

SciFinder检索工具介绍



SciFinder[®]

美国化学文摘社 中国代表处
陈东亮

15989176146



CAS is a division of the American Chemical Society

SciFinder[®]

joe@igroup.com.cn

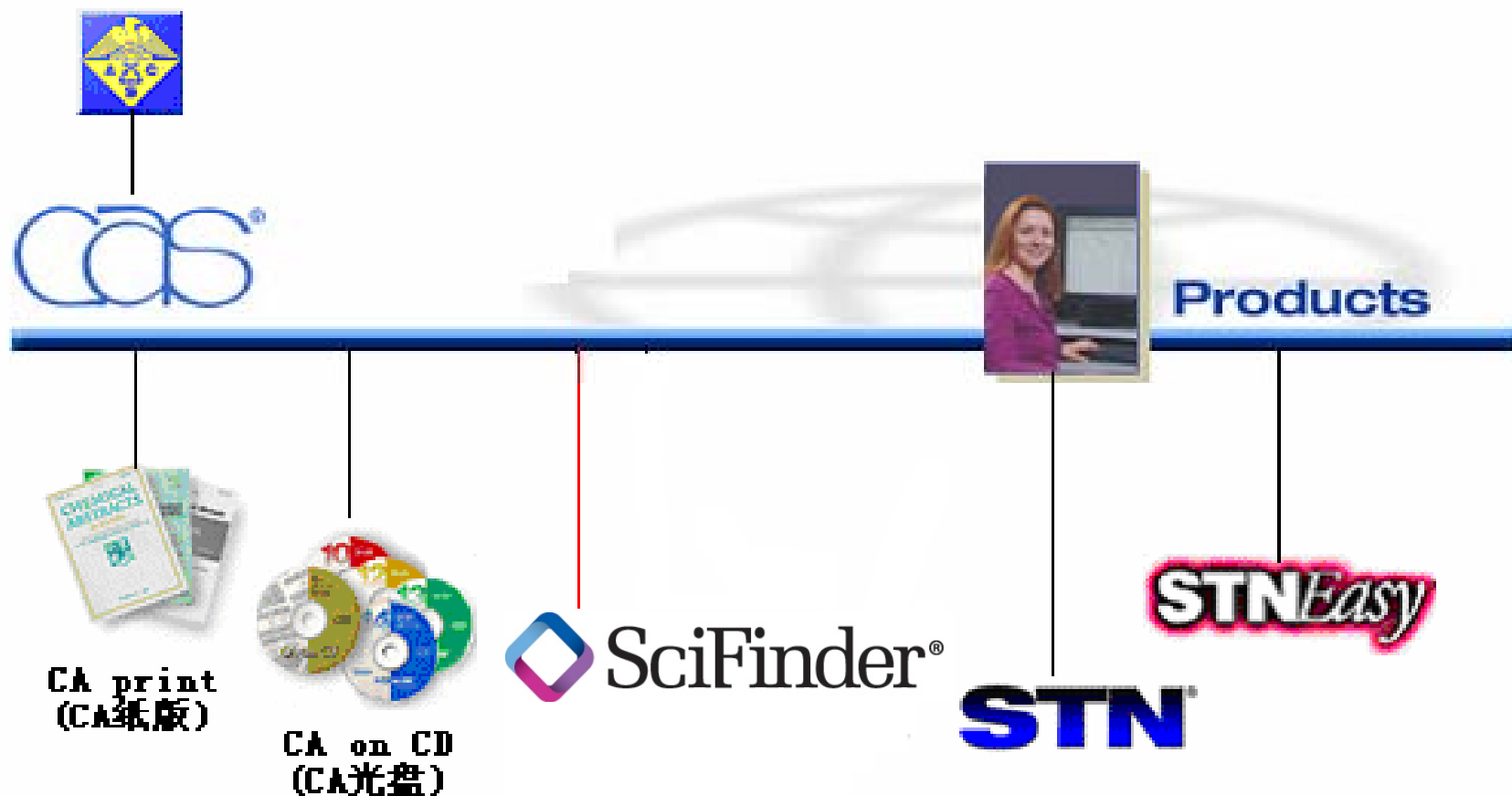
1
www.cas.org

- 美国化学文摘服务社（CAS）



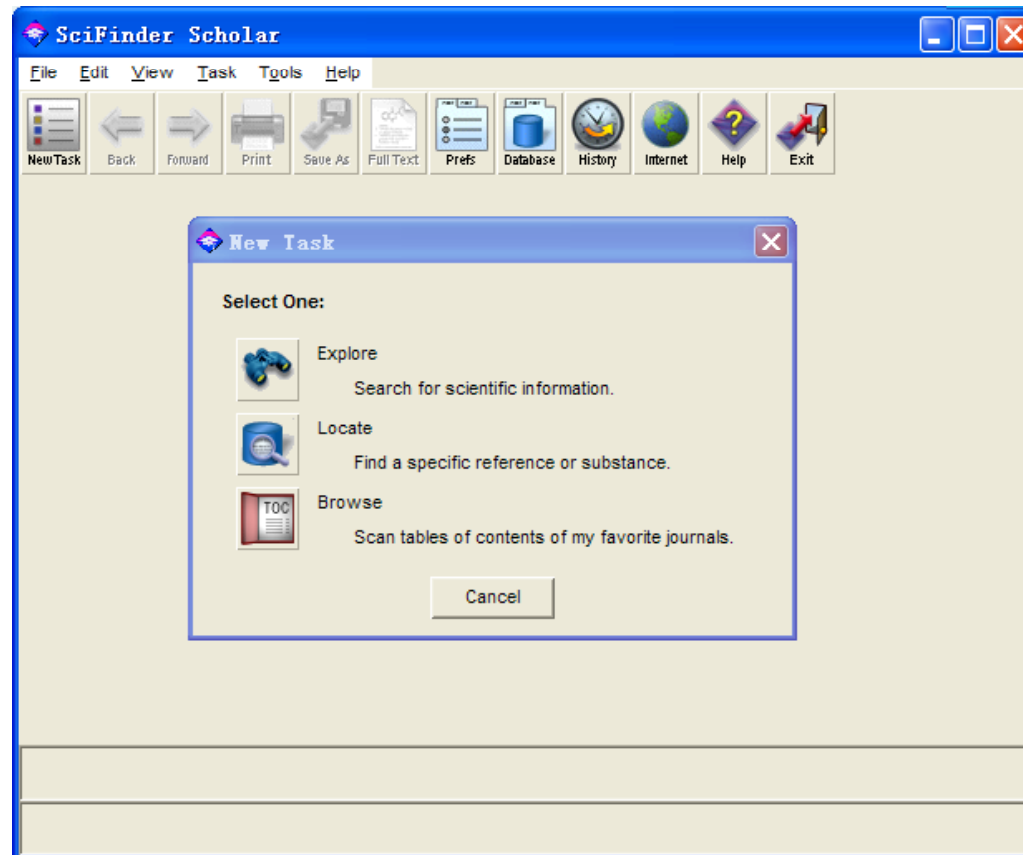
- 1907年 美国化学学会（ACS）分支机构
 - 全球最大的科学协会组织
 - 非盈利组织
 - >1000 PHD从事文献编辑工作

SciFinder的背景---CAS主要产品



SciFinder scholar VS SciFinder Web





SciFinder登陆界面

Scifinder.cas.org

The image shows the SciFinder login page. At the top left is the SciFinder logo with the tagline "Essential content. Proven results.™". Below the logo is a "Sign In" form. The form contains two input fields: "Username" and "Password", both of which are highlighted with a red rectangular box. Below these fields are a checkbox for "Remember my username", a link for "Forgot Username or Password?", and a "Sign In" button. A note below the button states: "Your SciFinder username and password are assigned to you alone and may not be shared with anyone else." To the right of the sign-in form is a "Welcome to SciFinder!" section. It includes a heading "Are you an outstanding PhD Chemistry student?" followed by a sub-heading "We want to hear from you with our SciFinder Academic Exchange Program!". The text describes an opportunity for students to exchange ideas with CAS staff and mentions a \$1,000 stipend. It also states that application materials are due April 30, 2011. Below this is a section for "SciFinder Mobile" which describes a mobile platform for accessing CAS databases. In the center of the page, there is a large, semi-transparent image of a person's face with chemical structures overlaid. A red rectangular box is drawn over this image, containing the Chinese text "输入SciFinder帐号和密码" (Enter SciFinder account and password).

SciFinder® Essential content. Proven results.™

Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

What is SciFinder? SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

Welcome to SciFinder!

Are you an outstanding PhD Chemistry student?

We want to hear from you with our **SciFinder Academic Exchange Program!**

This extraordinary opportunity is for outstanding PhD chemistry students to exchange ideas about chemical informatics with CAS senior management, editorial scientists, and technical specialists in Columbus, Ohio.

Participants are also invited to join their chemistry colleagues at the 242nd ACS National Meeting and Exposition, to be held in Denver, Colorado, in August 2011. All expenses are paid for this unique experience, and participants receive a \$1,000 stipend.

Don't miss out on your chance to apply - **all application materials are due April 30, 2011.**

SciFinder Mobile

With no need to download a special app, the new SciFinder Mobile platform allows researchers to use web-enabled smartphones to access CAS databases through SciFinder, the preferred research tool for chemical and related sciences. SciFinder Mobile is available to all SciFinder subscribers in commercial, academic, and government organizations and can be accessed at [scifinder.cas.org/mobile](#) with most mobile devices.

输入SciFinder帐号和密码

点击URL创建SciFinder账号



SciFinder®

Welcome to User Registration for SciFinder®!

Would you like to:

- Create a new username and password?
- Use an existing username and password? [Examples](#)

Next>>

开始创建SciFinder帐号

每个用户必须输入各自信息

SciFinder[®]

Please provide the following information:
(**bold*** = required)

CONTACT INFORMATION

First Name*:

Last Name*:

E-mail*:

Confirm E-mail*:

Phone Number:

Fax number:

Area of Research: Select one

Job Title: Select one

USERNAME AND PASSWORD

Username*: [Tips](#)

Password*:

Re-enter Password*:

SECURITY INFORMATION

Security Question*: Select one [Why?](#)

Answer*:

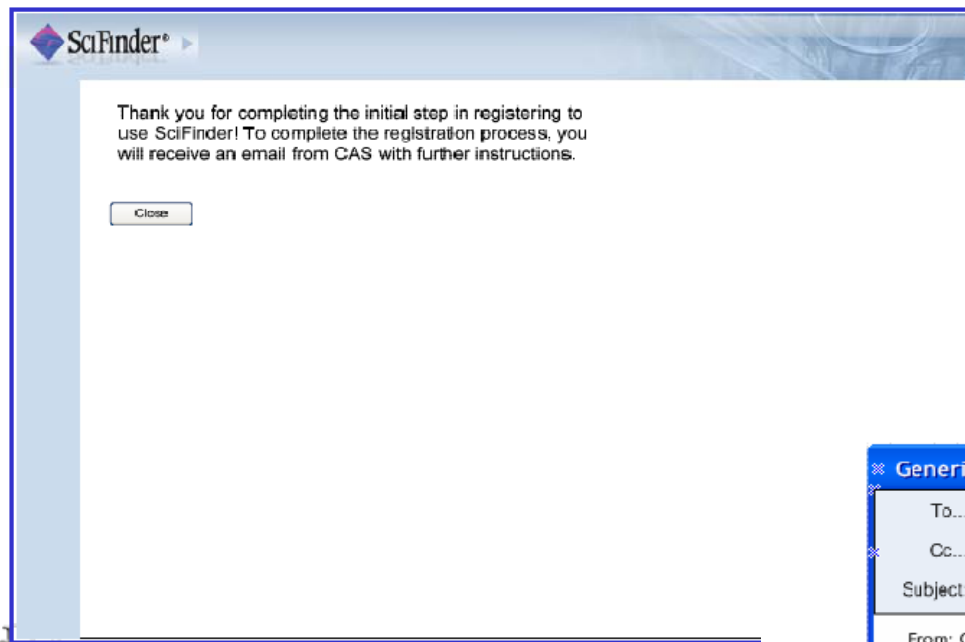
Register >> Clear All

Email domain must match valid domain(s) and the entire address must be unique.

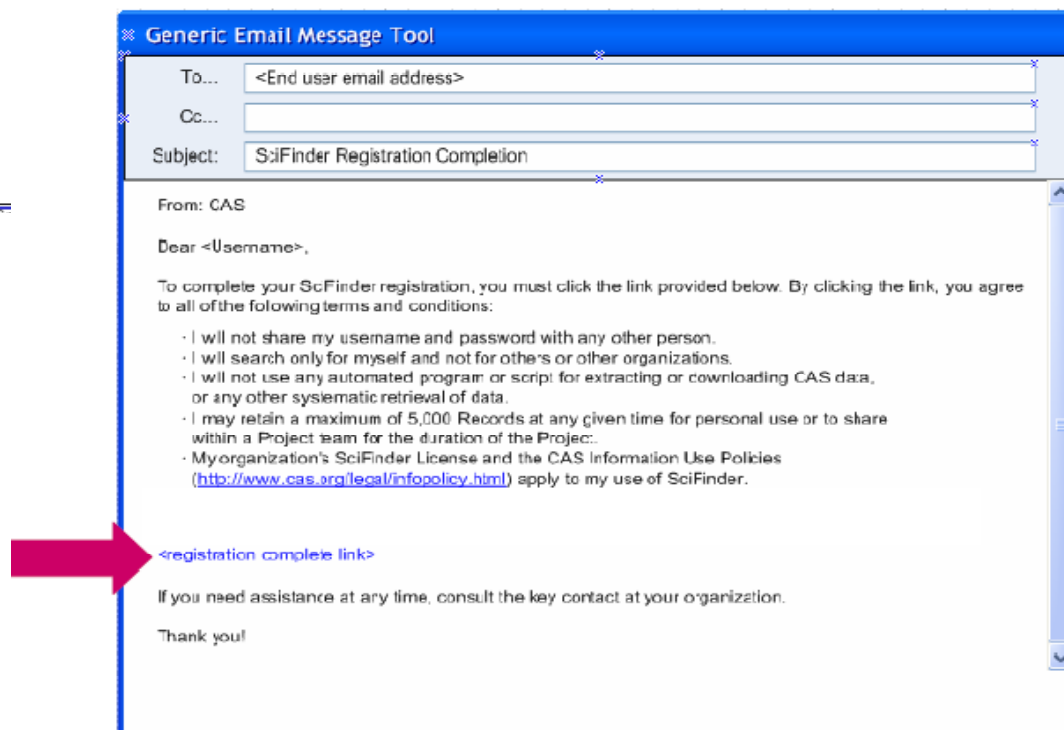
Username and password must meet minimum requirements and be unique.

- What is your favorite color?
- What is the name of the city where you grew up?
- What is the name of your favorite pet?
- What is your favorite musical instrument?
- What is your ideal vacation location?

