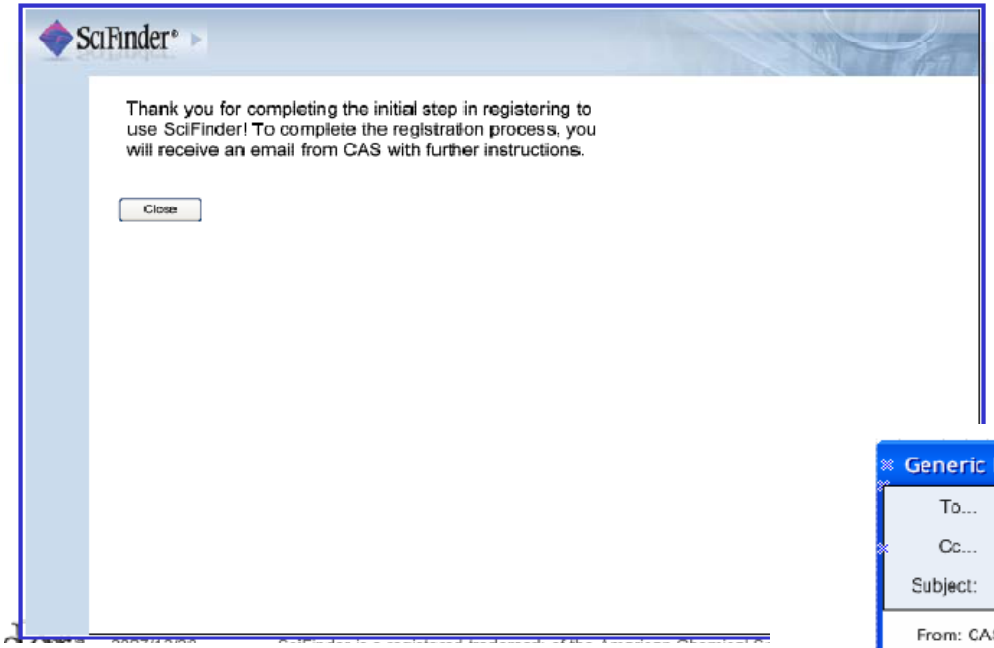


点击URL创建SciFinder账号

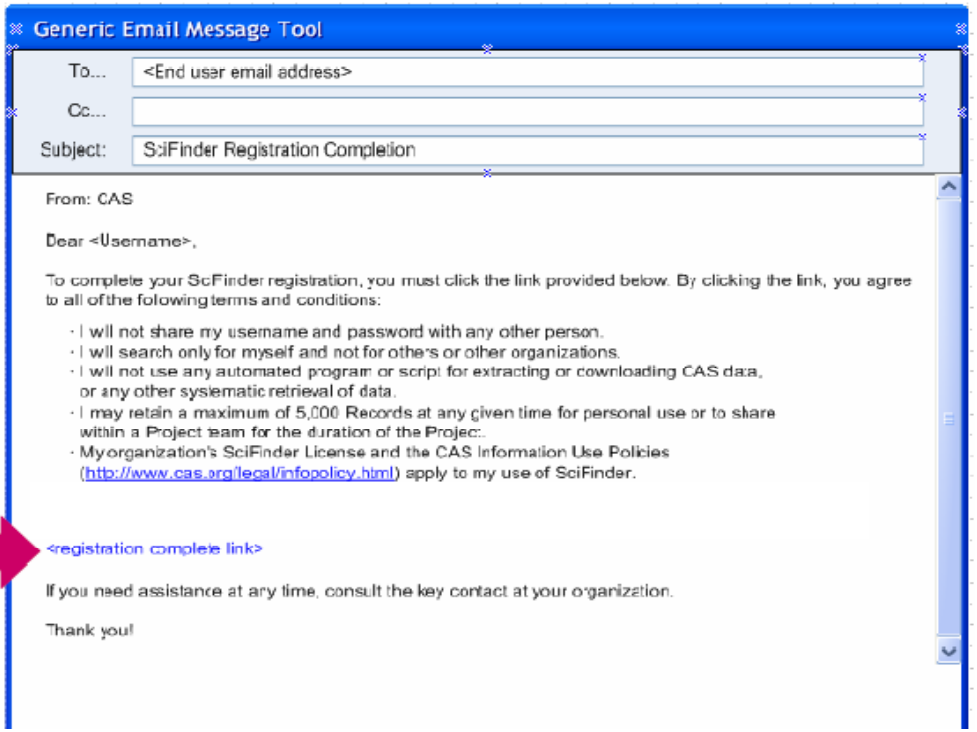
每个用户必须输入各自信息



对新ID的Email确认



需要点击邮件中的确认链接



使用这个链接登陆SciFinder

SciFinder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）

Scifinder scholar与scifinder 2007在2012年将停止使用。

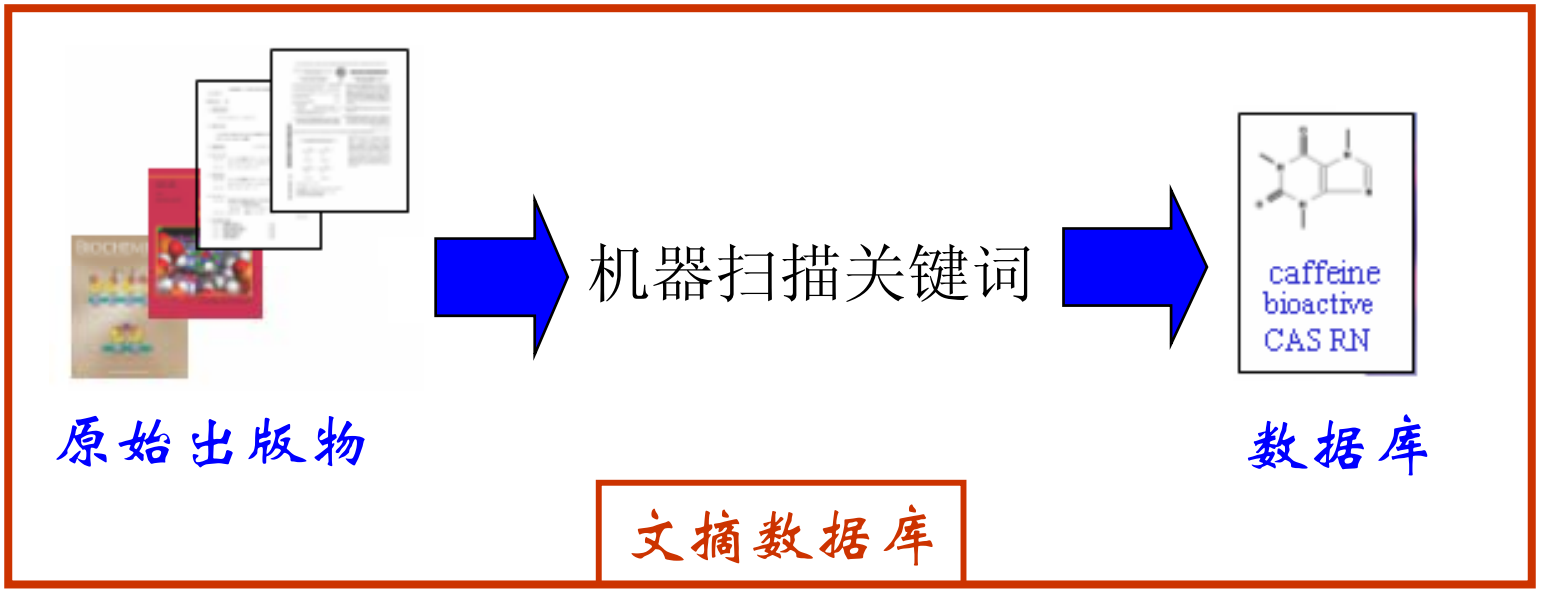
除了操作界面外，scifinder web功能更为丰富。

在图书馆相关页面上找到SciFinder Web注册用的网址

SciFinder的定位——二次文献数据库

- 二次文献是对一次文献进行加工整理后所产生的文献，如书目、题录、简介、文摘等形式的检索工具书。它是查找一次文献的线索。
- **SciFinder**覆盖化学界**98%**的文献，内容由**CAS**编者人工编目，文献中的重要信息被提炼总结，成为可检索和分析的条目。
- **SciFinder**提供对所有文献的分析、精选、分类功能，根据用户需要筛选众多信息，迅速锁定兴趣点。

目前流行的文摘数据库索引过程



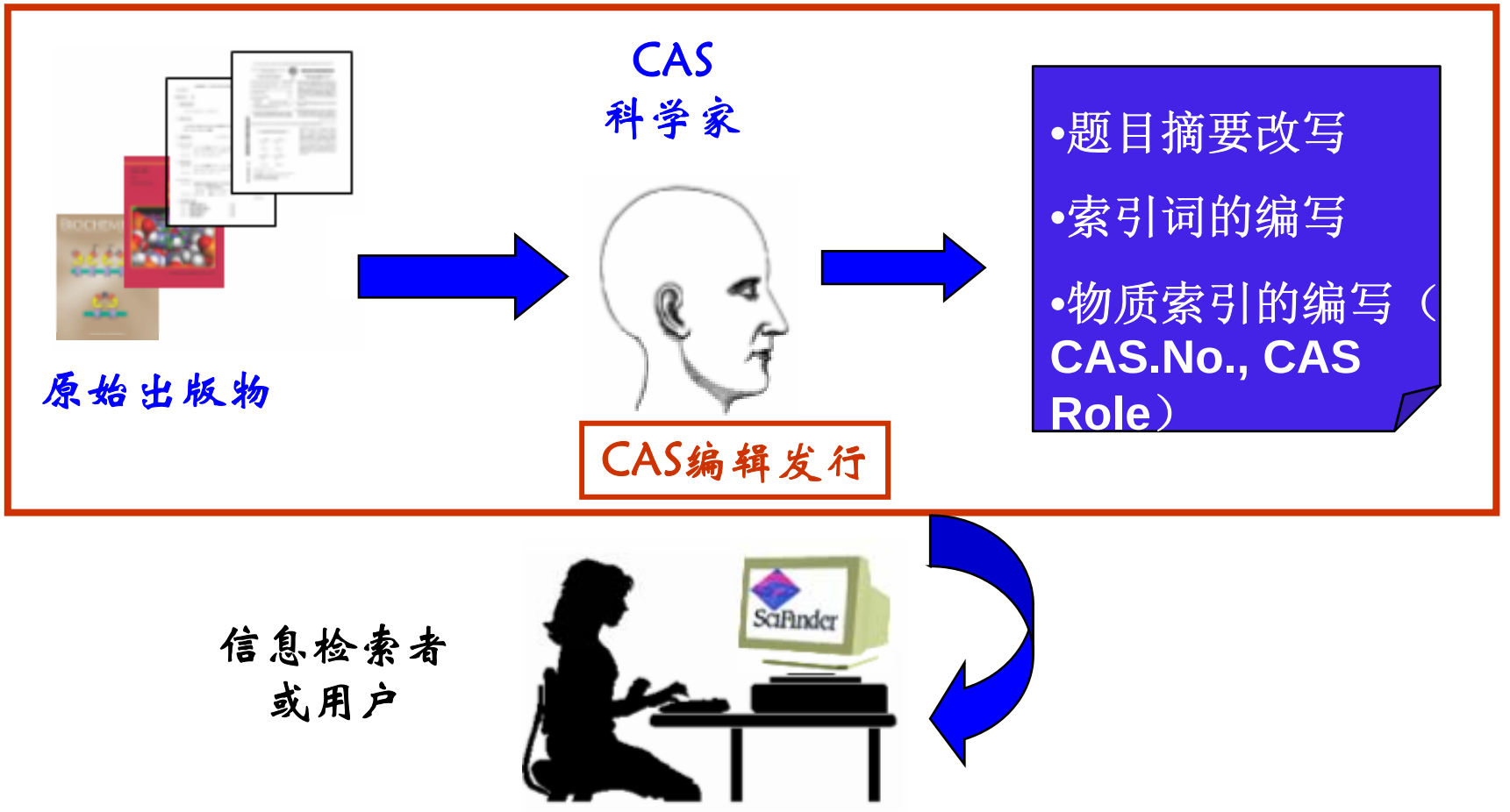
机器扫描的优点：

快速，节省时间

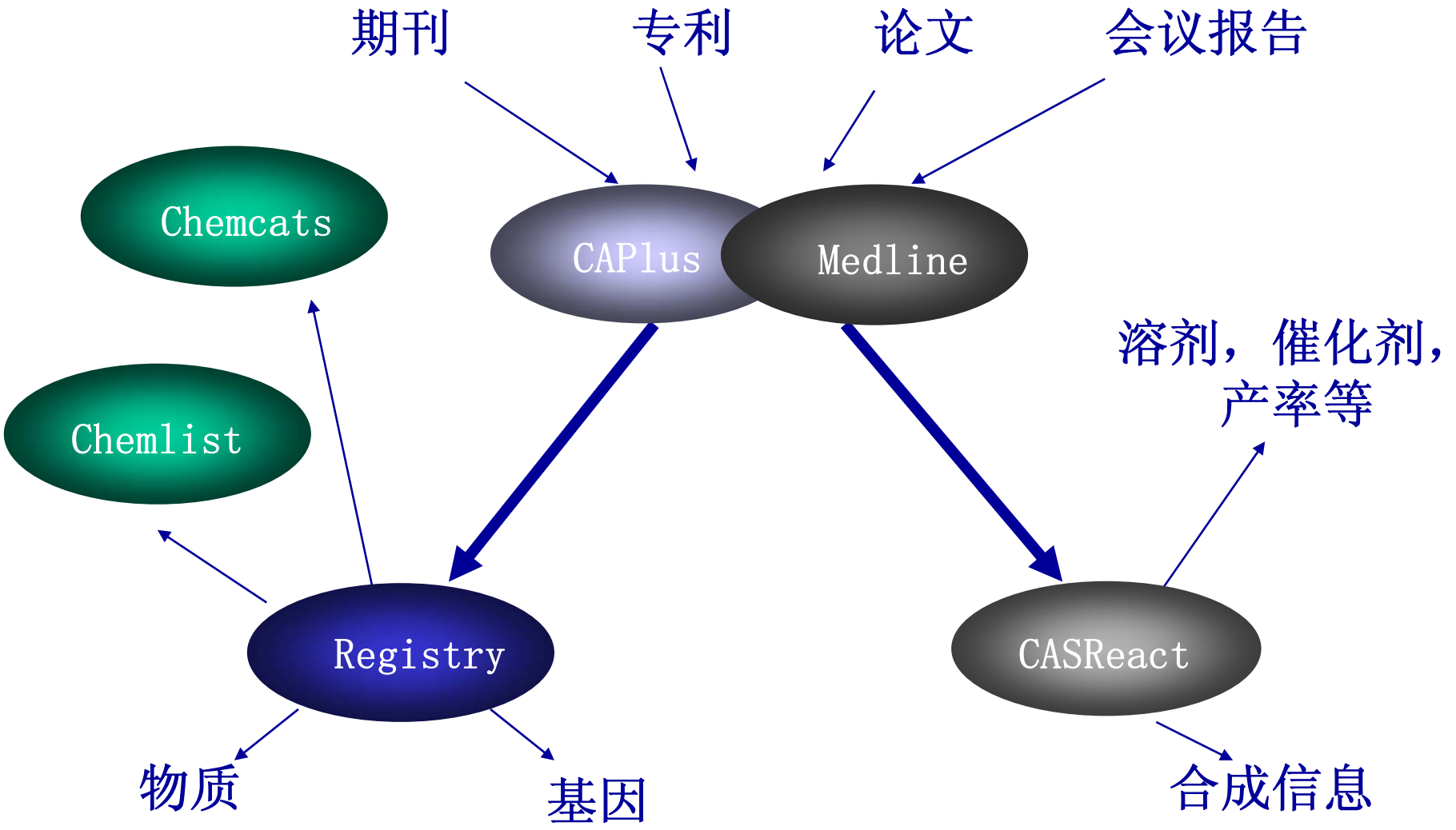
机器扫描的缺点：

1. 语言差异：日文？英文？中文？德文？….
2. 作者习惯：antitumor=anticancer

SciFinder科学索引过程



SciFinder介绍----组成



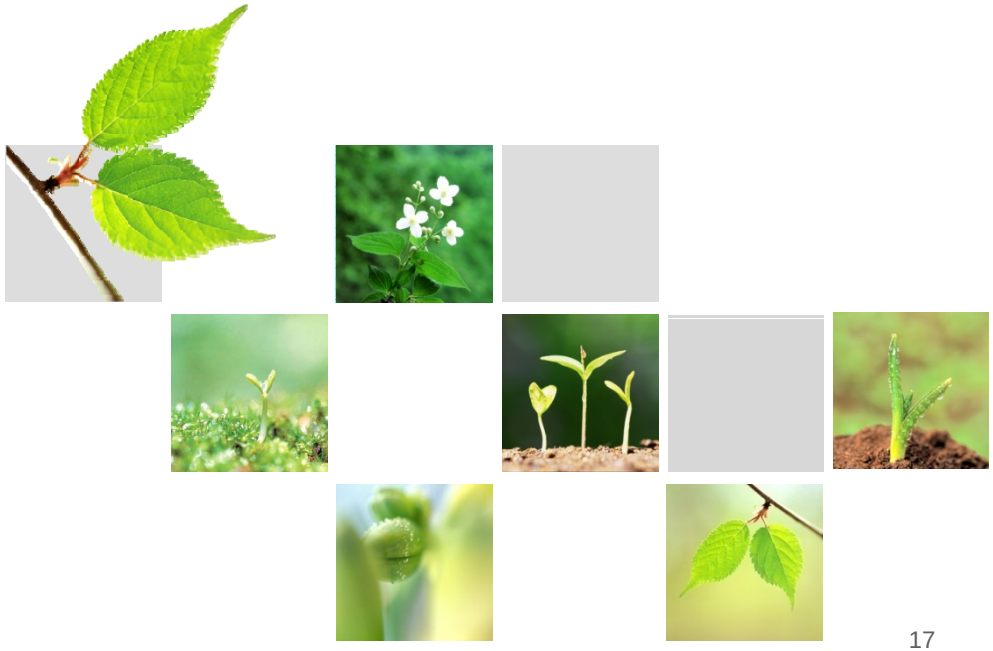
提纲

SciFinder®

- **SciFinder Web 文献及物质检索介绍**

检索天然产物抗菌研究的相关文献

来自天然的化合物具有特殊的生理活性，许多具有特殊治疗作用的药物已经被开发成药用。由于天然药物化学研究所提供的活性物质结构新颖，疗效高，不良反应少，所以它已成为制药工业中新药研究的主要方向.....



天然产物抗菌研究

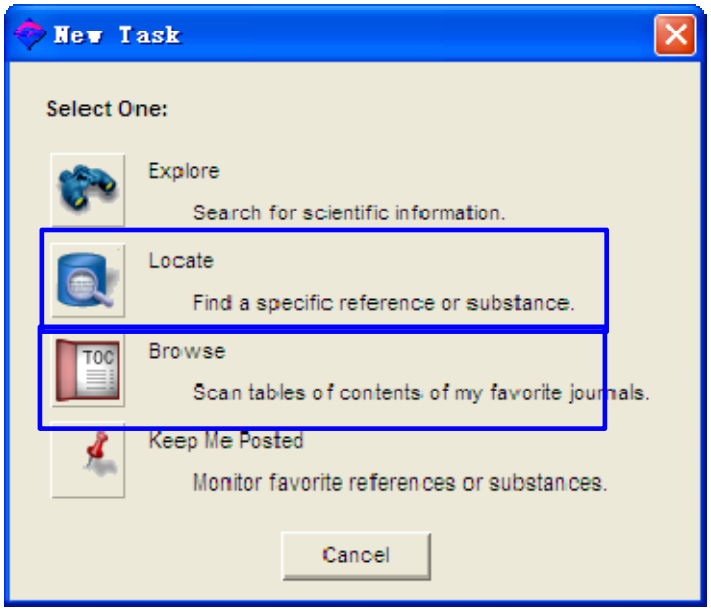
↓

来自哪些植物？方法学？

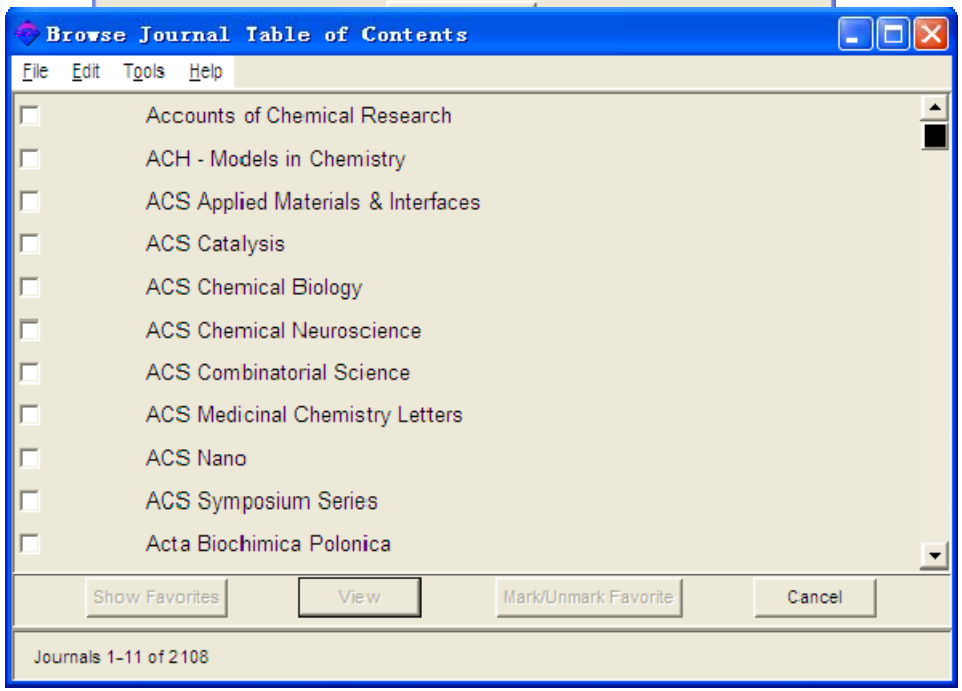
↓

有生物活性的具体物质？

Scifinder网页版取消序列检索功


New Task
Select One:
Explore
Search for scientific information.
Locate
Find a specific reference or substance.
Browse
Scan tables of contents of my favorite journals.
Keep Me Posted
Monitor favorite references or substances.
Cancel

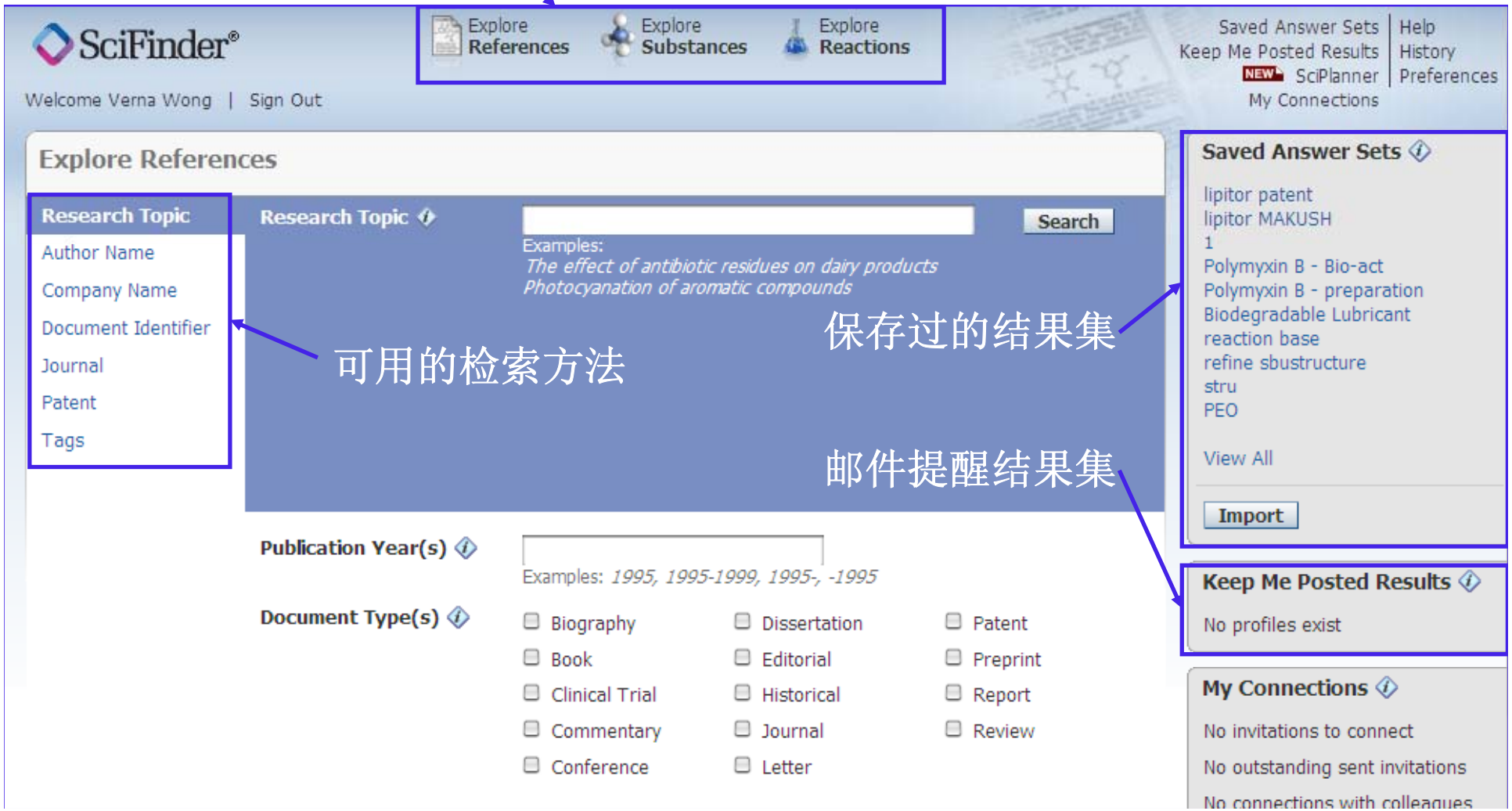

Locate
Select One:
Locate Literature
Bibliographic Information
Examples: journal name, title
Document Identifier
Examples: patent number, CA abstract number
Locate Substances
534-23
trimet
Substance Identifier
Examples: chemical name, CAS Registry Number


