

朱传娴

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hzhu@acs-i.org

如何使用SciFinder获取医药信息

中国药科大学

2019.10.09



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

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



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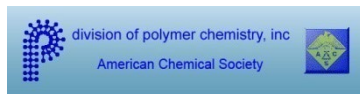
arXiv.org

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OF ORGANIC CHEMISTRY



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THE JOURNAL OF
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Letters

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CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水

染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学




CAS数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751  PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing


Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

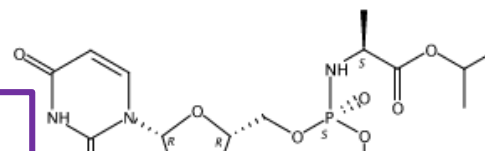
Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

Substances

1190307-88-0P Sofosbuvir 
Absolute stereochemistry.

Page 2 in PATENTPAK



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term, CAS RN, CAS Role），提高效率，启发思路。

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
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 - SciPlanner
- SciFinder常见问题及解决

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SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder web interface. At the top left is the CAS Solutions logo and the SciFinder logo. The top right contains links for Preferences, SciFinder Help, and a Sign Out button. Below the header is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' options. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with example text: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A 'Search' button and an 'Advanced Search' link are located below the input field. On the left side, a sidebar menu is open, showing categories: REFERENCES (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), SUBSTANCES (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and REACTIONS (with sub-item: Reaction Structure). On the right side, a 'SAVED ANSWER SETS' panel lists several saved sets: CSF1R, jmc, EP 19870107847, Daclatasvir-1, SUB result, EX result, MF result, polymer1, polymer1, structure search, and Autosaved Substance Set. Below this panel is a 'KEEP ME POSTED' section with the text 'You have no promises. Learn how to: Create Keep Me Posted'.

已保存的结果集

检索入口

定题追踪

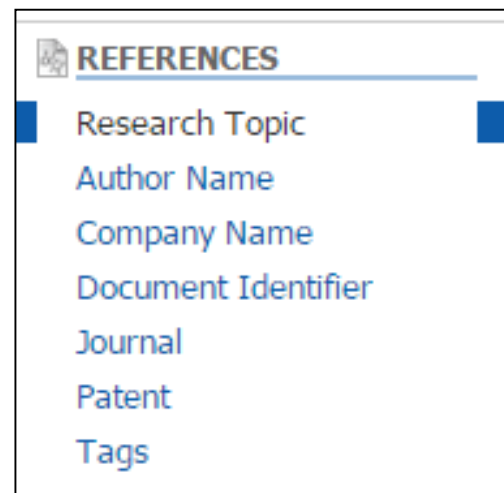
SciFinder检索——文献检索

■ 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献

■ 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索



文献检索——主题

主题检索：MMP抑制剂在肝癌治疗中的应用

检索式：MMP Inhibitor **in** Liver Cancer

The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the breadcrumb path reads 'Research Topic "MMP Inhibitor in Liver Cancer" > references (247)'. On the left side, there is a sidebar menu with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', the 'Research Topic' option is highlighted with a pink box. Other options include Author Name, Company Name, Document Identifier, Journal, Patent, Tags, Chemical Structure, and Markush. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'MMP Inhibitor in Liver Cancer'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples, and an 'Advanced Search' link is located at the bottom of the main area.

关键词之间用介词连接：in, with, of...

主题检索的候选项

Explore ▼ Saved Searches ▼ SciPlanner

Research Topic "MMP Inhibitor in Liver Cancer"

REFERENCES ?

Select All Deselect All

1 of 7 Research Topic Candidates Selected

	References
<input type="checkbox"/> 305 references were found containing the two concepts "MMP Inhibitor" and "Liver Cancer" closely associated with one another.	305
<input checked="" type="checkbox"/> 1607 references were found where the two concepts "MMP Inhibitor" and "Liver Cancer" were present anywhere in the reference.	1607
<input type="checkbox"/> 45632 references were found containing the concept "Liver Cancer", and either the concept "MMP" or the concept "Inhibitor". The concepts found were closely associated with one another.	45632
<input type="checkbox"/> 126253 references were found containing the concept "Liver Cancer", and either the concept "MMP" or the concept "Inhibitor". The concepts found were present anywhere (perhaps widely separated) within the reference.	126253
<input type="checkbox"/> 41826 references were found containing the concept "MMP Inhibitor".	41826
<input type="checkbox"/> 6281870 references were found containing either the concept "MMP" or the concept "Inhibitor".	6281870
<input type="checkbox"/> 478647 references were found containing the concept "Liver Cancer".	478647

Get References

“Concepts”表示对主题词做了同义词的扩展；

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

“were present anywhere in the reference”表示同时出现在一篇文献中；



按被引次数排序— Citing References

CAS Solutions

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Research Topic "MMP Inhibitor in Liver Cancer" > references (1197)

REFERENCES

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Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Citing References

Analyze by: Author Name

Kim Cheorl Ho 13

Saiki Ikuo 10

Hu Miao Lin 9

Lee Young Choon 8

Li Tao 8

Chen Zhi Nan 7

Chung Tae Wook 7

Lee Hyong Joo 7

Li Yan 7

Wang Li 7

Show More

Sort by: Citing References

Accession Number

Author Name

Citing References

Publication Year

Title

1. **Anticancer effect of caffeic acid and caffeic acid phenethyl ester on hepatocarcinoma cells: complete regression of hepatic growth and metastasis by dual mechanism**

By Chung, Tae-Wook; Moon, Sung-Kwon; Chang, Young-Chae; Ko, Jeong-Heon; Lee, Young-Choon; Cho, Gun; Kim, Soo-Hyun; Kim, Jong-Guk; Kim, Cheorl-Ho
From FASEB Journal (2004), 18(14), 1670-1681, 10.1096/fj.04-2126com. | Language: English, Database: CAPLUS

Our previous studies have clearly shown that the angiogenic enzymes, matrix metalloproteinase (MMP) -2/9, are directly involved in human hepatic tumorigenesis and metastasis and suggest that the MMP-2/9 inhibitors, which have dual inhibitory activities on enzyme activity and transcription, represent the best candidates for achieving tumor regression. Many anti-cancer drugs have strong cellular cytotoxicity and side effects, indicating that strong anti-cancer drugs that have no or minimal cytotoxicity and side effects need to be developed. The specific aim of the present study was to develop ...

2. **The role and regulation of hepatic stellate cell apoptosis in reversal of liver fibrosis**

By Elsharkawy, A. M.; Oakley, F.; Mann, D. A.
From Apoptosis (2005), 10(5), 927-939. | Language: English, Database: CAPLUS

A review. Liver fibrosis and its end-stage disease cirrhosis are major world health problems arising from chronic injury of the liver by a variety of etiol. factors including viruses, alc. and drug abuse, the metabolic syndrome, autoimmune disease and hereditary disorders of metab. Fibrosis is a progressive pathol. process in which wound-healing myofibroblasts of the liver respond to injury by promoting replacement of the normal hepatic tissue with a scar-like matrix composed of cross-linked collagen. Until recently it was believed that this process was irreversible. However emerging exptl...

3. **Expression patterns of matrix metalloproteinases and their inhibitors in parenchymal and non-parenchymal cells of rat liver: regulation by TNF- α and TGF- β 1**

By Knittel, Thomas; Mehde, Mirko; Kobold, Dominik; Saile, Bernhard; Dinter, Christina; Ramadori, Giuliano
From Journal of Hepatology (1999), 30(1), 48-60. | Language: English, Database: CAPLUS

Although matrix metalloproteinases (MMPs) and their specific inhibitors (TIMPs) play an essential role in liver injury assocd. with tissue remodeling, the cellular origin of MMPs/TMPs within the liver has not been well defined. Different transcriptional patterns of MMPs and TIMPs have been reported in various models of liver injury. In this study we investigated the expression patterns of MMPs and TIMPs in parenchymal and non-parenchymal cells of rat liver. We found that the expression of MMPs and TIMPs was up-regulated in parenchymal cells and down-regulated in non-parenchymal cells in response to liver injury. These results suggest that the expression of MMPs and TIMPs is regulated differently in parenchymal and non-parenchymal cells of rat liver. This finding may be important for understanding the role of MMPs and TIMPs in liver injury and for developing new therapeutic strategies for liver disease.