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。

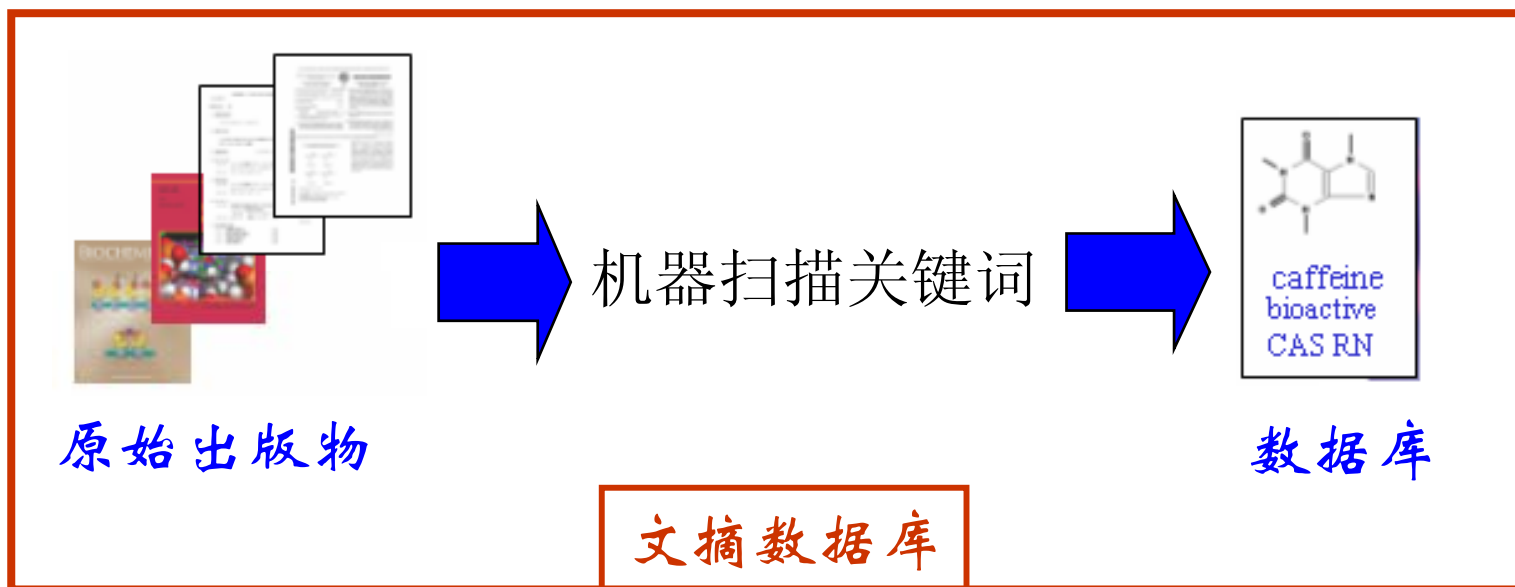
除了操作界面外，scifinder web功能更为丰富。

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



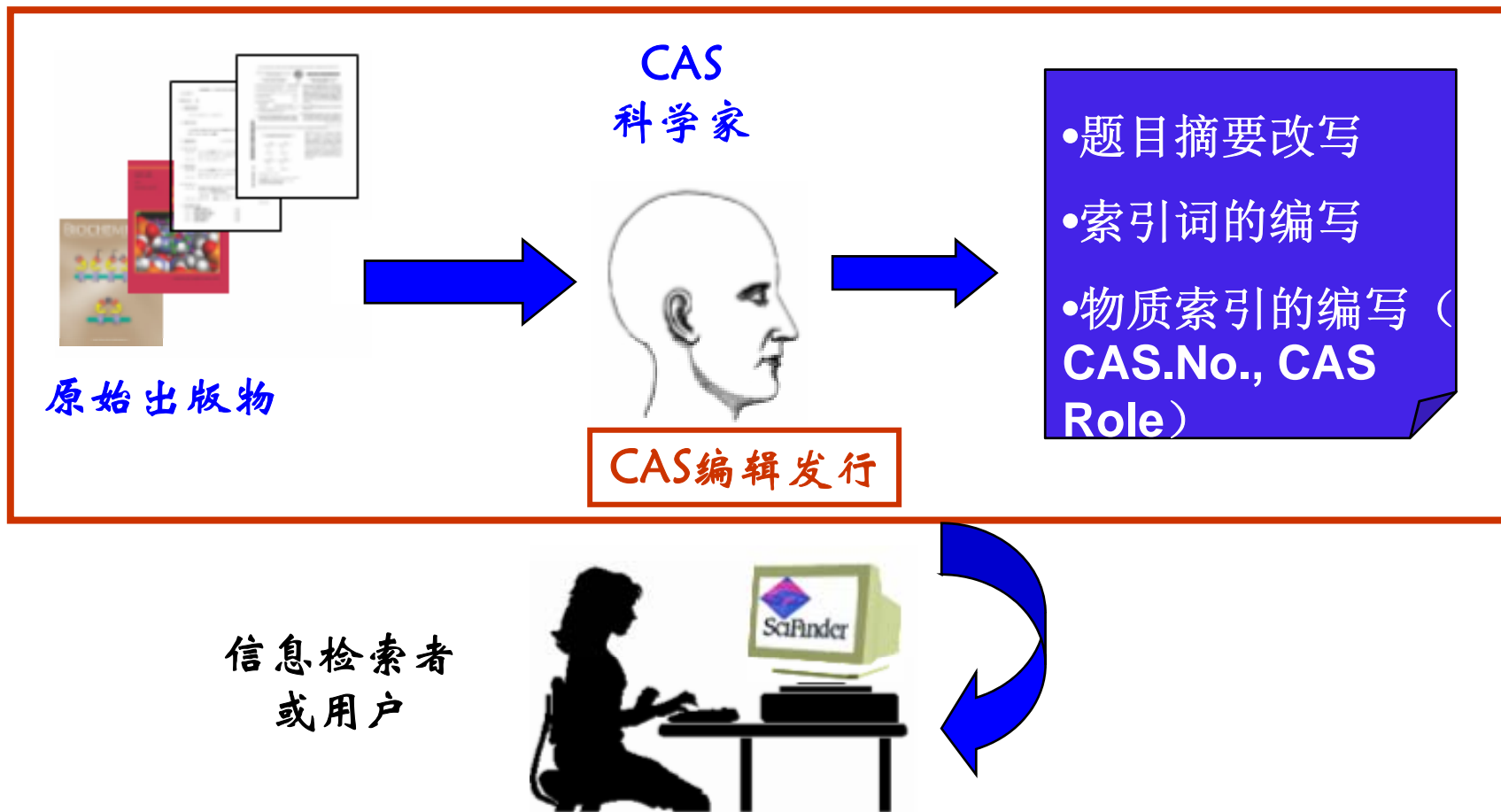
机器扫描的优点:

快速, 节省时间

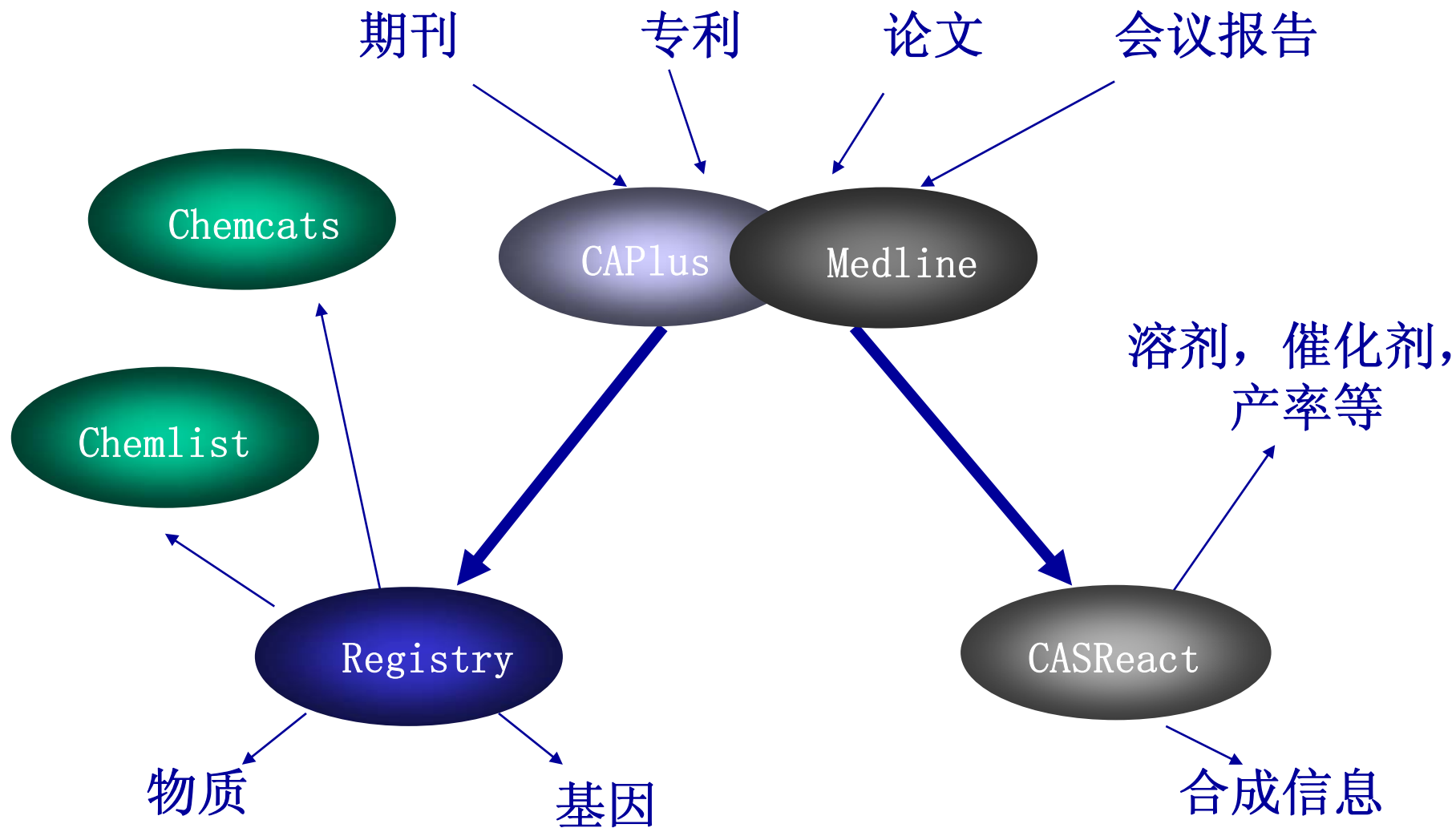
机器扫描的缺点:

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



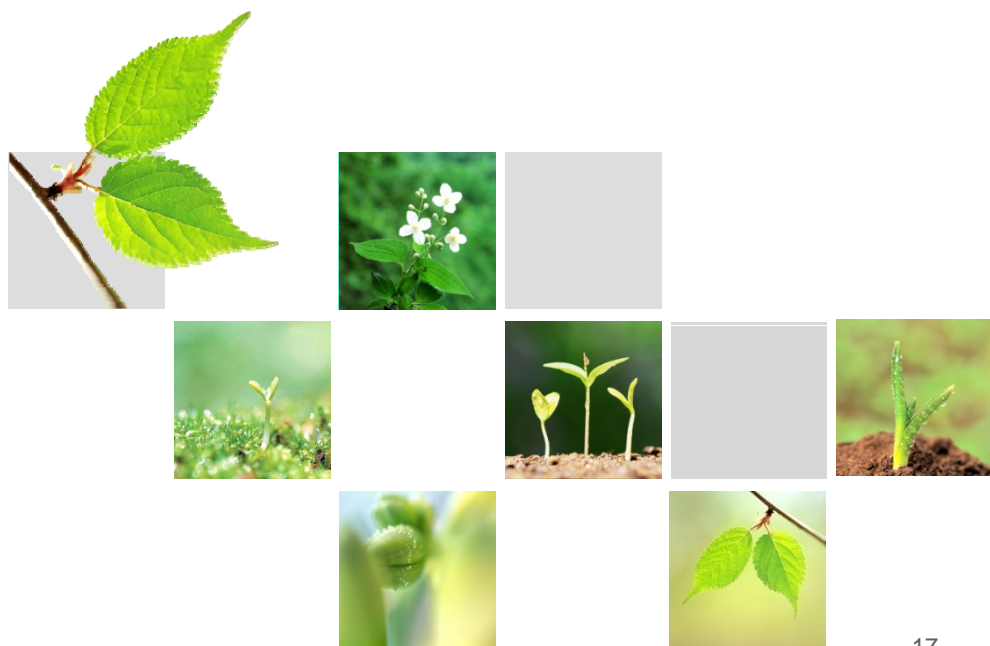
提纲



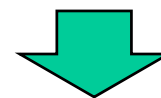
- **SciFinder Web** 文献及物质检索介绍

检索天然产物抗菌研究的相关文献

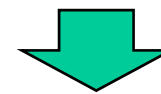
来自天然的化合物具有特殊的生理活性，许多具有特殊治疗作用的药物已经被开发成药用。由于天然药物化学研究所提供的活性物质结构新颖，疗效高，不良反应少，所以它已成为制药工业中新药研究的主要方向.....



天然产物抗菌研究



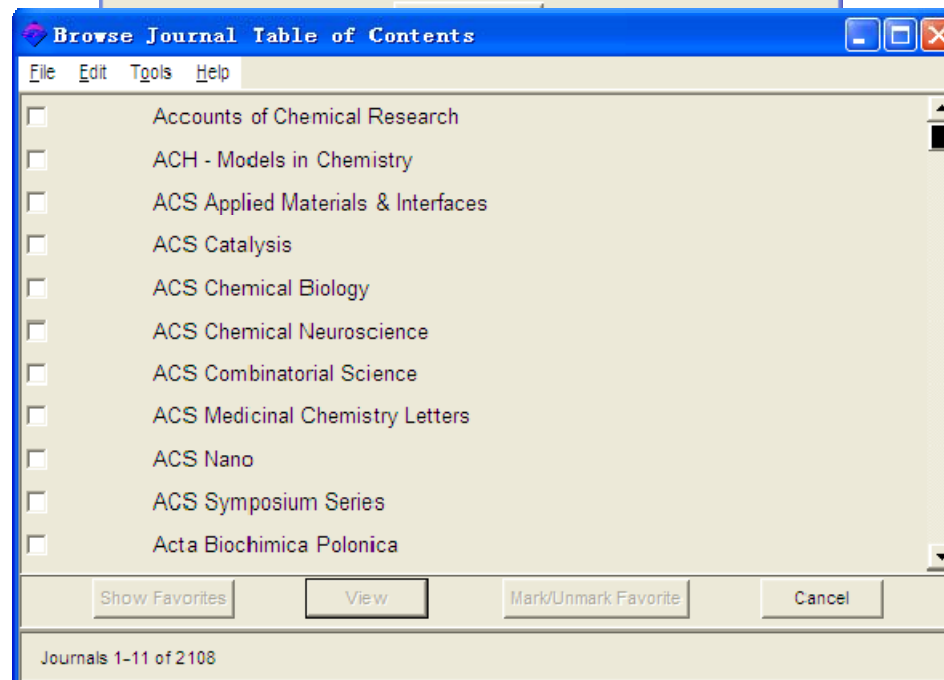
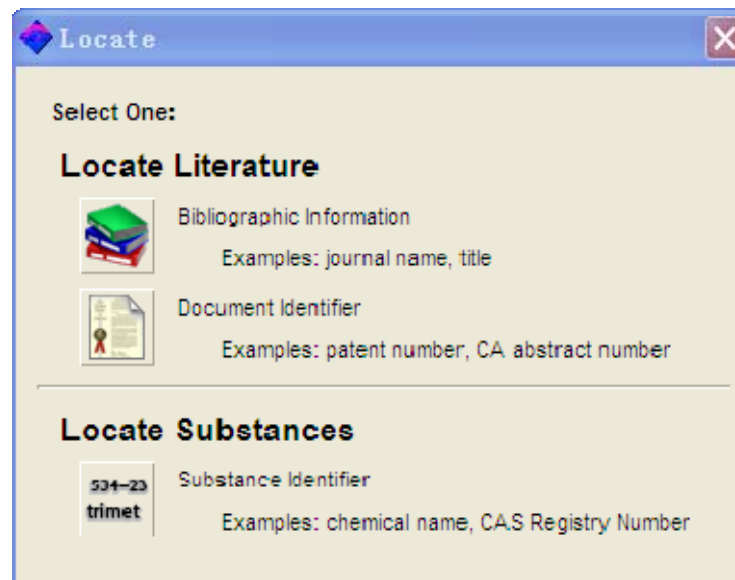
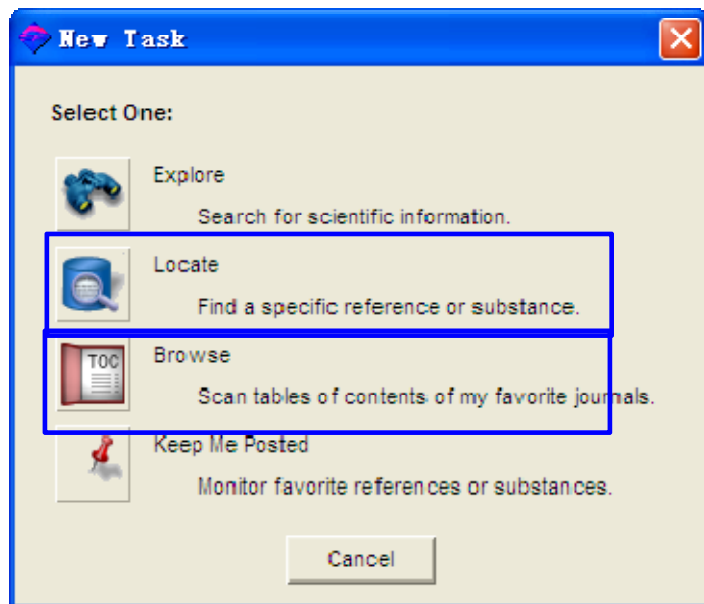
来自哪些植物？方法学？



有生物活性的具体物质？



Scifinder网页版取消序列检索功能



登陆网址: **scifinder.cas.org**



Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

输入用户名, 密码

What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

Welcome to SciFinder!

Fast forward from ideas to results with the power of SciPlanner

CAS is excited to announce enhancements to your SciFinder experience. These enhancements are now available to you and all SciFinder users at your organization. As the new features are designed to improve efficiency and productivity, we encourage you to log in and try them out today!

SciFinder enhancements include:

- SciPlanner - a groundbreaking interactive workspace that allows researchers to more quickly identify synthesis options to design the best pathways and approaches.
- Sorting reference answer sets by citing References.
- Copy/paste ISIS/Draw structures into the SciFinder structure drawing editor.