Browse Journal Table of Contents
File Edit Tools Help
Accounts of Chemical Research
ACH - Models in Chemistry
ACS Applied Materials & Interfaces
ACS Catalysis
ACS Chemical Biology
ACS Chemical Neuroscience
ACS Combinatorial Science
ACS Medicinal Chemistry Letters
ACS Nano
ACS Symposium Series
Acta Biochimica Polonica
Show Favorites
View
Mark/Unmark Favorite
Cancel
Journals 1-11 of 2108

登陆网址：scifinder.cas.org

SciFinder 的主检索界面

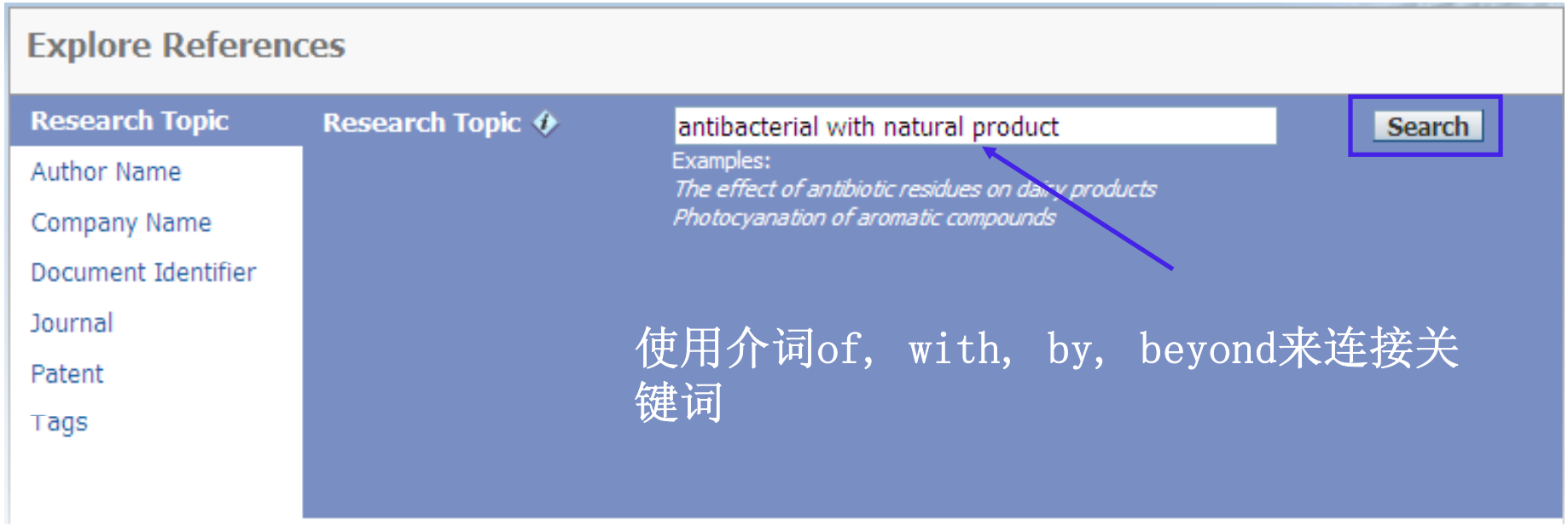
文献，物质，反应检索入口，
默认开始检索文献



设置合适的关键词获得最为全面和相关的文献

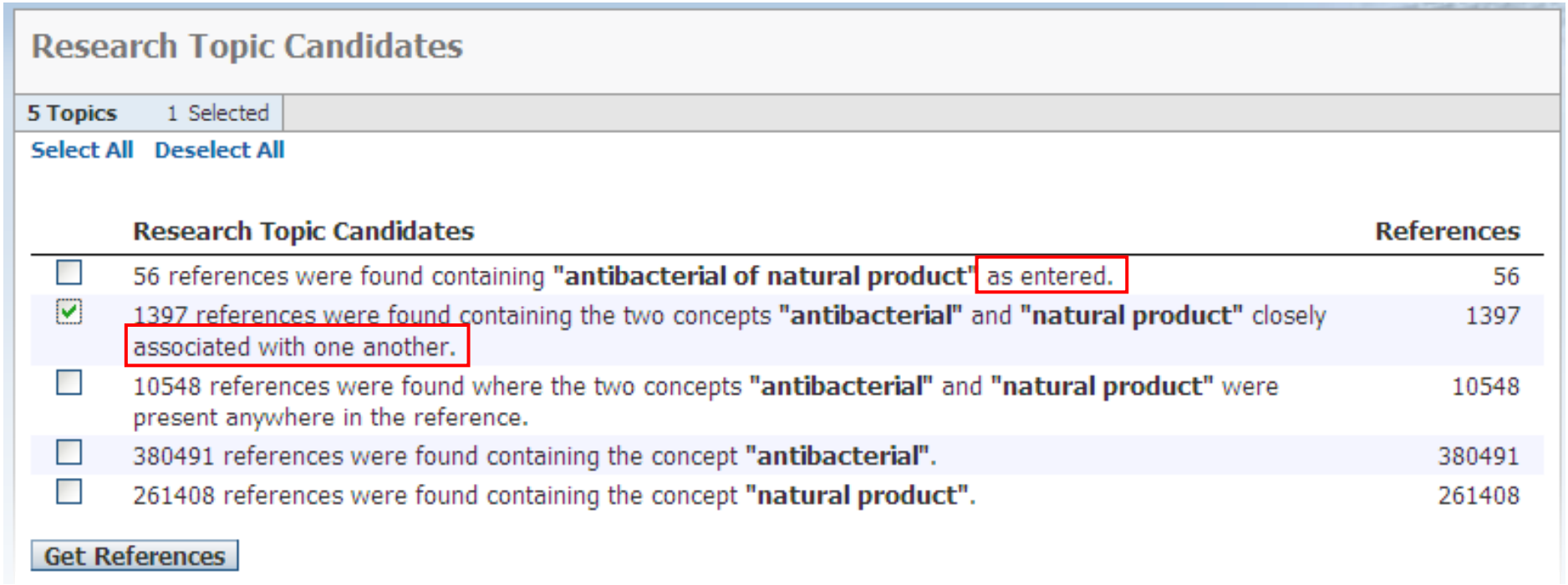
天然产物的抗菌研究

Antibacterial of nature product



Scifinder智能识别介词，将介词前后的单词或词组作为关键词进行检索。
3-5个关键词是比较适合的检索开始。

检索结果输出：



Research Topic Candidates

5 Topics 1 Selected

Select All Deselect All

	Research Topic Candidates	References
☐	56 references were found containing **"antibacterial of natural product"** as entered.	56
☑	1397 references were found containing the two concepts **"antibacterial"** and **"natural product"** closely associated with one another.	1397
☐	10548 references were found where the two concepts **"antibacterial"** and **"natural product"** were present anywhere in the reference.	10548
☐	380491 references were found containing the concept **"antibacterial"**.	380491
☐	261408 references were found containing the concept **"natural product"**.	261408

Get References

“concept” 表示做了同义词的扩展------ 全面

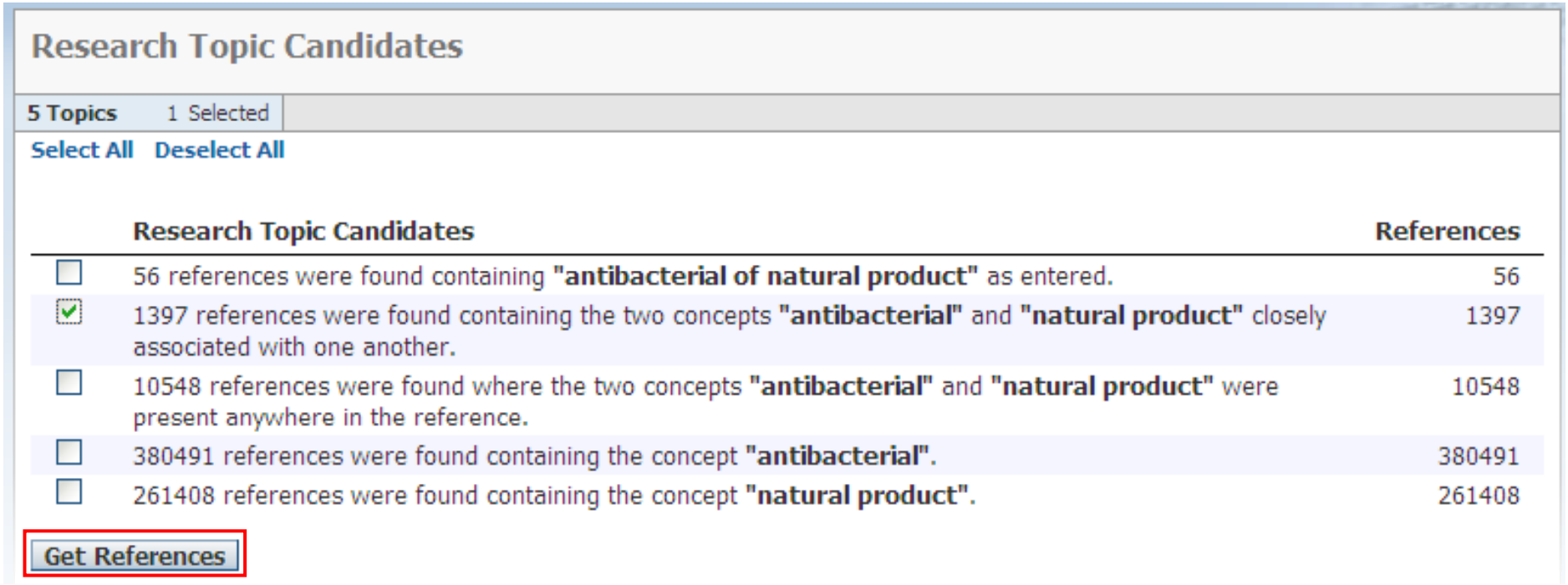
“as entered ” 表示检索结果与有输入的词组一致------ 精确

“closely associated with one another” 表示关键词联系最紧密

帮助您获取最全面最有效的文献信息！

只有两个候选选项。

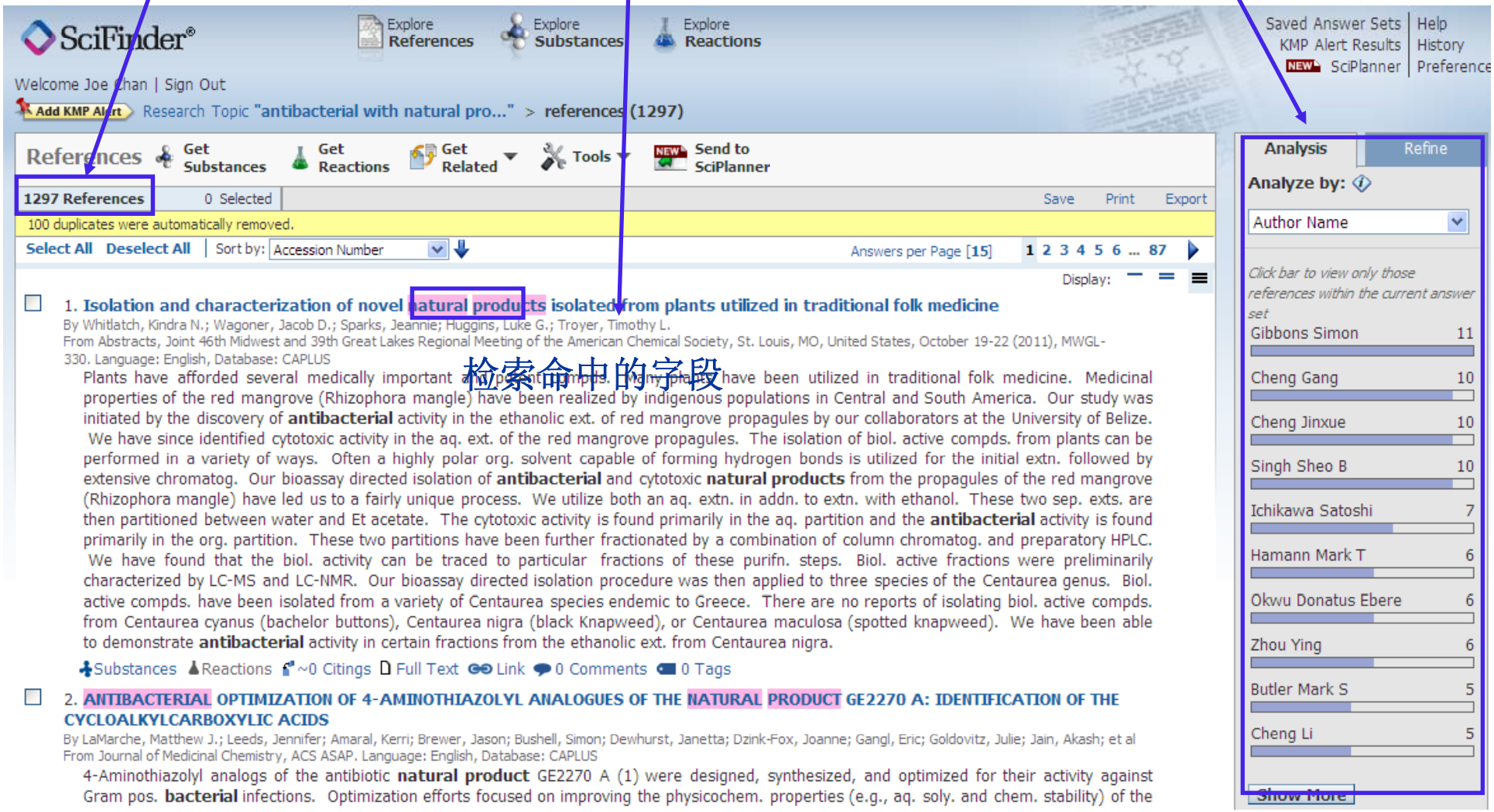
检索结果输出：



文献记录数

可以快速阅览文献的内容，是否符合要求

文献分析限定工具

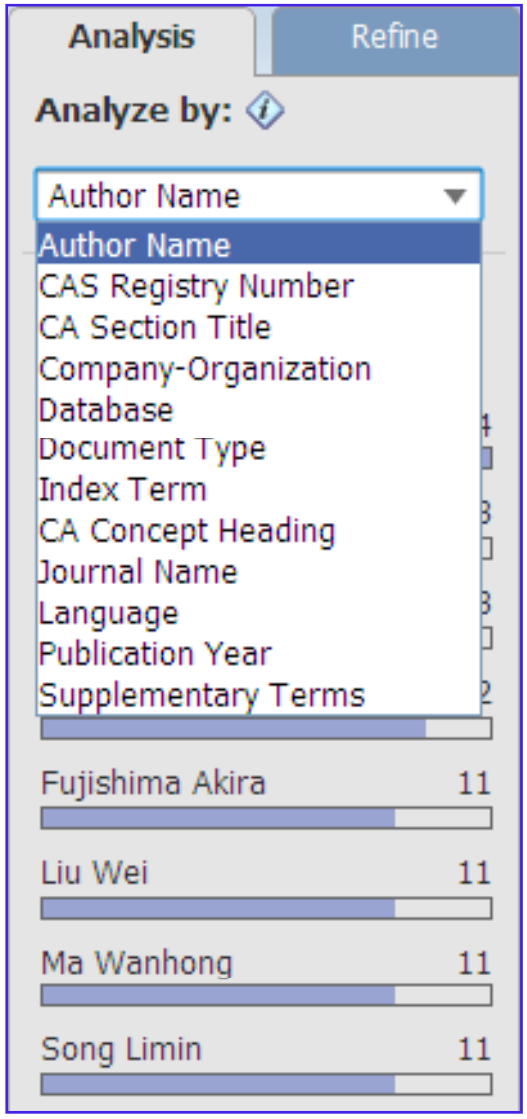


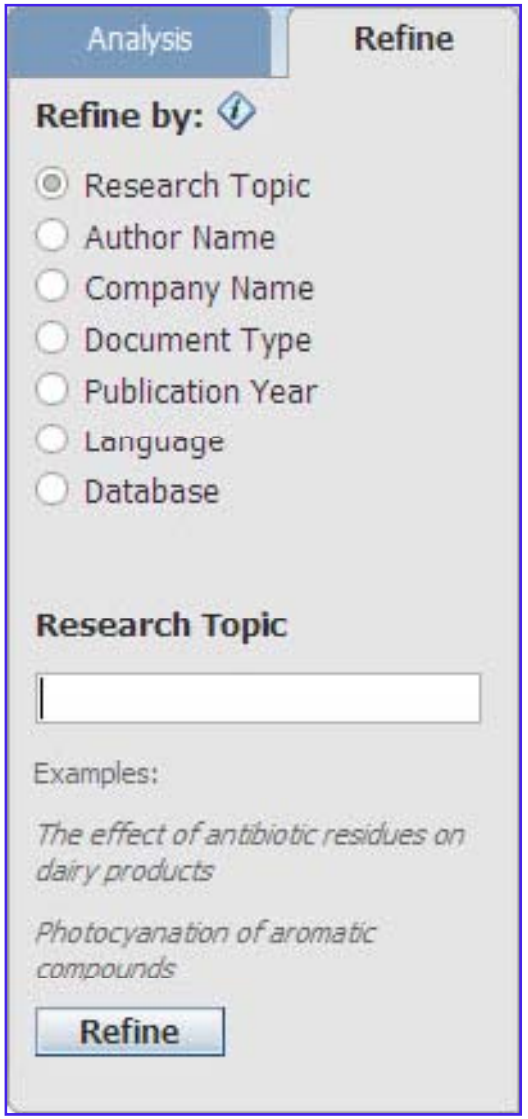
SciFinder中强大的文献的后处理功能，帮助我们缩小文献范围

SciFinder为文献分析提供：

12种分析方法
7种限定工具

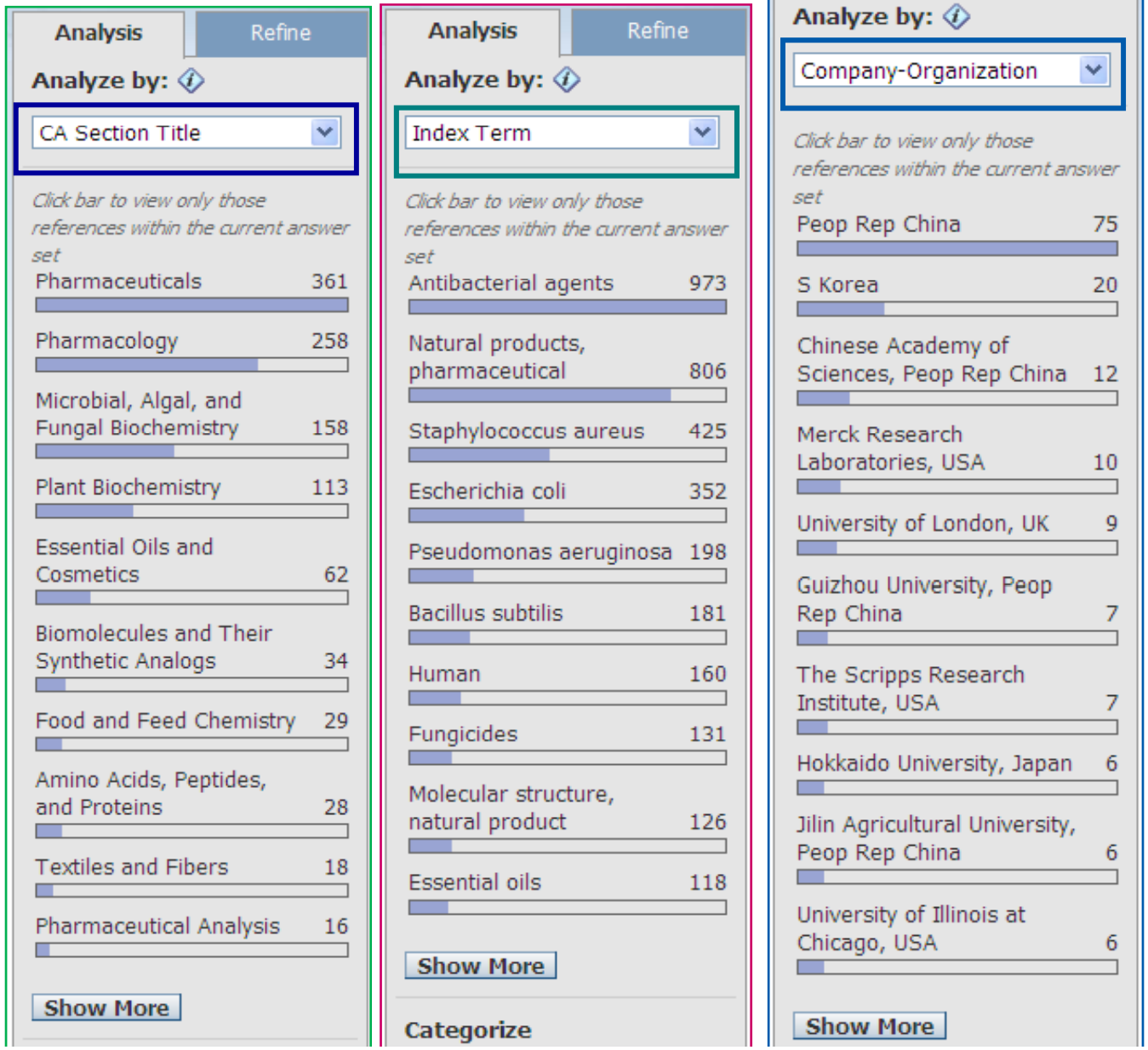
包括索引词，学科，作者名，机构名，文献类型，期刊名称，出版年限，出版语言等。





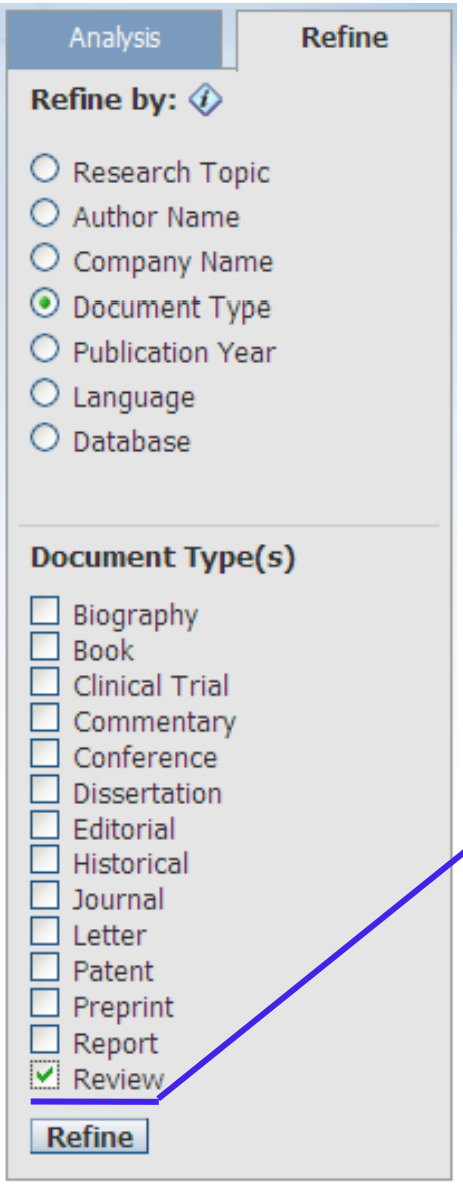
对文献进行多角度分析

- 这些文献涉及了哪些领域？
- 文献中出现了哪些重要概念？
- 哪些机构的研究处于领先水平？

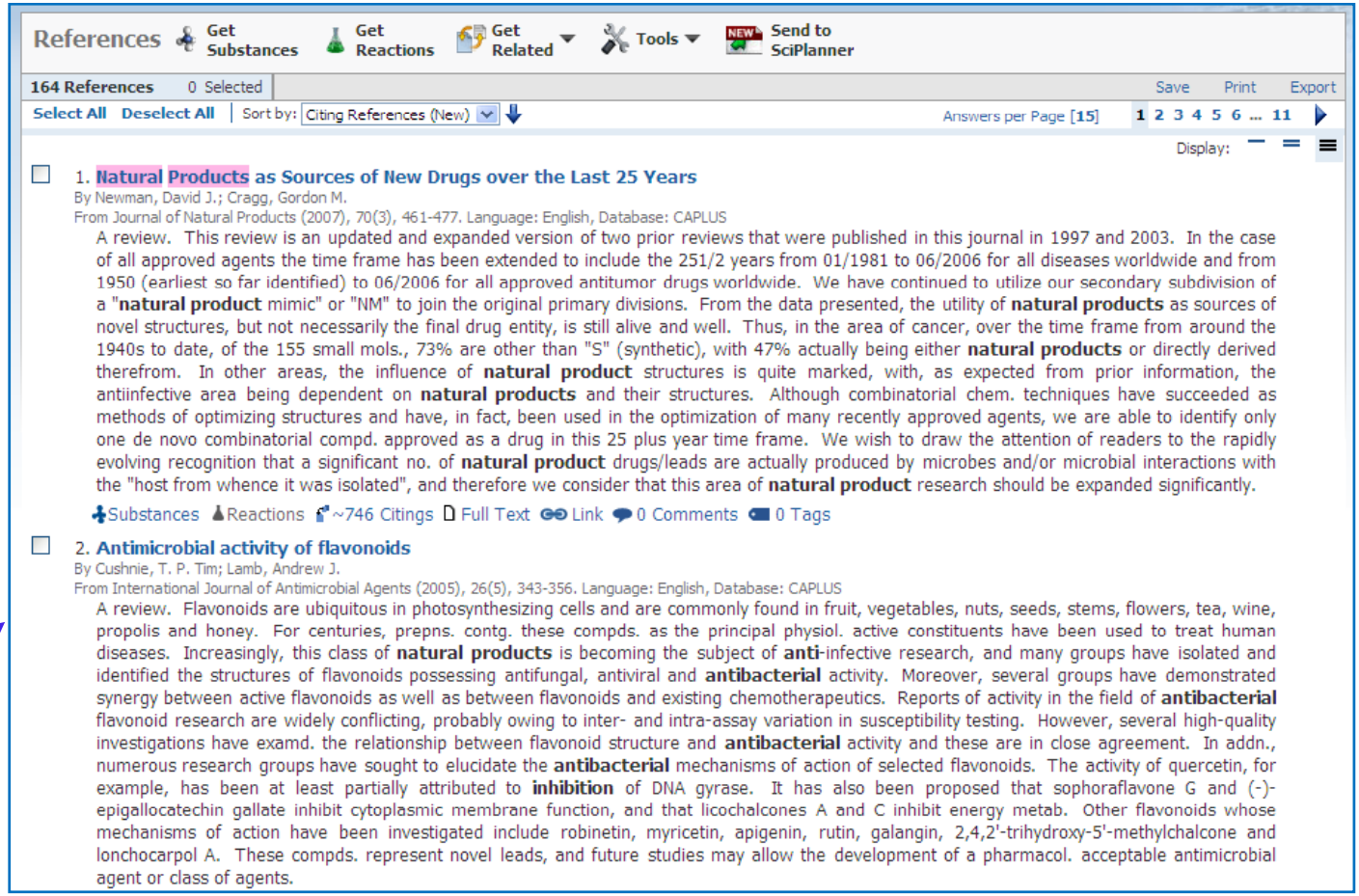


SCIFINDER

对文献进行限定，缩小范围



通过文献类型直接获取综述类文章



References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

1297 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Citing References (New) | Answers per Page [15] | 1 2 3 4 5 6 ... 87

Display:

1. **Natural Products as Sources of New Drugs over the Last 25 Years**

By Newman, David J.; Cragg, Gordon M.