Citing Reference: 帮助找到最重要的文献

文献检索结果

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Research Topic "MMP Inhibitor in Liver Cancer" > re

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REFERENCES

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Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Citing References

0 of 1197 References Selected

Page: 1 of 60

Analyze by:

- Author Name
- Kim Cheorl Ho 13
- Saiki Ikuro 10
- Hu Miao Lin 9
- Lee Young Choon 8
- Li Tao 8
- Chen Zhi Nan 7
- Chung Tae Wook 7
- Lee Hyong Joo 7
- Li Yan 7
- Wang Li 7

1. **Novel and therapeutic effect of caffeic acid and caffeic acid phenethyl ester on hepatocarcinoma cells: complete regression of hepatoma growth and metastasis by dual mechanism**

Quick View | Other Sources

By Chung, Tae-Wook; Moon, Sung-Kwon; Chang, Young-Chae; Ko, Jeong-Heon; Lee, Young-Choon; Cho, Gun; Kim, Soo-Hyun; Kim, Jong-Guk; Kim, Cheorl-Ho
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From Journal of Hepatology (1999), 30(1), 48-60. | Language: English, Database: CAPLUS

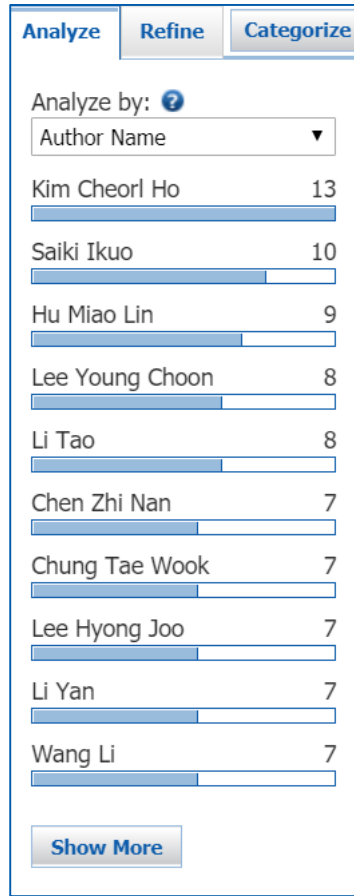
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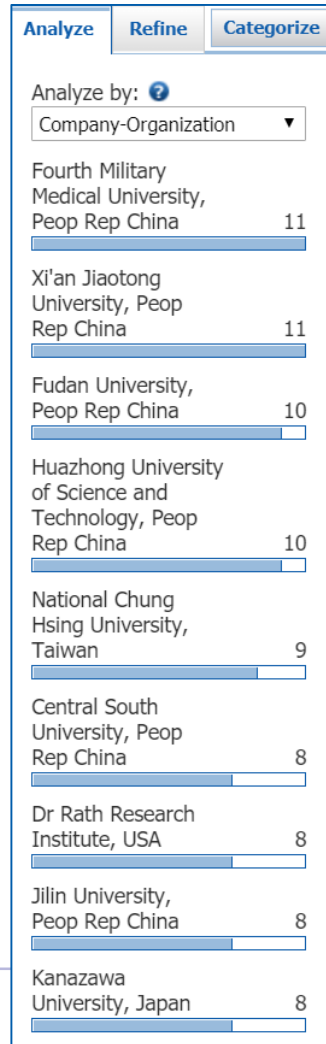


文献检索结果的Analyze

本领域研究人员



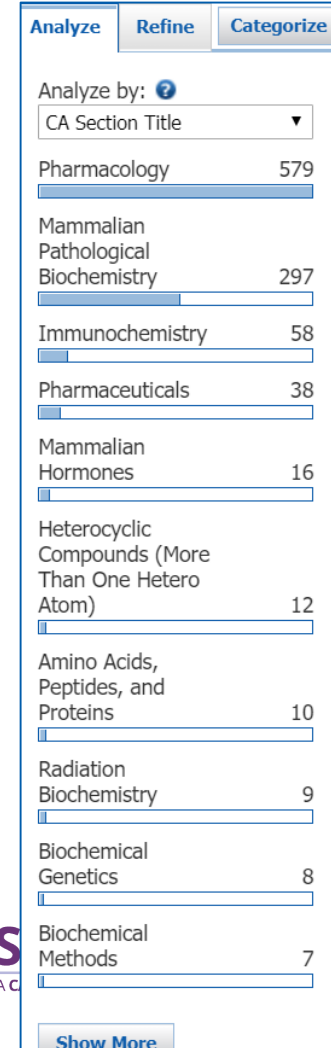
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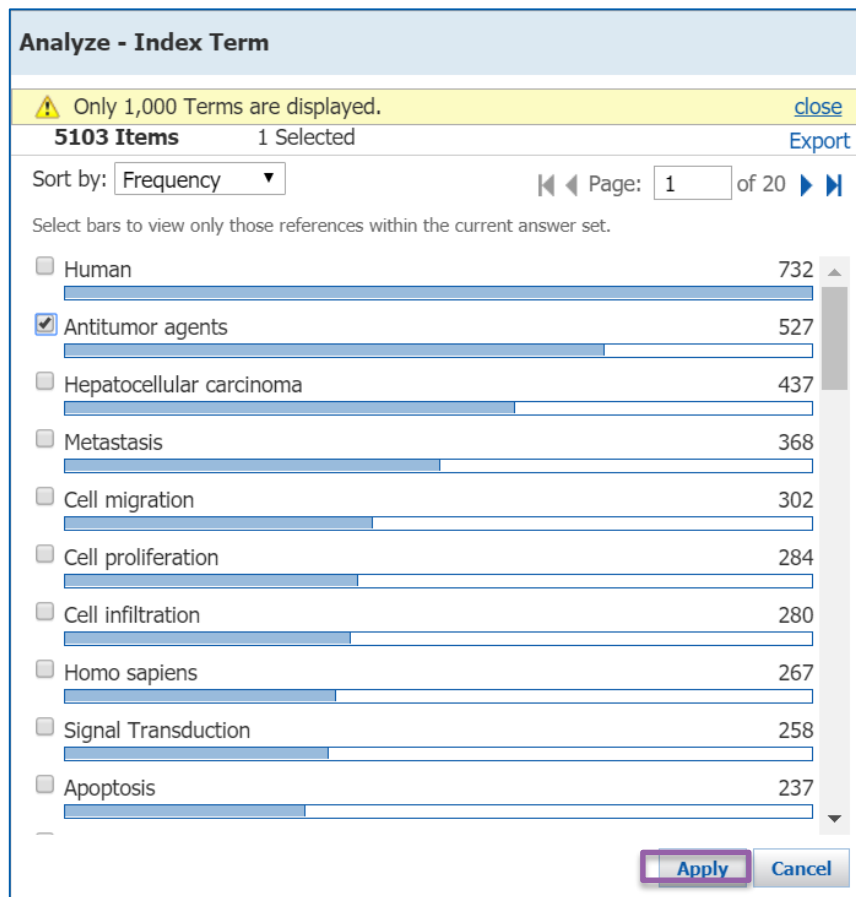
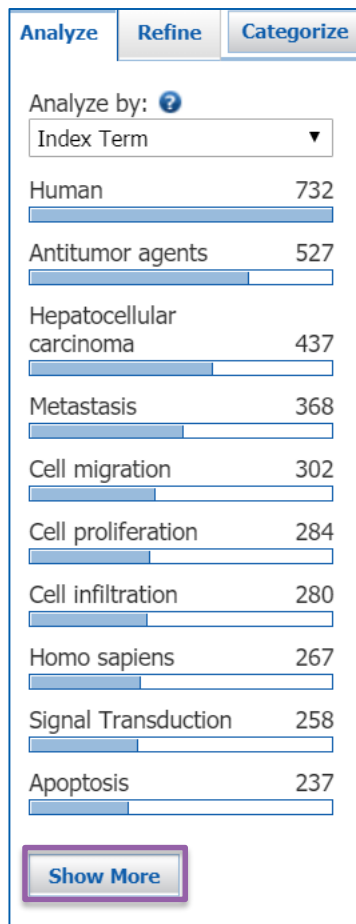
涉及学科领域



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Index Term:

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文献检索结果的Refine

Analyze Refine Categorize

Refine by: ?

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

Research Topic

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

[Refine](#)

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Sort by: Citing References

0 of 24 References Selected

1. **Baicalein inhibits the invasion and metastatic capabilities of hepatocellular carcinoma cells via down-regulation of the ERK pathway**

Quick View Other Sources

By Chen, Kunlun; Zhang, Shu; Ji, Yuan Yuan; Li, Jun; An, Peng; Ren, Hongtao; Liang, Rongrui; Yang, Jun; Li, Zongfang
From PLoS One (2013), 8(9), e72927. | Language: English, Database: CAPLUS

Baicalein, a widely used **Chinese herbal medicine**, has historically been used in anti-inflammatory and anti-cancer therapies. However, the anti-metastatic effect and mol. mechanism(s) of baicalein on **hepatocellular carcinoma** (HCC) remain poorly understood. Therefore, the purpose of this study was to assess the anti-metastatic effects of baicalein and related mechanism(s) on HCC. Based on assays utilized in both HCC cell lines and in an animal model, we found that baicalein **inhibited tumor** cell metastasis in vivo and in vitro. Furthermore, after treatment with baicalein for 24 h, there was a...