SciFinder Mobile

With no need to download a special app, the new SciFinder Mobile platform allows researchers to use web-enabled smartphones to access CAS databases through SciFinder, the preferred research tool for chemical and related sciences.

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

The screenshot shows the SciFinder main search interface. At the top, there are three navigation buttons: "Explore References", "Explore Substances", and "Explore Reactions". The "Explore References" button is highlighted with a blue box and an arrow pointing to the text "默认开始检索文献".

Below the navigation buttons, there is a "Research Topic" search box with a "Search" button. To the left of the search box is a dropdown menu for "Research Topic" with options: Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. This menu is highlighted with a blue box and an arrow pointing to the text "可用的检索方法".

Below the search box, there are two filter sections: "Publication Year(s)" and "Document Type(s)". The "Document Type(s)" section has a grid of checkboxes for various document types: Biography, Book, Clinical Trial, Commentary, Conference, Dissertation, Editorial, Historical, Journal, Letter, Patent, Preprint, Report, and Review.

On the right side of the interface, there are several panels:

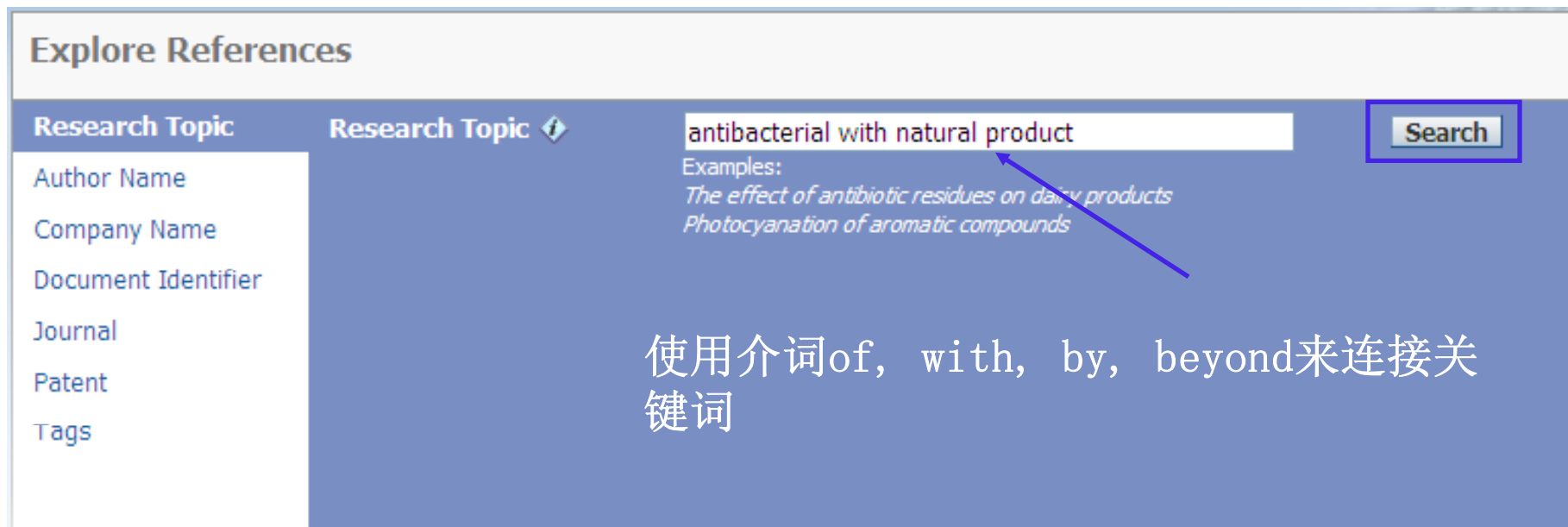
- "Saved Answer Sets" panel: Lists saved search results like "lipitor patent", "lipitor MAKUSH 1", "Polymyxin B - Bio-act", etc. It has an "Import" button. An arrow points to this panel with the text "保存过的结果集".
- "Keep Me Posted Results" panel: Shows "No profiles exist". An arrow points to this panel with the text "邮件提醒结果集".
- "My Connections" panel: Shows "No invitations to connect", "No outstanding sent invitations", and "No connections with colleagues".

At the top right, there are links for "Saved Answer Sets", "Keep Me Posted Results", "NEW! SciPlanner", "My Connections", "Help", "History", and "Preferences".

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



The screenshot shows the Scifinder search interface. On the left, there is a sidebar with the following options: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The main search area has a search bar containing the text "antibacterial with natural product". To the right of the search bar is a "Search" button. Below the search bar, there are two example search results: "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds". A blue arrow points from the text "使用介词of, with, by, beyond来连接关键词" to the search bar. The text "使用介词of, with, by, beyond来连接关键词" is written in white on a blue background.

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	
<input type="checkbox"/> 56 references were found containing "antibacterial of natural product" as entered.	56	
<input checked="" type="checkbox"/> 1397 references were found containing the two concepts "antibacterial" and "natural product" closely associated with one another.	1397	
<input type="checkbox"/> 10548 references were found where the two concepts "antibacterial" and "natural product" were present anywhere in the reference.	10548	
<input type="checkbox"/> 380491 references were found containing the concept "antibacterial".	380491	
<input type="checkbox"/> 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!

Explore References

Research Topic Search

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Author Name
Company Name
Document Identifier
Journal
Patent
Tags

Research Topic Candidates

2 Topics 0 Selected
Select All Deselect All

Research Topic Candidates	References
<input type="checkbox"/> 35 references were found containing "antibacterial natural product" as entered.	35
<input type="checkbox"/> 1397 references were found containing the concept "antibacterial natural product".	1397

Get References

不使用介词连接关键词

只有两个候选选项。

检索结果输出:

Research Topic Candidates

5 Topics 1 Selected

[Select All](#) [Deselect All](#)

Research Topic Candidates	References
<input type="checkbox"/> 56 references were found containing " antibacterial of natural product " as entered.	56
<input checked="" type="checkbox"/> 1397 references were found containing the two concepts " antibacterial " and " natural product " closely associated with one another.	1397
<input type="checkbox"/> 10548 references were found where the two concepts " antibacterial " and " natural product " were present anywhere in the reference.	10548
<input type="checkbox"/> 380491 references were found containing the concept " antibacterial ".	380491
<input type="checkbox"/> 261408 references were found containing the concept " natural product ".	261408

[Get References](#)

文献记录数

可以快速浏览文献的内容，是
否符合要求

文献分析限定工具

1297 References

100 duplicates were automatically removed.

Select All Deselect All | Sort by: Accession Number | Answers per Page [15] 1 2 3 4 5 6 ... 87 | Display: [icon]

1. **Isolation and characterization of novel natural products isolated from plants utilized in traditional folk medicine**
By Whitlatch, Kindra N.; Wagoner, Jacob D.; Sparks, Jeannie; Huggins, Luke G.; Troyer, Timothy L.
From Abstracts, Joint 46th Midwest and 39th Great Lakes Regional Meeting of the American Chemical Society, St. Louis, MO, United States, October 19-22 (2011), MWGL-330. Language: English, Database: CAPLUS

Plants have afforded several medically important **natural products** that have been utilized in traditional folk medicine. Medicinal properties of the red mangrove (*Rhizophora mangle*) have been realized by indigenous populations in Central and South America. Our study was initiated by the discovery of **antibacterial** activity in the ethanolic ext. of red mangrove propagules by our collaborators at the University of Belize. We have since identified cytotoxic activity in the aq. ext. of the red mangrove propagules. The isolation of biol. active compds. from plants can be performed in a variety of ways. Often a highly polar org. solvent capable of forming hydrogen bonds is utilized for the initial extn. followed by extensive chromatog. Our bioassay directed isolation of **antibacterial** and cytotoxic **natural products** from the propagules of the red mangrove (*Rhizophora mangle*) have led us to a fairly unique process. We utilize both an aq. extn. in addn. to extn. with ethanol. These two sep. exts. are then partitioned between water and Et acetate. The cytotoxic activity is found primarily in the aq. partition and the **antibacterial** activity is found primarily in the org. partition. These two partitions have been further fractionated by a combination of column chromatog. and preparatory HPLC. We have found that the biol. activity can be traced to particular fractions of these purifn. steps. Biol. active fractions were preliminarily characterized by LC-MS and LC-NMR. Our bioassay directed isolation procedure was then applied to three species of the *Centaurea* genus. Biol. active compds. have been isolated from a variety of *Centaurea* species endemic to Greece. There are no reports of isolating biol. active compds. from *Centaurea cyanus* (bachelor buttons), *Centaurea nigra* (black Knapweed), or *Centaurea maculosa* (spotted knapweed). We have been able to demonstrate **antibacterial** activity in certain fractions from the ethanolic ext. from *Centaurea nigra*.

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

2. **ANTIBACTERIAL OPTIMIZATION OF 4-AMINOTHIAZOLYL ANALOGUES OF THE NATURAL PRODUCT GE2270 A: IDENTIFICATION OF THE CYCLOALKYLCARBOXYLIC ACIDS**
By LaMarche, Matthew J.; Leeds, Jennifer; Amaral, Kerri; Brewer, Jason; Bushell, Simon; Dewhurst, Janetta; Dzink-Fox, Joanne; Gangl, Eric; Goldovitz, Julie; Jain, Akash; et al
From Journal of Medicinal Chemistry, ACS ASAP. Language: English, Database: CAPLUS

4-Aminothiazolyl analogs of the antibiotic **natural product** GE2270 A (1) were designed, synthesized, and optimized for their activity against Gram pos. **bacterial** infections. Optimization efforts focused on improving the physicochem. properties (e.g., aq. soly. and chem. stability) of the

Analysis Refine

Analyze by: Author Name

Gibbons Simon	11
Cheng Gang	10
Cheng Jinxue	10
Singh Sheo B	10
Ichikawa Satoshi	7
Hamann Mark T	6
Okwu Donatus Ebere	6
Zhou Ying	6
Butler Mark S	5
Cheng Li	5

Show More

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。

The screenshot shows the 'Analysis' tab in SciFinder. The 'Analyze by' dropdown menu is open, displaying a list of analysis categories. Below the menu, a list of authors is shown with their respective counts and progress bars.

Author Name	Count
Fujishima Akira	11
Liu Wei	11
Ma Wanhong	11
Song Limin	11

The screenshot shows the 'Refine' tab in SciFinder. The 'Refine by' section contains several radio button options for refining search results. Below this is a 'Research Topic' input field with examples of search terms and a 'Refine' button.

Refine by:

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

Examples:

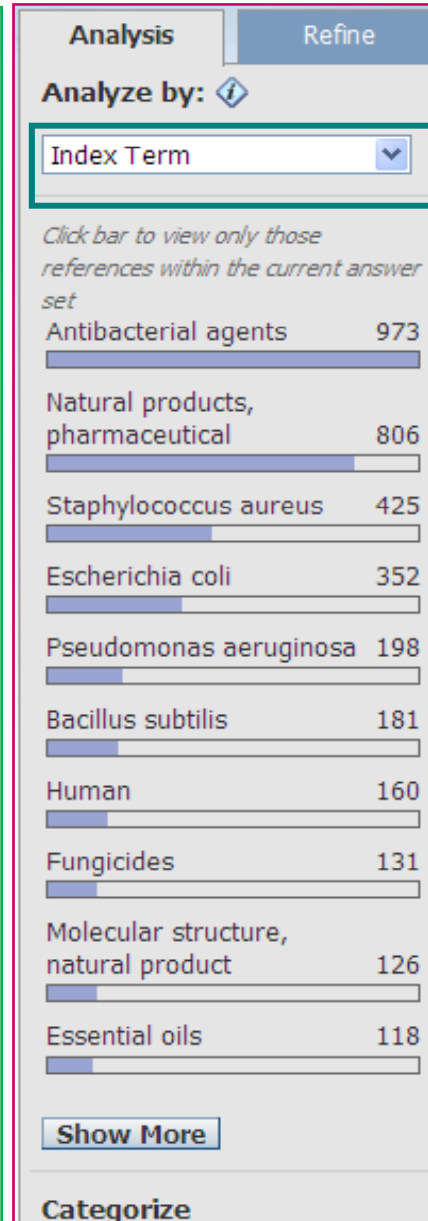
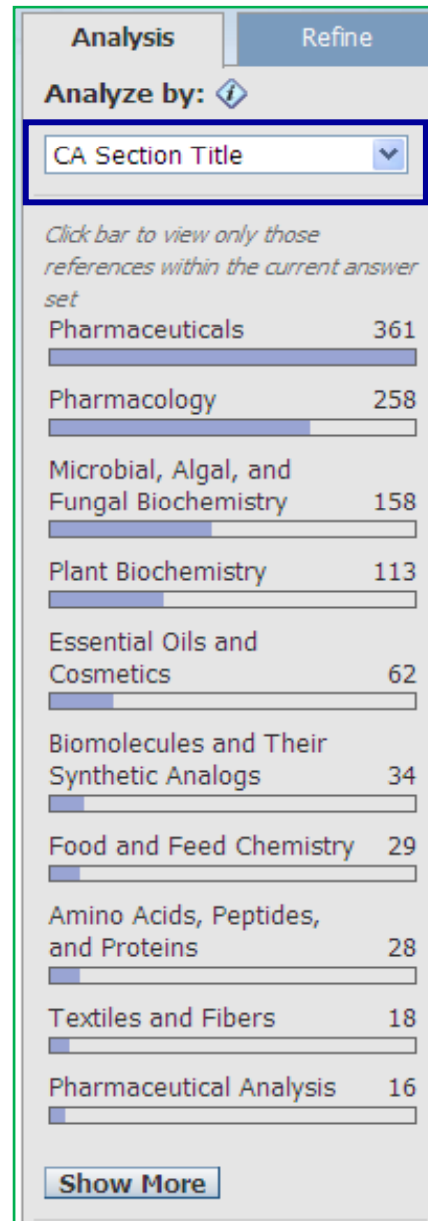
The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

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？



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

Analysis
Refine

Refine by:

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

References
Get Substances
Get Reactions
Get Related
Tools
Send to SciPlanner

164 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 ... 11 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, prepn. 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.

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

1297 References 0 Selected Save Print Export

100 duplicates were automatically removed.

Select All Deselect All | Sort by: Accession Number ↓ Answers per Page [15] 1 2 3 4 5 6 ... 87

1. **Isolation and characterization of natural products isolated from plants utilized in traditional folk medicine**
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From Abstracts, Joint 46th Midwest and 59th Great Lakes Regional Meeting of the American Chemical Society, St. Louis, MO, United States, October 19-22 (2011), MWGL-330. Language: English, Database: CAPLUS

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Plants have afforded several medically important and potent compds. Many plants have been utilized in traditional folk medicine. Medicinal properties of the red mangrove (*Rhizophora mangle*) have been realized by indigenous populations in Central and South America. Our study was initiated by the discovery of **antibacterial** activity in the ethanolic ext. of red mangrove propagules by our collaborators at the University of Belize. We have since identified cytotoxic activity in the aq. ext. of the red mangrove propagules. The isolation of biol. active compds. from plants can be performed in a variety of ways. Often a highly polar org. solvent capable of forming hydrogen bonds is utilized for the initial extrn. followed by extensive chromatog. Our bioassay directed isolation of **antibacterial** and cytotoxic **natural products** from the propagules of the red mangrove (*Rhizophora mangle*) have led us to a fairly unique process. We utilize both an aq. extrn. in addn. to extrn. with ethanol. These two sep. exts. are then partitioned between water and Et acetate. The cytotoxic activity is found primarily in the aq. partition and the **antibacterial** activity is found primarily in the org. partition. These two partitions have been further fractionated by a combination of column chromatog. and preparatory HPLC. We have found that the biol. activity can be traced to particular fractions of these purifn. steps. Biol. active fractions were preliminarily characterized by LC-MS and LC-NMR. Our bioassay directed isolation procedure was then applied to three species of the *Centaurea* genus. Biol. active compds. have been isolated from a variety of *Centaurea* species endemic to Greece. There are no reports of isolating biol. active compds. from *Centaurea cyanus* (bachelor buttons), *Centaurea nigra* (black Knapweed), or *Centaurea maculosa* (spotted knapweed). We have been able to demonstrate **antibacterial** activity in certain fractions from the ethanolic ext. from *Centaurea nigra*.