From Journal of Natural Products (2007), 70(3), 461-477. Language: English, Database: CAPLUS

A review. This review is an updated and expanded version of two prior reviews that were published in this journal in 1997 and 2003. In the case of all approved agents the time frame has been extended to include the 251/2 years from 01/1981 to 06/2006 for all diseases worldwide and from 1950 (earliest so far identified) to 06/2006 for all approved antitumor drugs worldwide. We have continued to utilize our secondary subdivision of a "**natural product** mimic" or "NM" to join the original primary divisions. From the data presented, the utility of **natural products** as sources of novel structures, but not necessarily the final drug entity, is still alive and well. Thus, in the area of cancer, over the time frame from around the 1940s to date, of the 155 small mols., 73% are other than "S" (synthetic), with 47% actually being either **natural products** or directly derived therefrom. In other areas, the influence of **natural product** structures is quite marked, with, as expected from prior information, the antiinfective area being dependent on **natural products** and their structures. Although combinatorial chem. techniques have succeeded as methods of optimizing structures and have, in fact, been used in the optimization of many recently approved agents, we are able to identify only one de novo combinatorial compd. approved as a drug in this 25 plus year time frame. We wish to draw the attention of readers to the rapidly evolving recognition that a significant no. of **natural product** drugs/leads are actually produced by microbes and/or microbial interactions with the "host from whence it was isolated", and therefore we consider that this area of **natural product** research should be expanded significantly.

Substances | Reactions | ~746 Citings | Full Text | Link | 0 Comments | 0 Tags

2. **Antimicrobial activity of flavonoids**

By Cushnie, T. P. Tim; Lamb, Andrew J.

From International Journal of Antimicrobial Agents (2005), 26(5), 343-356. Language: English, Database: CAPLUS

A review. Flavonoids are ubiquitous in photosynthesizing cells and are commonly found in fruit, vegetables, nuts, seeds, stems, flowers, tea, wine, propolis and honey. For centuries, prepns. contg. these compds. as the principal physiol. active constituents have been used to treat human diseases. Increasingly, this class of **natural products** is becoming the subject of **anti**-infective research, and many groups have isolated and identified the structures of flavonoids possessing antifungal, antiviral and **antibacterial** activity. Moreover, several groups have demonstrated synergy between active flavonoids as well as between flavonoids and existing chemotherapeutics. Reports of activity in the field of **antibacterial** flavonoid research are widely conflicting, probably owing to inter- and intra-assay variation in susceptibility testing. However, several high-quality investigations have examd. the relationship between flavonoid structure and **antibacterial** activity and these are in close agreement. In addn., numerous research groups have sought to elucidate the **antibacterial** mechanisms of action of selected flavonoids. The activity of quercetin, for example, has been at least partially attributed to **inhibition** of DNA gyrase. It has also been proposed that sophoraflavone G and (-)-epigallocatechin gallate inhibit cytoplasmic membrane function, and that licochalcones A and C inhibit energy metab. Other flavonoids whose mechanisms of action have been investigated include robinetin, myricetin, apigenin, rutin, galangin, 2,4,2'-trihydroxy-5'-methylchalcone and lonchocarpol A. These compds. represent novel leads, and future studies may allow the development of a pharmacol. acceptable antimicrobial agent or class of agents.

Substances | Reactions | ~262 Citings | Full Text | Link | 0 Comments | 0 Tags

按被引用的次数排序

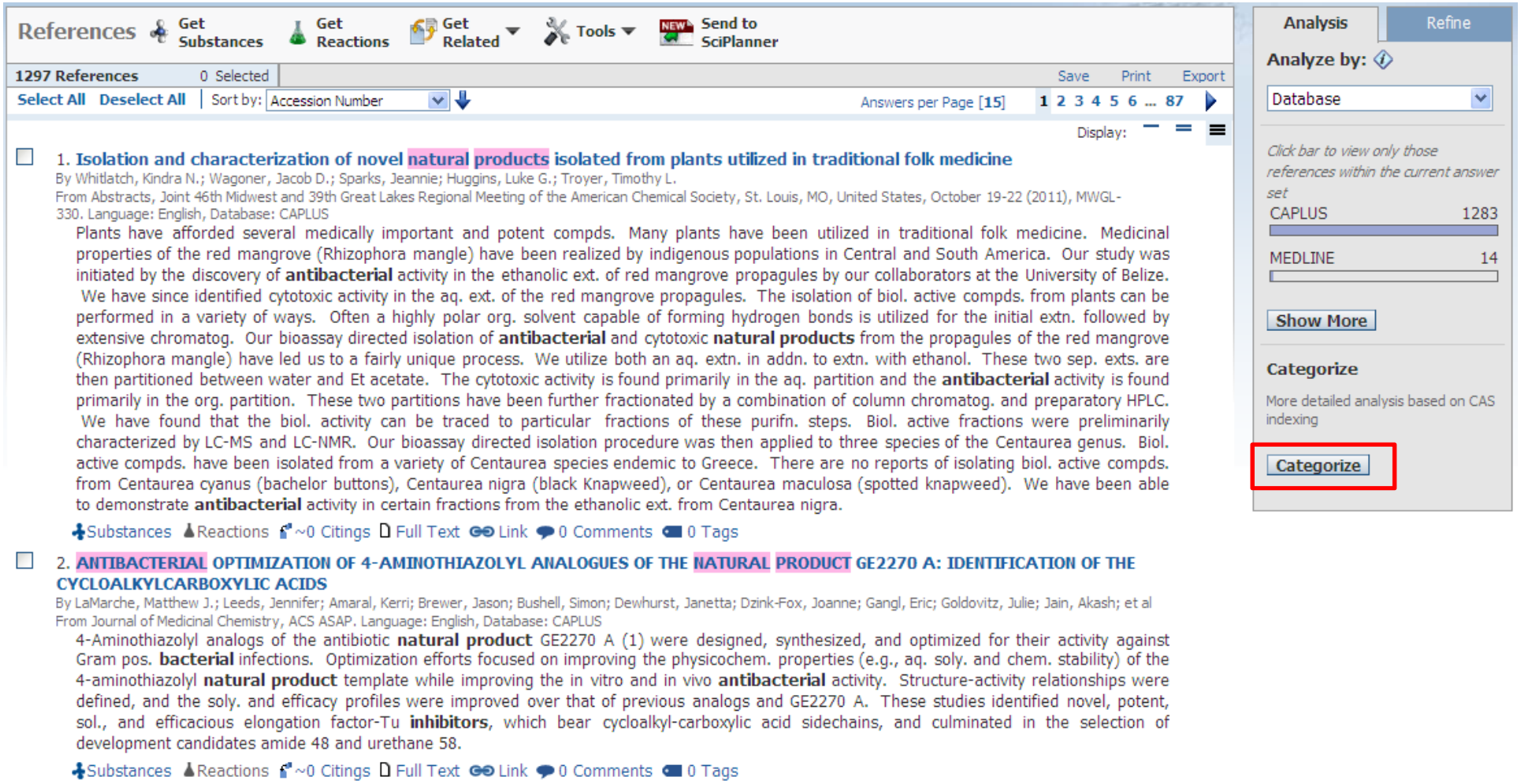
针对课题的思考：

- 阅读综述，重要的文章（引用次数多）对全局有基本了解。
- 来自哪些植物？方法学？
- 具体到哪些药物？

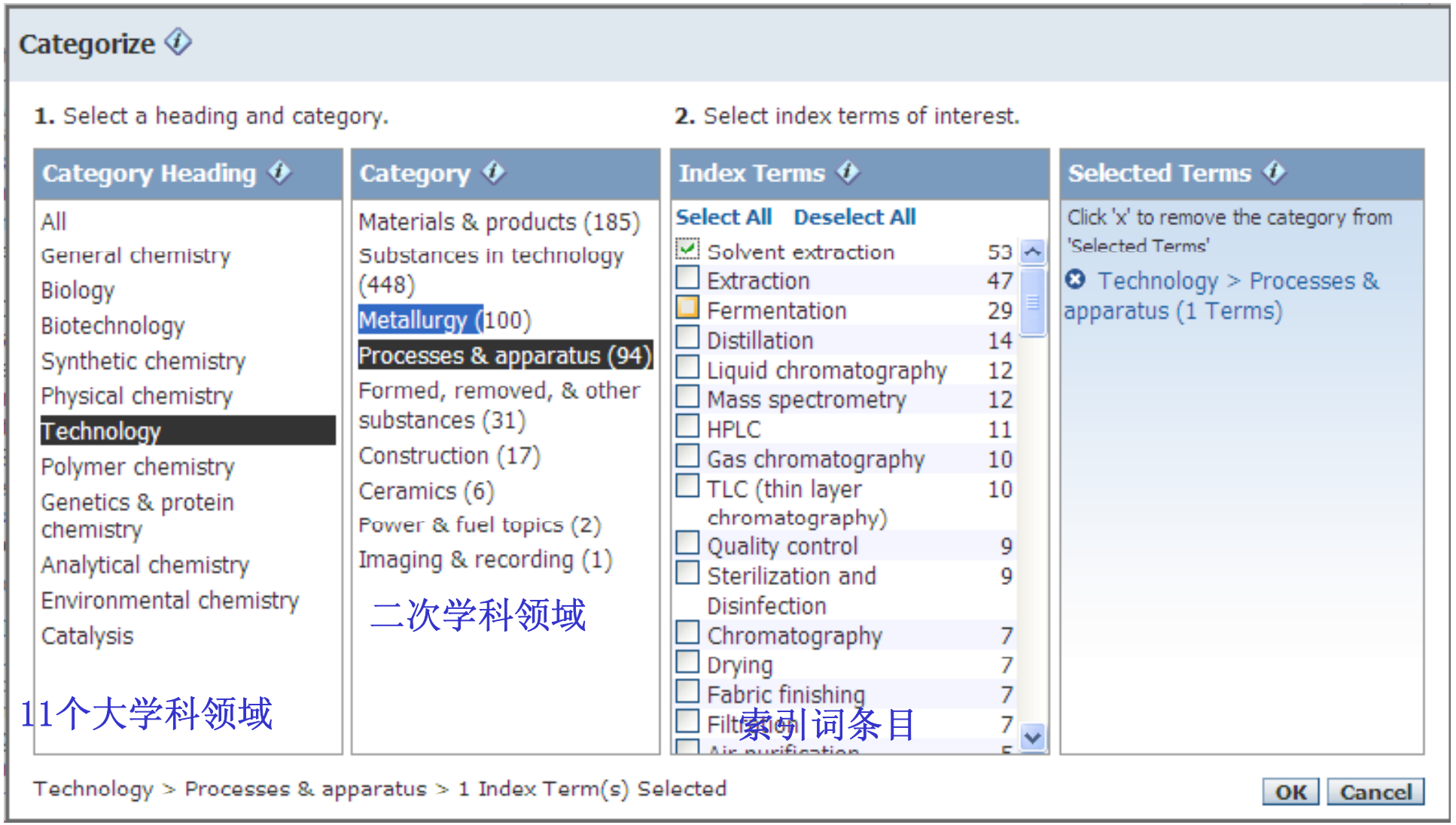
✓当有明确的目标，可以利用二次检索分析/后处理功能细分。

✓当没有明确的目标？

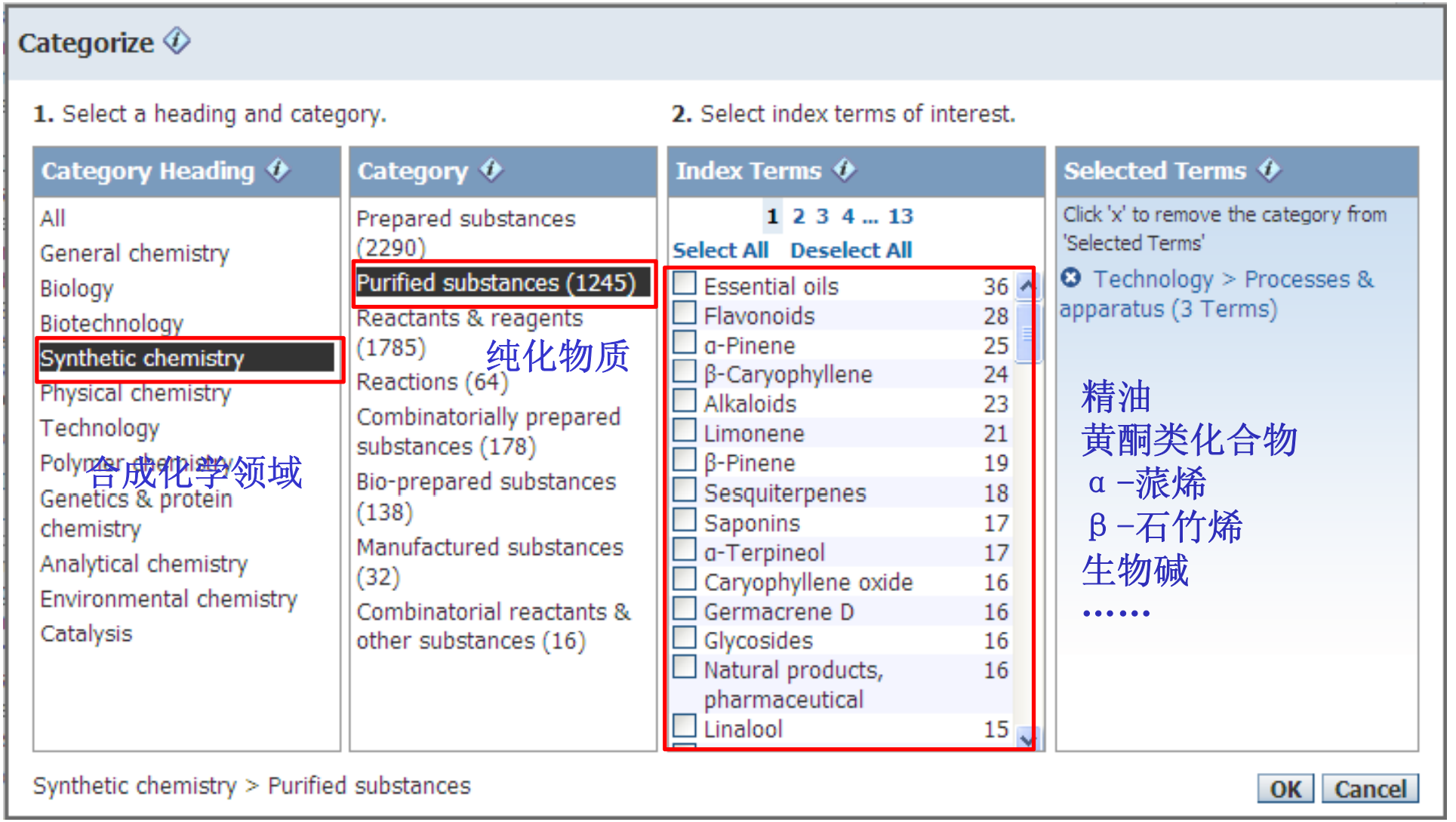
Categorize 功能：针对文献细分为72个学科领域

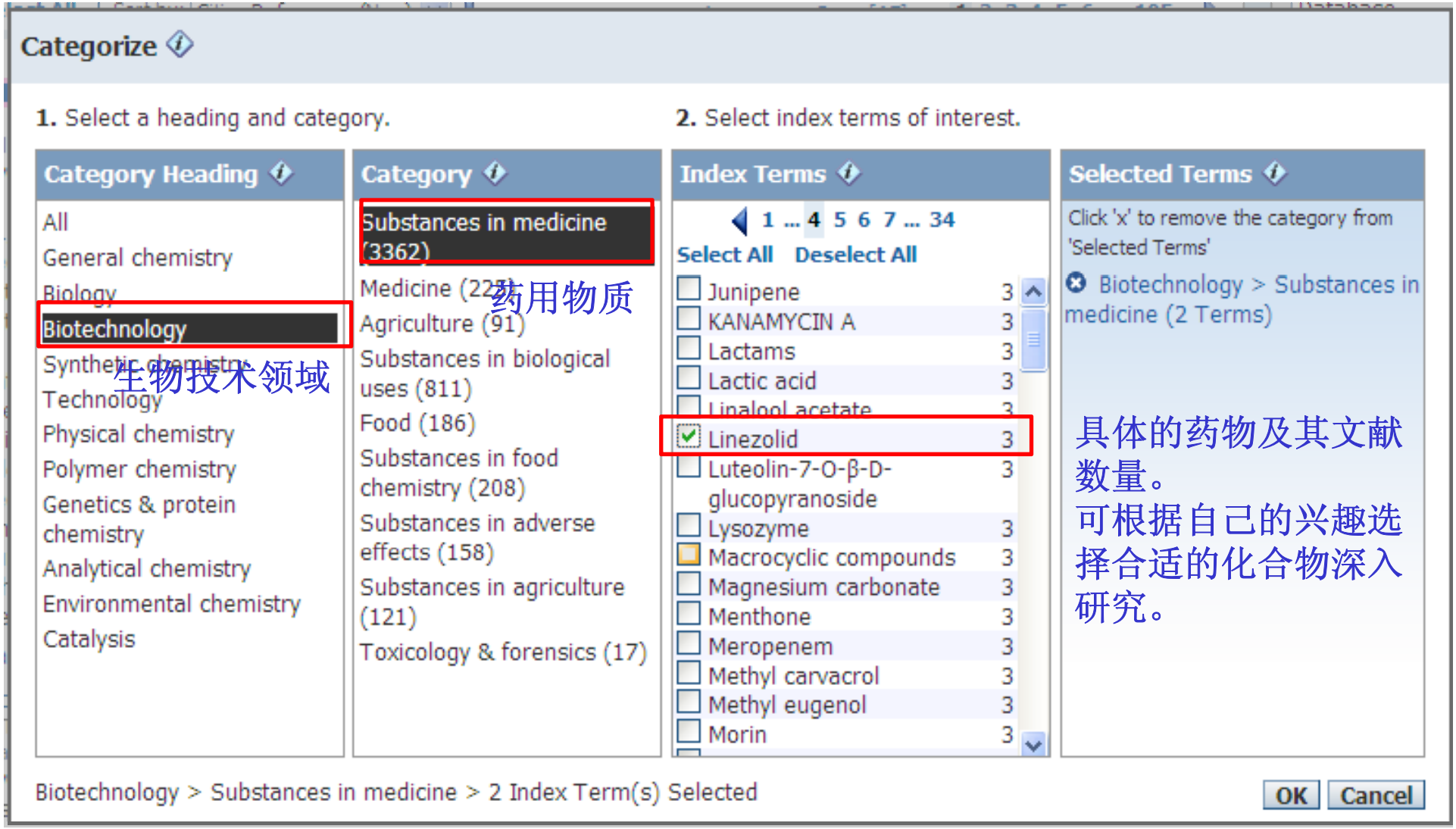


Categorize 功能：针对文献细分为72个学科领域



查看通过纯化手段获得哪些物质。





药用物质

生物技术领域

具体的药物及其文献数量。
可根据自己的兴趣选择合适的化合物深入研究。

除了SciFinder，其他数据库均无法做到如此精确的分类。

获得Linezolid（利奈唑胺）相应的文献

媲美原文内容的文摘信息：

物质的详细信息

Substance Detail | Get References | Get Reactions | Get Commercial Sources | Get Regulatory Info | Send to SciPlanner

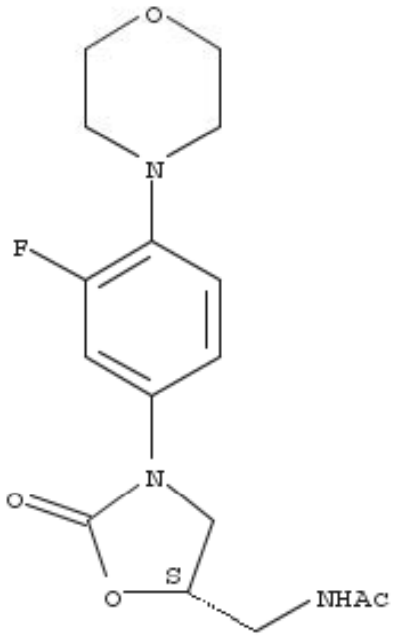
Link | Save | Print | Export

CAS Registry Number: 165800-03-3

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

Acetamide, N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-, (S)-; (S)-Linezolid; Linezolid; Linospan; Linox; N-[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide; N-[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide; PNU 100766; U 100766; Zyvox; Zyvoxid

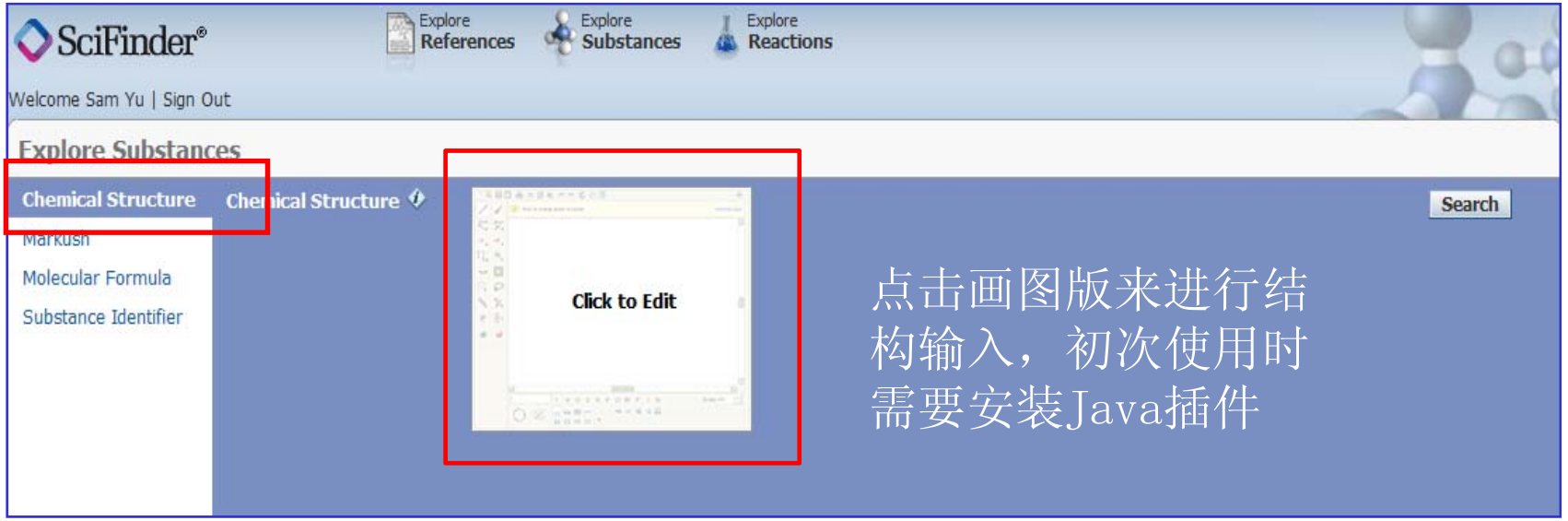


Absolute stereochemistry. Rotation (-).

Source of Registration: US Adopted Names Council (USAN)

~2,545 References

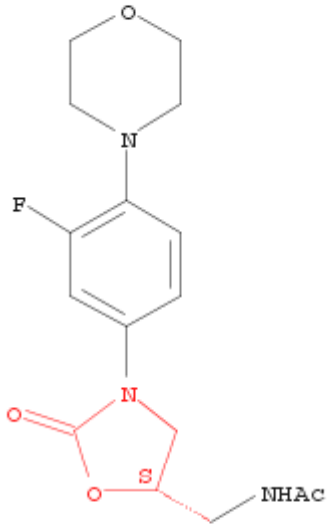
Document Types: Book, Conference, Dissertation, Journal, Patent



点击画图版来进行结构输入，初次使用时需要安装Java插件

这里可以通过输入物质的名称，CA号，俗名，商品名，来进行检索

1. **Substance Detail**
   165800-03-3



获得物质详细物理化学信息

Absolute stereochemistry.
Rotation (-).