2. **Celastrol targets mitochondrial respiratory chain complex I to induce reactive oxygen species-dependent cytotoxicity in tumor cells**

Quick View Other Sources

By Chen, Guozhu; Zhang, Xuhui; Zhao, Ming; Wang, Yan; Cheng, Xiang; Wang, Di; Xu, Yuanji; Du, Zhiyan; Yu, Xiaodan
From BMC Cancer (2011), 11, 170. | Language: English, Database: CAPLUS

Background: Celastrol is an active ingredient of the traditional **Chinese medicinal** plant Tripterygium Wilfordii, which exhibits significant antitumor activity in different **cancer** models in vitro and in vivo; however, the lack of information on the target and mechanism of action of this compd. have impeded its clin. application. In this study, we sought to det. the mode of action of celastrol by focusing on the processes that mediate its anticancer activity. Methods: The downregulation of heat shock protein 90 (HSP90) client proteins, phosphorylation of c-Jun NH2-terminal kinase (JNK), and cl...

3. **Isofraxidin, a coumarin component from Acanthopanax senticosus, inhibits matrix metalloproteinase-7 expression and cell invasion of human hepatoma cells**

Quick View Other Sources

By Yamazaki, Taisuke; Tokiwa, Takayoshi
From Biological & Pharmaceutical Bulletin (2010), 33(10), 1716-1722. | Language: English, Database: CAPLUS

7-Hydroxy-6,8-dimethoxy-2H-1-benzopyran-2-one (Isofraxidin) is a major coumarin component isolated from the stem bark of Acanthopanax senticosus, a widely used **Chinese medicinal** herb. We investigated isofraxidin in its anti-tumor effects on human **hepatoma** cell lines HuH-7 and HepG2. Isofraxidin significantly **inhibited hepatoma** cell invasion, without affecting cell attachment or growth. Expression of 12-O-tetradecanoylphorbol-13-acetate (TPA)-induced matrix metalloproteinase-7 (**MMP-7**) in **hepatoma** cells was **inhibited** by isofraxidin at the both mRNA and protein levels. This **inhibition** tended ...

4. **Shikonin inhibits thyroid cancer cell growth and invasiveness through targeting major signaling pathways**

Quick View Other Sources

By Yang, Qi; Ji, Meiju; Guan, Haixia; Shi, Bingyin; Hou, Peng
From Journal of Clinical Endocrinology and Metabolism (2013), 98(12), E1909-E1917. | Language: English, Database: CAPLUS

Context: Shikonin, which is an active naphthoquinone isolated from traditional **Chinese** herbal **medicine** Zi Cao, has been recently developed to use as an antitumor agent in colorectal **cancer**, melanoma, leukemia, breast **cancer**, and **hepatocellular cancer**. However, its antitumor effect in thyroid **cancer** remains largely unknown. Objectives: The aim of the study

Refine: 帮助用户迅速获得需要的文献

文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Medicine (16)
Biology	Substances in medicine (16)
Genetics & protein chemistry	Substances in adverse effects (2)
Biotechnology	Toxicology & forensics (2)
General chemistry	Agriculture (1)
Physical chemistry	
Polymer chemistry	
Synthetic chemistry	
Analytical chemistry	
Technology	

2. Select index terms of interest.

Index Terms	
Select All	Deselect All
<input type="checkbox"/> 1,4-Naphthalenedione	1
<input type="checkbox"/> Ardipusilloside I	1
<input checked="" type="checkbox"/> Baicalein	1
<input checked="" type="checkbox"/> Berberin	1
<input type="checkbox"/> Capecitabine	1
<input type="checkbox"/> Celastrol	1
<input type="checkbox"/> Cystathionine β -synthase	1
<input type="checkbox"/> Doxorubicin	1
<input type="checkbox"/> Flavonoids	1
<input type="checkbox"/> Isofraxidin	1
<input type="checkbox"/> Kang-Lai-Te	1
<input type="checkbox"/> Matrine	1
<input type="checkbox"/> Mitogen-activated protein kinase p38	1
<input type="checkbox"/> Osthole	1
<input type="checkbox"/> Saponins	1
<input type="checkbox"/> Shikonin	1

Selected Terms

Click 'x' to remove the category from 'Selected Terms'

- Biotechnology > Medicine (2 Terms)
- Biotechnology > Substances in medicine (2 Terms)

黄芩素
黄连素

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

OK Cancel

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

结果集的保存— Save, Print, Export

Searches ▾ SciPlanner Save Print Export

ably removed.

ver Cancer" > references (1197) > refine "chinese medicine" (24) > refine by categories

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0 of 2 References Selected

1. Baicalein inhibits the invasion and metastatic capabilities of hepatocellular carcinoma cells via down-regulation of the ERK pathway

Quick View Other Sources

By Chen, Kunlun; Zhang, Shu; Ji, Yuanyuan; Li, Jun; An, Peng; Ren, Hongtao; Liang, Rongrui; Yang, Jun; Li, Xiangfang

From PLoS One (2013), 8(9), e72927. | Language: English, Database: CAPLUS

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文献详细信息

2. Berberine inhibits invasion and metastasis of colorectal cancer cells via COX-2/PGE2 mediated JAK2/STAT3 signaling pathway

Quick View Other Sources

By Liu, Xuan; Ji, Qing; Ye, Najing; Sui, Hua; Zhou, Lihong; Zhu, Huirong; Fan, Zhongze; Cai, Jianfeng; Li, Qi

From PLoS One (2015), 10(5), e0123478/1-e0123478/18. | Language: English, Database: CAPLUS

Berberin, extd. from Chinese herbal medicine Coptis chinensis, has been found to have anti-tumor activities. However, the underlying mechanisms have not been fully elucidated. Our current study demonstrated that berberine inhibited the in vitro and in vivo growth, migration/invasion of CRC cells, via attenuating the expression levels of COX-2/PGE2, following by reducing the phosphorylation of JAK2 and STAT3, as well as the MMP-2/-9 expression. We further clarified that an increase of COX-2/PGE2 expression offset the repressive activity of Berberin on JAK2/STAT3 signaling, and a JAK2 inhibit...

Save: 保存在服务器上, 方便以后登陆查看, 每次可存2万条记录。

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For:

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Reference_06_19_2012_100848

Format:

Summary without abstracts

Summary with partial abstracts

Summary with full abstracts

Detail (full record)

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Task History

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文献信息—题录、摘要、索引

REFERENCE DETAIL

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获得相关文献

Previous Next

1. Baicalein inhibits the invasion and metastatic capabilities of hepatocellular carcinoma cells via down-regulation of the ERK pathway

By: Chen, Kunlun; Zhang, Shu; Ji, Yuanyuan; Li, Jun; An, Peng; Ren, Hongtao; Liang, Rongrui; Yang, Jun; Li, Zongfang

Baicalein, a widely used Chinese herbal medicine, has historically been used in anti-inflammatory and anti-cancer therapies. However, the anti-metastatic effect and mol. mechanism(s) of baicalein on hepatocellular carcinoma (HCC) remain poorly understood. Therefore, the purpose of this study was to assess the anti-metastatic effects of baicalein and related mechanism(s) on HCC. Based on assays utilized in both HCC cell lines and in an animal model, we found that baicalein inhibited tumor cell metastasis in vivo and in vitro. Furthermore, after treatment with baicalein for 24 h, there was a decrease in the levels of matrix metalloproteinase-2 (MMP-2), MMP-9 and urokinase-type plasminogen activator (u-PA) expression as well as proteinase activity in hepatocellular carcinoma MHCC97H cells. Meanwhile, the expression of tissue inhibitor of metalloproteinase-1 (TIMP-1) and TIMP-2 were increased in a dose-dependent fashion. Moreover, baicalein treatment dramatically decreased the levels of the phosphorylated forms of MEK1 and ERK1/2. MEK1 overexpression partially blocked the anti-metastatic effects of baicalein. Combined treatment with an ERK inhibitor (U0126) and baicalein resulted in a synergistic redn. in MMP-2, MMP-9 and u-PA expression and an increase in TIMP-1 and TIMP-2 expression; the invasive capabilities of MHCC97H cells were also inhibited. In conclusion, baicalein inhibits tumor cell invasion and metastasis by reducing cell motility and migration via the suppression of the ERK pathway, suggesting that baicalein is a potential therapeutic agent for HCC.