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

2. **ANTIBACTERIAL OPTIMIZATION OF 4-AMINOTHIAZOLYL ANALOGUES OF THE NATURAL PRODUCT GE2270 A: IDENTIFICATION OF THE CYCLOALKYLCARBOXYLIC ACIDS**
By LaMarche, Matthew J.; Leeds, Jennifer; Amaral, Kerri; Brewer, Jason; Bushell, Simon; Dewhurst, Janetta; Dzink-Fox, Joanne; Gangl, Eric; Goldovitz, Julie; Jain, Akash; et al
From Journal of Medicinal Chemistry, ACS ASAP. Language: English, Database: CAPLUS

4-Aminothiazolyl analogs of the antibiotic **natural product** GE2270 A (1) were designed, synthesized, and optimized for their activity against Gram pos. **bacterial** infections. Optimization efforts focused on improving the physicochem. properties (e.g., aq. soly. and chem. stability) of the 4-aminothiazolyl **natural product** template while improving the in vitro and in vivo **antibacterial** activity. Structure-activity relationships were defined, and the soly. and efficacy profiles were improved over that of previous analogs and GE2270 A. These studies identified novel, potent, sol., and efficacious elongation factor-Tu **inhibitors**, which bear cycloalkyl-carboxylic acid sidechains, and culminated in the selection of development candidates amide 48 and urethane 58.

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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 25 1/2 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** ← 按被引用的次数排序
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, prepsns. 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

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

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1. **Isolation and characterization of novel natural products isolated from plants utilized in traditional folk medicine**
 By Whitlatch, Kindra N.; Wagoner, Jacob D.; Sparks, Jeannie; Huggins, Luke G.; Troyer, Timothy L.
 From Abstracts, Joint 46th Midwest and 39th Great Lakes Regional Meeting of the American Chemical Society, St. Louis, MO, United States, October 19-22 (2011), MWGL-330. Language: English, Database: CAPLUS

Plants have afforded several medically important and potent compds. Many plants have been utilized in traditional folk medicine. Medicinal properties of the red mangrove (*Rhizophora mangle*) have been realized by indigenous populations in Central and South America. Our study was initiated by the discovery of **antibacterial** activity in the ethanolic ext. of red mangrove propagules by our collaborators at the University of Belize. We have since identified cytotoxic activity in the aq. ext. of the red mangrove propagules. The isolation of biol. active compds. from plants can be performed in a variety of ways. Often a highly polar org. solvent capable of forming hydrogen bonds is utilized for the initial extn. followed by extensive chromatog. Our bioassay directed isolation of **antibacterial** and cytotoxic **natural products** from the propagules of the red mangrove (*Rhizophora mangle*) have led us to a fairly unique process. We utilize both an aq. extn. in addn. to extn. with ethanol. These two sep. exts. are then partitioned between water and Et acetate. The cytotoxic activity is found primarily in the aq. partition and the **antibacterial** activity is found primarily in the org. partition. These two partitions have been further fractionated by a combination of column chromatog. and preparatory HPLC. We have found that the biol. activity can be traced to particular fractions of these purifn. steps. Biol. active fractions were preliminarily characterized by LC-MS and LC-NMR. Our bioassay directed isolation procedure was then applied to three species of the *Centaurea* genus. Biol. active compds. have been isolated from a variety of *Centaurea* species endemic to Greece. There are no reports of isolating biol. active compds. from *Centaurea cyanus* (bachelor buttons), *Centaurea nigra* (black Knapweed), or *Centaurea maculosa* (spotted knapweed). We have been able to demonstrate **antibacterial** activity in certain fractions from the ethanolic ext. from *Centaurea nigra*.

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2. **ANTIBACTERIAL OPTIMIZATION OF 4-AMINOTHIAZOLYL ANALOGUES OF THE NATURAL PRODUCT GE2270 A: IDENTIFICATION OF THE CYCLOALKYLCARBOXYLIC ACIDS**
 By LaMarche, Matthew J.; Leeds, Jennifer; Amaral, Kerri; Brewer, Jason; Bushell, Simon; Dewhurst, Janetta; Dzink-Fox, Joanne; Gangl, Eric; Goldovitz, Julie; Jain, Akash; et al
 From Journal of Medicinal Chemistry, ACS ASAP. Language: English, Database: CAPLUS

4-Aminothiazolyl analogs of the antibiotic **natural product** GE2270 A (1) were designed, synthesized, and optimized for their activity against Gram pos. **bacterial** infections. Optimization efforts focused on improving the physicochem. properties (e.g., aq. soly. and chem. stability) of the 4-aminothiazolyl **natural product** template while improving the in vitro and in vivo **antibacterial** activity. Structure-activity relationships were defined, and the soly. and efficacy profiles were improved over that of previous analogs and GE2270 A. These studies identified novel, potent, sol., and efficacious elongation factor-Tu **inhibitors**, which bear cycloalkyl-carboxylic acid sidechains, and culminated in the selection of development candidates amide 48 and urethane 58.

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Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Materials & products (185)	Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Substances in technology (448)	<input checked="" type="checkbox"/> Solvent extraction 53	<input checked="" type="checkbox"/> Technology > Processes & apparatus (1 Terms)
Biology	Metallurgy (100)	<input type="checkbox"/> Extraction 47	
Biotechnology	Processes & apparatus (94)	<input checked="" type="checkbox"/> Fermentation 29	
Synthetic chemistry	Formed, removed, & other substances (31)	<input type="checkbox"/> Distillation 14	
Physical chemistry	Construction (17)	<input type="checkbox"/> Liquid chromatography 12	
Technology	Ceramics (6)	<input type="checkbox"/> Mass spectrometry 12	
Polymer chemistry	Power & fuel topics (2)	<input type="checkbox"/> HPLC 11	
Genetics & protein chemistry	Imaging & recording (1)	<input type="checkbox"/> Gas chromatography 10	
Analytical chemistry	二次学科领域	<input type="checkbox"/> TLC (thin layer chromatography) 10	
Environmental chemistry		<input type="checkbox"/> Quality control 9	
Catalysis		<input type="checkbox"/> Sterilization and Disinfection 9	
		<input type="checkbox"/> Chromatography 7	
		<input type="checkbox"/> Drying 7	
		<input type="checkbox"/> Fabric finishing 7	
		<input type="checkbox"/> Filtration 7	
		<input type="checkbox"/> Air purification 5	

Technology > Processes & apparatus > 1 Index Term(s) Selected

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查看通过纯化手段获得哪些物质。

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1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Prepared substances (2290)	1 2 3 4 ... 13 Select All Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Purified substances (1245)	<input type="checkbox"/> Essential oils 36	✖ Technology > Processes & apparatus (3 Terms)
Biology	Reactants & reagents (1785)	<input type="checkbox"/> Flavonoids 28	精油
Biotechnology	Reactions (64)	<input type="checkbox"/> α -Pinene 25	黄酮类化合物
Synthetic chemistry	Reactions (64) 纯化物质	<input type="checkbox"/> β -Caryophyllene 24	α -蒎烯
Physical chemistry	Combinatorially prepared substances (178)	<input type="checkbox"/> Alkaloids 23	β -石竹烯
Technology	Bio-prepared substances (138)	<input type="checkbox"/> Limonene 21	生物碱
Polymer chemistry	Manufactured substances (32)	<input type="checkbox"/> β -Pinene 19
Genetics & protein chemistry	Combinatorial reactants & other substances (16)	<input type="checkbox"/> Sesquiterpenes 18	
Analytical chemistry		<input type="checkbox"/> Saponins 17	
Environmental chemistry		<input type="checkbox"/> α -Terpineol 17	
Catalysis		<input type="checkbox"/> Caryophyllene oxide 16	
		<input type="checkbox"/> Germacrene D 16	
		<input type="checkbox"/> Glycosides 16	
		<input type="checkbox"/> Natural products, pharmaceutical 16	
		<input type="checkbox"/> Linalool 15	

Synthetic chemistry > Purified substances

OK Cancel

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Selected Terms ⓘ
All	Substances in medicine (3362)	◀ 1 ... 4 5 6 7 ... 34	Click 'x' to remove the category from 'Selected Terms'
General chemistry	Medicine (225)	Select All Deselect All	✖ Biotechnology > Substances in medicine (2 Terms)
Biology	Agriculture (91)	<input type="checkbox"/> Junipene 3	
Biotechnology	Substances in biological uses (811)	<input type="checkbox"/> KANAMYCIN A 3	
Synthetic chemistry	Food (186)	<input type="checkbox"/> Lactams 3	
Technology	Substances in food chemistry (208)	<input type="checkbox"/> Lactic acid 3	
Physical chemistry	Substances in adverse effects (158)	<input type="checkbox"/> Linalool acetate 3	
Polymer chemistry	Substances in agriculture (121)	<input checked="" type="checkbox"/> Linezolid 3	
Genetics & protein chemistry	Toxicology & forensics (17)	<input type="checkbox"/> Luteolin-7-O-β-D-glucopyranoside 3	
Analytical chemistry		<input type="checkbox"/> Lysozyme 3	
Environmental chemistry		<input checked="" type="checkbox"/> Macrocyclic compounds 3	
Catalysis		<input type="checkbox"/> Magnesium carbonate 3	
		<input type="checkbox"/> Menthone 3	
		<input type="checkbox"/> Meropenem 3	
		<input type="checkbox"/> Methyl carvacrol 3	
		<input type="checkbox"/> Methyl eugenol 3	
		<input type="checkbox"/> Morin 3	

Biotechnology > Substances in medicine > 2 Index Term(s) Selected

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1. In vitro activities of U-100592 and U-100766, novel oxazolidinone antibacterial agents

By Zurenko, Gary E.; Yagi, Betty H.; Schaadt, Ronda D.; Allison, John W.; Kilburn, James O.; Glickman, Suzanne E.; Hutchinson, Douglas K.; Barbachyn, Michael R.; Brickner, Steven J.

From Antimicrobial Agents and Chemotherapy (1996), 40(4), 839-45. [View Full Text](#) [View Abstract](#) [View Citations](#)

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Oxazolidinones make up a relatively new class of antimicrobial agents which possess a unique mechanism of **bacterial** protein synthesis **inhibition**. U-100592 {(S)-N-[[3-[3-fluoro-4-[4-(hydroxyacetyl)-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]-acetamide} and U-100766 {(S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-acetamide} are novel **oxazolidinone** analogs from a directed chem. modification program. MICs were detd. for a variety of **bacterial** clin. isolates; the resp. MICs of U-100592 and U-100766 at which 90% of isolates were inhibited were as follows: methicillin-susceptible Staphylococcus aureus, 4 and 4 µg/mL; methicillin-resistant S. aureus, 4 and 4 µg/mL; methicillin-susceptible Staphylococcus epidermidis, 2 and 2 µg/mL; methicillin-resistant S. epidermidis, 1 and 2 µg/mL; Enterococcus faecalis, 2 and 4 µg/mL; Enterococcus faecium, 2 and 4 µg/mL; Streptococcus pyogenes, 1 and 2 µg/mL; Streptococcus pneumoniae, 0.50 and 1 µg/mL; Corynebacterium spp., 0.50 and 0.50 µg/mL; Moraxella catarrhalis, 4 and 4 µg/mL; Listeria monocytogenes, 8 and 2 µg/mL; and Bacteroides fragilis, 16 and 4 µg/mL. Most strains of Mycobacterium tuberculosis and the gram-pos. anaerobes were inhibited in the range of 0.50 to 2 µg/mL. Enterococcal strains resistant to vancomycin (VanA, VanB, and VanC resistance phenotypes), pneumococcal strains resistant to penicillin, and M. tuberculosis strains resistant to common antitubercular agents (isoniazid, streptomycin, rifampin, ethionamide, and ethambutol) were not cross-resistant to the **oxazolidinones**. The presence of 10, 20, and 40% pooled human serum did not affect the **antibacterial** activities of the **oxazolidinones**. Time-kill studies demonstrated a bacteriostatic effect of the analogs against staphylococci and enterococci but a bactericidal effect against streptococci. The spontaneous mutation frequencies of S. aureus ATCC 29213 were 3.8×10^{-10} and 8×10^{-11} for U-100592 and U-100766, resp. Serial transfer of three staphylococcal and two enterococcal strains on drug gradient plates produced no evidence of rapid resistance development. Thus, these new **oxazolidinone** analogs demonstrated in vitro **antibacterial** activities against a variety of clin. important human pathogens.

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2. Mechanism of action of oxazolidinones: effects of linezolid and eperezolid on translation reactions

By Shinabarger, Dean L.; Marotti, Keith R.; Murray, Robert W.; Lin, Alice H.; Melchior, Earline P.; Swaney, Steve M.; Duniyak, Donna S.; Demyan, William F.;

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1. In vitro activities of U-100592 and U-100766, novel oxazolidinone antibacterial agents

By: Zurenko, Gary E.; Yagi, Betty H.; Schaadt, Ronda D.; Allison, John W.; Kilburn, James O.; Glickman, Suzanne E.; Hutchinson, Douglas K.; Barbachyn, Michael R.; Brickner, Steven J.

Oxazolidinones make up a relatively new class of antimicrobial agents which possess a unique mechanism of bacterial protein synthesis inhibition. U-100592 {(S)-N-[[3-[3-fluoro-4-[4-(hydroxyacetyl)-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]-acetamide} and U-100766 {(S)-N-[[3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-acetamide} are novel oxazolidinone analogs from a directed chem. modification program. MICs were detd. for a variety of bacterial clin. isolates; the resp. MICs of U-100592 and U-100766 at which 90% of isolates are inhibited were as follows: methicillin-susceptible *Staphylococcus aureus*, 4 and 4 µg/mL; methicillin-resistant *S. aureus*, 4 and 4 µg/mL; Streptococcus pneumoniae, 4 and 4 µg/mL; anaerobic bacteria, 4 and 4 µg/mL; phenotypically diverse streptococci, 4 and 4 µg/mL; pooled strains of the anaerobic bacteria of *S. aureus* and two strains of *Streptococcus pneumoniae*.

Microbial, Algal, and Fungal Biochemistry (Section 10-5)

Concepts

Bacteroides	Corynebacterium
Listeria	Moraxella
Mycobacterium	Staphylococcus
Streptococcus	

in vitro activities of U-100592 and U-100766, novel oxazolidinone antibacterial agents

Indexing Terms

Streptococcus
intestinal, in vitro activities of U-100592 and U-100766, novel oxazolidinone antibacterial agents

Supplementary Terms

U 100592 100766 oxazolidinone antibacterial activity

Substances

165800-03-3 U 100766
165800-04-4 U 100592

in vitro activities of U-100592 and U-100766, novel oxazolidinone antibacterial agents

Biological activity or effector, except adverse; Biological study, unclassified; Therapeutic use; Biological study; Uses

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Source

Antimicrobial Agents and Chemotherapy
Volume 40
Issue 4
Pages 839-45
Journal
1996
CODEN: AMACCC
ISSN: 0066-4804

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Kalamazoo, MI, USA 49001

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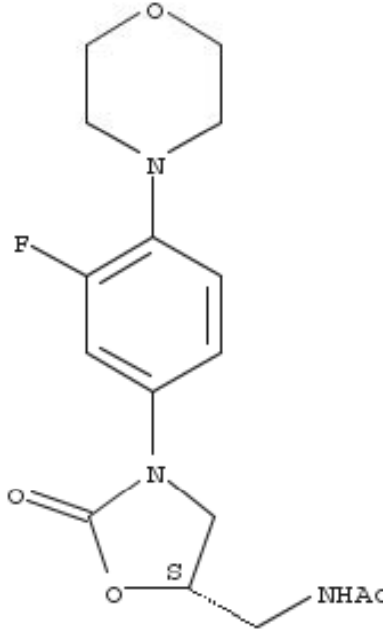
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CAS Registry Number: 165800-03-3

C₁₆ H₂₀ F N₃ O₄

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)

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

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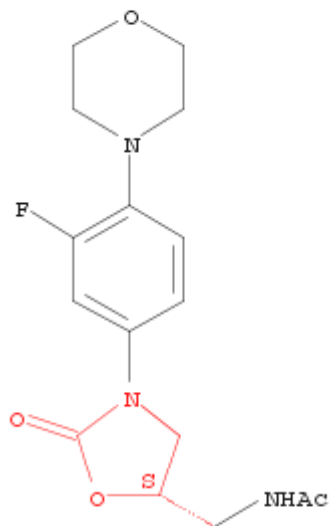
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1. Substance Detail
165800-03-3



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Absolute stereochemistry.
Rotation (-).