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

- ~2,545 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

物质的详细信息

Substance Detail | Get References | Get Reactions | Get Commercial Sources | Get Regulatory Info | Send to SciPlanner

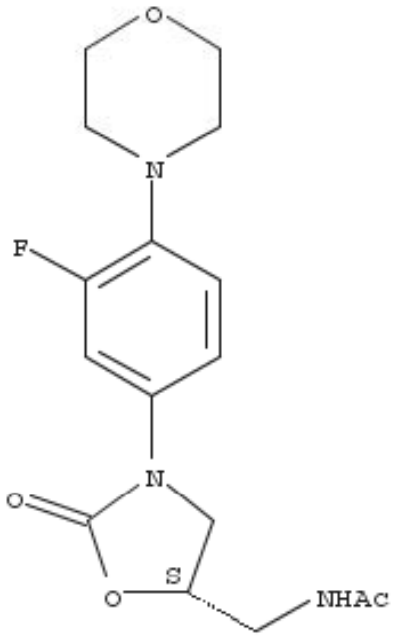
Link | Save | Print | Export

CAS Registry Number: 165800-03-3

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

Acetamide, N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-, (S)-; (S)-Linezolid; Linezolid; Linospan; Linox; N-[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide; N-[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide; PNU 100766; U 100766; Zyvox; Zyvoxid



Absolute stereochemistry. Rotation (-).

Source of Registration: US Adopted Names Council (USAN)

~2,545 References

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

Source of Registration: US Adopted Names Council (USAN)

~2,545 References

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

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

物质角色：已研究的领域

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

Biological Properties	Value	Condition	Note
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(18)
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(18)
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(18)
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(18)
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(18)
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(18)
Bioconcentration Factor	1.22	pH 7 Temp: 25 °C	(18)
Bioconcentration Factor	1.28	pH 8 Temp: 25 °C	(18)

Top

Experimental Properties: Biological Chemical 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 of 17	(1) CAS	
Half-Life (Biological)	See full text	1 of 8	(6) CAS	
LD50	See full text		(7) CAS	
Minimum Inhibitory Concentration	See full text	1 of 125	(15) CAS	

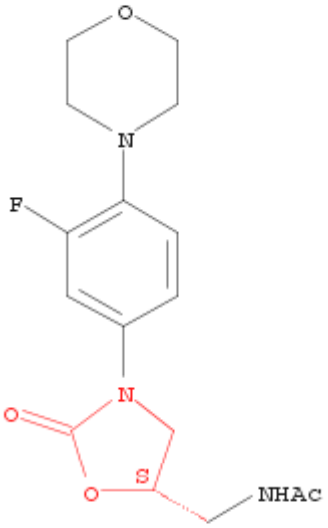
Chemical Properties	Value	Condition	Note	Top
logP	See full text		(8) CAS	
Solubility	See full text		(8) CAS	

Lipinski and Related Properties	Value	Condition	Note	Top
logP	See full text		(8) CAS	

Optical and Scattering Properties	Value	Condition	Note	Top
Optical Rotatory Power	-8.8 °	Conc: 1.0 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 20 °C	(2) CAS	
Optical Rotatory Power	-9 °	Conc: 1.52 g/100mL; Solv: chloroform (67-66-3); Wavlen: 589.3 nm; Temp: 20 °C	(12) CAS	
Melting Point	73-76 °C		(14) CAS	

(1) Goteti, Kosalaram; Journal of Pharmaceutical Sciences 2010, V99(3), P1601-1613 CAPLUS
(2) Moran-Ramallal, Roberto; Organic Letters 2008, V10(10), P1935-1938 CAPLUS
(3) Tanaka, Rumiko; Analytical Sciences: X-Ray Structure Analysis Online 2008, V24(3), PNo pp. given CAPLUS
(4) Bielejewska, A.; Acta Chromatographica 2005, V15, P183-191 CAPLUS
(5) Ramgren, Stephen D.; Angewandte Chemie, International Edition 2011, V50(9), P2171-2173, S2171/1-S2171/43 CAPLUS
(6) Stein, Gary E.; Annals of Pharmacotherapy 2005, V39(3), P427-432 CAPLUS
(7) Dehghanyar, Pejman; Antimicrobial Agents and Chemotherapy 2005, V49(6), P2367-2371 CAPLUS
(8) Germani, Massimiliano; European Journal of Pharmaceutical Sciences 2007, V31(3-4), P190-201 CAPLUS

1. **Substance Detail**
165800-03-3



Absolute stereochemistry.
Rotation (-).

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

~2,545 References
Reactions
Commercial Sources
Regulatory Information
Link

从物质到文献：获得各研究领域文献

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.

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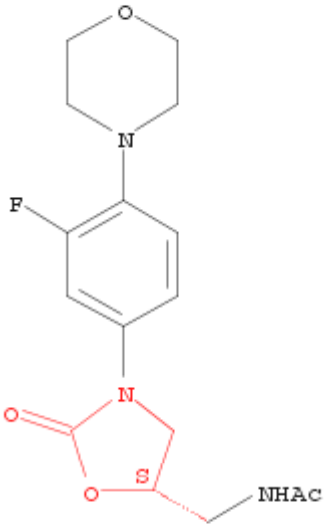
1. **Substance Detail**
165800-03-3



Absolute stereochemistry.
Rotation (-).

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

- ~2,545 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

Commercial Sources

82 Commercial Sources | 0 Selected | Keep Selected | Remove Selected | Print | Export

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Select All Deselect All | Sort by: Catalog Name | Answers per Page [20] | 1 2 3 4 5

1. **9W Pharmaceutical Technology Product List**
Supplier Name: 9W Pharmaceutical Technology Co., Ltd., Catalog Publication Date: 19 Feb 2011
Order Number: 9W-07708, Quantity: on request
165800-03-3 Linezolid
Link

2. **A.S. Chemical Laboratories Product List**
Supplier Name: A.S. Chemical Laboratories Inc., Catalog Publication Date: 17 May 2010
Order Number: L-070530, Quantity: Various
165800-03-3 Linezolid
Link

3. **Abby PharmaTech Product List**
Supplier Name: Abby PharmaTech, LLC, Catalog Publication Date: 31 Mar 2011
Order Number: AP-34-3188, Quantity: N/A
165800-03-3 Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-
Link

4. **AC Scientific Products Listing**
Supplier Name: AvaChem Scientific LLC, Catalog Publication Date: 1 Apr 2011
Order Number: 2446, Quantity: 100mg, 1g, 10g
165800-03-3 Linezolid
Link

5. **ACC Corp. Catalog**
Supplier Name: American Custom Chemicals Corp., Catalog Publication Date: 28 Feb 2011
Order Number: API0003178, Quantity: 10 MG, 100 MG, 1 G, 5 G, 10 G
165800-03-3 LINEZOLID, ≥95%
Link

Analyze by:
Country

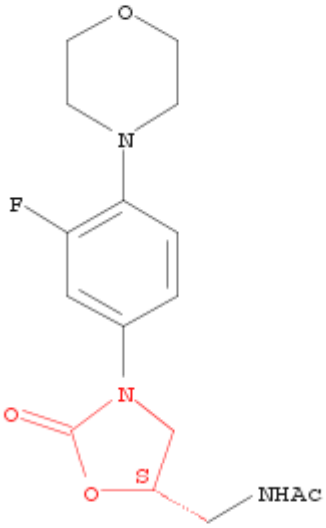
Click bar to view only those commercial sources within the current answer set

People's Republic of China	43
USA	26
Canada	6
United Kingdom	4
Germany	2
Hong Kong	2
Austria	1
Belgium	1
FRANCE	1
UNITED KINGDOM	1

Show More

1. **Substance Detail**
165800-03-3

管制信息



Absolute stereochemistry.
Rotation (-).

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

- ~2,545 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

Regulatory Information Detail

Print Export

CAS Registry Number: 165800-03-3

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]- (REACH)
(S)-Linezolid
Acetamide, N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-, (S)-
Linezolid
Linospan
Linox
N-[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide
PNU 100766
U 100766
Zyvox
Zyvoxid

File Segment

EU: REACH

Confidentiality Status

Public

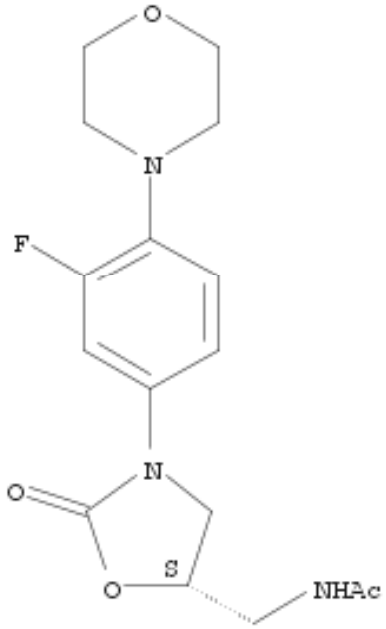
Regulatory List Number

EC No.: 605-416-1

Inventory Status

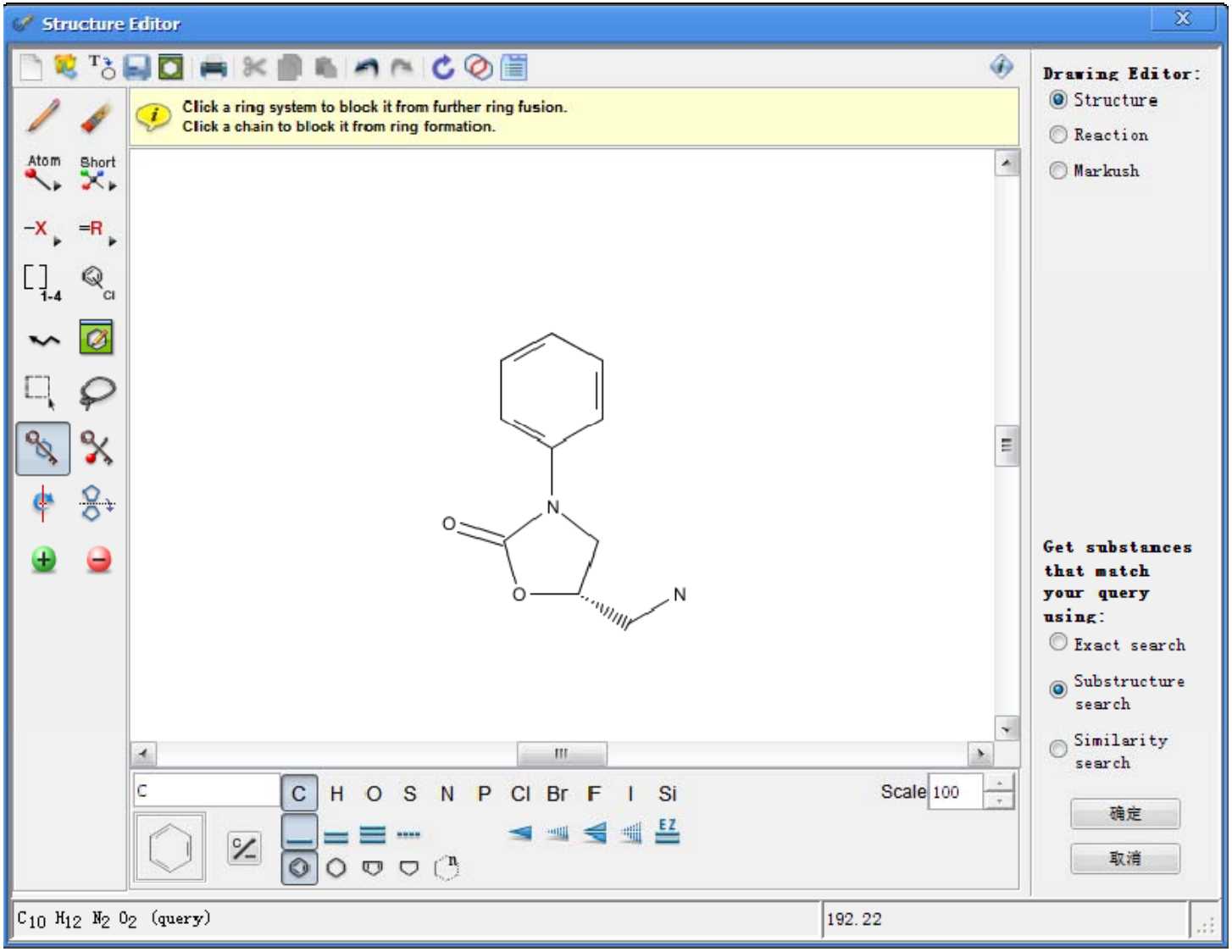
On REACH
List of Pre-Registered Substances, March 2009
Registration Date: 31-MAY-2018.

针对课题的思考：

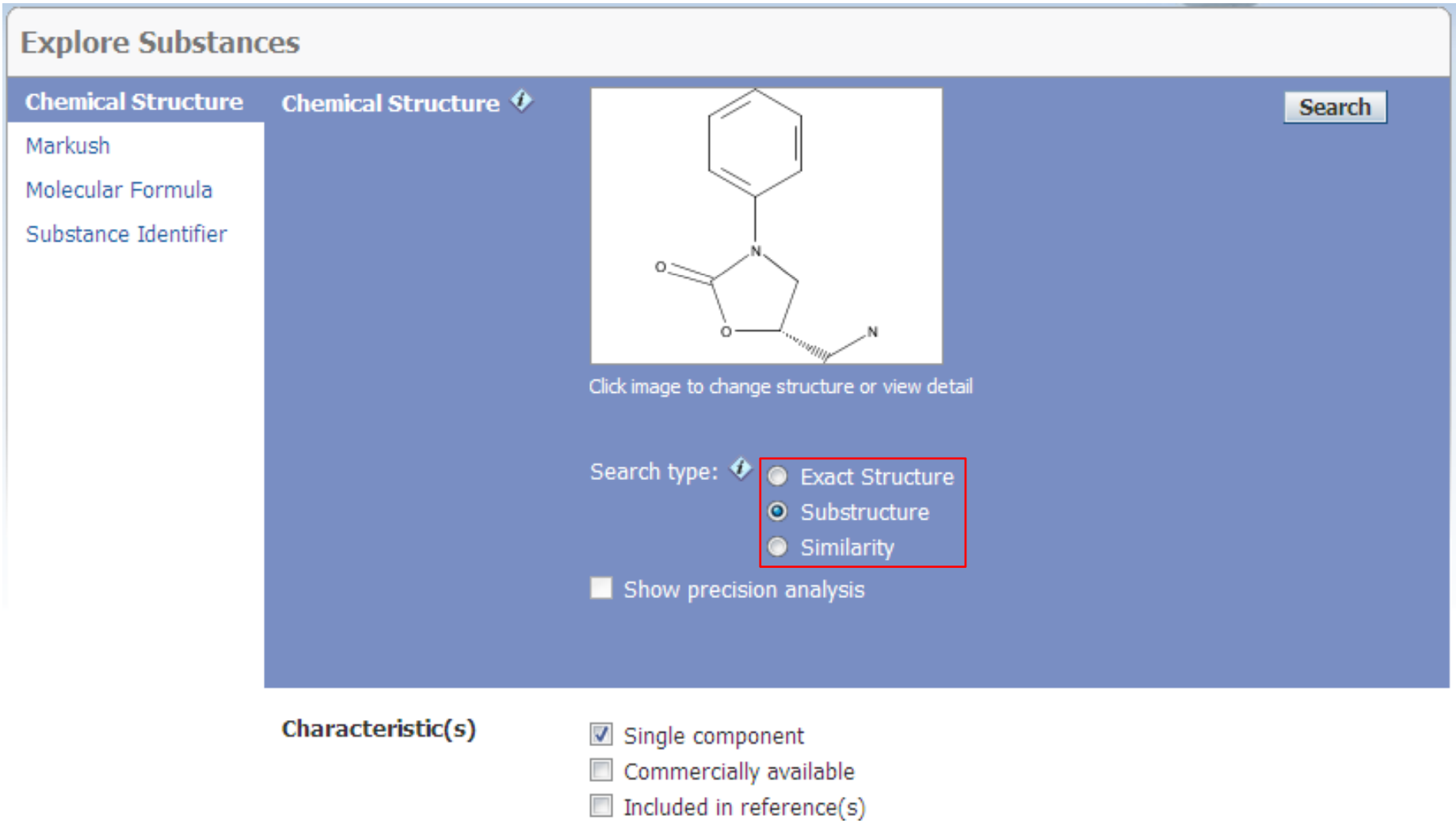


- 含有噁唑烷酮母核的化合物？结构修饰情况？
- 结构相似的化合物？

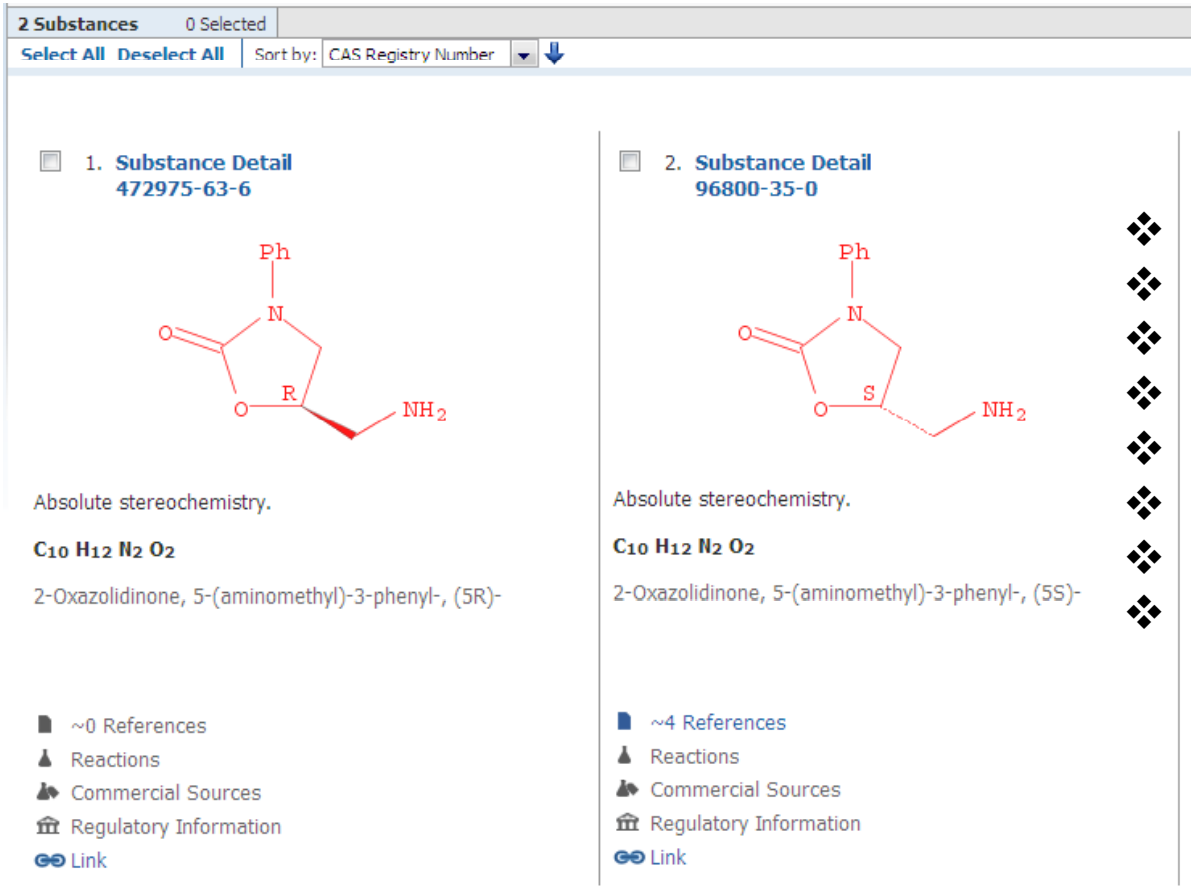
通过绘图面板绘制噁唑烷酮类药物的母核结构



三种检索方式：

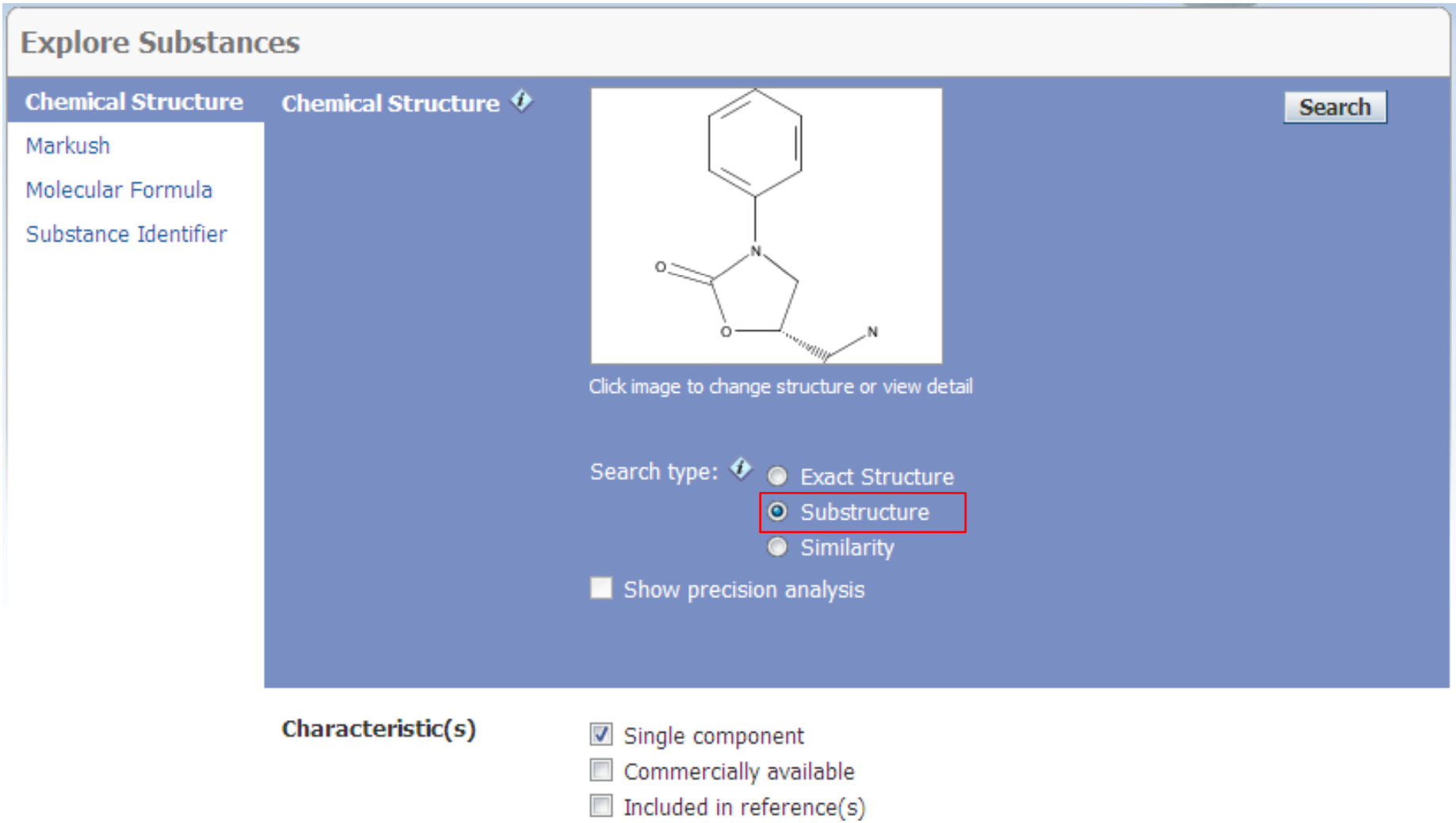


Exact Structure

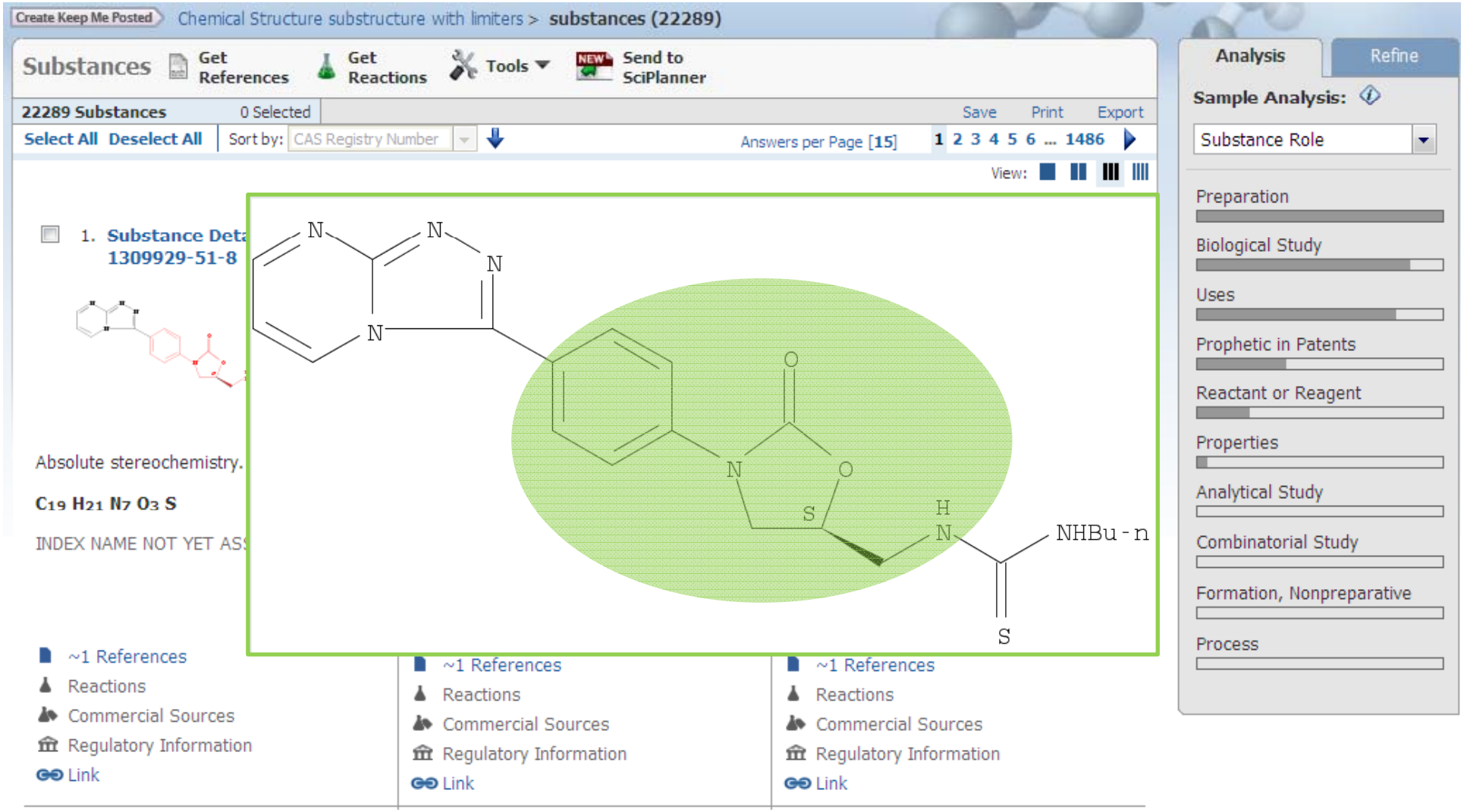


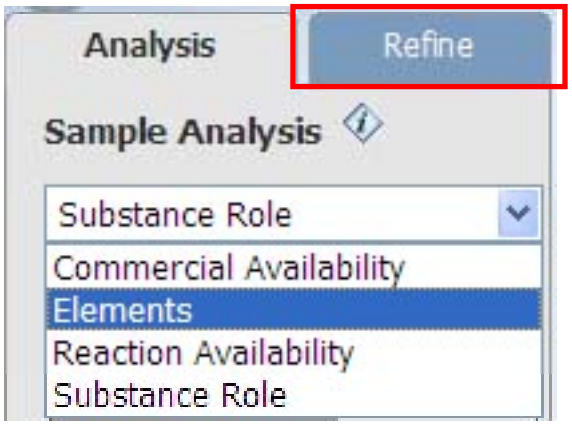
- 与已绘画的化学结构相同：
- 构造异构体
- 互变异构(包括酮-烯醇互变异构)
- 配位化合物
- 离子化合物
- 原子基和离子基
- 含同位素的物质
- 单体组成之聚合物