Indexing

Pharmacology

重要概念

Concepts

Antitumor agents
Cell migration
Hepatocellular carcinoma
Human
Phosphorylation
Scutellaria baicalensis
Cell infiltration
Cell proliferation
Homo sapiens
Pharmaceutical natural products
Root
Signal transduction

baicalein inhibits the invasion and metastatic capabilities of hepatocellular carcinoma cells via

文献详情界面包括:

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质, 反应
7. 参考文献
8. 链接原文

重要物质

Substances

9039-53-6 Urokinase-type plasminogen activator
124861-55-8 TIMP2
137632-07-6 Extracellular signal-regulated kinase 1
137632-08-7 Extracellular signal-regulated kinase 2
140208-24-8 Tissue inhibitor of metalloproteinase-1
146480-35-5 Matrix metalloproteinase-2
146480-36-6 Matrix metalloproteinase-9
1818417-67-2 MEK1

baicalein inhibits the invasion and metastatic capabilities of hepatocellular carcinoma cells via down-regulation of the extracellular signal-regulated kinase pathway

Biological study, unclassified; Biological study

491-67-8 Baicalein

QUICK LINKS

0 Tags, 0 Comments

SOURCE

PLoS One
Volume8
Issue9
Page9272927
Journal; Online Computer File
2013
CODEN:POLNCL
ISSN:1932-6203
DOI:10.1371/journal.pone.0072927

COMPANY/ORGANIZATION

General Surgeon Department of Cadre's Ward, The Second Affiliated Hospital, School of Medicine
Xi'an Jiaotong University
Xi'an, Peop. Rep. China

ACCESSION NUMBER

2013:1468635
CAN160:113210
CAPLUS

PUBLISHER

Public Library of Science

LANGUAGE



文献检索小结

- 主题检索时，使用介词 **in, with, of** 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的**Analyze/Refine**功能来缩小检索的范围
- 尝试将不同的**Analyze/Refine**功能组合起来用，会有更多的收益
- 使用**Categorize**可以让系统来实现自动分类



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder检索选项——物质检索

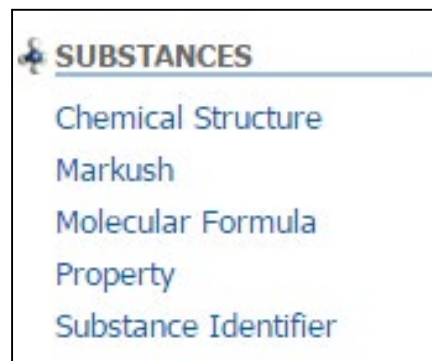
■ 物质检索方法

—结构式检索

—分子式检索

—理化性质检索

—物质标识符检索：化学名称，CAS RN



■ 物质检索策略推荐

—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

物质检索——标识符检索

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Research Topic "MMP Inhibitor in Liver Cancer" > references (1197) > refine "chinese medicine" (24) > refine by categories >

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier**

SUBSTANCES: SUBSTANCE IDENTIFIER ?

berberin

Enter one per line.
Examples:
50-00-0
999815
Acetaminophen

Search

提示:

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 2086-83-1

~8533 ~61

C₂₀H₁₈NO₄
Benzo[*g*]-1,3-benzodioxolo[5,6-*a*]quinolinizinium,
5,6-dihydro-9,10-dimethoxy-

▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

» CAS Registry Number: 63968-64-9

- View Substance Detail
- Explore by Structure ▶
- Synthesize this...
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
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- Export as molfile
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SciFinder中的物质记录

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Substance Identifier "berberin " > substances (1) > 2086-83-1

SUBSTANCE DETAIL ?

 Get References  Get Reactions  Get Commercial Sources

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CAS Registry Number 2086-83-1

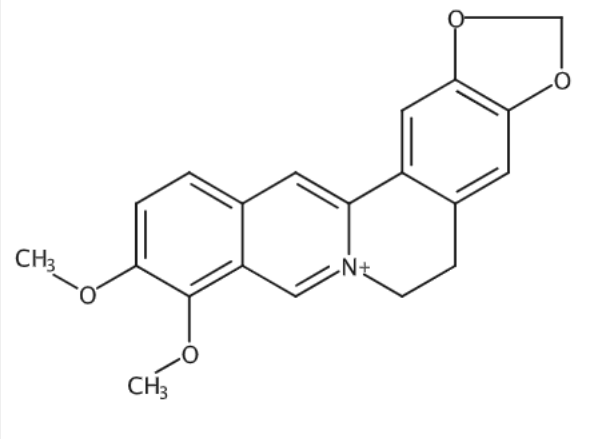
~8,533  ~61 

C₂₀ H₁₈ N O₄
Benzo[*g*]-1,3-benzodioxolo[5,6-*a*]quinolizinium, 5,6-dihydro-9,10-dimethoxy-

Melting Point (Experimental)
Value: 145 °C

Other Names
Berbinium, 7,8,13,13a-tetrahydro-9,10-dimethoxy-2,3-(methylenedioxy)- (8CI)
Umbellatine (6CI)
5,6-Dihydro-9,10-dimethoxybenzo[*g*]-1,3-benzodioxolo[5,6-*a*]quinolizinium
Berbericine
Berberin
[View more...](#)

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物质详情

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All substances
 Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Process
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Prophetic in Patents
<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.

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生物研究

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谱图数据

用途



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A CAS SOLUTION

EXPERIMENTAL PROPERTIES

Biological Chemical Lipinski Optical and Scattering Thermal

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 10	(1)CAS
Half-Life (Biological)	See full text	1 of 5	(9)CAS
LC50	See full text		(13)CAS
Median Lethal Dose(LD50)	50 mg/kg	Organism: mouse Route: intraperitoneal	(16)CAS
Median Lethal Dose(LD50)	15 mg/kg	Organism: mouse Route: intraperitoneal	(16)CAS
Minimum Inhibitory Concentration	See full text	1 of 7	(14)CAS

Notes

- (1) Wang, Xueli; Neuroscience Letters 2005, V379(2), P132-137 CAPLUS [Q](#)
- (9) Ye, Minzhong; Journal of Pharmacy and Pharmacology 2009, V61(7), P831-837 CAPLUS [Q](#)
- (13) Amatya, Sajjan; Zeitschrift fuer Naturforschung, B: Chemical Sciences 2008, V60(9), P1006-1011 CAPLUS [Q](#)
- (14) Zloh, Mire; Theoretical Chemistry Accounts 2007, V117(2), P231-238 CAPLUS [Q](#)
- (16) Anis, K. V.; Pharmacy and Pharmacology Communications 1999, V5(12), P697-700 CAPLUS [Q](#)

实验数据与实验谱图

EXPERIMENTAL SPECTRA

REGULATORY INFORMATION

BIOACTIVITY INDICATORS

TARGET INDICATORS

CAS REFERENCE ROLES

ADDITIONAL DETAILS

利用SciFinder鉴定天然产物的结构

MS谱显示分子离子峰为400

获得分子量在390-410之间的物质

The screenshot displays the SciFinder interface with the following elements:

- Search Criteria:** Sort by: CAS Registry Number. 0 of 5892125 Substances Selected. Page: 1 of 117843.
- Search Results Grid:**
 - 1. 2147485-36-5**: C16H12ClN3O4S2 2-Thiophenecarboxamide, *N*-[4-(4-chloro-3-ethoxyphenyl)-2-thiazolyl]-5-nitro-
[Key Physical Properties](#)
 - 2. 2147485-35-4**: C15H10ClN3O4S2 2-Thiophenecarboxamide, *N*-[4-(4-chloro-3-methoxyphenyl)-2-thiazolyl]-5-nitro-
[Key Physical Properties](#)
 - 3. 2147485-34-3**: C15H9F2N3O4S2 2-Thiophenecarboxamide, *N*-[4-(2,4-difluoro-5-methoxyphenyl)-2-thiazolyl]-5-nitro-
[Key Physical Properties](#)
 - 4. 2147485-30-9**: C15H9F2N3O4S2 2-Thiophenecarboxamide, *N*-[4-(3,4-difluoro-5-methoxyphenyl)-2-thiazolyl]-5-nitro-
[Key Physical Properties](#)
 - 5. 2147485-21-8**: C14H7F3N4O3S2 2-Thiophenecarboxamide, 5-nitro-*N*-[4-[6-(trifluoromethyl)-3-pyridinyl]-2-thiazolyl]-
[Key Physical Properties](#)
 - 6. 2147485-15-0**: C15H11N3O5S3 2-Thiophenecarboxamide, *N*-[4-[4-(methylsulfonyl)phenyl]-2-thiazolyl]-5-nitro-
[Key Physical Properties](#)
 - 7. 2147485-05-8**: C17H25N3O4S2 Hydrazinecarboxylic acid, 2-[(2*R*)-2-(acetylamino)-1-oxo-3-[(phenylmethyl)dithio]propyl]-, 1,1-dimethylethyl ester
[Key Physical Properties](#)
 - 8. 2147484-88-4**: Absolute stereochemistry.
[Key Physical Properties](#)
- Right Panel:** SUBSTANCES: PROPERTY. Experimental. Send to SciPlanner.