C₁₆ H₂₀ F N₃ O₄

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

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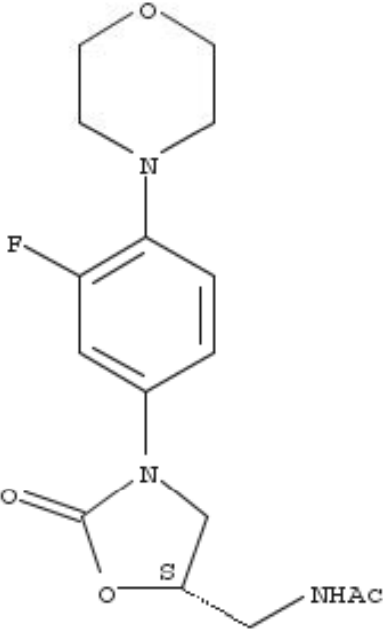
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CAS Registry Number: 165800-03-3

C₁₆ H₂₀ F N₃ O₄

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	Top
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)	

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

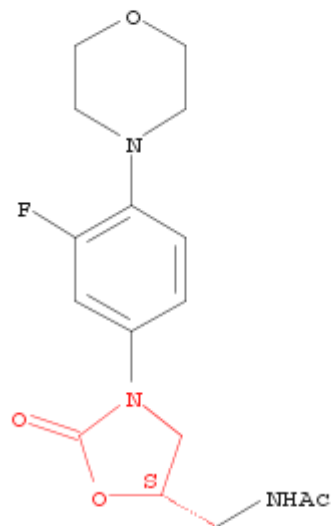
(5) Ramgren, Stephen D.; Angewandte Chemie, International Edition 2011, V50(9), P2171-2173, S2171/1-S2171/43 CAPLUS

(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 (-).

C₁₆ H₂₀ F N₃ O₄

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:

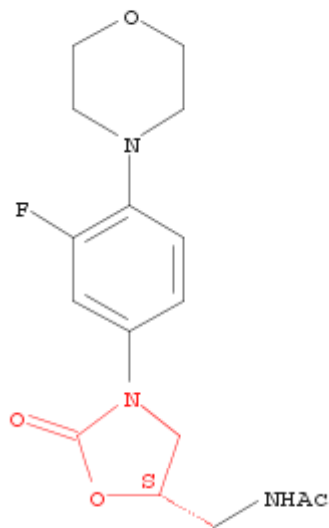
- | | |
|---|--|
| <input type="checkbox"/> Adverse Effect, including toxicity | <input type="checkbox"/> Prophetics in Patents |
| <input type="checkbox"/> Analytical Study | <input type="checkbox"/> Preparation |
| <input type="checkbox"/> Biological Study | <input type="checkbox"/> Process |
| <input type="checkbox"/> Combinatorial Study | <input type="checkbox"/> Properties |
| <input type="checkbox"/> Crystal Structure | <input type="checkbox"/> Reactant or Reagent |
| <input type="checkbox"/> Formation, nonpreparative | <input type="checkbox"/> Spectral Properties |
| <input type="checkbox"/> Miscellaneous | <input type="checkbox"/> Uses |
| <input type="checkbox"/> Occurrence | |

For each sequence, retrieve:

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

Get Cancel

1. Substance Detail
165800-03-3



Absolute stereochemistry.
Rotation (-).

C₁₆ H₂₀ F N₃ O₄

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

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

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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

<input type="checkbox"/> 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
<input type="checkbox"/> 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
<input type="checkbox"/> 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-oxazolidinylmethyl]-
<input type="checkbox"/> 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
<input type="checkbox"/> 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:

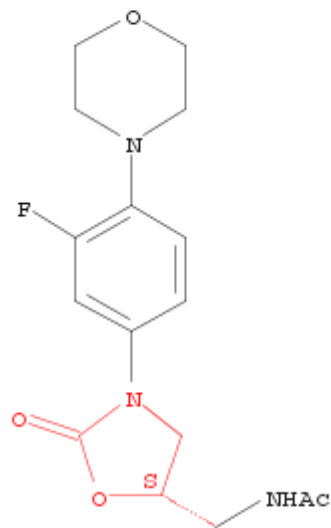
Country ▼

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



Absolute stereochemistry.
Rotation (-).

C₁₆ H₂₀ F N₃ O₄

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

~2,545 References

Reactions

Commercial Sources

Regulatory Information

Link

管制信息

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

Linospam

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

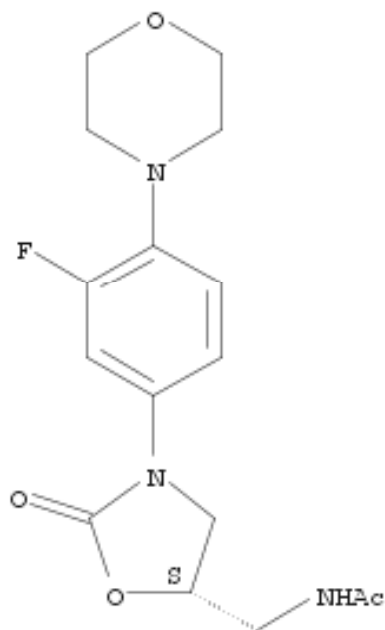
Inventory Status

On REACH

List of Pre-Registered Substances, March 2009

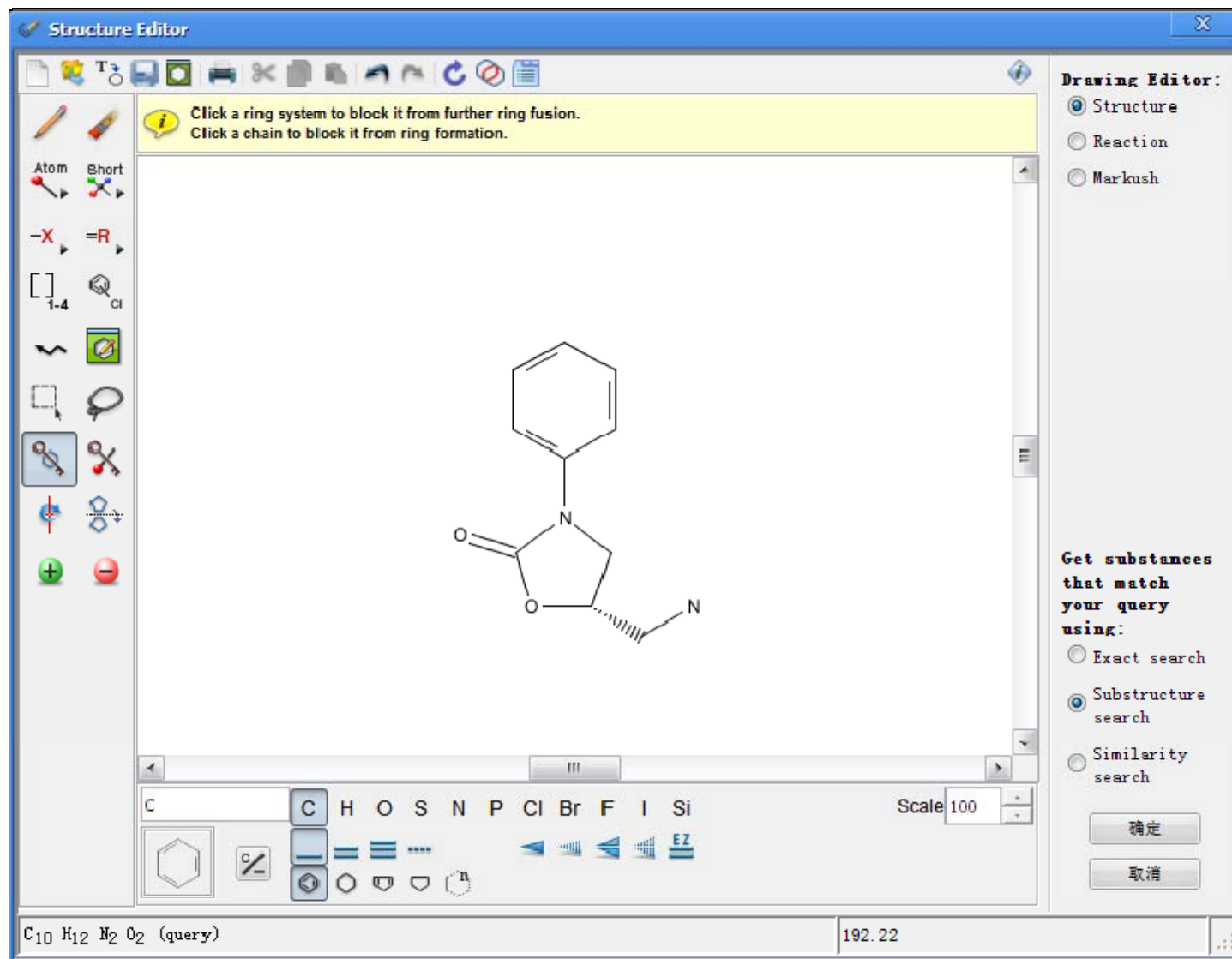
Registration Date: 31-MAY-2018.

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



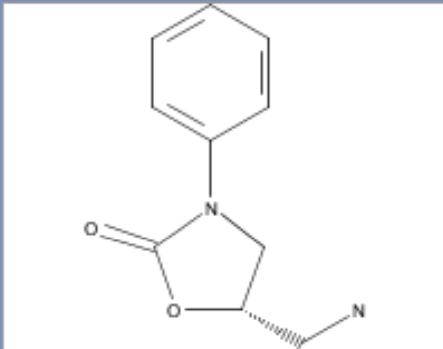
三种检索方式:

Explore Substances

Chemical Structure **Chemical Structure** ⓘ

Markush
Molecular Formula
Substance Identifier

Search



Click image to change structure or view detail

Search type: ⓘ

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Characteristic(s)

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



Exact Structure

2 Substances 0 Selected

Select All Deselect All Sort by: CAS Registry Number

1. Substance Detail
472975-63-6

Absolute stereochemistry.

C₁₀ H₁₂ N₂ O₂

2-Oxazolidinone, 5-(aminomethyl)-3-phenyl-, (5R)-

~0 References

Reactions

Commercial Sources

Regulatory Information

Link

2. Substance Detail
96800-35-0

Absolute stereochemistry.

C₁₀ H₁₂ N₂ O₂

2-Oxazolidinone, 5-(aminomethyl)-3-phenyl-, (5S)-

~4 References

Reactions

Commercial Sources

Regulatory Information

Link

- ❖ 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

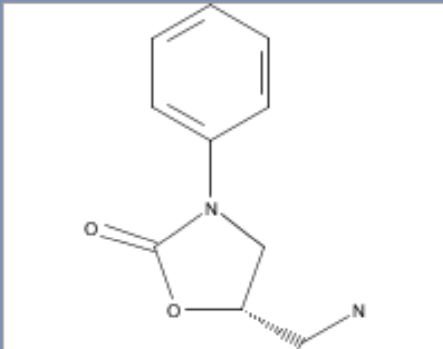
亚结构检索方式:

Explore Substances

Chemical Structure **Chemical Structure** ⓘ

Markush
Molecular Formula
Substance Identifier

Search



Click image to change structure or view detail

Search type: ⓘ

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Characteristic(s)

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

查看具有噁唑烷酮母核的所有已经报道的物质结构：

Create Keep Me Posted Chemical Structure substructure with limiters > substances (22289)

Substances Get References Get Reactions Tools NEW Send to SciPlanner

22289 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number ↓ Answers per Page [15] 1 2 3 4 5 6 ... 1486 View:

1. Substance Details
1309929-51-8

Absolute stereochemistry.
C₁₉ H₂₁ N₇ O₃ S
INDEX NAME NOT YET ASSIGNED

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

~1 References
Reactions
Commercial Sources
Regulatory Information
Link

Analysis Refine

Sample Analysis: ⓘ

Substance Role

Preparation

Biological Study

Uses

Prophetic in Patents

Reactant or Reagent

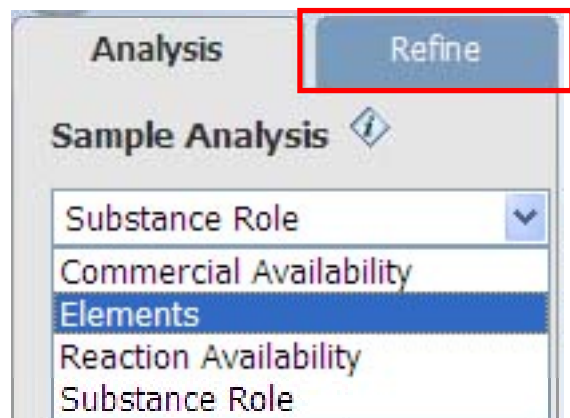
Properties

Analytical Study

Combinatorial Study

Formation, Nonpreparative

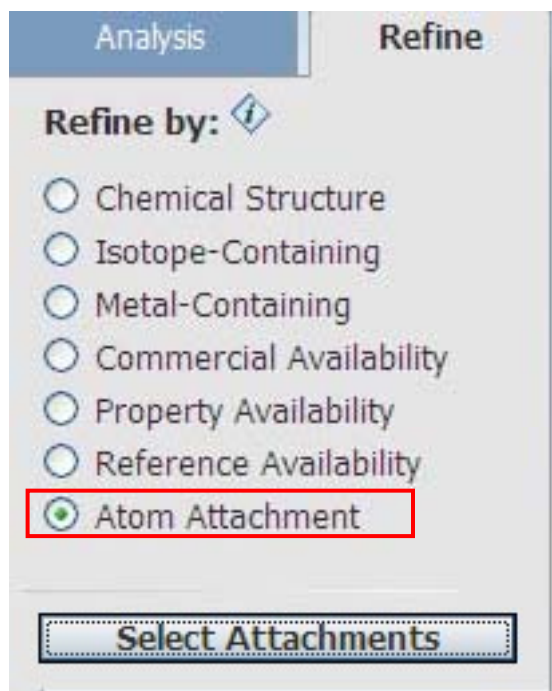
Process



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

Analysis **Refine**

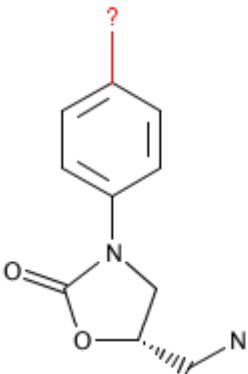
Refine by: **Refine by Atom Attachment** ⓘ

Chemical
 Isotope-C
 Metal-Co
 Commer
 Property
 Property
 Referenc
 Atom Atta

Select

1. Click an atom to display the attachments present at that site. 2. Select attachment(s) of interest.

Substructure



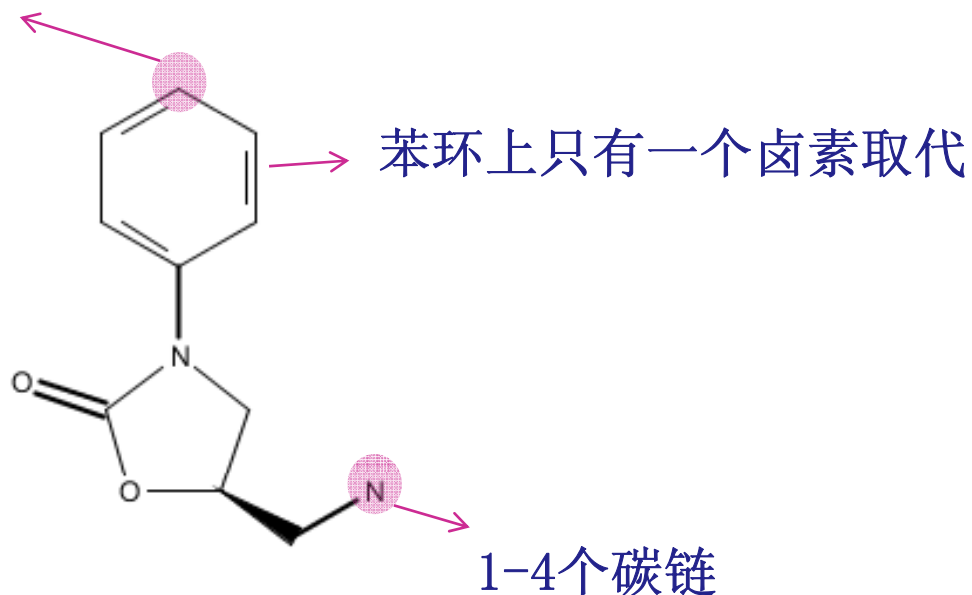
Atom Attachments

Select All Deselect All

<input type="checkbox"/> H or None	86
<input type="checkbox"/> N	9156
<input type="checkbox"/> C	4862
<input type="checkbox"/> O	369
<input type="checkbox"/> S	172
<input type="checkbox"/> Cl	102
<input type="checkbox"/> I	47
<input type="checkbox"/> B	25
<input type="checkbox"/> Br	17
<input type="checkbox"/> F	11
<input type="checkbox"/> Sn	6
<input type="checkbox"/> A - Any (not H)	14767
<input type="checkbox"/> Q - Any (not C,H)	9905
<input type="checkbox"/> Hy - Heterocycle	9829
<input type="checkbox"/> Cb - Carbocycle	997
<input type="checkbox"/> Ak - Alkyl chain	637
<input type="checkbox"/> X - Halogen	177
<input type="checkbox"/> M - Metal	6