亚结构检索方式：



查看具有噁唑烷酮母核的所有已经报道的物质结构：

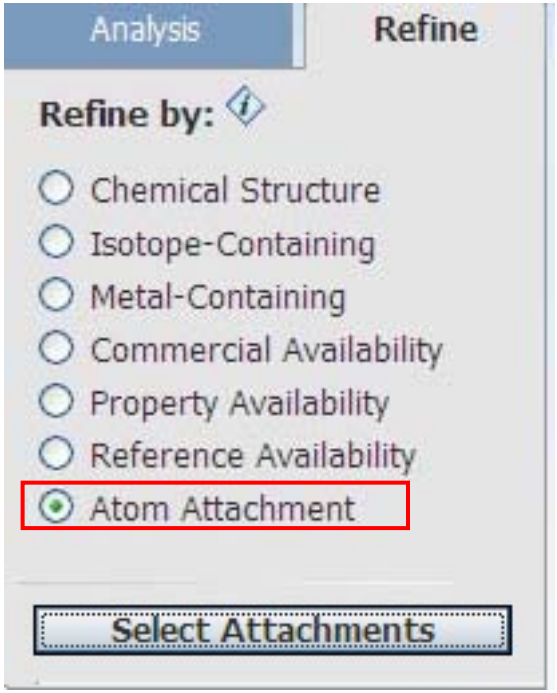




一共有4种分析功能

提供结构物质角色分析，元素分析，商业可购买性分析，反应提供性分析等。

通常可以通过物质角色分析（Substance Role）去看看这些物质都存在哪些应用



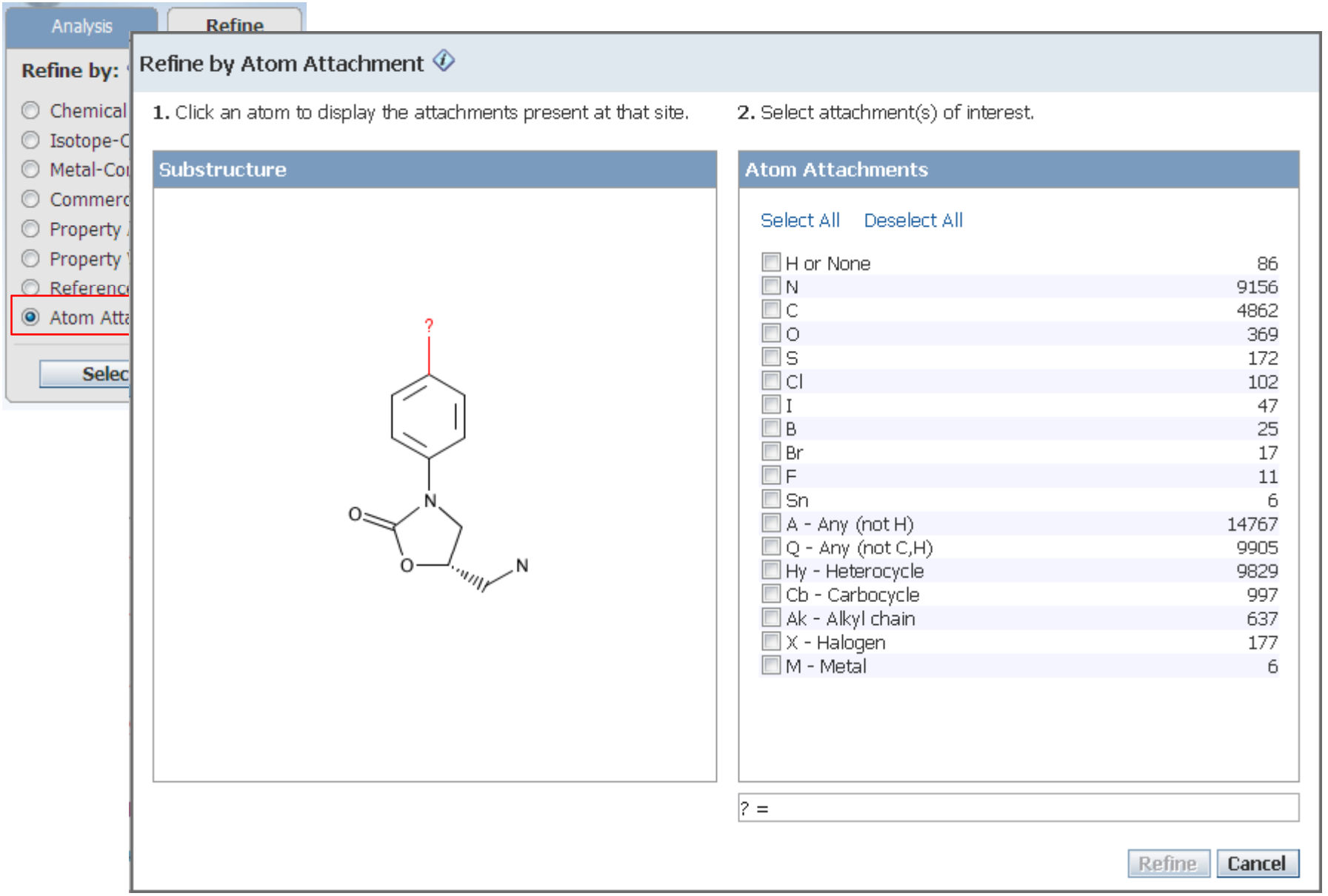
一共有7种限定功能

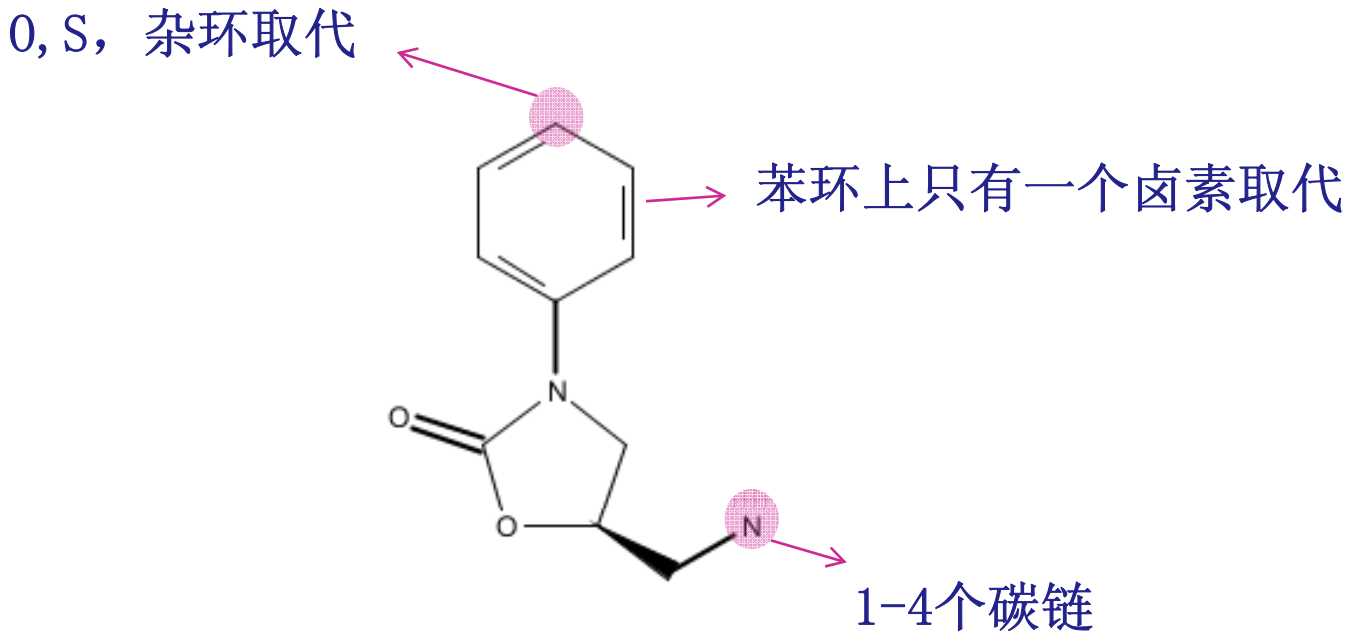
提供结构再次限定，同位素是否包含限定，金属是否包含限定，理化性质限定等。

通常可以通过结构的再次限定（Chemical Structure）去对结构再次修饰

或者通过理化性质（Property Date）去找到符合理化性质要求的物质

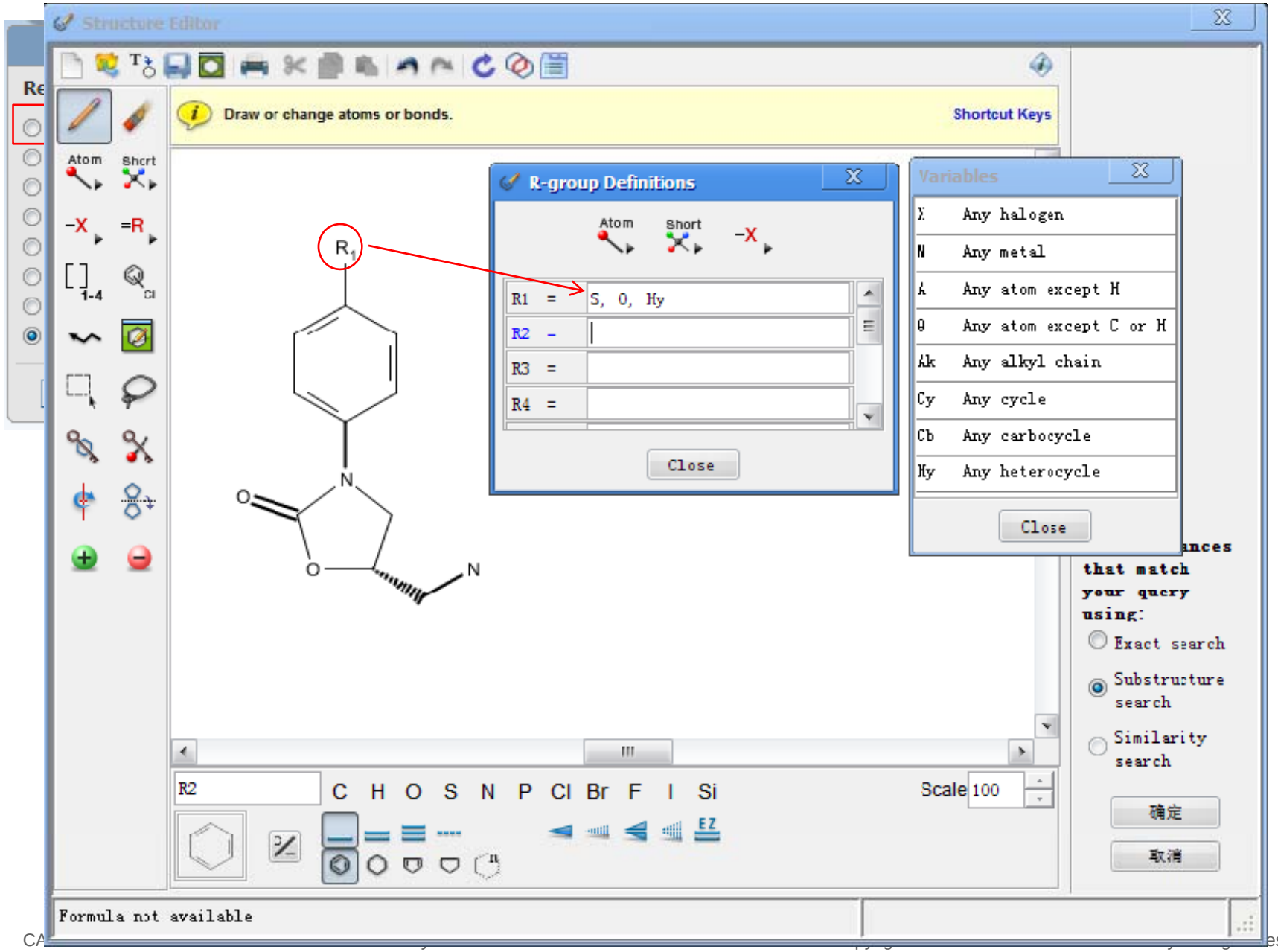
还可以通过原子附属性（Atom Attachment）去分析结构上的修饰情况

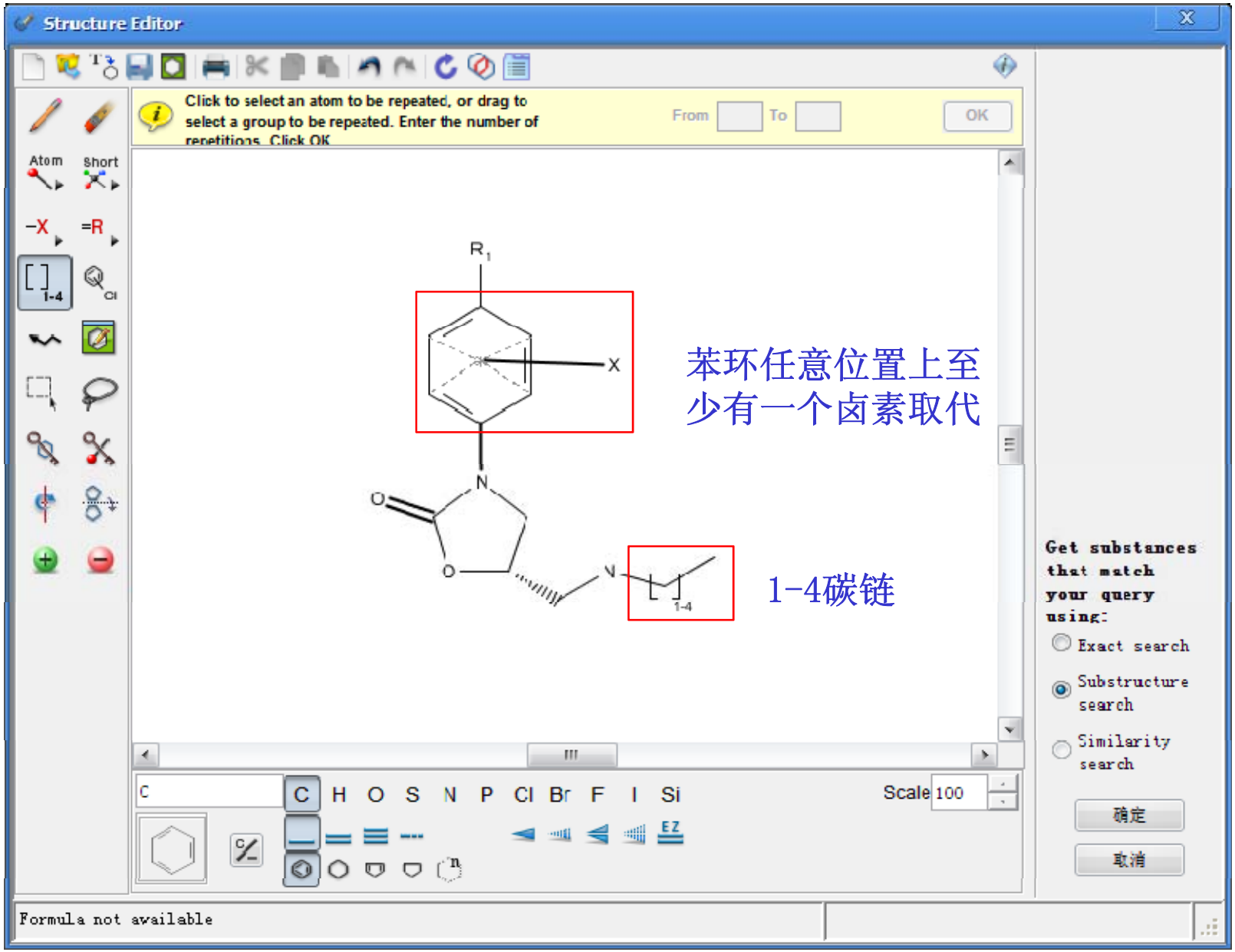




当我们用**Atom Attachment**限定工具分析完全部位点的原子附属性后，我们想去获得：苯环对位为硫，氧或杂环取代， 苯环上只有一个卤素取代，同时还想限定N链上是1-4个碳链的化合物。

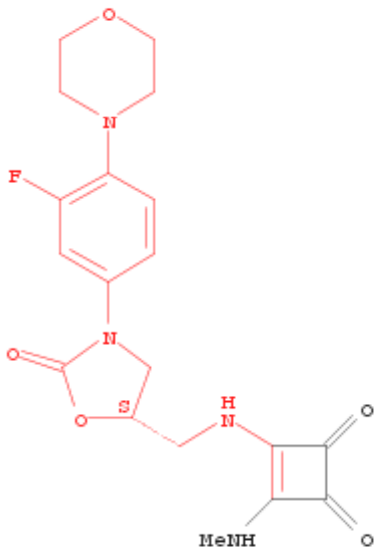
那我们应该如何去做呢？


Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
Atom
Short
-X
=R
1-4
R-group Definitions
Atom
Short
-X
R1 = S, O, Hy
R2 -
R3 =
R4 =
Close
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any alkyl chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Close
that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
R2
C H O S N P Cl Br F I Si
Scale 100
Formula not available



获得符合设计要求的化合物

7. **Substance Detail**
1308299-22-0

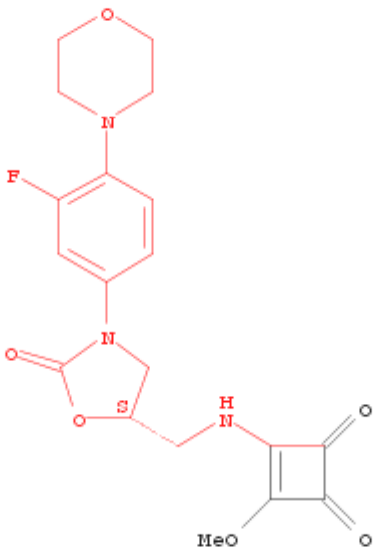


Absolute stereochemistry.

$C_{19}H_{21}FN_4O_5$

3-Cyclobutene-1,2-dione, 3-[[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]amino]-4-(methylamino)-

8. **Substance Detail**
1308299-21-9

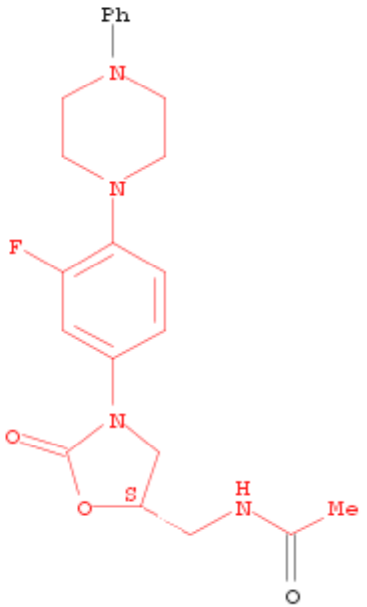


Absolute stereochemistry.

$C_{19}H_{20}FN_3O_6$

3-Cyclobutene-1,2-dione, 3-[[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]amino]-4-methoxy-

9. **Substance Detail**
1303962-95-9
(Component: 465520-11-0)



• 3/4 H_2O

Absolute stereochemistry.

提纲

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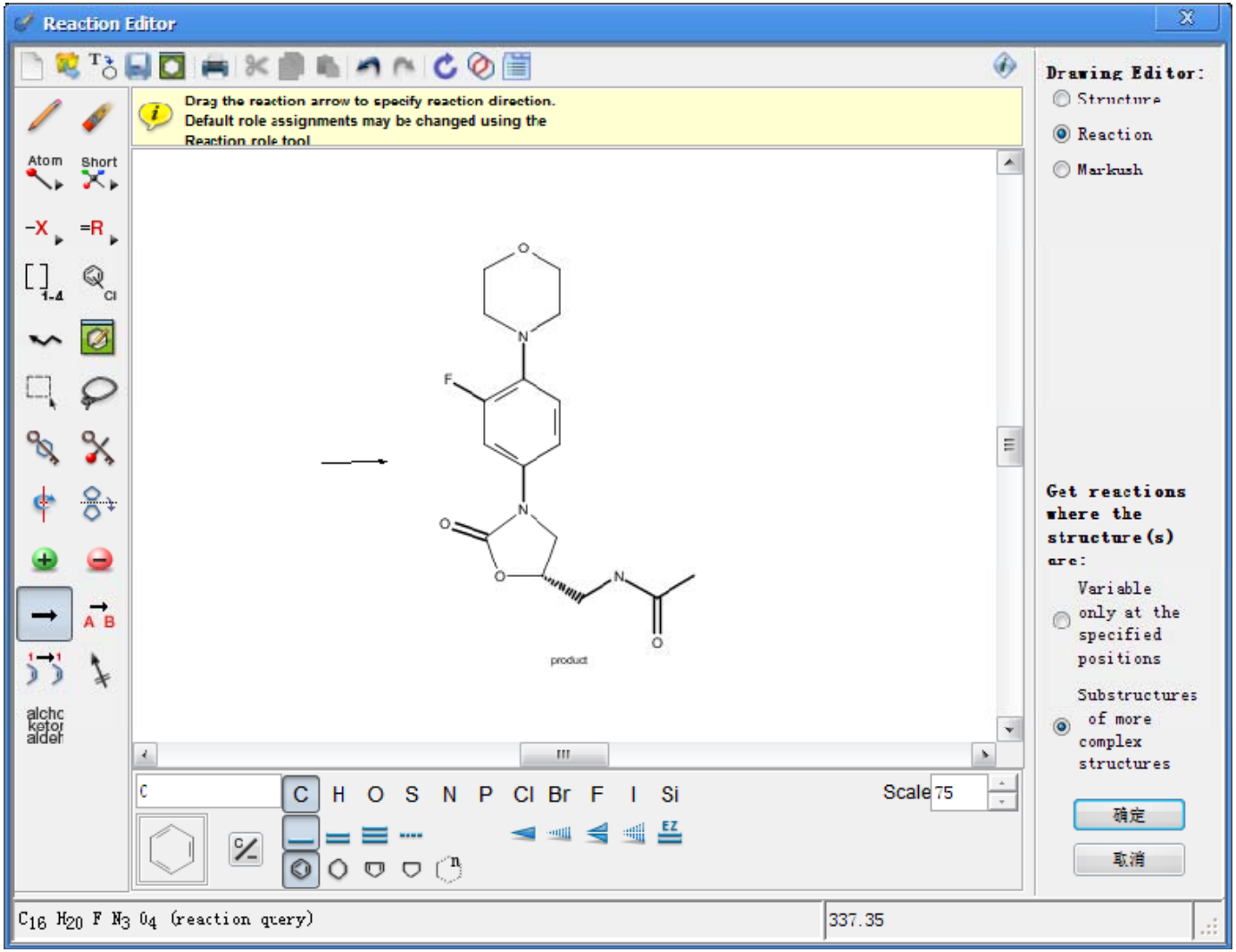
SciFinder检索反应信息