利用SciFinder鉴定天然产物结构

利用已知信息和从MS、HNMR、CNMR中获得的碎片信息逐渐缩小范围

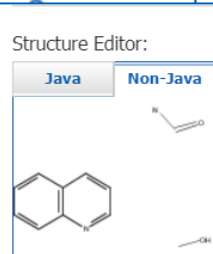
Analyze Refine

Refine by: Analyze Refine

- Chemical
- Isotope
- Metal-Complex
- Comment
- Property
- Reference
- Atom

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Java Non-Java



Click image to change structure or view detail.

Search type: **Substructure**

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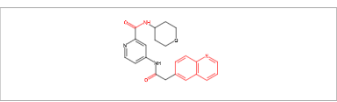
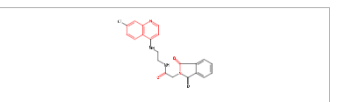
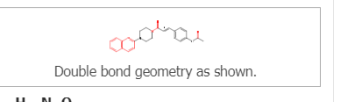
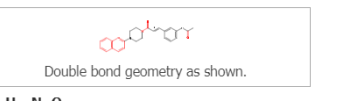
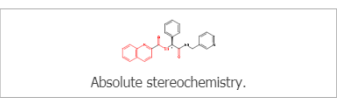
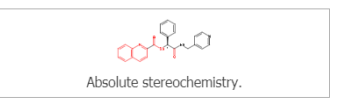
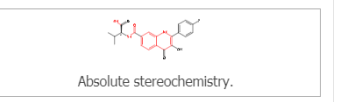
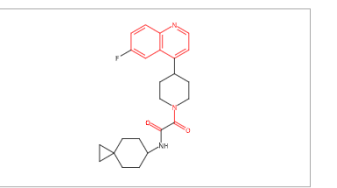
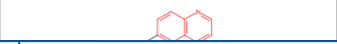



- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
 - Alloys
 - Coordination compounds
 - Incompletely defined
 - Mixtures
 - Polymers
 - Organics, and others not listed
- Are in specific types of studies
 - Analytical
 - Biological
 - Preparation
 - Reactant or reagent

Refine

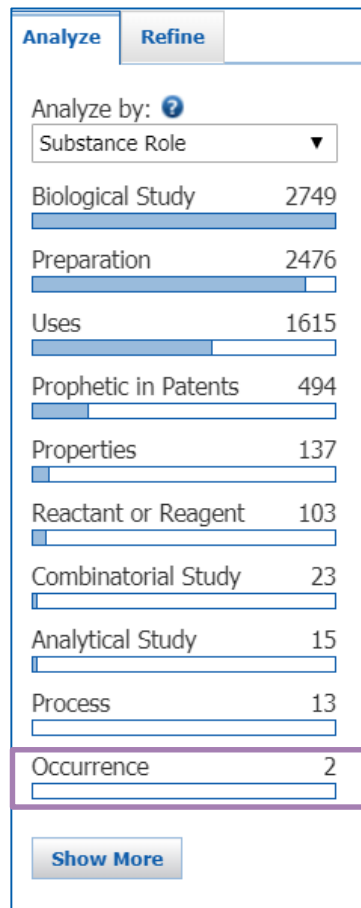
Sort by: CAS Registry Number

0 of 2755 Substances Selected


Page: 1 of 138


<p>1. 2367646-05-5</p>  <p>C₂₂H₂₂N₄O₃ 6-Quinolinesacetamide, <i>N</i>-[2-[[[(tetrahydro-2H-pyran-4-yl)amino]carbonyl]-4-pyridinyl]-</p> <p>▶ Key Physical Properties</p>	<p>2. 2365363-29-5</p>  <p>C₂₁H₁₇ClN₄O₃ 2<i>H</i>-Isoindole-2-acetamide, <i>N</i>-[2-[(7-chloro-4-quinolinyl)amino]ethyl]-1,3-dihydro-1,3-dioxo-</p> <p>▶ Key Physical Properties</p>	<p>3. 2365304-27-2</p>  <p>C₂₄H₂₃N₃O₃ 2-Propen-1-one, 3-[4-(acetyloxy)phenyl]-1-[4-(2-quinolinyl)-1-piperazinyl]-, (2<i>E</i>)-</p> <p>▶ Key Physical Properties</p>	<p>4. 2365304-25-0</p>  <p>C₂₄H₂₃N₃O₃ 2-Propen-1-one, 3-[3-(acetyloxy)phenyl]-1-[4-(2-quinolinyl)-1-piperazinyl]-, (2<i>E</i>)-</p> <p>▶ Key Physical Properties</p>
<p>5. 2360547-65-3</p>  <p>Absolute stereochemistry.</p> <p>C₂₄H₂₀N₄O₂ 2-Quinolinescarboxamide, <i>N</i>-[(1<i>S</i>)-2-oxo-1-phenyl-2-[(3-pyridinylmethyl)amino]ethyl]-</p> <p>▶ Key Physical Properties</p>	<p>6. 2360547-62-0</p>  <p>Absolute stereochemistry.</p> <p>C₂₄H₂₀N₄O₂ 2-Quinolinescarboxamide, <i>N</i>-[(1<i>S</i>)-2-oxo-1-phenyl-2-[(4-pyridinylmethyl)amino]ethyl]-</p> <p>▶ Key Physical Properties</p>	<p>7. 2351924-87-1</p>  <p>Absolute stereochemistry.</p> <p>C₂₁H₁₉FN₃O₃ L-Valine, <i>N</i>-[[2-(4-fluorophenyl)-1,4-dihydro-3-hydroxy-4-oxo-7-quinolinyl]carbonyl]-</p> <p>▶ Key Physical Properties</p>	<p>8. 2351199-95-4</p>  <p>C₂₄H₂₈FN₃O₂ INDEX NAME NOT YET ASSIGNED</p> <p>▶ Key Physical Properties</p>
<p>9. 2351199-90-9</p> 	<p>10. 2351199-71-6</p> 	<p>11. 2351199-42-1</p> 	<p>12. 2351199-38-5</p> 

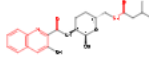
利用SciFinder鉴定天然产物结构



0 of 2755 Substances Selected

639. 1985663-76-0 


~1 




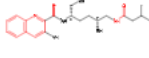
Rotation (-), Absolute stereochemistry unknown., Currently available stereo shown.

$C_{21}H_{27}N_3O_5$
INDEX NAME NOT YET ASSIGNED

▶ Key Physical Properties

640. 1985663-75-9 

~1 



Rotation (+), Absolute stereochemistry unknown., Currently available stereo shown.

$C_{21}H_{29}N_3O_5$
INDEX NAME NOT YET ASSIGNED

▶ Key Physical Properties

从Analyze的Substance Role判断
是否有来源于天然产物的物质

利用SciFinder鉴定天然产物结构

639. CAS Registry Number 1985663-76-0

~1

C₂₁ H₂₇ N₃ O₅

INDEX NAME NOT YET ASSIGNED

Molecular Weight

401.46

Boiling Point (Predicted)

Value: 725.1±60.0 °C | Condition: Press: 760 Torr

Density (Predicted)

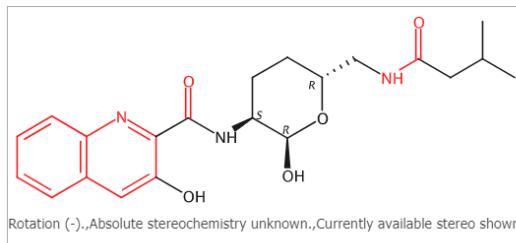
Value: 1.31±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