? =

0, S, 杂环取代



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？

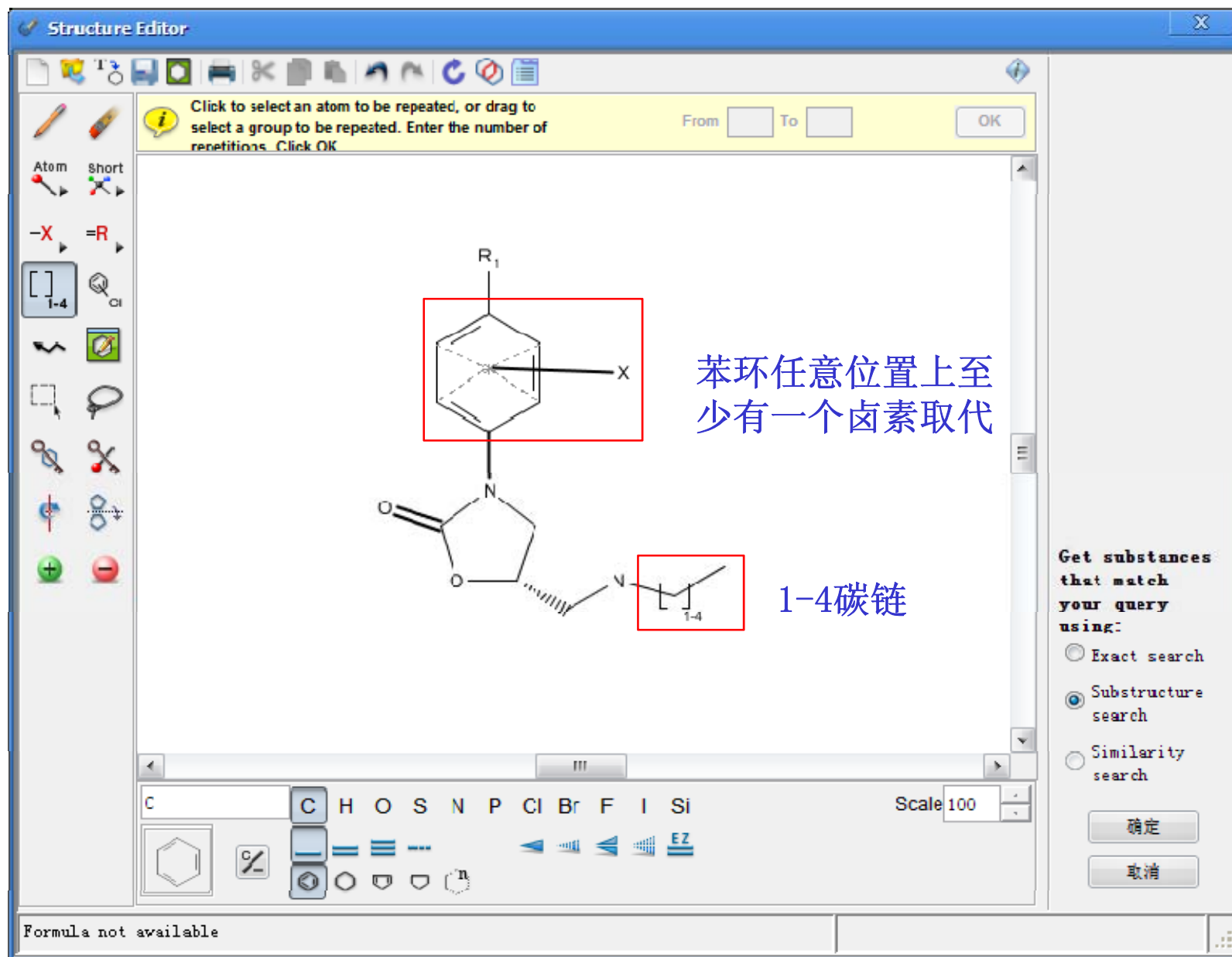
The screenshot shows the SCIFINDER Structure Editor interface. The main window displays a chemical structure of a benzimidazole derivative with an R-group attached to the benzene ring. Two dialog boxes are open:

- R-group Definitions:** A dialog box with a table for defining R-groups.

R-group	Definition
R1	S, O, Hy
R2	
R3	
R4	
- Variables:** A dialog box listing predefined variables.

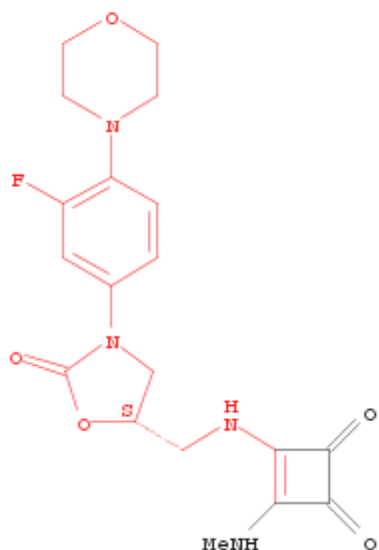
X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Alk	Any alkyl chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

The interface also includes a toolbar on the left, a status bar at the bottom with the text "Formula not available", and search options on the right for "Exact search", "Substructure search", and "Similarity search".



获得符合设计要求的化合物

7. Substance Detail
1308299-22-0

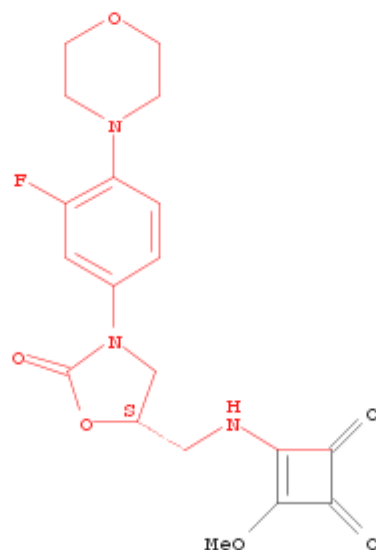


Absolute stereochemistry.

C₁₉ H₂₁ F N₄ O₅

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

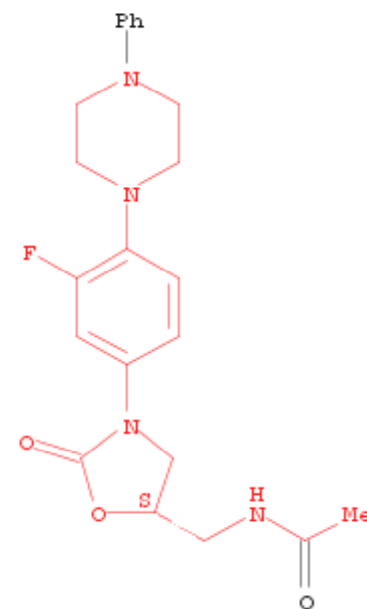


Absolute stereochemistry.

C₁₉ H₂₀ F N₃ O₆

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 H₂O

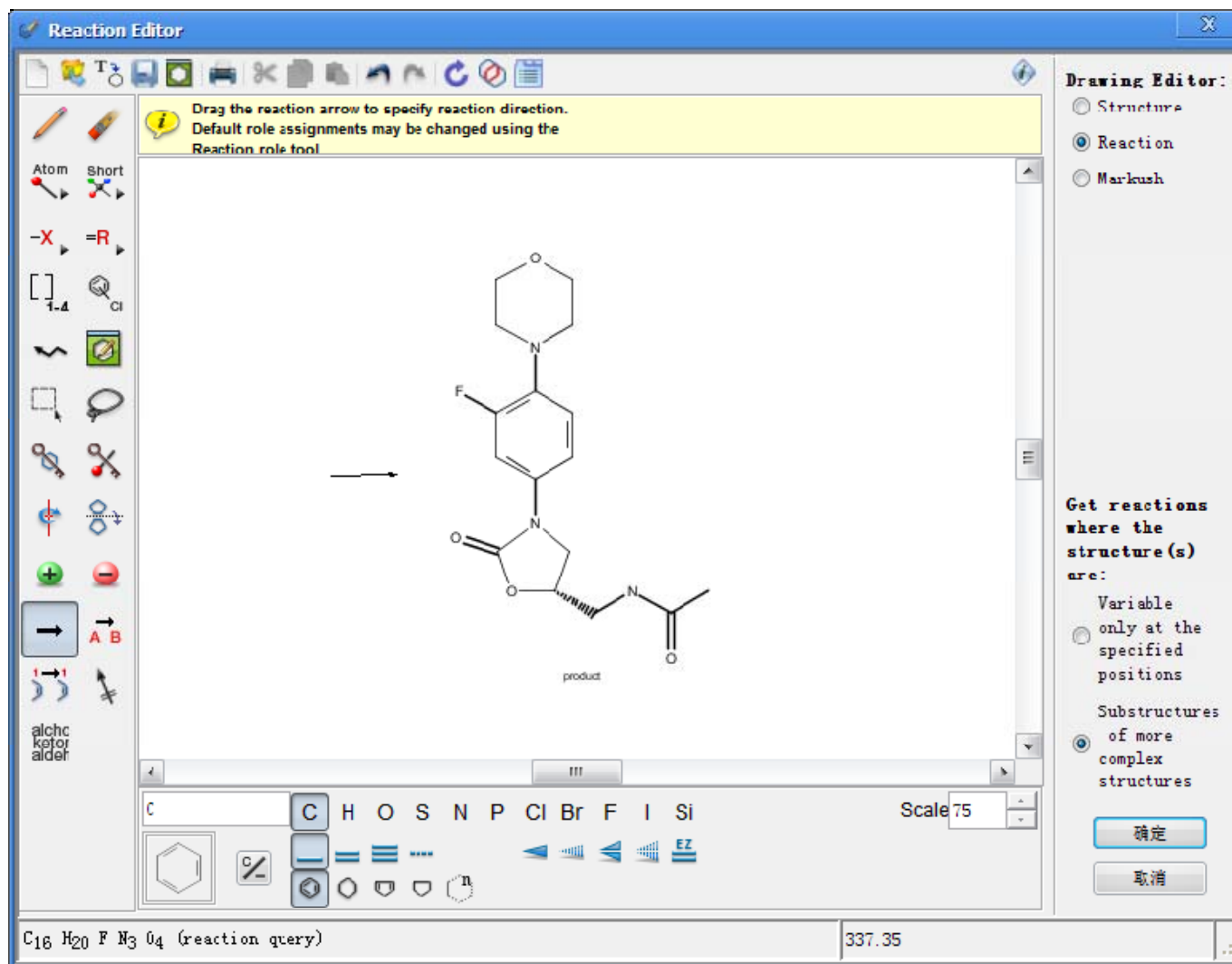
Absolute stereochemistry.

提纲



- **SciFinder Web 反应sciplanner介绍**

SciFinder检索反应信息



Reactions [Get References](#) [Tools](#) [Send to SciPlanner](#)

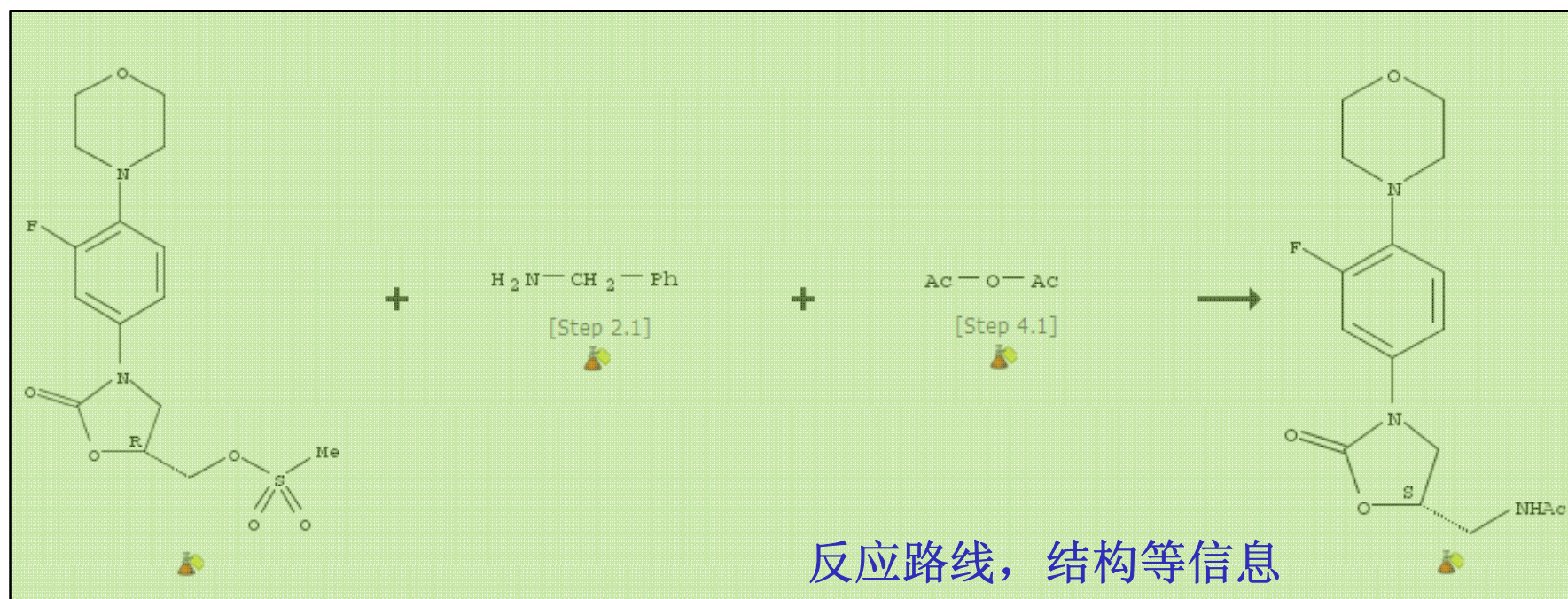
221 Reactions 1 Selected Save Print Export

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 **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.*

Steps/Stages

- 1.1 R:LiBr, S:THF, 27-30°C; 30°C → reflux; 8-9 h, reflux
- 2.1 rt → 150°C; 1-2 h, 150°C; 150°C → 60°C
- 3.1 R:H₂, C:Pd, S:AcOH, S:MeOH, rt → 40°C; 8-10 h, 40°C, 10-12 kg/cm²
- 4.1 S:AcOEt, S:H₂O, 25-30°C
- 4.2 R:NH₃, S:H₂O, 2 h, 25-30°C, pH 6-8

Notes

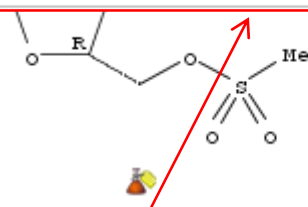
Reactants: 3, Reagents: 3, Catalysts: 1, Solvents: 5, Steps: 4, Stages: 5, Most stages in any one step: 2

References

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

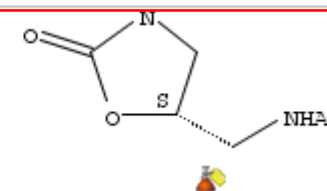
By Ramakrishnan, Arul et al
 From PCT Int. Appl., 2010084514, 29 Jul 2010

Full Text



[▶ Overview](#)

[▶ Experimental Procedure](#)



Reactions **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: Preparation of (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 3

Example-6: Preparation of (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 4

Example-8: Preparation of (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

Experimental Procedure



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

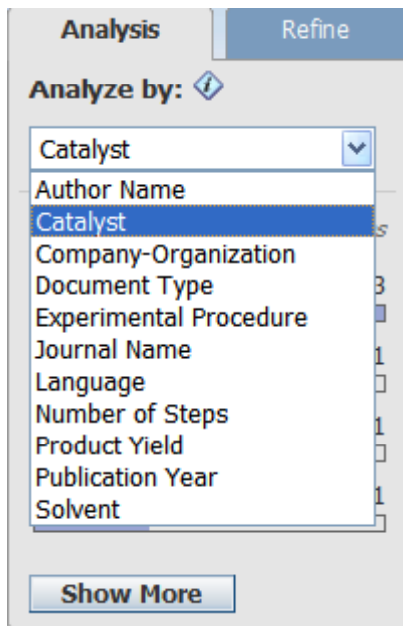
(CDCl₃, 400 MHz): δ 6.83 (t, J = 8.8 Hz, 1H), 6.38 (m, 2H), 4.34 (m, 1H), 4.09 (m, 1H), 3.85 (t, J = 4.4 Hz, 4H), 3.75 (m, 1H), 3.24 (d, J = 4 Hz, 1H), 3.13 (d, J = 4 Hz, 1H), 2.96 (t, J = 4.4 Hz, 4H), 1.44 (s, 3H), 1.37 (s, 3H). ¹³C NMR (CDCl₃): δ 25.27, 26.70, 26.88, 46.93, 51.66, 63.01, 65.81, 67.10, 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-Pr₂NET (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 MgSO₄, 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 (CDCl₃, 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); ¹³C NMR (CDCl₃): 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).