Reactions | Get References | Tools | Send to SciPlanner

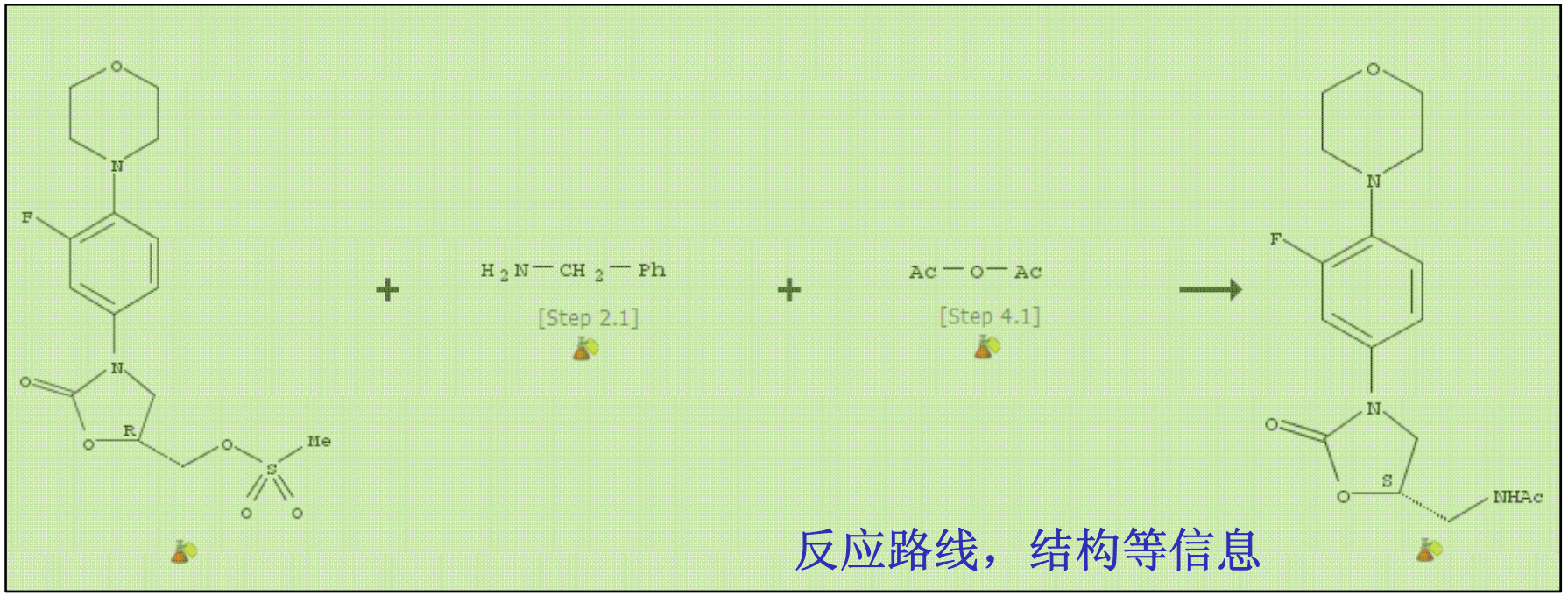
221 Reactions | 1 Selected | Save | Print | Export

80 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15] | 1 2 3 4 5 6 | Display:

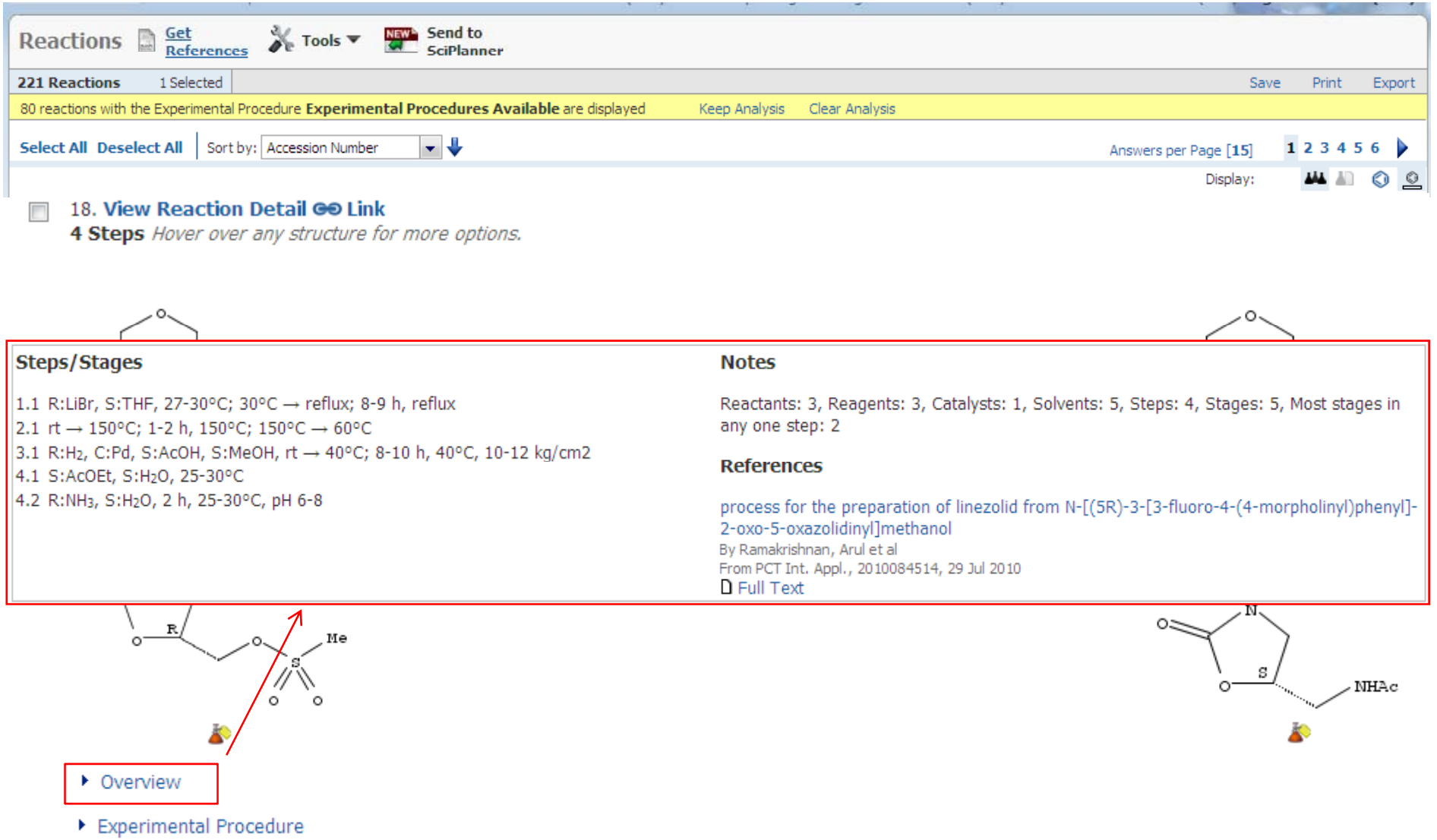
18. **View Reaction Detail Link**

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



▸ Overview

▸ Experimental Procedure



Reactions | Get References | Tools | Send to SciPlanner

221 Reactions | 1 Selected | Save | Print | Export

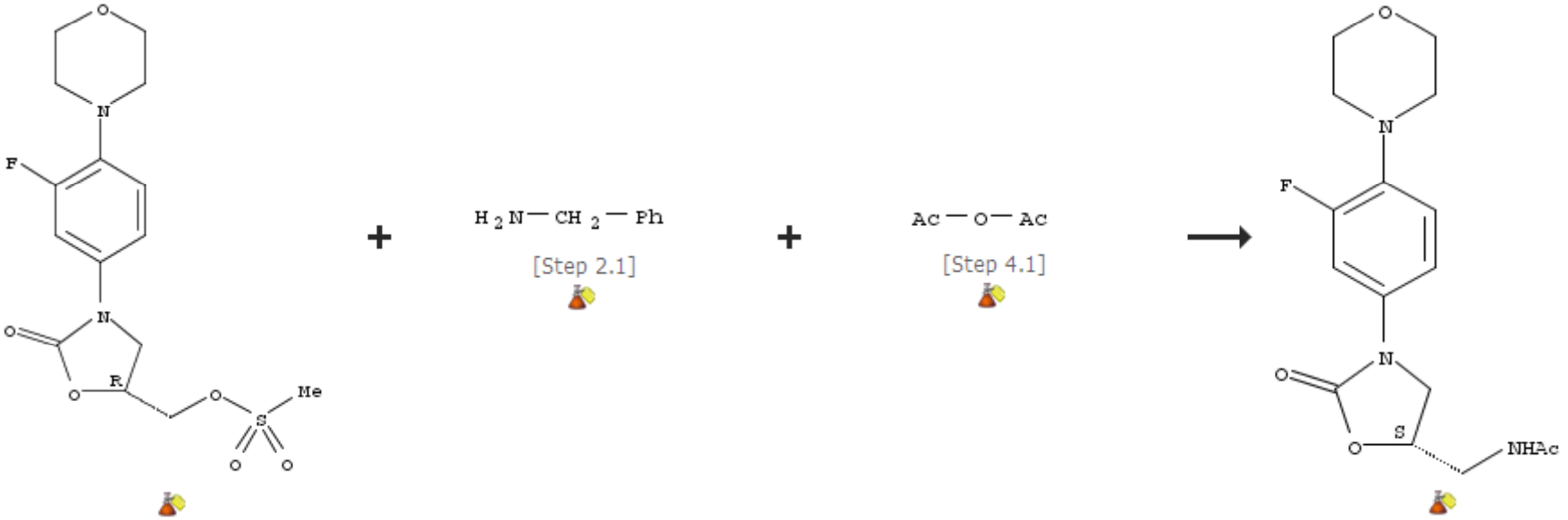
80 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15] | 1 2 3 4 5 6

Display:

18. **View Reaction Detail Link**

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



▸ Overview

▸ Experimental Procedure

来自原文的详细反应操作

Step 1

Example-2: Preparation of (5R)-(N)-[[3-fluoro-(4-morpholinylphenyl)-2-oxo-5-oxazolidinyl]methyl]bromide. (5R)-(N)-[3-fluoro-(4-morpholinylphenyl)-2-oxo-5-oxazolidinyl]methyl]sulphonate (1 mole eq, 100 g) and lithium bromide (2.0 mole eq, 46.36 g) were taken in tetrahydrofuran (1.0 L) under nitrogen at 27 - 30°C and heated to reflux for 8-9 hours. The reaction mixture was cooled to room temperature and distilled out completely. To the residue was added water (350 ml), stirred for 1hr

Step 2

Example-4: Prepar
oxazolidinyl]methy
was cooled to 60°
and dried to obtair
temperature, filter

Step 3

Example-6: Prepar
oxazolidinyl]benzyl
hydrogen pressure
acetate (750 ml) a

Step 4

Example-8: Prepar
morpholinylphenyl
acetic anhydride (1
mixture was then f

▾ Experimental Procedure

Organic LETTERS

Step 1

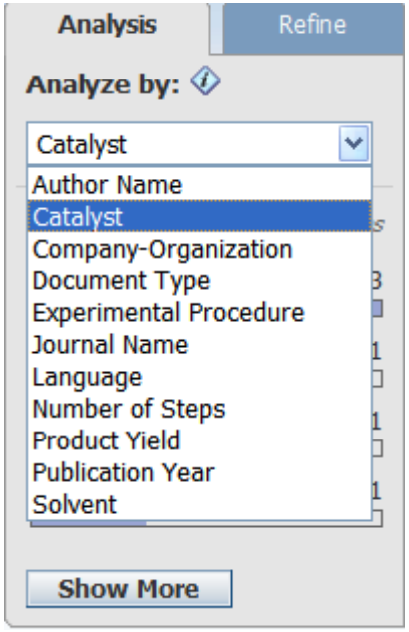
N-((2, 2-Dimethyl-1, 3-dioxolan-4-yl) methyl)-3-fluoro-4-morpholinobenzenamine (8) To a solution of 1.96 g of 6 (0.01 mol) in 30 mL of THF was slowly added 1.97 g of 2, 2-dimethyl-1, 3-dioxolane-4-carbaldehyde 7 (0.015 mol) and 6 g of $NaBH(OAc)_3$ (0.028 mol). The mixture was stirred overnight and was purified on medium pressure silica gel column to give 2.52 g of product. Yield: 82%. ^1H NMR ($CDCl_3$, 400 MHz): δ 6.83 (t, J = 8.8 Hz, 1H), 6.38 (m, 2H), 4.34 (m, 1H), 4.09 (m, 1H), 3.85 (t, J = 4.4 Hz, 4H), 3.75 (m, 1H), 3.24 (d, J = 4 Hz, 1H), 3.13 (d, J = 4 Hz, 1H), 2.96 (t, J = 4.4 Hz, 4H), 1.44 (s, 3H), 1.37 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 25.27, 26.70, 26.88, 46.93, 51.66, 63.01, 65.81, 67.10, 74.35, 76.20, 101.40, 101.80, 109.30, 109.48, 120.33, 136.50, 144.90, 158.18. MS (EI): m/e (%) = 310 (77) $[M]^+$, 209 (100), 151 (11).

来自原文的谱图信息

Step 2

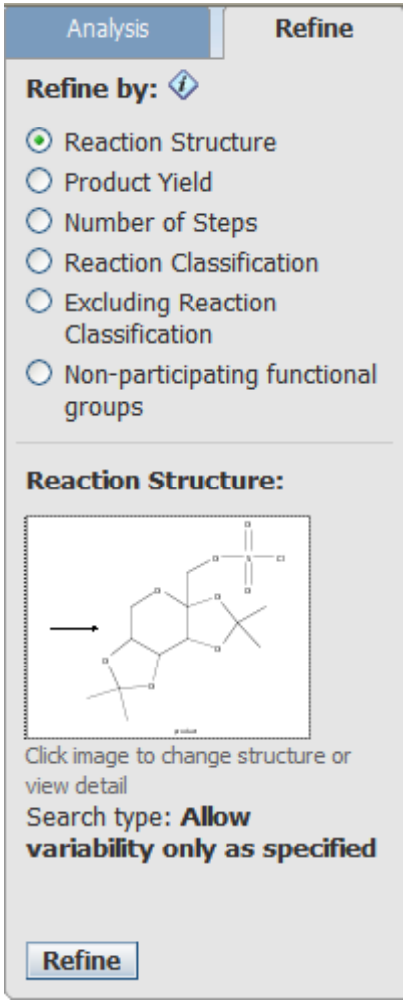
Ethyl (2,2-dimethyl-1,3-dioxolan-4-yl)methyl(3-fluoro-4-morpholinophenyl)carbamate (9) To a solution of 1.55 g of 8 (4 mmol) and 0.5 g of i-Pr_2NEt (4 mmol) in 15 mL of MeCN was added 0.64 g of ethyl chloroformate (5 mmol). The mixture was stirred at room temperature for 2 h. Then water was added. The solution was extracted with ethyl acetate. The combined organic layers were dried over $MgSO_4$, filtered and concentrated to afford the crude product. The pure product was obtained after purification by column chromatography on silica gel. Yield: 94%. ^1H NMR ($CDCl_3$, 500 MHz): δ 6.91 (m, 3H), 4.23 (m, 1H), 4.11 (m, 2H), 3.95 (m, 1H), 3.81 (t, J = 4.4 Hz, 4H), 3.72 (m, 2H), 3.58 (m, 1H), 3.03 (d, J = 4.4 Hz, 4H), 1.28 (s, 3H), 1.25 (s, 3H), 1.15 (m, 3H); ^{13}C NMR ($CDCl_3$): δ 14.49, 25.24, 25.42, 26.67, 26.73, 51.03, 62.04, 62.98, 65.71, 66.67, 67.46, 73.96, 76.15, 109.37, 120.33, 136.50, 144.90, 158.18; MS (EI): m/e (%) = 382 (100) $[M]^+$, 296 (10), 281 (14), 237 (12), 209 (40), 150 (19), 101 (12).

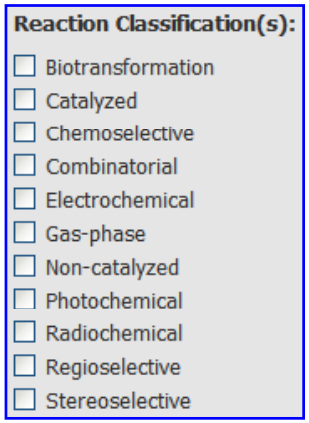
反应结果集的Analyze/ Refine功能

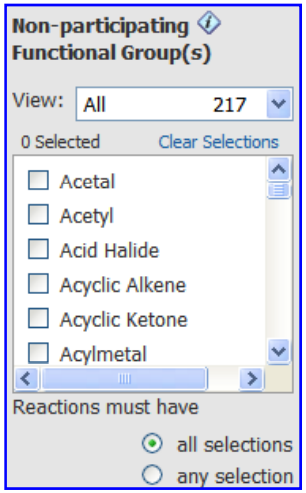


Analyze:

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







Refine:

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

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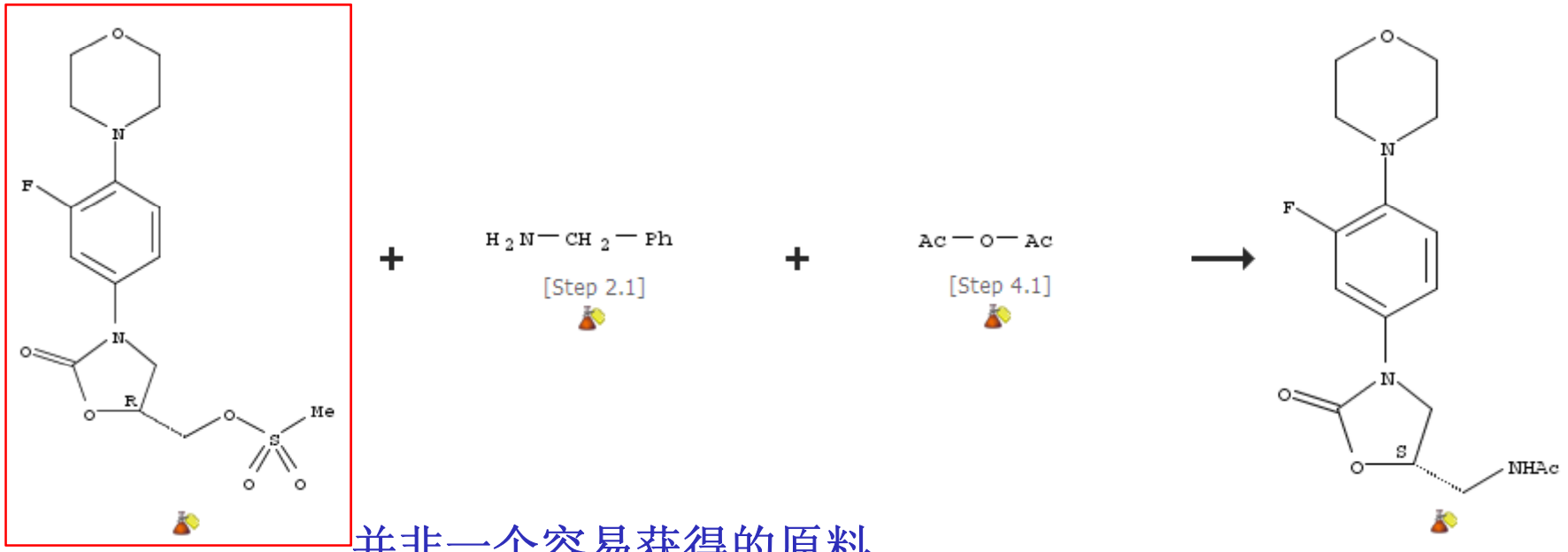
4 Steps *Hover over any structure for more options.*

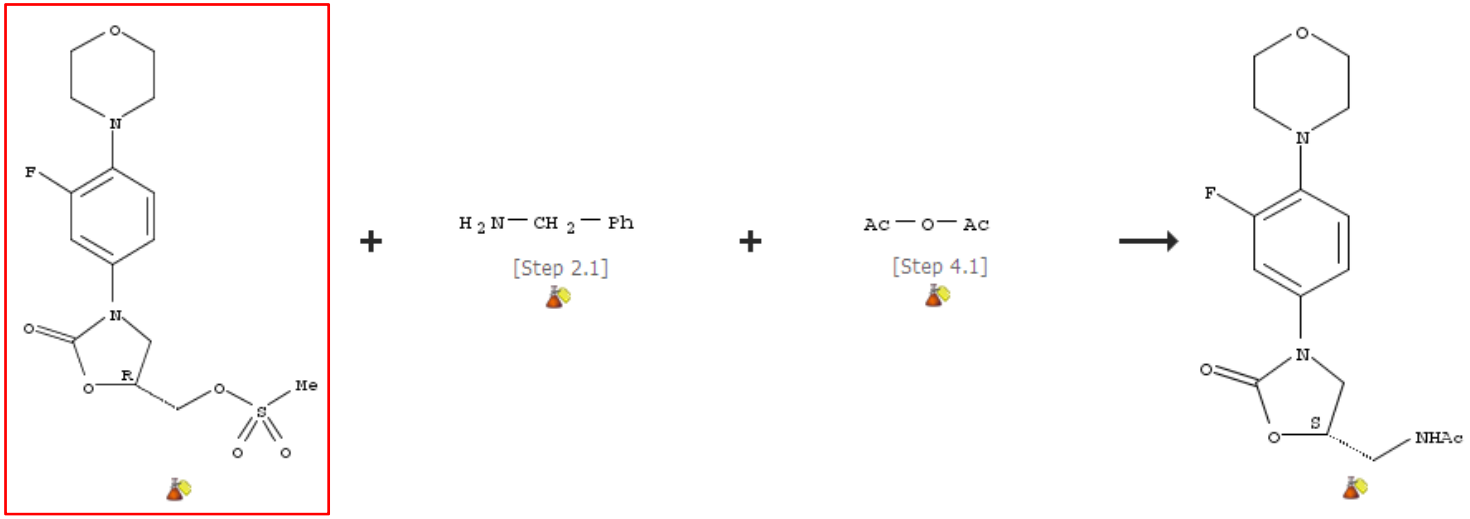


并非一个容易获得的原料

▸ Overview

▸ Experimental Procedure

18. **View Reaction Detail Link**
4 Steps *Hover over any structure for more options.*



▸ Overview

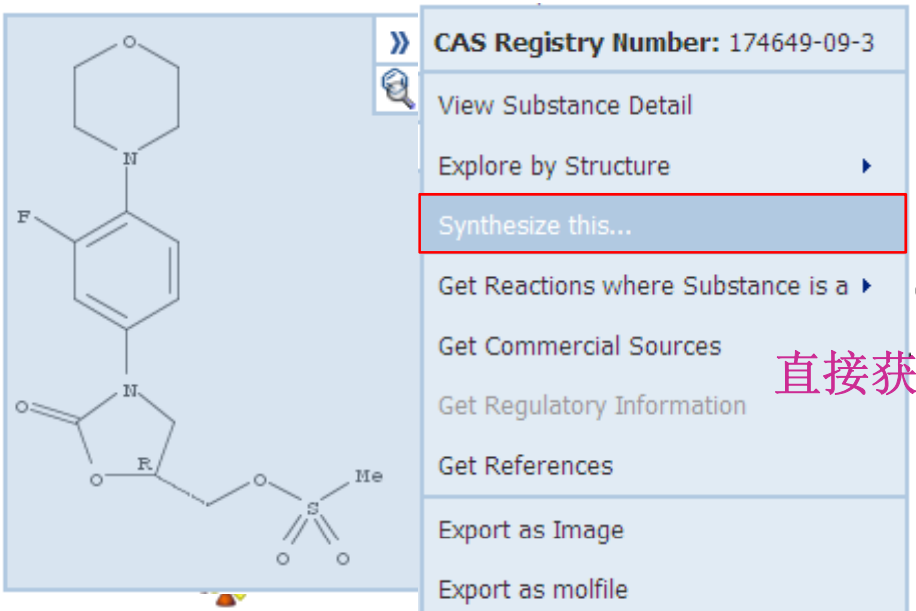
▸ Experimental Procedure

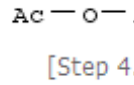
➢如何通过此反应物向前延伸，推导最合适的起始原料？

➢如何利用SciFinder编写完整的合成路线报告？
✓物质的基本理化性质。
✓合适的起始原料，详细的反应条件。
✓具体的反应操作步骤。
✓参考文献。

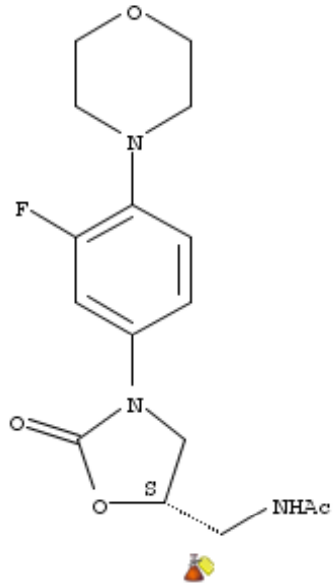
利用sciplanner编写完整的合成报告

18. **View Reaction Detail Link**
4 Steps *Hover over any structure for more options.*





直接获得合成此物质的反应



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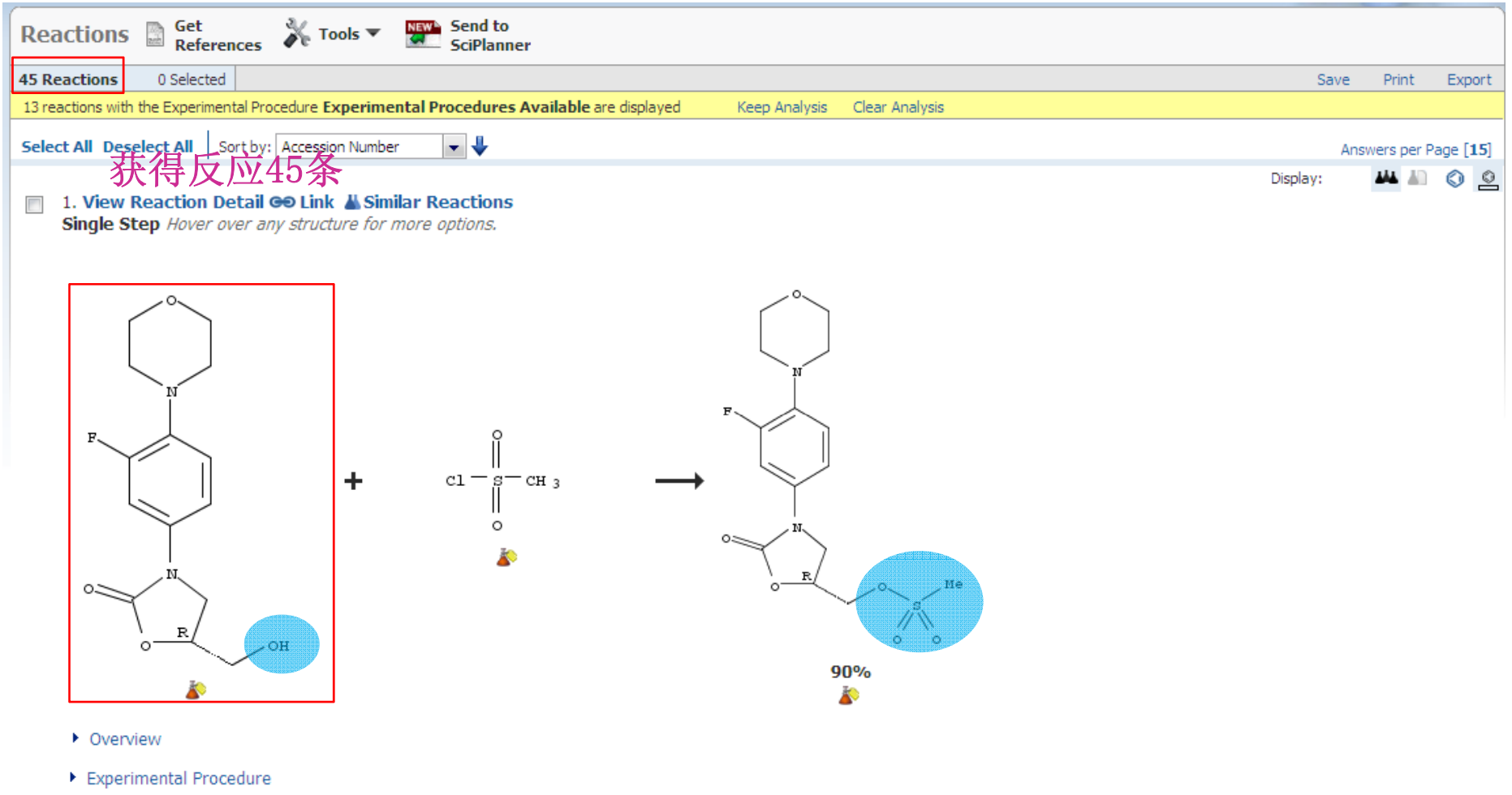