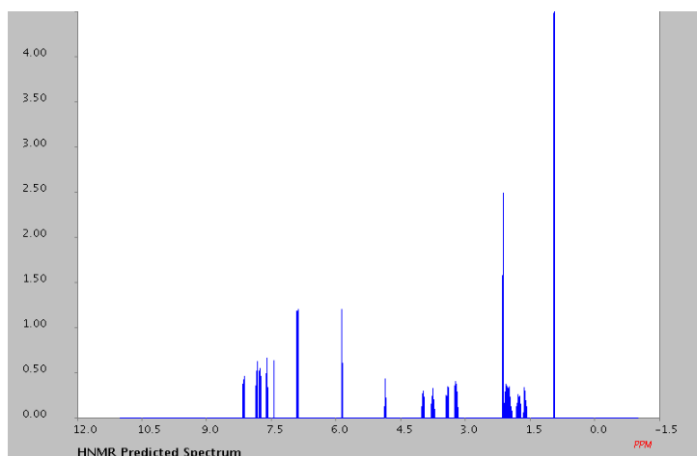
Value: 7.27±0.40 | Condition: Most Acidic Temp: 25 °C

Other Names

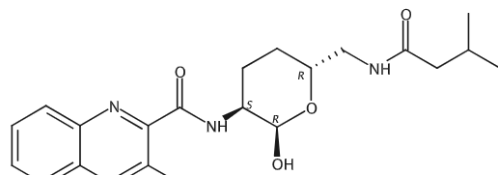
Actinoquinoline B



Proton NMR Spectrum



[View High Resolution Image](#) (Opens in a new window)



CAS REGISTRY NUMBER

1985663-76-0

FORMULA

C₂₁ H₂₇ N₃ O₅

CAS INDEX NAME

INDEX NAME NOT YET ASSIGNED

Note

(2)

WORKING FREQUENCY

400 MHz

STANDARD

tetramethylsilane (75-76-3)

NUCLEUS

¹H

TEMPERATURE

25 °C

SOURCE

Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2019 ACD/Labs)

尽量寻找实验谱图进行比对，若无，可用预测谱图



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A CAS SOLUTION

物质检索——结构

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure**
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or re

Import CXF

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[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface also features a command line at the bottom with the text 'C H O S N P Cl Br F I Si' and a 'Scale 100' indicator. The labels point to the following features:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 碳链工具 (Carbon Chain Tool)
- 选择工具 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C Atom and Single Bond Restoration Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Lasso Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 负电子 (Negatron)
- 常见环, 多元环工具 (Common Ring, Polycyclic Ring Tool)

物质检索——精确结构检索

The screenshot displays the Structure Editor interface. At the top, a toolbar contains various icons, with a callout box pointing to the 'I' icon (representing CAS RN input) and containing the text: "通过CAS RN转换结构: CAS RN: 50-36-2". The main workspace shows a chemical structure of a complex molecule, specifically a bicyclic amine derivative with a benzoyl group and a methoxy group. On the right side, the 'Drawing Editor' panel is visible, with 'Structure' selected. Below it, the search options are listed: 'Exact search' (selected), 'Substructure search', and 'Similarity search'. A callout box highlights the 'Exact search' option with the text: "精确结构检索". At the bottom of the interface, the molecular formula $C_{17}H_{21}NO_4$ and the molecular weight 303.36 are displayed.

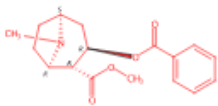
精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**



Absolute stereochemistry.

C₁₇H₂₁N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

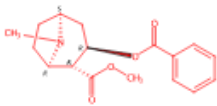
▶ Key Physical Properties
Spectra

可卡因

2. **114599-38-1**

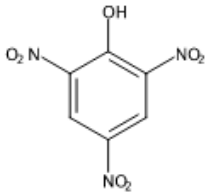
可卡因组合物

668-19-9
C₁₇H₂₁N O₄



Absolute stereochemistry.

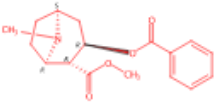
88-89-1
C₆H₃N₃O₇



C₁₇H₂₁N O₄ · C₆H₃N₃O₇
Alcocaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)



* HCl

Absolute stereochemistry.

C₁₇H₂₁N O₄ · Cl H
Alcocaine, hydrochloride (6CI)

盐酸可卡因

物质检索——精确结构检索

精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

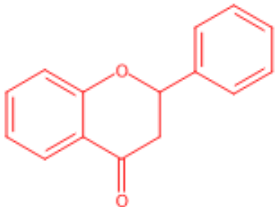
The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a phenyl group. The interface includes a toolbar on the left with various drawing tools, a top toolbar with standard editing functions, and a right-hand panel with search options. The search options are: 'Exact search', 'Substructure search' (which is selected and highlighted with a purple box), and 'Similarity search'. Below the search options are 'OK' and 'Cancel' buttons. At the bottom of the window, the molecular formula $C_{15}H_{12}O_2$ and the molecular weight 224.26 are displayed.

物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

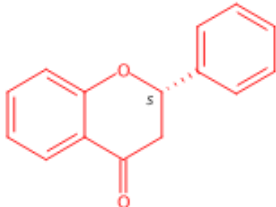


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



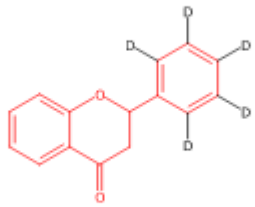
Absolute stereochemistry: Rotation (-).

$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5



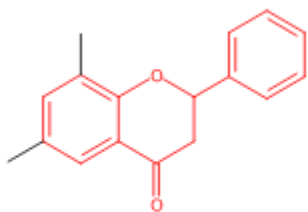
$C_{15}H_7D_5O_2$
4-(2,3,4,5-tetradeuteriophenyl)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl-*d*)- (9CI)

Spectra

同位素

亚结构检索结果

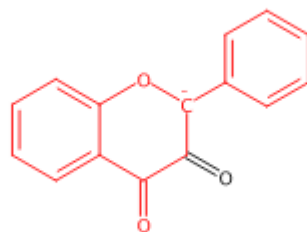
取代物



$C_{17}H_{16}O_2$
4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

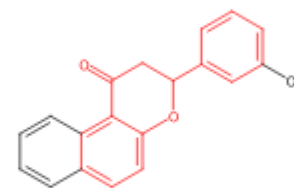
▶ Key Physical Properties
Experimental Properties

离子



$C_{15}H_9O_3$
2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

稠环物质



$C_{19}H_{14}O_3$
1H-Naphtho[2,1-b]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

▶ Key Physical Properties

亚结构检索结果的限定

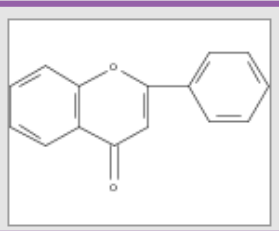
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

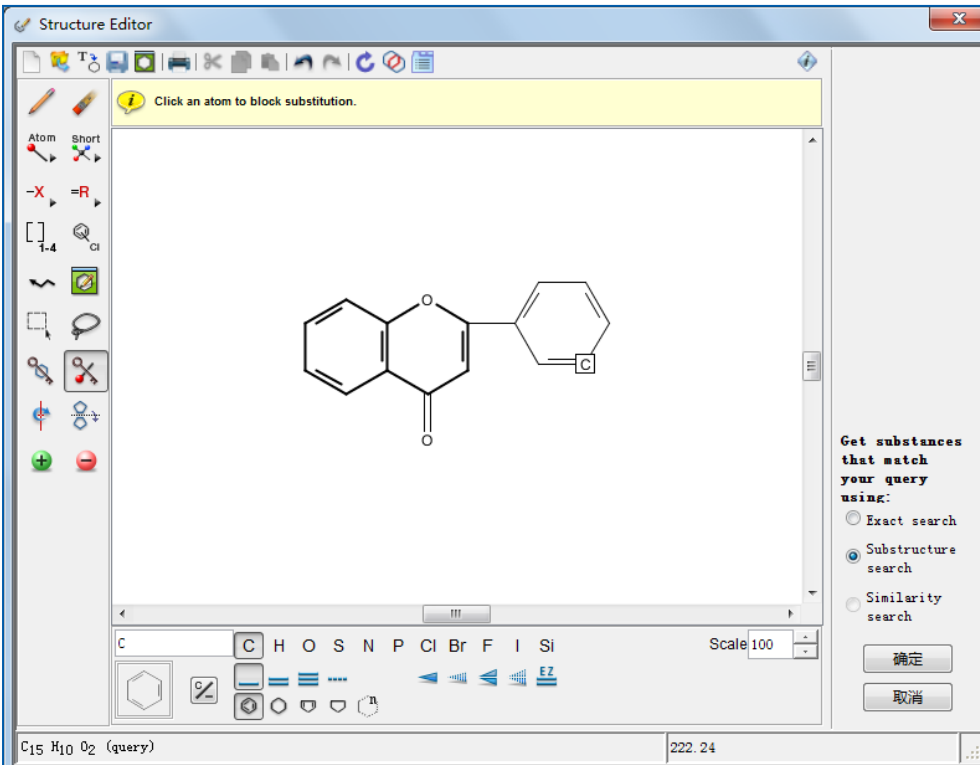


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C₁₅ H₁₀ O₂ (query) 222.24



环锁定

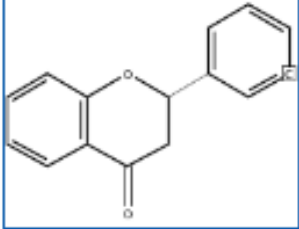


原子锁定

亚结构检索结果的限定

Structure Editor:

Java Non-Java



Click image to change structure or view detail.
Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

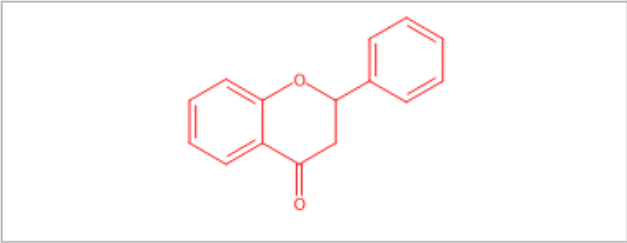
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

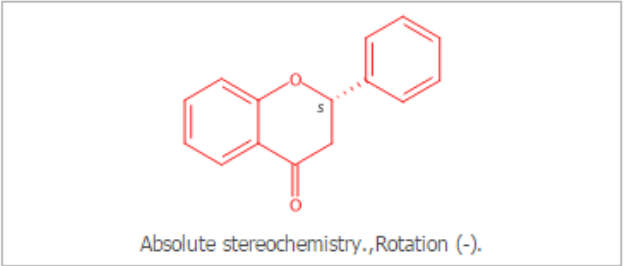
1. 487-26-3
~2093



$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2
~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

Key Physical Properties
Experimental Properties

4. 104550-32-5
~3

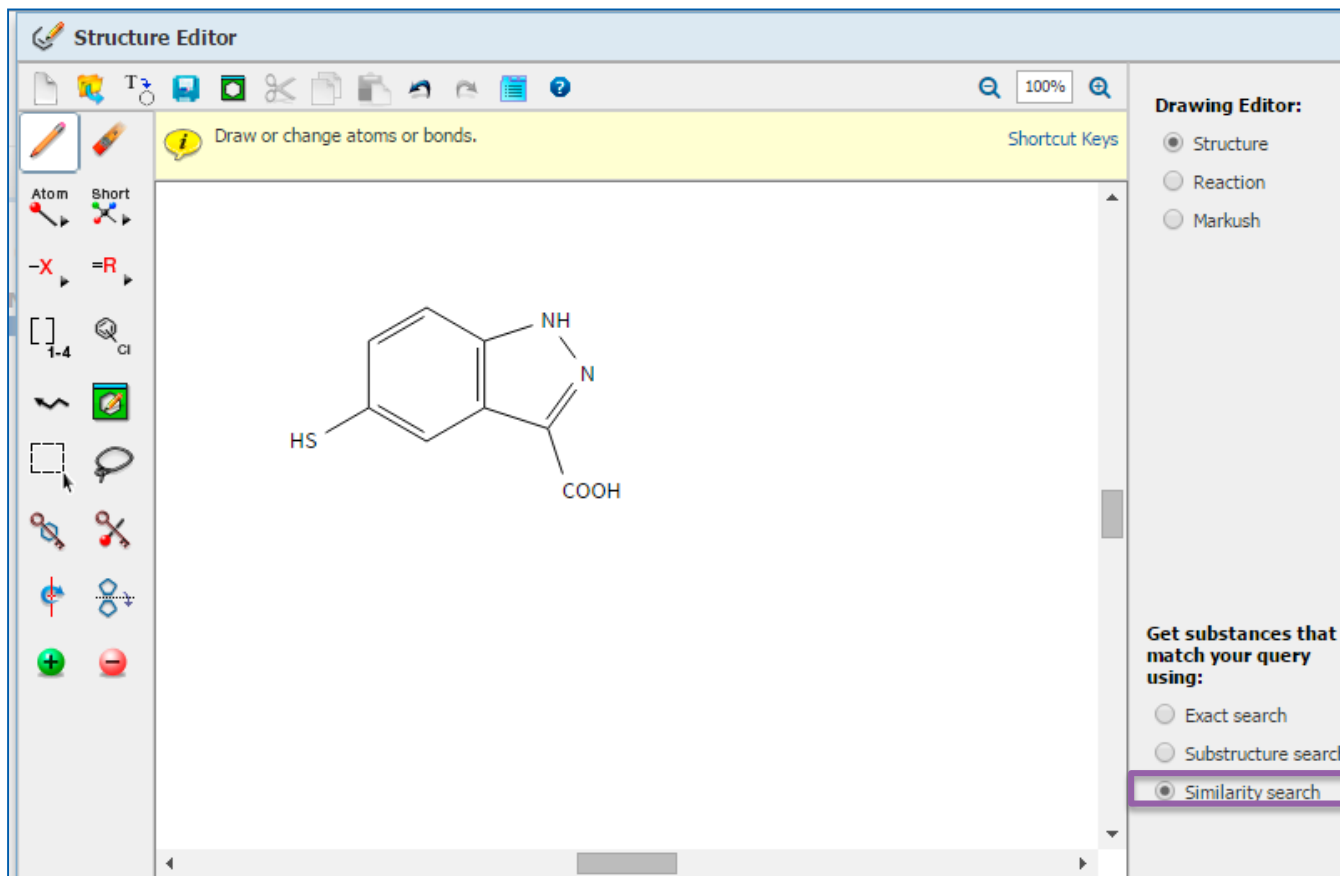
5. 75524-43-5
~2

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

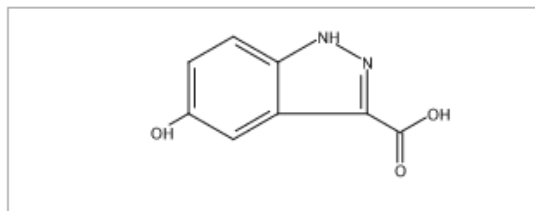
相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

1H-Indazole-3-carboxylic acid, 5-hydroxy-

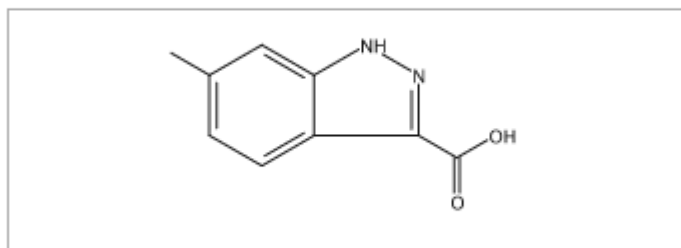
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

1H-Indazole-3-carboxylic acid, 6-methyl-

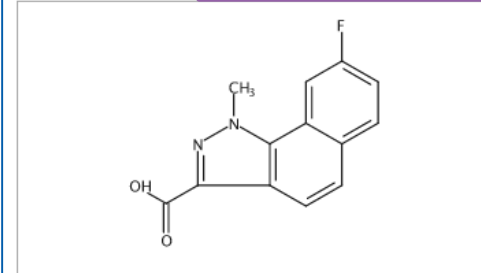
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[σ]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties



SCIFINDER®
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

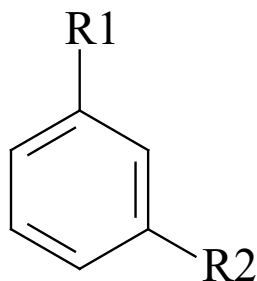
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
 - 案例分析
- SciFinder常见问题及解决

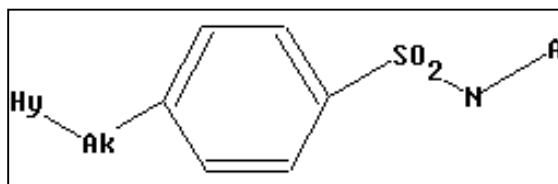
Markush检索

- 具体物质[Specific Substance]:
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance]:
 - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质，不会被分配CAS RN
 - 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—halogen,
|
CH₃



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

Structure Editor interface showing the chemical structure and the Markush search options.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:


- Structure
- Reaction
- Markush

Get Markush patents where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK
Cancel

Markush检索



WELCOME Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Markush substructure > references (1969) > Compounds and methods for anti...