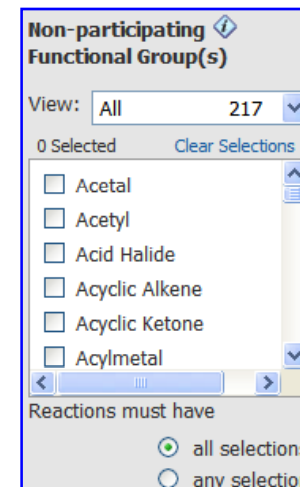
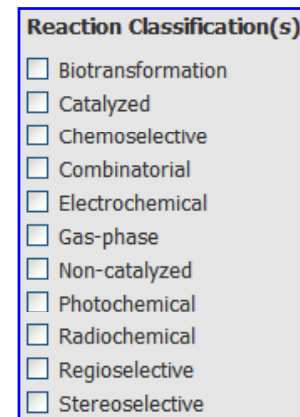
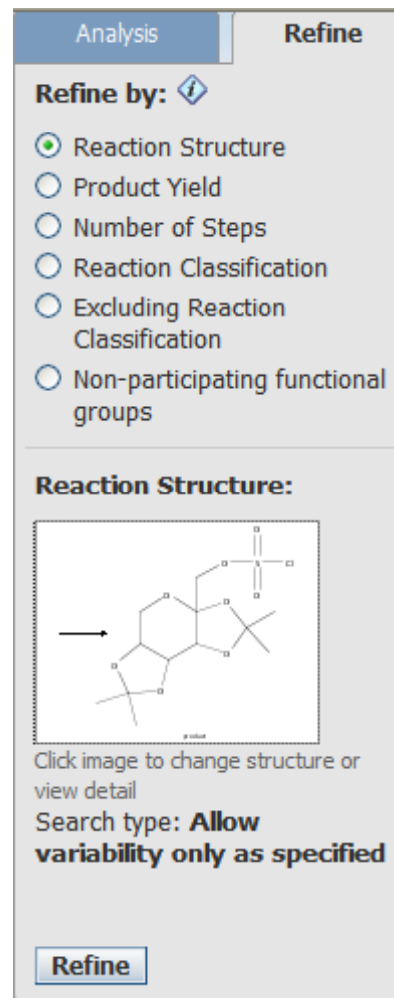
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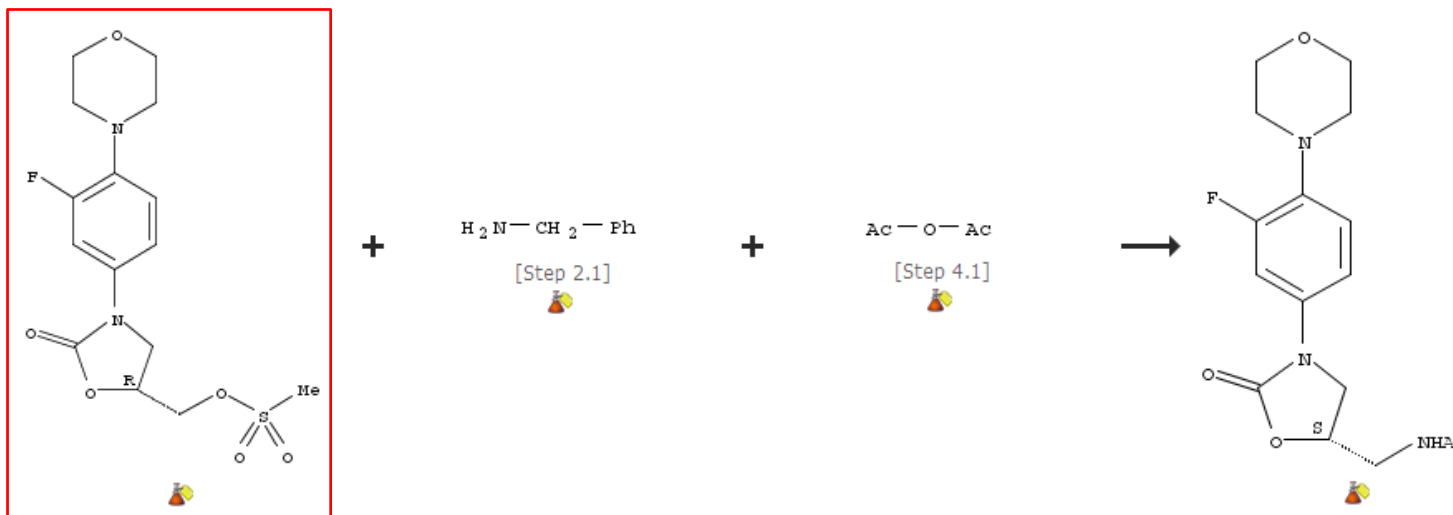
Analyze:
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溶剂
机构名称
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期刊名称
实验步骤

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出版年代
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产率
催化剂

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产率
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反应类型
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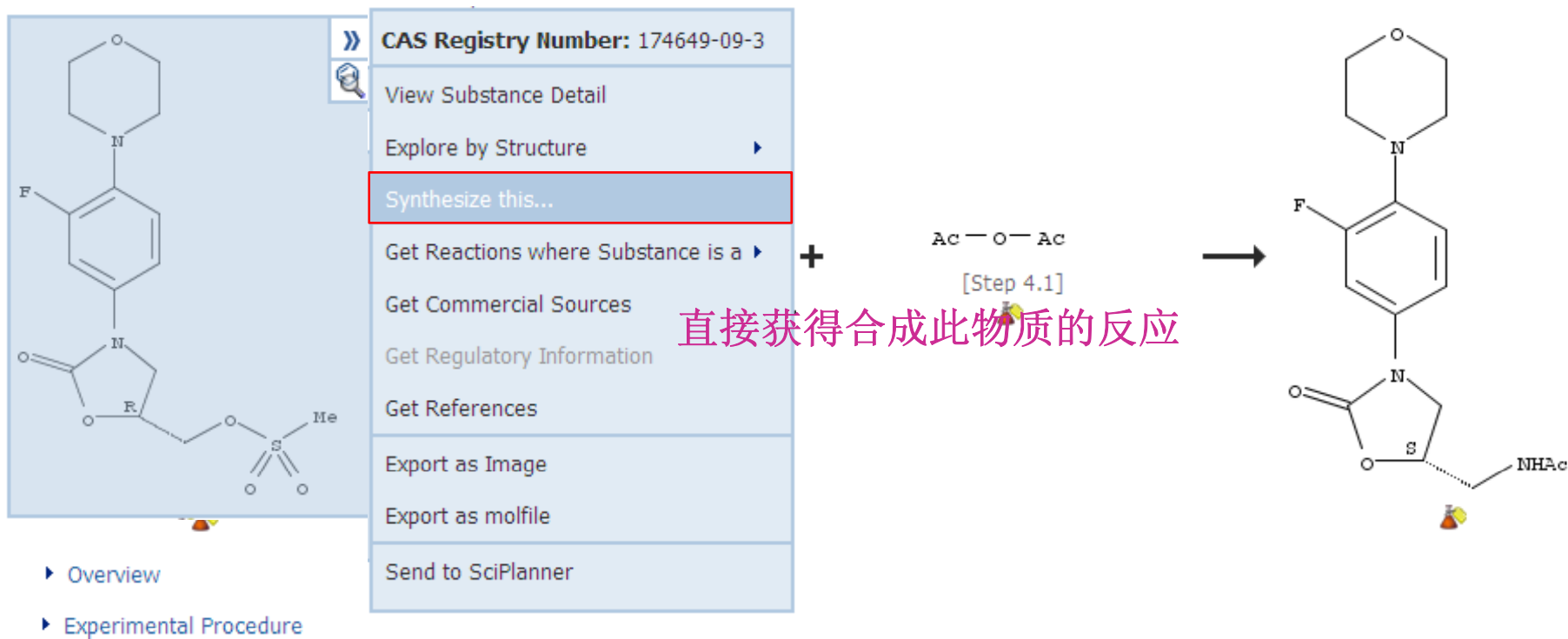
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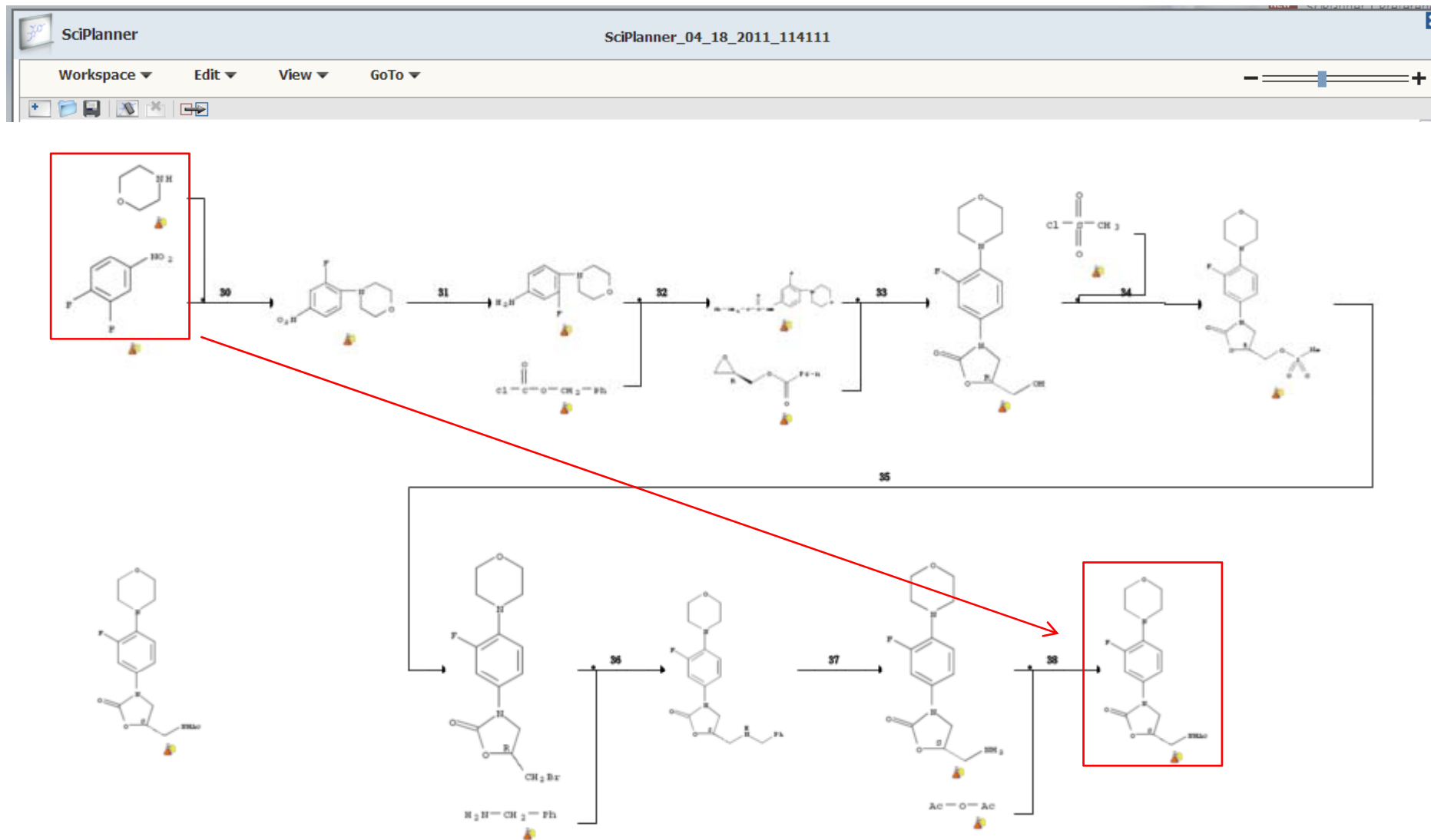
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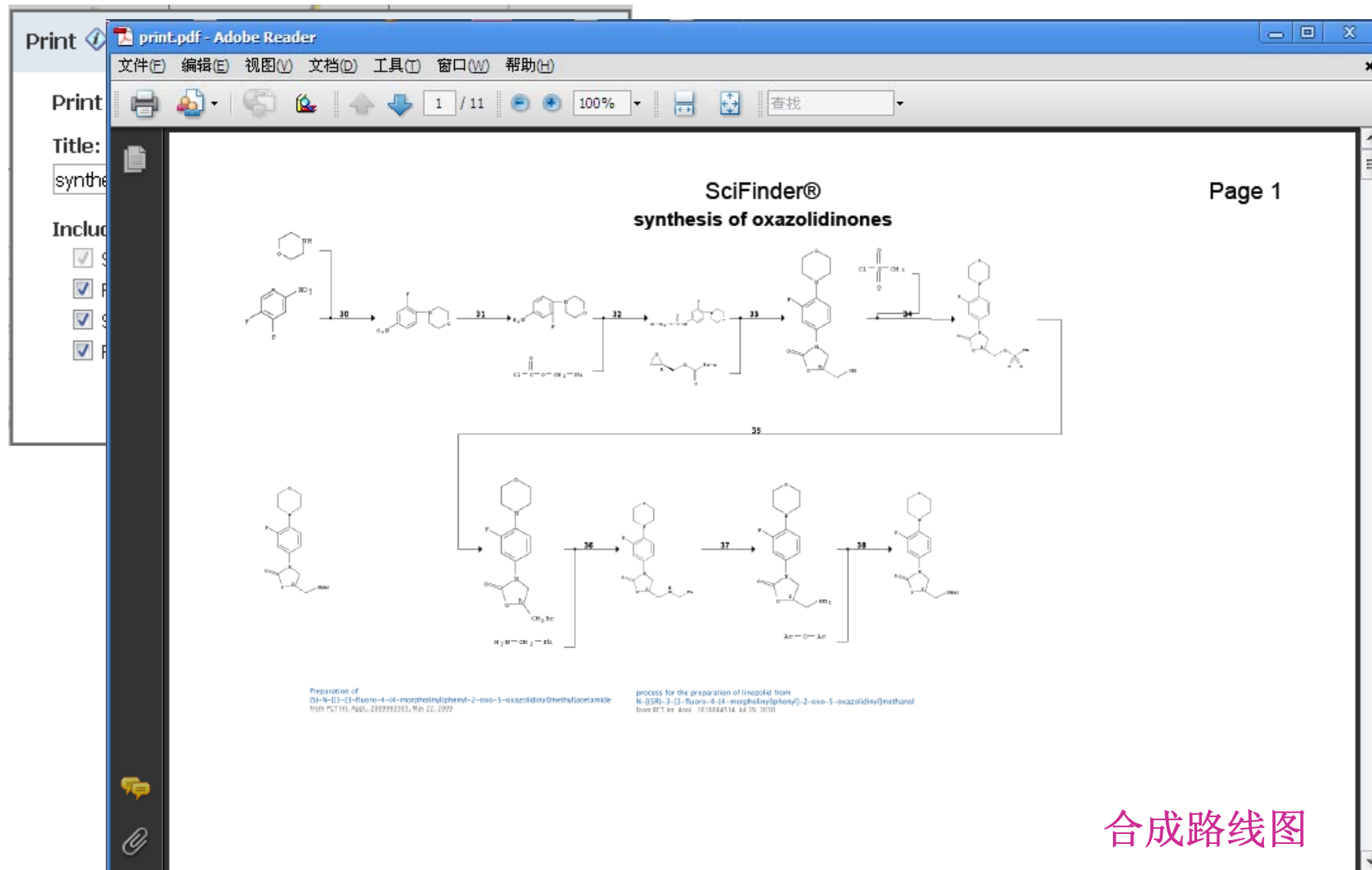
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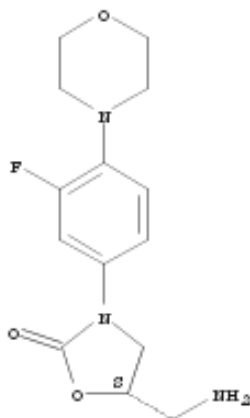
1. **process for the preparation of linezolid from N-[(5R)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methanol**
By Ramakrishnan, Arul; Wadekar, Kashyap Ravindrabhai; Kapkoti, Gobind Singh; Narayana, Venugopala Rao
From PCT Int. Appl. (2010), WO 2010084514 A2 20100729. Language: English, 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 hydrochloride, the free base of which was acetylated with Ac2O in H2O/EtOAc to give 68% linezolid form II.
Substances Reactions Citings Full Text Link Comments Tags

2. **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-(4-morpholinyl)phenyl]-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-morpholinyl)phenyl]-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.
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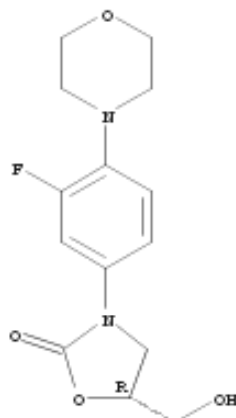
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1. Substance Detail
168828-90-8

Absolute stereochemistry.
Rotation (-).