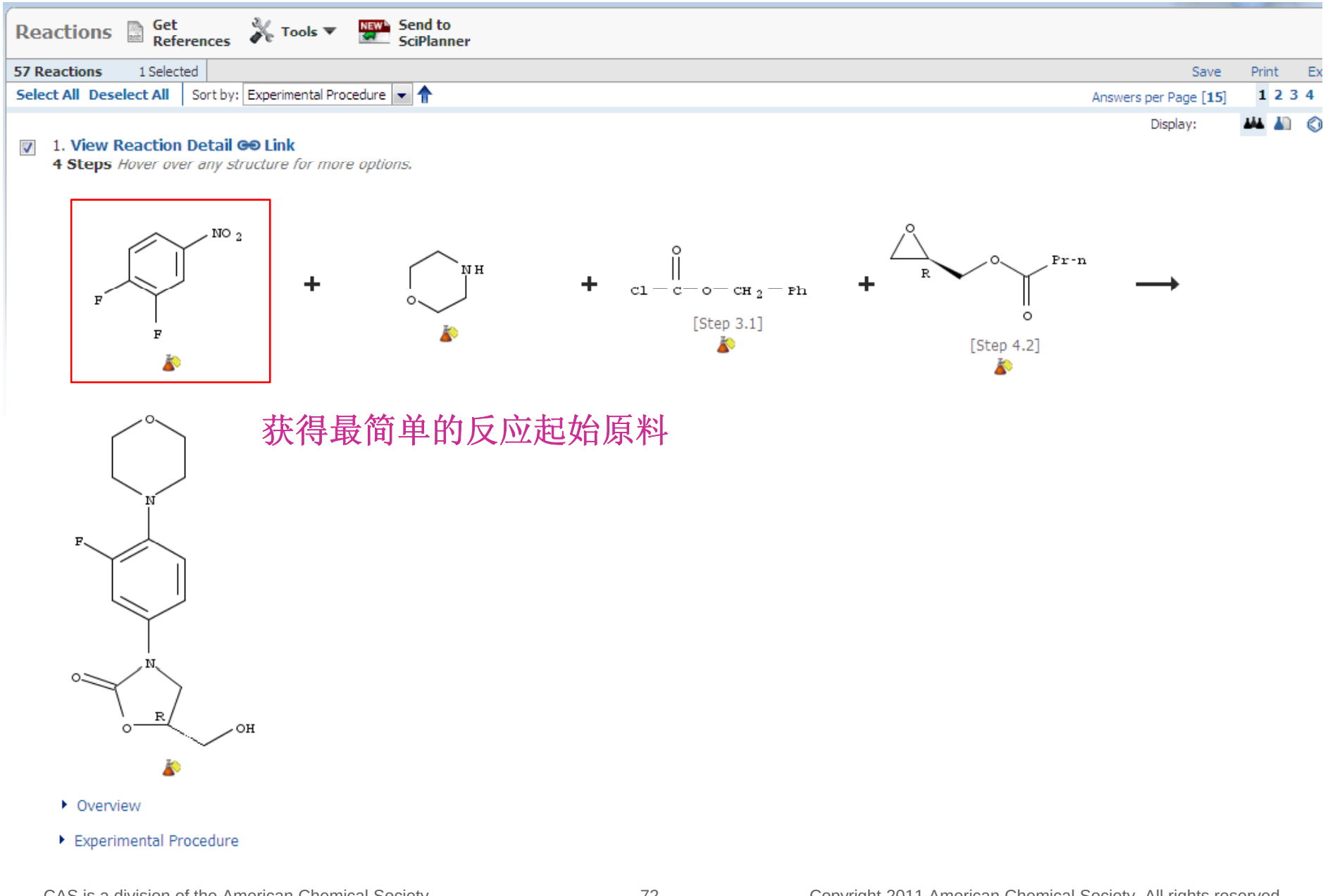

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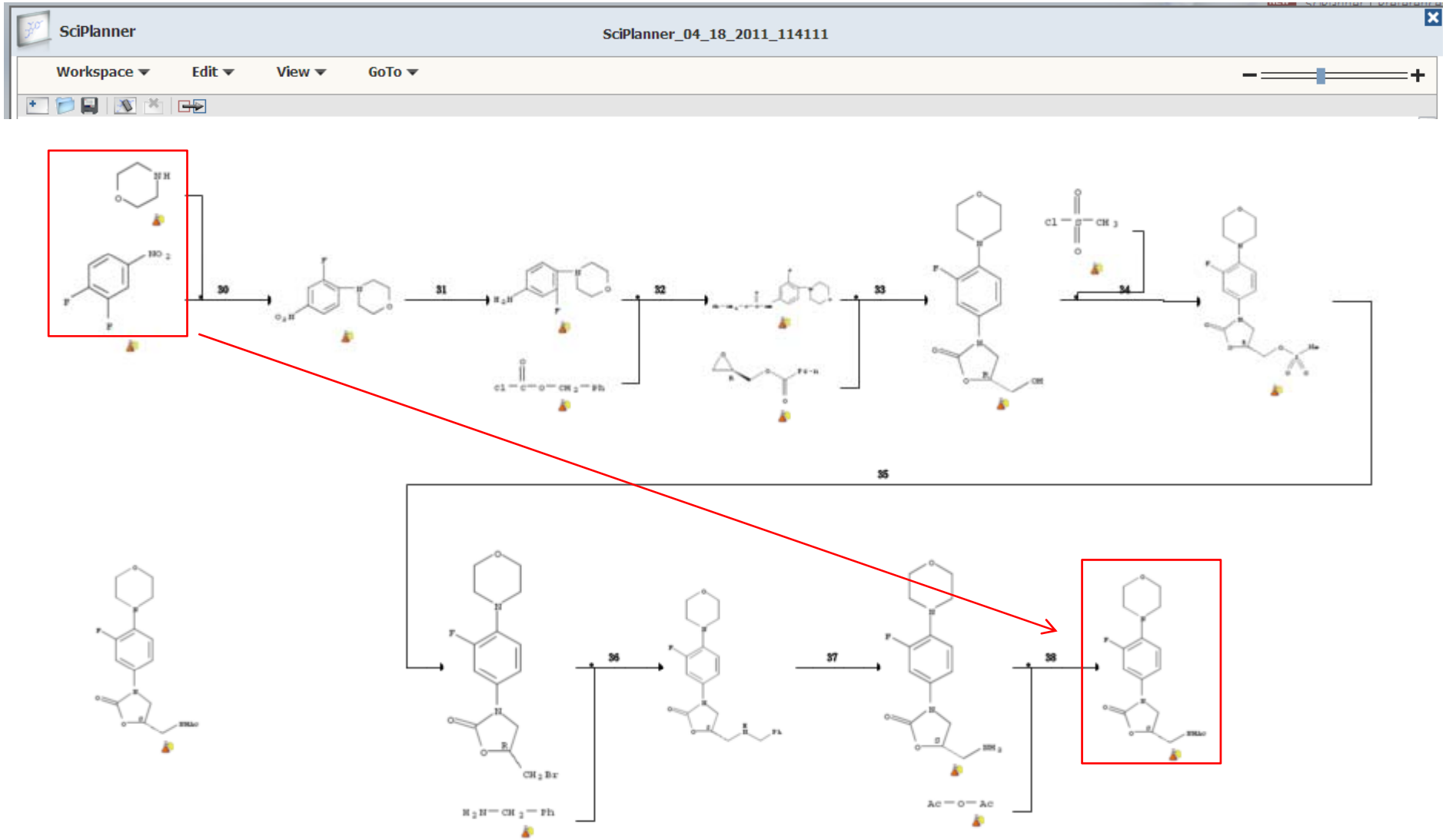
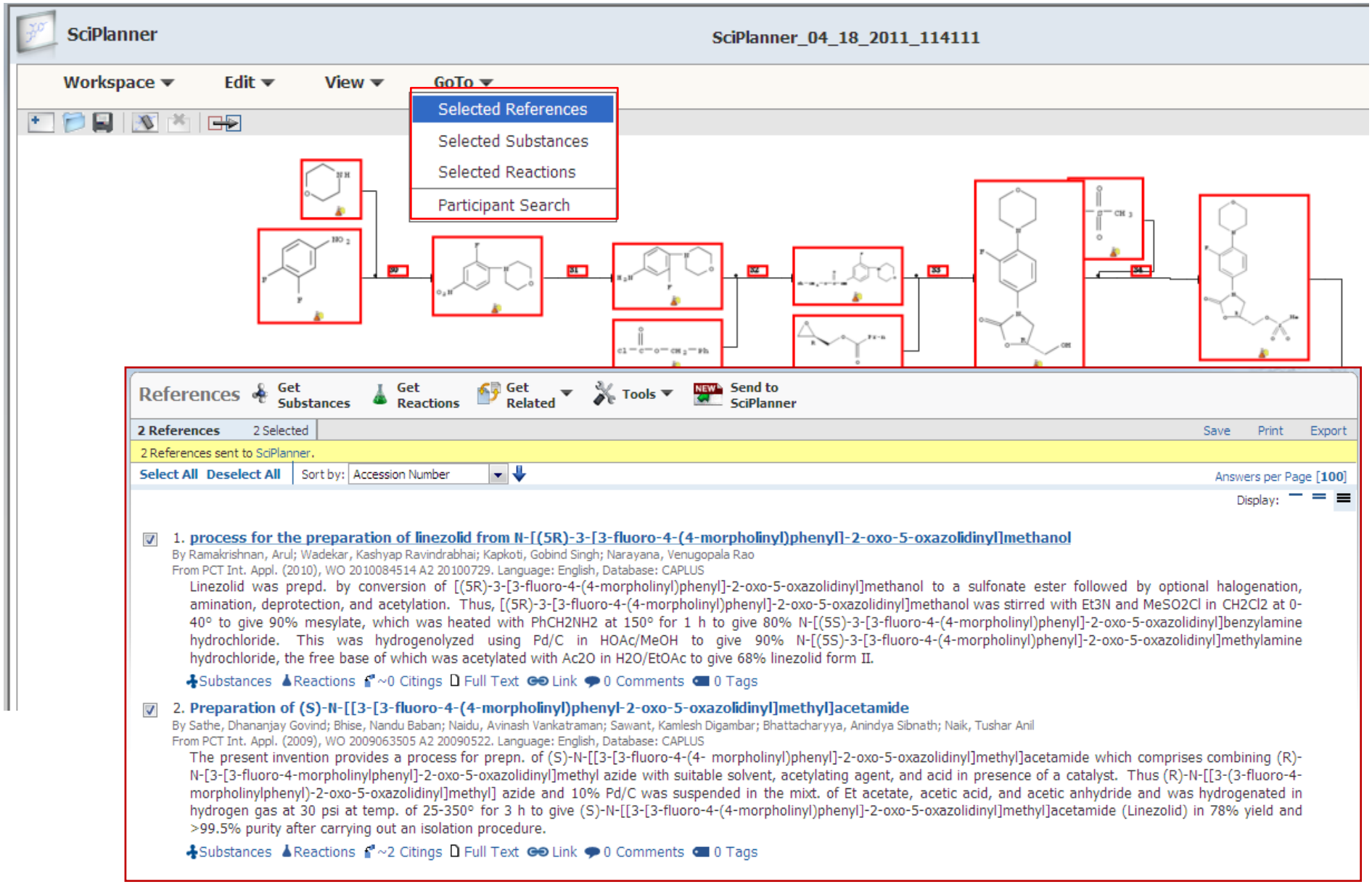
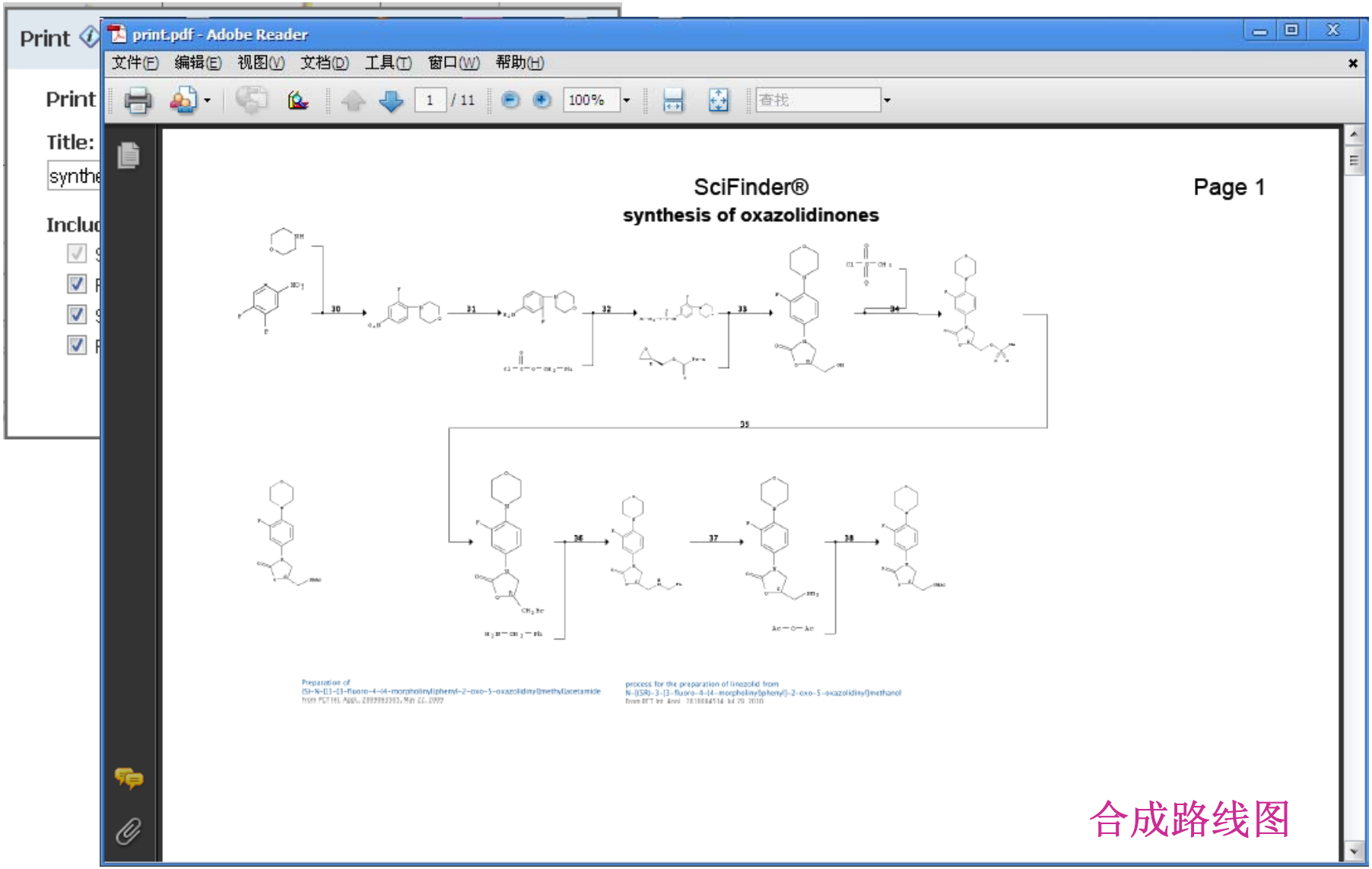




利用sciplanner编写完整的合成报告



涉及的物质的信息：

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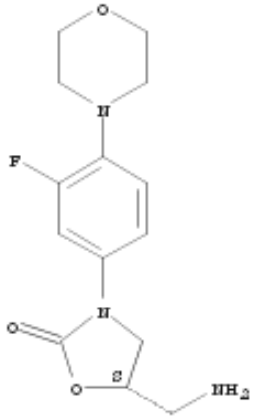
168828-90-8

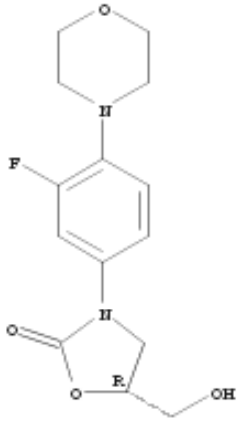


Absolute stereochemistry.
Rotation (-).

$C_{14}H_{18}FN_3O_3$

2-Oxazolidinone, 5-(aminomethyl)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-, (5S)-

2. **Substance Detail**
168828-82-8

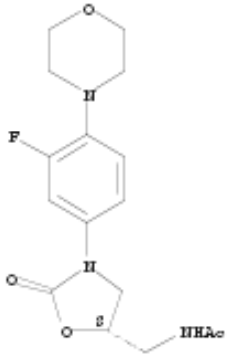


Absolute stereochemistry.

$C_{14}H_{17}FN_2O_4$

2-Oxazolidinone, 3-[3-fluoro-4-(4-morpholinyl)phenyl]-5-(hydroxymethyl)-, (5R)-

3. **Substance Detail**
165800-03-3



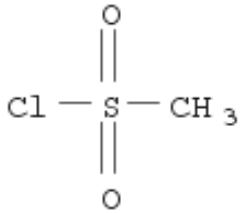
Absolute stereochemistry.
Rotation (-).

$C_{16}H_{20}FN_3O_4$

Acetamide, N-[[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-

~2,595 References

4. **Substance Detail**
124-63-0

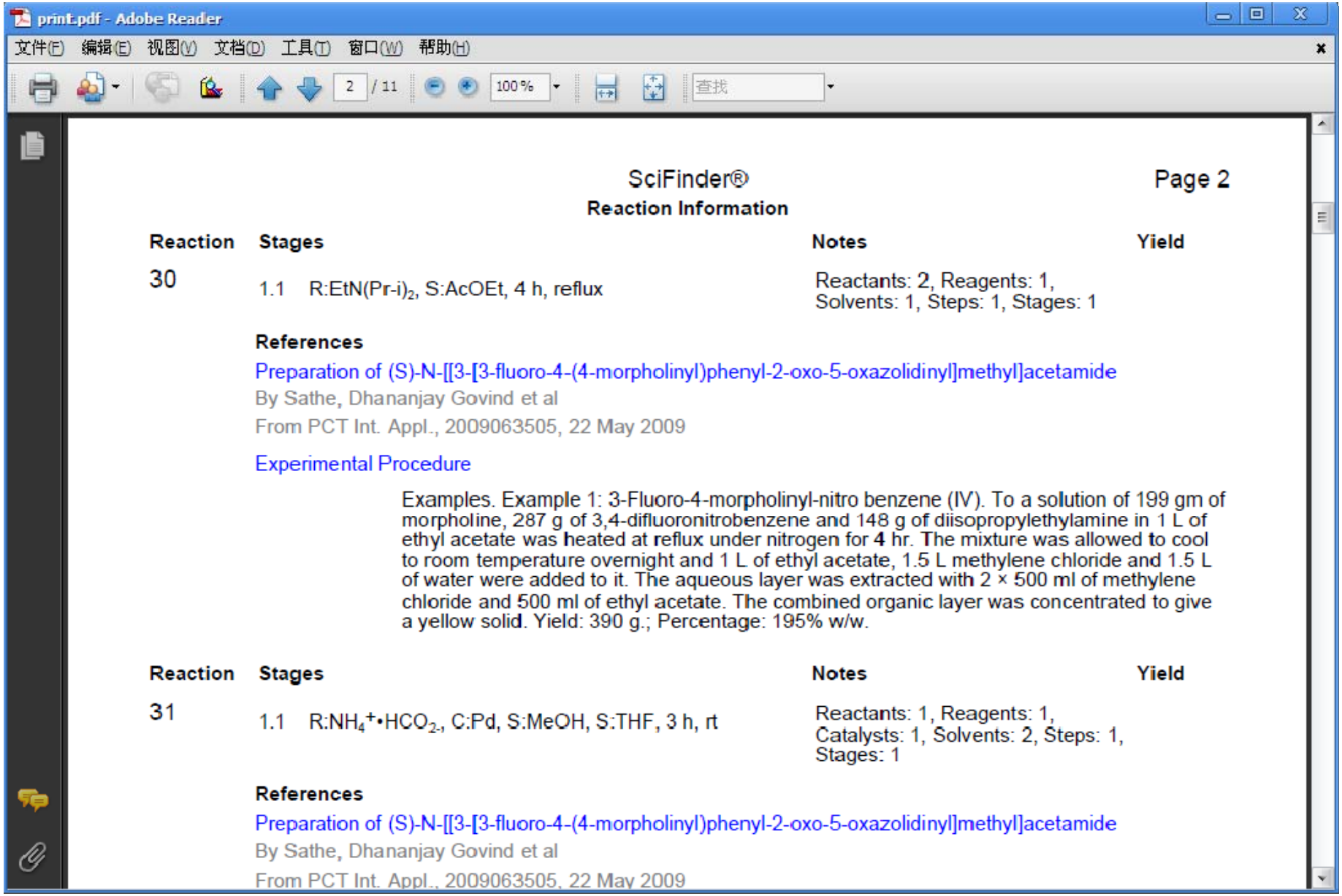


CH_3ClO_2S

Methanesulfonyl chloride

~7,725 References
Reactions
Commercial Sources
Regulatory Information
Link

每步反应的条件，详细操作步骤



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Reaction Information

Reaction	Stages	Notes	Yield
30	1.1 R:EtN(Pr-i)$_2$, S:AcOEt, 4 h, reflux	Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1	

References

Preparation of (S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl-2-oxo-5-oxazolidinyl]methyl]acetamide

By Sathe, Dhananjay Govind et al

From PCT Int. Appl., 2009063505, 22 May 2009

Experimental Procedure

Examples. Example 1: 3-Fluoro-4-morpholinyl-nitro benzene (IV). To a solution of 199 gm of morpholine, 287 g of 3,4-difluoronitrobenzene and 148 g of diisopropylethylamine in 1 L of ethyl acetate was heated at reflux under nitrogen for 4 hr. The mixture was allowed to cool to room temperature overnight and 1 L of ethyl acetate, 1.5 L methylene chloride and 1.5 L of water were added to it. The aqueous layer was extracted with 2 × 500 ml of methylene chloride and 500 ml of ethyl acetate. The combined organic layer was concentrated to give a yellow solid. Yield: 390 g.; Percentage: 195% w/w.