C₁₄ H₁₈ F N₃ O₃

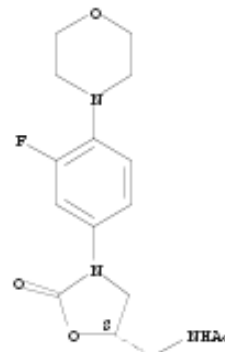
2-Oxazolidinone, 5-(aminomethyl)-3-[3-fluoro-4-(4-morpholinyl)phenyl]-, (5S)-

2. Substance Detail
168828-82-8

Absolute stereochemistry.

C₁₄ H₁₇ F N₂ O₄

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

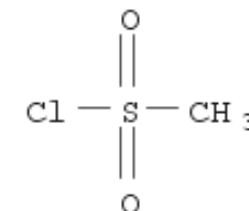
3. Substance Detail
165800-03-3

Absolute stereochemistry.
Rotation (-).

C₁₆ H₂₀ F N₃ O₄

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

~2,595 References

4. Substance Detail
124-63-0

C H₃ Cl O₂ S

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 ⁺ •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

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Page 11

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.

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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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1. Composition and light emitting element using the composition
 By Nakatani, Tomoya; Kawaguchi, Keiko; Sasaki, Shigeru
 From PCT Int. Appl. (2011), WO 2011078387 A1 20110630. Language: Japanese, Database: CAPLUS
 The compn. contains (i) a crosslinkable high-mol.-wt. compd. that has a crosslinkable group and exhibits either light emitting properties and/or charge transporting properties, and (ii) a crosslinkable low-mol.-wt. compd. that has a crosslinkable group and exhibits either light emitting properties and/or charge transporting properties. Thus, heating divinylcarbinol with tri-Et orthoacetate and propionic acid while removing ethanol at 130° for 4 h gave CH₂:CHCH:CHCH₂CH₂C(O)OEt which was reduced with LiAlH₄ to its alc., mixed with CH₃SO₂Cl in the presence of Et₃N in CH₂Cl₂ at 0°, extd. as a yellow oil then heated with LiBr in THF at reflux to give CH₂:CHCH:CHCH₂CH₂CH₂Br (I). Condensing I with 2,7-dibromofluorene gave a 9,9-di-substituted dibromofluorene.
 Substances Reactions ~0 Citings Full Text Link 0 Comments 0 Tags

2. Chemo- and stereospecific solid-state dimerization of lithium trans-2-butenolate and lithium trans-2-butenolate formamide solvate
 By Shang, Wen; Hickey, Magali B.; Enkelmann, Volker; Snider, Barry B.; Foxman, Bruce M.
 From CrystEngComm (2011), 13(13), 4339-4350. Language: English, Database: CAPLUS
 60Co γ -irradn. of both lithium trans-2-butenolate (11) and lithium trans-2-butenolate·formamide (12) affords the same dimer, dilithium trans-5-methyl-2-heptenedioate (13). However, stereochem. anal. of products 22 and 24 from the analogous trans-2-butenolate-2-d salts 21 and 23 established that C-C and C-H bond formation occur stereospecifically by syn addn. to the double bond in lithium trans-2-butenolates 11 and 21 and anti addn. to the double bond in lithium trans-2-butenolate·formamide complexes 12 and 23. These reactions, which provide an unprecedented, chemospecific one step synthesis of dicarboxylate 13, add significantly to the synthetic scope of the γ -ray induced reactions of cryst. metal trans-2-butenolates that lead to cyclic and acyclic dimers and acyclic trimers by γ -ray initiated radical chain reactions. The stereochem. of products 22 and 24 is that predicted by anal. of crystal packing, consistent with least-motion principles of the topochem. postulate as shown in Fig. 12 and 13. Anal. of the crystal structures, with respect to nearest neighbors, is consistent with the hypothesis that formation of carbon-carbon bonds in propagation step 1 and hydrogen atom transfer in propagation step 2 are topochem. and controlled by the crystal lattice. Anal. of the packing diagrams provides a pathway for chain propagation throughout the crystal that consumes all the mols. in the unit cell. The dimerization of 12 is much more rapid and proceeds in much higher yield than that of 11, probably as a result of significantly shorter C...C contacts and a more robust pathway for hydrogen transfer.

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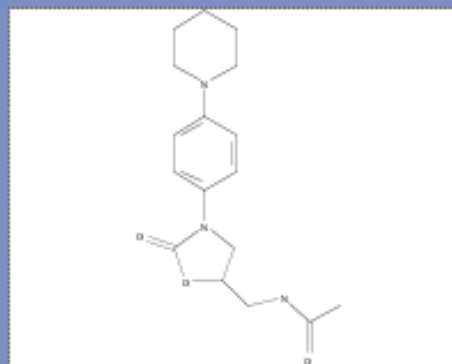
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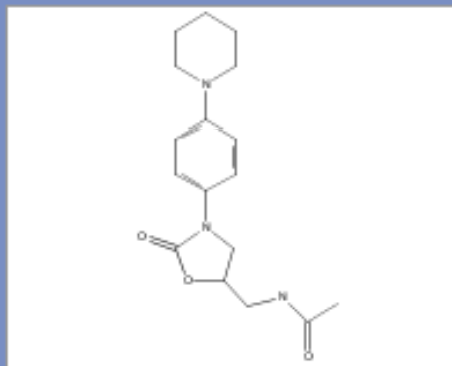
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1. Preparation of (piperidinophenyl)oxazolidinone derivatives as antimicrobial agents
By Yamada, Hiroyoshi; Munesada, Kiyotaka; Taniguchi, Mikio
From PCT Int. Appl. (1995), WO 9525106 A1 19950921. Language: English, Database: CAPLUS
Novel oxazolidinone derivs. represented by chem. formula (I; R = H, alkyl, cycloalkyl, NH2, alkylamino, dialkylamino, alkoxy, haloalkyl; R1, R3 = H, alkyl cycloalkyl, O-(un)substituted hydroxyalkyl or carboxyalkyl, CHO, hydroxyalkanoyl, alkanoyl, acyloxymethoxycarbonyl; X, Y = H, halo; R4, R5 = H, alkyl, alkoxy, alkylthio, O-(un)substituted hydroxyalkyl or hydroxyalkoxy, (un)substituted NH2, N-(un)substituted N-(aminomethylene)amino, (un)substituted carbamoyl, formyl-, O-(un)substituted hydroxyalkanoyl-, alkoxy-carbonyl-, acyloxymethoxycarbonyl-, or O-(un)substituted (carboxyalkanoyl)alkyl, or ...
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2. Preparation of pharmaceutically active (S)-2-oxo-5-oxazolidinylmethylacetamides via a one step process from (S)-acetamidoacetoxypromanes and N-aryl-O-alkylcarbamates
By Perrault, William R.; Pearlman, Bruce A.; Godrej, Delara B.
From PCT Int. Appl. (2002), WO 2002085849 A2 20021031. Language: English, Database: CAPLUS
Title compds. I [X, Y = H, F; Q = II, III, IV, etc. or Q and X together = dihydropyrrolidine (un)substituted with R5; R1 = CH3 optionally substituted by 1-3 F or Cl atoms; R3 = H, CH3; R4 = H, OH, alkyl, etc.; R5 = COCH3, CHO, COCHCl2, etc.; Z1 = CH2(CH2)p, CH(OH)(CH2)p, CO; Z2 = S, SO, SO2, etc.; m = 0-1; n = 1-3; p= 0-2] were prepd via a one step process from (S)-acetamidoacetoxypromanes and N-aryl-O-alkylcarbamates. For example, to a soln. of N-carbobenzoxy-3-fluoro-4-morpholinylaniline (3.125 mmol) in DMF (2.0 mL) and MeOH (6.32 mmol) was added a soln. of lithium tert-butoxide in THF (9.3...
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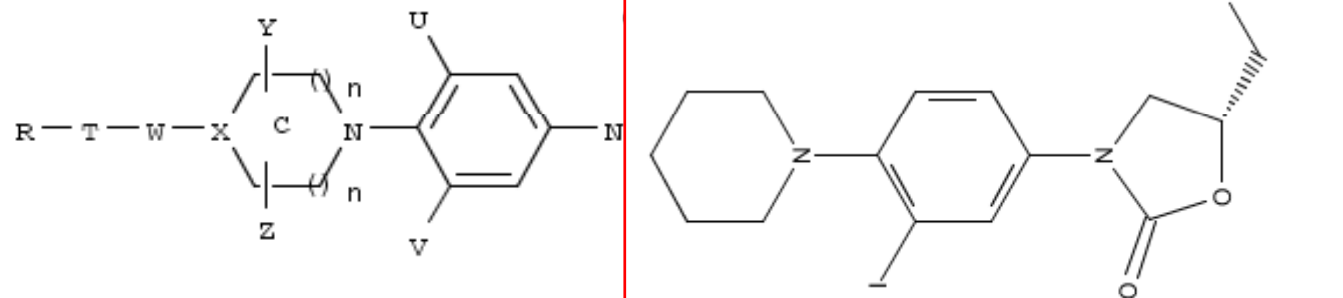
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1. Preparation of oxazolidinone derivatives as antimicrobial agents

By: Mehta, Anita; Rudra, Sonali; Rao, Ajjarapu Venkata Subrahmanya Raju; 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 as multiply-resistant staphylococci, streptococci and enterococci as well as ana species, and acid fast organisms such as *Mycobacterium tuberculosis*, *Mycoba*



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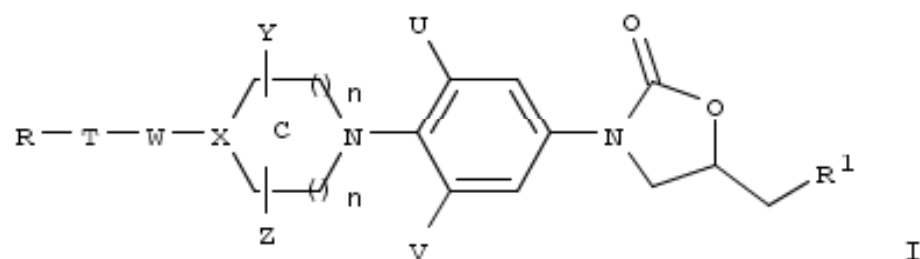
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1. Preparation of oxazolidinone derivatives as antimicrobial agents

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Substances

776296-79-8P
776296-89-0Pprepn. of oxazolidi
agentsPharmacological a
Therapeutic use; B
or reagent776296-76-5P
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
776296-93-6Pprepn. of oxazolidi
agentsPharmacological a
use; Biological stud

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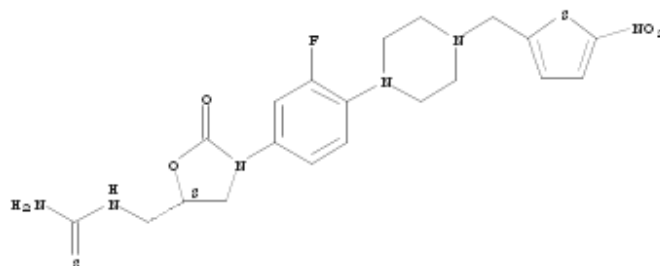
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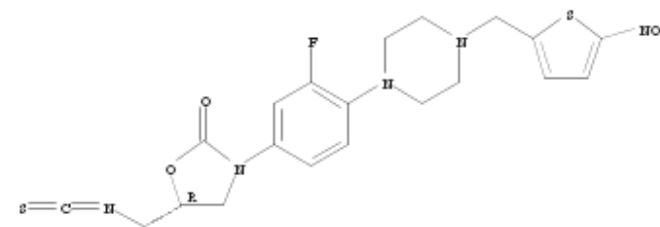
 1. **Substance Detail**
776296-93-6

Absolute stereochemistry.

C₂₀ H₂₃ F N₆ O₄ S₂

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
- Link

 2. **Substance Detail**
776296-92-5

Absolute stereochemistry.

C₂₀ H₂₀ F N₅ O₄ S₂

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

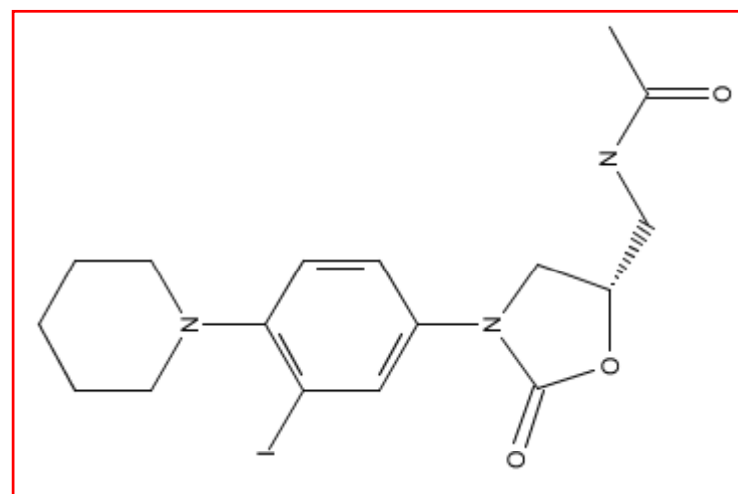
prepn. of oxazolidinone derivs. as antimicrobial/antibacterial agents

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
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776296-86-7P
776296-87-8P
776296-88-9P
776296-90-3P
776296-91-4P
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776296-93-6P

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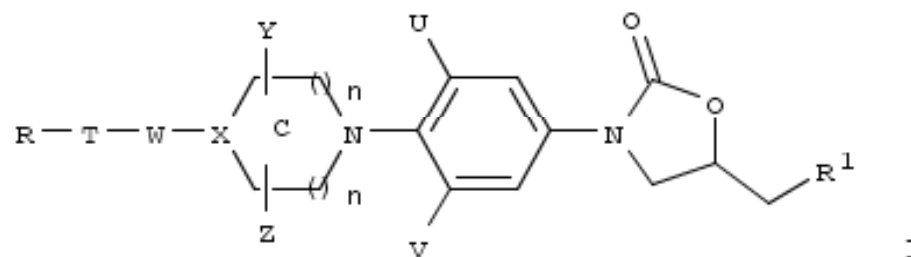
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只合成一类物质，通过各种可能的取代基团保护可能的物质-----Markush结构通式。

在专利中描述物质的方式

➤ 特定物质[Specific Substance]:

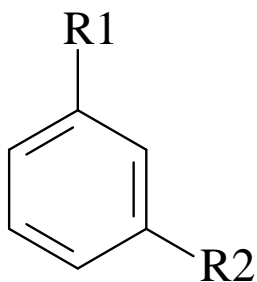
以特定化学结构所陈述的特定物质，会被标示**CAS No.**

➤ 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

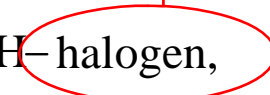
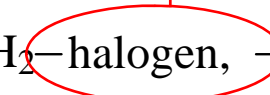


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH(CH₃)—halogen,

Br, Cl, F, I

Br, Cl, F, I



SciFinder中的Markush检索

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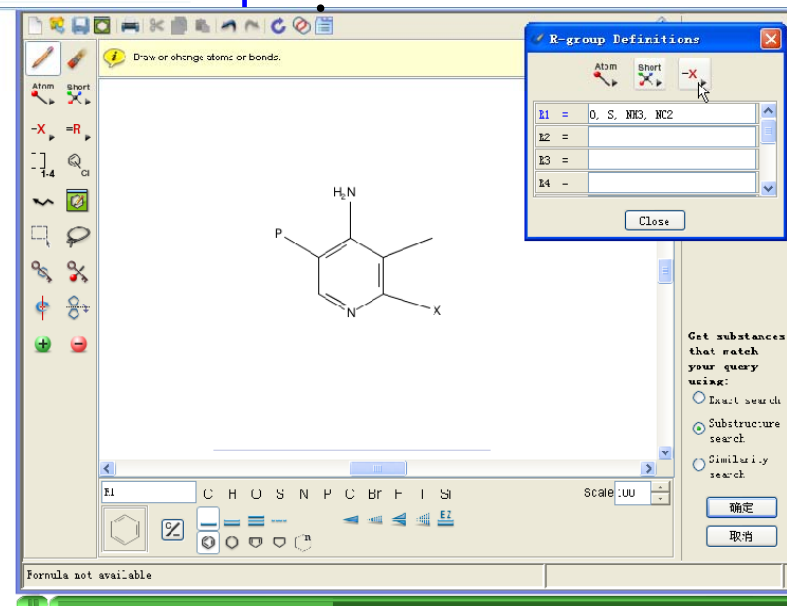


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文献检索	Web版机构名检索	
结构物质检索	Web版结构检索	
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反应检索	Web版反应检索	
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*For more information please contact :
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