Reaction	Stages	Notes	Yield
31	1.1 R:$NH_4^+ \cdot HCO_2^-$, C:Pd, S:MeOH, S:THF, 3 h, rt	Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1	

References

Preparation of (S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl-2-oxo-5-oxazolidinyl]methyl]acetamide

By Sathe, Dhananjay Govind et al

From PCT Int. Appl., 2009063505, 22 May 2009

每步反应涉及的参考文献信息：

References

Preparation of (S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl-2-oxo-5-oxazolidinyl]methyl]acetamide

By Sathe, Dhananjay Govind; Bhise, Nandu Baban; Naidu, Avinash Vankatraman; Sawant, Kamlesh Digambar; Bhattacharyya, Anindya Sibnath; Naik, Tushar Anil

From PCT Int. Appl. (2009), WO 2009063505 A2 20090522. , Language: English, Database: CAPLUS

The present invention provides a process for prepn. of (S)-N-[[3-[3-fluoro-4-(4- morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide which comprises combining (R)-N-[3-[3-fluoro-4-morpholinylphenyl]-2-oxo-5-oxazolidinyl]methyl azide with suitable solvent, acetylating agent, and acid in presence of a catalyst. Thus (R)-N-[[3-(3-fluoro-4-morpholinylphenyl)-2-oxo-5-oxazolidinyl]methyl] azide and 10% Pd/C was suspended in the mixt. of Et acetate, acetic acid, and acetic anhydride and was hydrogenated in hydrogen gas at 30 psi at temp. of 25-350° for 3 h to give (S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide (Linezolid) in 78% yield and >99.5% purity after carrying out an isolation procedure.

process for the preparation of linezolid from N-[(5R)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methanol

By Ramakrishnan, Arul; Wadekar, Kashyap Ravindrabhai; Kapkoti, Gobind Singh; Narayana, Venugopala Rao

From PCT Int. Appl. (2010), WO 2010084514 A2 20100729. , Language: English, Database: CAPLUS

Linezolid was prepd. by conversion of [(5R)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methanol to a sulfonate ester followed by optional halogenation, amination, deprotection, and acetylation. Thus, [(5R)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methanol was stirred with Et3N and MeSO2Cl in CH2Cl2 at 0-40° to give 90% mesylate, which was heated with PhCH2NH2 at 150° for 1 h to give 80% N-[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]benzylamine hydrochloride. This was hydrogenolyzed using Pd/C in HOAc/MeOH to give 90% N-[(5S)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methylamine

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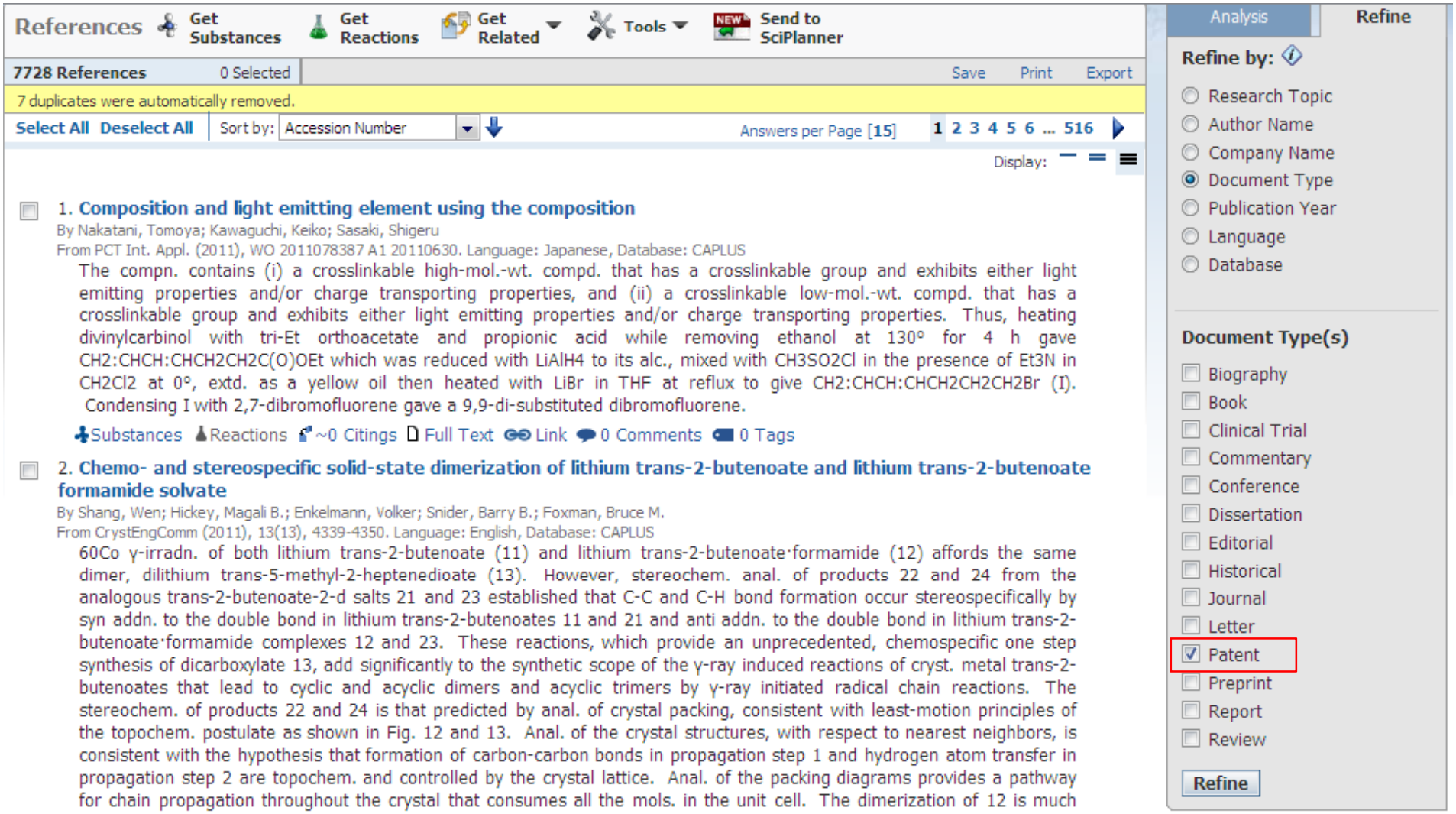

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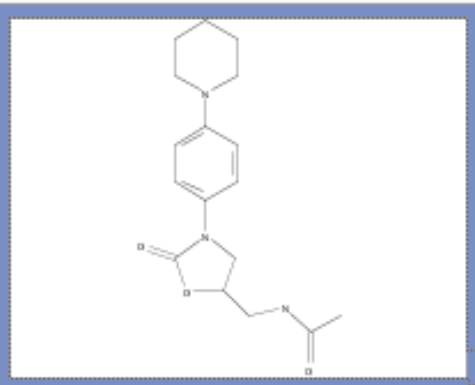

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Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

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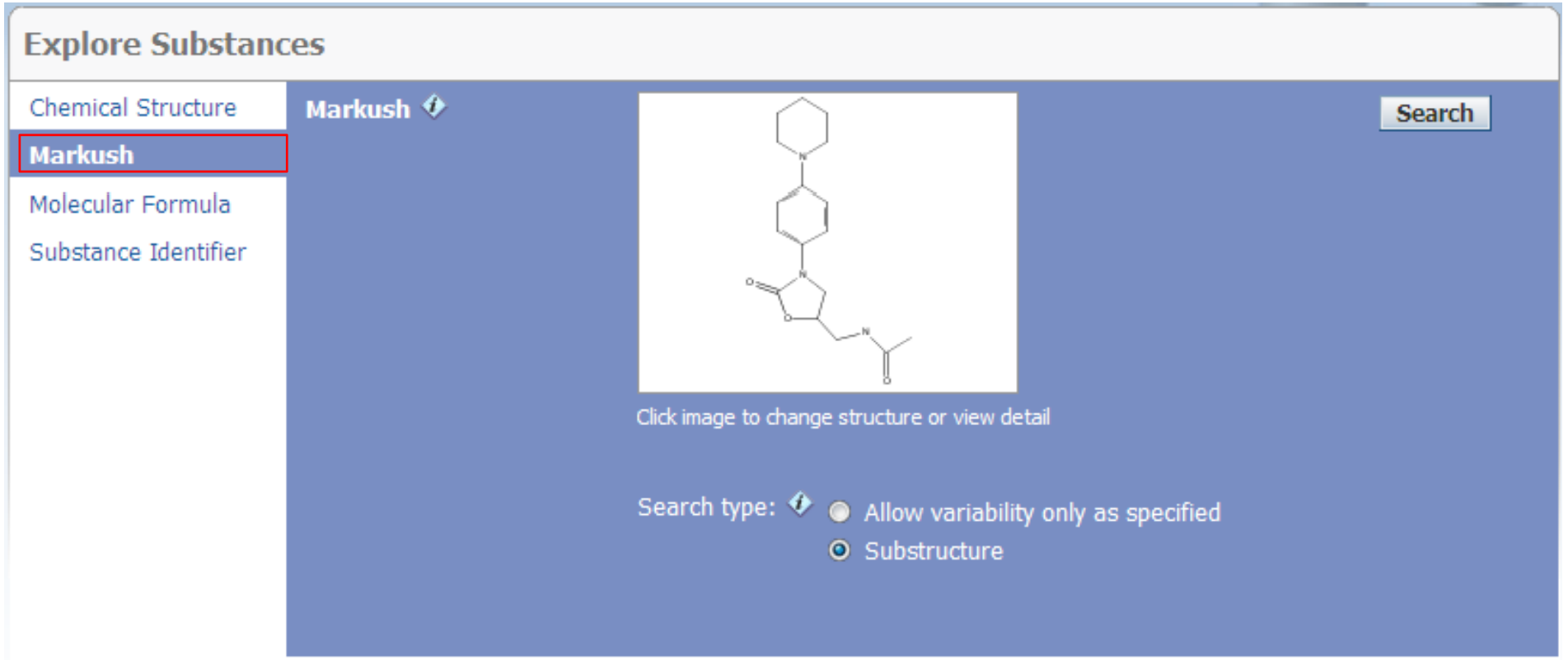

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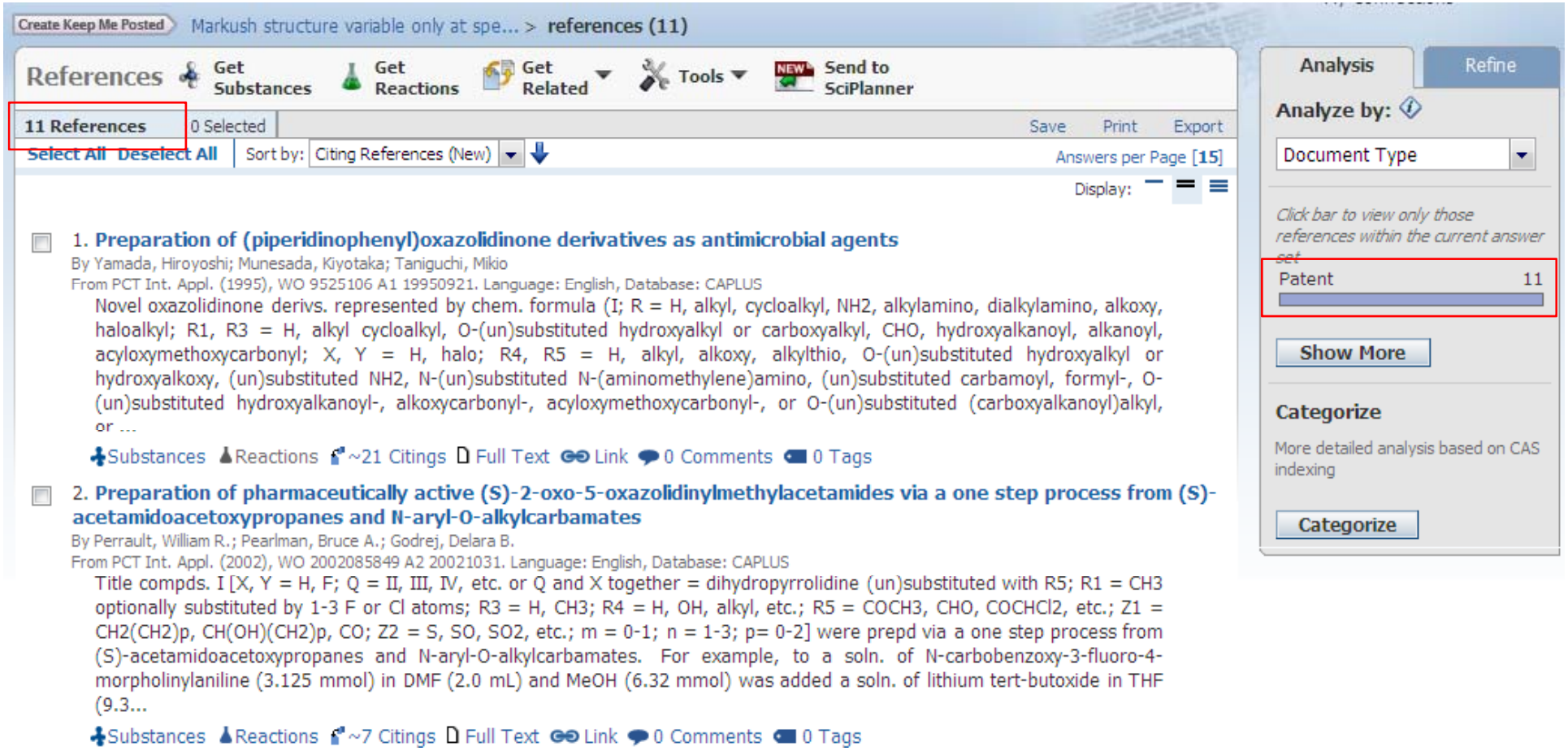

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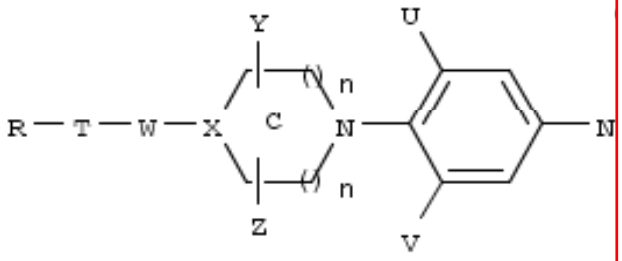
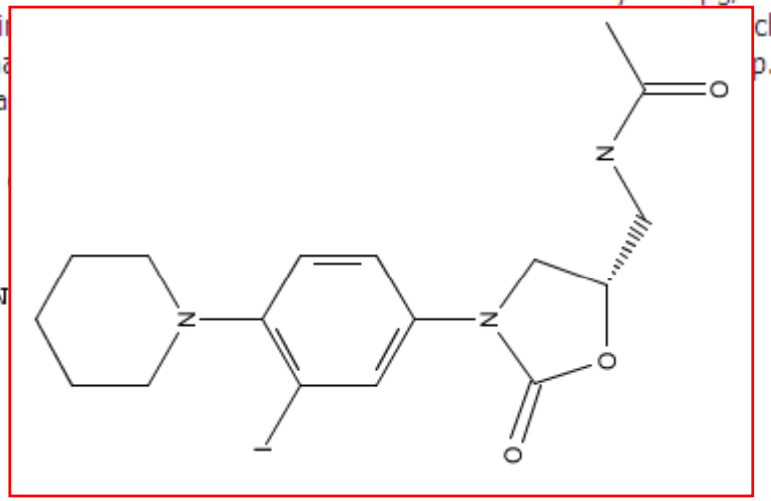
1. Preparation of oxazolidinone derivatives as antimicrobial agents

By: Mehta, Anita; Rudra, Sonali; Rao, Ajjarapu Venkata Subrahmanya Rajo; Yadav, Ajay Singh; Rattan, Ashok

Assignee: Ranbaxy Laboratories Limited, India

Title compds. I [T = 5-7 membered heterocycle, aryl, etc.; R = H, alkyl, F, Cl, Br, etc.; n = 0-3; X = H, CH, CHS, etc.; Y, Z = H, alkyl, cycloalkyl, etc.; U, V = H, alkyl, F, Cl, Br, I, etc.; W = CH2, CO, CH2NH, etc.; R1 = amido, thioamido, etc.] are prepd. For instance, II is prepd. from (S)-5-(((isoxazol-3-yl)oxy)methyl)-3-[3-fluoro-4-(piperazin-1-yl)phenyl]oxazolidin-2-one.bul.HCl and 4-bromo-5-nitrothiophene-2-carboxaldehyde (THF, NaHB(OAc)3, 17 h). Selected compds. of the invention exhibited antibacterial activity of 1 μg/mL against S. aureus (259231). I are effective against a no. of human and veteri ch as multiply-resistant staphylococci, streptococci and enterococci as well as ana p. species, and acid fast organisms such as Mycobacterium tuberculosis, Mycoba





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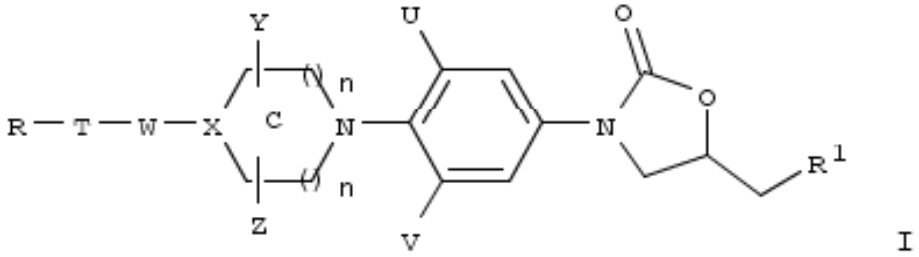
1. Preparation of oxazolidinone derivatives as antimicrobial agents

By: Mehta, Anita; Rudra, Sonali; Rao, Ajjarapu Venkata Subrahmanya Rajo; Yadav, Ajay Singh; Rattan, Ashok

Assignee: Ranbaxy Laboratories Limited, India

Title compds. I [T = 5-7 membered heterocycle, aryl, etc.; R = H, alkyl, F, Cl, Br, etc.; n = 0-3; X = H, CH, CHS, etc.; Y, Z = H, alkyl, cycloalkyl, etc.; U, V = H, alkyl, F, Cl, Br, I, etc.; W = CH2, CO, CH2NH, etc.; R1 = amido, thioamido, etc.] are prepd. For instance, II is prepd. from (S)-5-(((isoxazol-3-yl)oxy)methyl)-3-[3-fluoro-4-(piperazin-1-yl)phenyl]oxazolidin-2-one.bul.HCl and 4-bromo-5-nitrothiophene-2-carboxaldehyde (THF, NaHB(OAc)3, 17 h). Selected compds. of the invention exhibited antibacterial activity of 1 μg/mL against S. aureus (259231). I are effective against a no. of human and veterinary pathogens, including gram-pos. aerobic bacteria such as multiply-resistant staphylococci, streptococci and enterococci as well as anaerobic organisms as Bacterioides spp. and Clostridia spp. species, and acid fast organisms such as Mycobacterium tuberculosis, Mycobacterium avium and Mycobacterium spp.



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776296-89-0P

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Therapeutic use; B
or reagent

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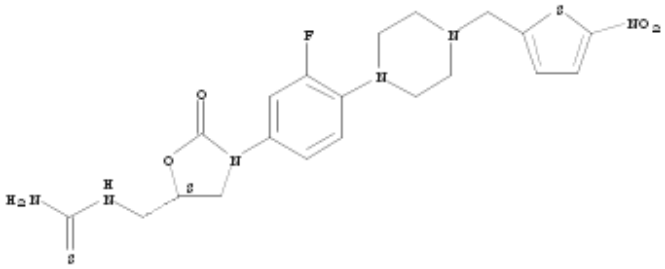
1. **Substance Detail**
776296-93-6



Absolute stereochemistry.

$C_{20}H_{23}FN_6O_4S_2$

Thiourea, N-[[(5S)-3-[3-fluoro-4-[4-[(5-nitro-2-thienyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]-

~1 References
Reactions
Commercial Sources
Regulatory Information
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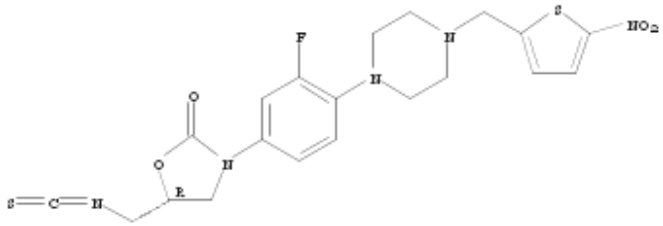
2. **Substance Detail**
776296-92-5



Absolute stereochemistry.

$C_{20}H_{20}FN_5O_4S_2$

2-Oxazolidinone, 3-[3-fluoro-4-[4-[(5-nitro-2-thienyl)methyl]-1-piperazinyl]phenyl]-5-(isothiocyanatomethyl)-, (5R)-

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

Substances

776296-79-8P
776296-89-0P

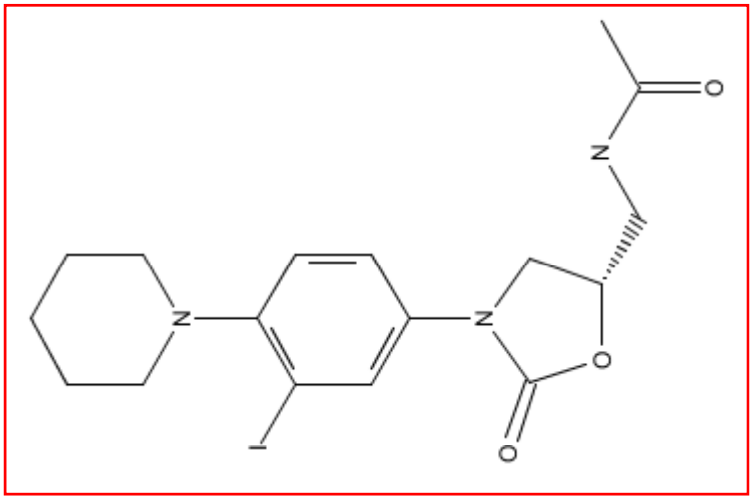
prepn. of oxazolidinone derivs. as antimicrobial/antibacterial agents

Pharmacological activity; Reactant; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses; Reactant or reagent

776296-76-5P
776296-77-6P
776296-78-7P
776296-80-1P
776296-81-2P
776296-82-3P
776296-83-4P
776296-84-5P
776296-85-6P
776296-86-7P
776296-87-8P
776296-88-9P
776296-90-3P
776296-91-4P
776296-92-5P
776296-93-6P

prepn. of oxazolidinone derivs. as antimicrobial/antibacterial agents

Pharmacological activity; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses



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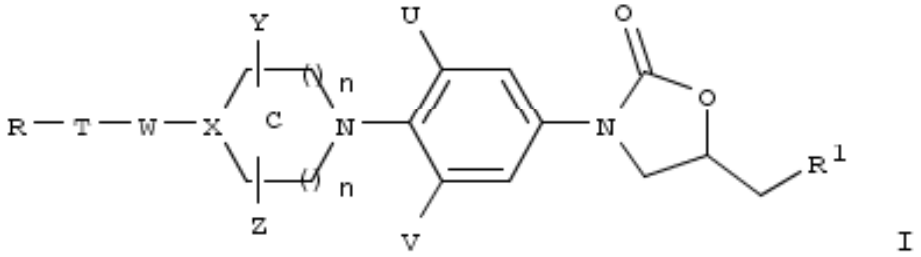
1. Preparation of oxazolidinone derivatives as antimicrobial agents

By: Mehta, Anita; Rudra, Sonali; Rao, Ajjarapu Venkata Subrahmanya Rajo; Yadav, Ajay Singh; Rattan, Ashok

Assignee: Ranbaxy Laboratories Limited, India

Title compds. I [T = 5-7 membered heterocycle, aryl, etc.; R = H, alkyl, F, Cl, Br, etc.; n = 0-3; X = H, CH, CHS, etc.; Y, Z = H, alkyl, cycloalkyl, etc.; U, V = H, alkyl, F, Cl, Br, I, etc.; W = CH2, CO, CH2NH, etc.; R1 = amido, thioamido, etc.] are prepd. For instance, II is prepd. from (S)-5-(((isoxazol-3-yl)oxy)methyl)-3-[3-fluoro-4-(piperazin-1-yl)phenyl]oxazolidin-2-one.bul.HCl and 4-bromo-5-nitrothiophene-2-carboxaldehyde (THF, NaHB(OAc)3, 17 h). Selected compds. of the invention exhibited antibacterial activity of 1 μg/mL against S. aureus (259231). I are effective against a no. of human and veterinary pathogens, including gram-pos. aerobic bacteria such as multiply-resistant staphylococci, streptococci and enterococci as well as anaerobic organisms as Bacterioides spp. and Clostridia spp. species, and acid fast organisms such as Mycobacterium tuberculosis, Mycobacterium avium and Mycobacterium spp.



I

只合成一类物质，通过各种可能的取代基团保护可能的物质-----Markush结构通式。

在专利中描述物质的方式

- 特定物质**[Specific Substance]**：

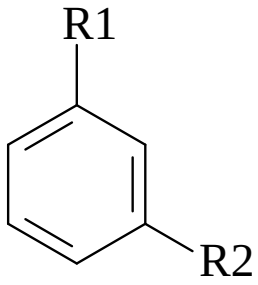
  以特定化学结构所陈述的特定物质，会被标示**CAS No.**

- 预测性物质**[Prophetic Substance]**：

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

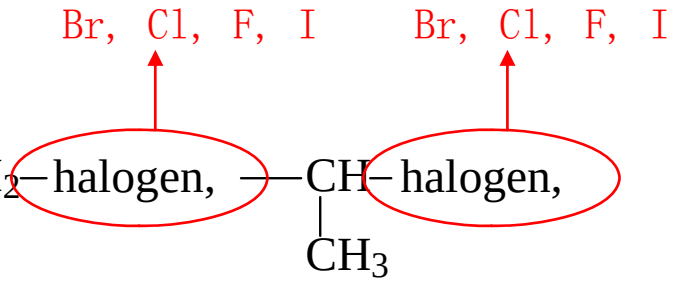
  Patent 中所陈述的预测物质，不会被标示**CAS No.**

Markush检索，能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

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



SciFinder中的Markush检索

1. SciFinder的用户对于专利信息的需求逐渐增大，Markush 检索是对REGISTRY的一个补充。

2. Markush检索通过预先设定一些检索参数，提供了简易的MARPAT检索。

3. Markush检索会给出一类相关的Markush结构相关的专利文献，可用于专利全景的初步评估。

4. 更专业的专利检索数据库：STN

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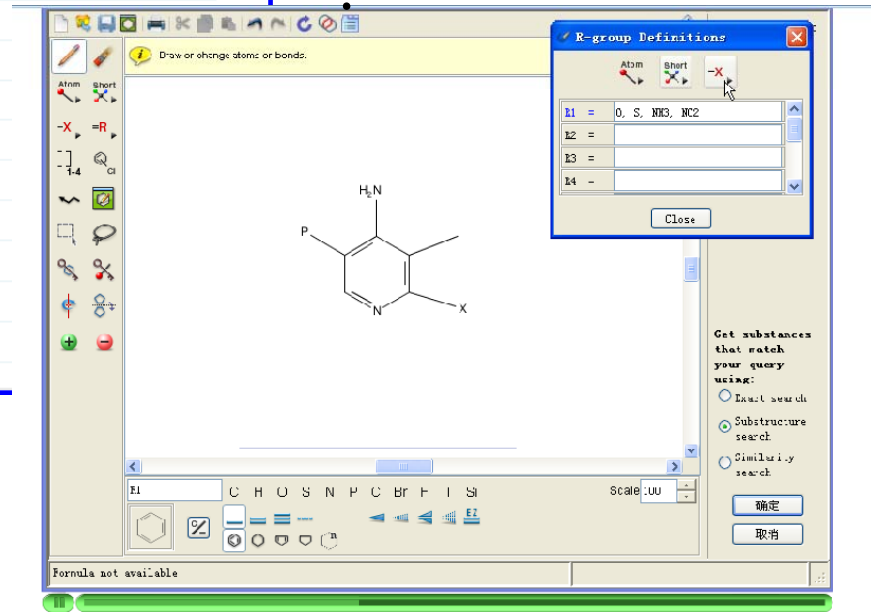
在线演示：Flash演示

网络培训：不定期的网络专题培训

Flash演示

在线演示，录制了不同检索类型下的检索步骤，帮助了解更加细节的内容



Thanks for attention!

For more information please contact：

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iGroup广州办公室

广州市越秀区东风中路318号嘉业大厦2705

邮编：510030

陈东亮

Tel:(020)83274076 15989176146

Email: joe@igroup.com.cn