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

Analyze | Refine | Categorize | Sort by: Accession Number | Display Options

0 of 1969 References Selected

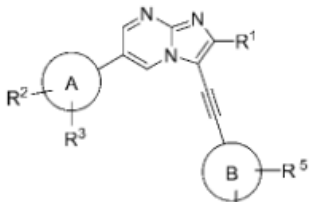
Analyze by: Document Type

Patent	1969
Journal	1

Show More

1. **Compounds and methods for anticoagulation therapy**
PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS
The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**
PATENTPAK
By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

全部是专利

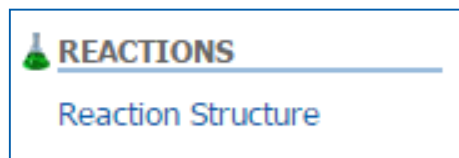
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

结构式



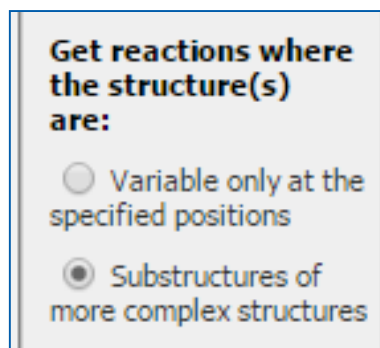
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

The screenshot shows the 'Structure Editor' window. The top toolbar includes icons for file operations and a search bar. Below the toolbar is a yellow instruction bar: 'Draw or change atoms or bonds.' To the right of the main workspace is a 'Drawing Editor' panel with radio buttons for 'Structure', 'Reaction' (selected), and 'Markush'. Below that is a section for finding reactions based on structure(s). The main workspace contains a chemical structure of a benzene ring. The bottom toolbar has a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si) and various bond types. A status bar at the bottom shows 'CH₄' and '16.04'.

Annotations in Chinese:

- 反应箭头 (Reaction Arrow)
- 反应原子标记工具 (Reaction Atom Marking Tool)
- 官能团列表 (Functional Group List)
- 反应角色工具 (Reaction Role Tool)
- 反应位置标记工具 (Reaction Position Marking Tool)

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with a nitro group (NO_2) at the bottom position, and the product is a benzene ring with an amino group (NH_2) at the bottom position. An arrow points from the reactant to the product.

The interface includes a drawing toolbar on the left with various tools for creating and editing structures. A yellow banner at the top of the workspace reads "Draw or change atoms or bonds." The right side of the interface features a "Drawing Editor" panel with three radio buttons: "Structure", "Reaction" (which is selected), and "Markush". Below this, a section titled "Get reactions where the structure(s) are:" contains two radio buttons: "Variable only at the specified positions" (which is highlighted by a purple callout box) and "Substructures of more complex structures". At the bottom of the panel are "OK" and "Cancel" buttons.

At the bottom of the editor, there is a search bar containing "NH2" and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si. The status bar at the very bottom shows the molecular formula $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_7\text{N}$ and the coordinates 137.14 . 107.16.

精确反应检索

反应检索结果

浏览记录，发现很多反应来自同一篇文章，
通过Group by Document合并。

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

Cc1ccc([N+](=O)[O-])cc1 → Cc1ccc(N)cc1

~102 100%
~122

Overview
Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制:

Broad: 仅反应中心相似

Medium: 反应中心及附属原子和键

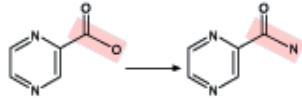
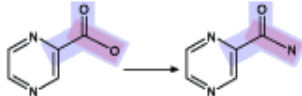
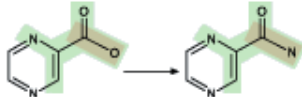
Narrow: 反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (2934)

- Medium - Reaction centers plus adjacent atoms and bonds (109)

- Narrow - Reaction centers plus extended atoms and bonds (95)


按照反应类型排序

Group by: Transformation ▼ Sort by: Frequency ▼ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS

Get References Tools

Analyze Refine

Analyze by: Reagent

H ₂	148
NaBH ₄	51
N ₂ H ₄ -H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ •HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~102 ~122

100%

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

Experimental Procedure



General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

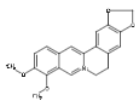
不用阅读全文，直接获得包含实验过程的反应记录

天然产物的结构修饰反应

寻找对黄连素 (berberin) 进行结构修饰的反应

1. 2086-83-1

~8533   ~61 



$C_{20}H_{18}NO_4$
Benzo[*g*]-1,3-benzodioxolo[5,6-*a*]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-

Key Physical Properties

Regulatory Information
Spectra
Experimental Properties

CAS Registry Number: 2086-83-1

View Substance Detail

Explore by Structure

Chemical Structure

Synthesize this...

Markush Patents by Structure

Get Reactions where Substance is a

Reactions

Get Commercial Sources

Get Regulatory Information

Get References

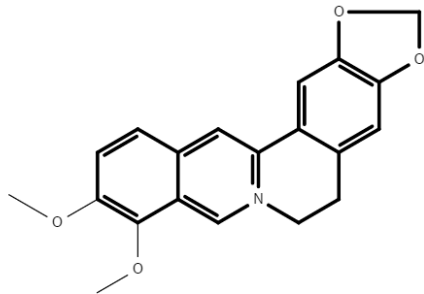
Export as Image

Export as molfile

Send to SciPlanner

Structure Editor

Click an object to delete. Click and drag to delete multiple objects.



Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

ACS / Propriet

$C_{20}H_{18}NO_4$ 336.37

天然产物的结构修饰反应

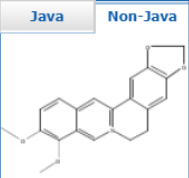
Analyze **Refine**

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java **Non-Java**



Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

Refine

Analyze **Refine**

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure substructure > substances (3011) > refine "exclude isotope-containing" (2983) > refine "substructure" (1281)

SUBSTANCES **Analyze** **Refine**

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 1281 Substances Selected

1. 2086-83-1	2. 1586251-17-3	3. 1465825-15-3	4. 2260637-67-8
~8533	~1	~2	~1
C₂₀H₁₈N₂O₄ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-	C₂₀H₁₈N₂O₄ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-, radical ion(1+)	C₂₀H₁₈N₂O₅ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-, mnohydroxy deriv.	C₂₀H₁₈N₂O₄ INDEX NAME NOT YET ASSIGNED
Key Physical Properties Regulatory Information Spectra Experimental Properties			
5. 2363120-02-7	6. 26292-84-2	7. 1065849-20-8	8. 1065849-22-0
~1	~15	~1	~1
C₂₀H₁₈N₂O₆ INDEX NAME NOT YET ASSIGNED	C₂₁H₂₀N₂O₄ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 9-ethoxy-5,6-dihydro-10-methoxy-	C₂₁H₂₀N₂O₄ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 10-ethoxy-5,6-dihydro-9-methoxy-	C₂₂H₂₂N₂O₄ Benzo[<i>g</i>]-1,3-benzodioxolo[5,6- <i>a</i>]quinolinizinium, 9,10-diethoxy-5,6-dihydro-
9. 1596803-31-4	10. 1830356-36-9	11. 5058-45-7	12. 38691-92-8
~0	~1	~39	~61

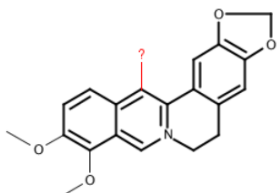
Select Attachments

天然产物的结构修饰反应

Refine by Atom Attachment

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	862
<input type="checkbox"/> C	372
<input type="checkbox"/> O	35
<input type="checkbox"/> Br	6
<input type="checkbox"/> N	4
<input type="checkbox"/> I	1
<input type="checkbox"/> Cl	1
<input type="checkbox"/> A - Any (not H)	419
<input checked="" type="checkbox"/> Ak - Alkyl chain	367
<input type="checkbox"/> Q - Any (not C,H)	47
<input type="checkbox"/> X - Halogen	8

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Sort by: Relevance

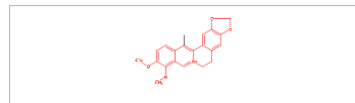
Display Options

0 of 367 Substances Selected

Page: 1 of 19

1. 38691-92-8

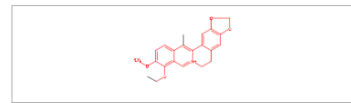
~61



C₂₁H₂₀N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-13-methyl-

2. 357213-72-0

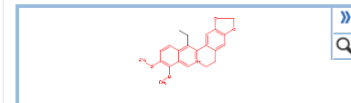
~1



C₂₂H₂₂N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 9-ethoxy-5,6-dihydro-10-methoxy-13-methyl- (9CI)

3. 55582-53-1

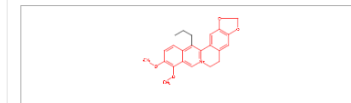
~19



C₂₂H₂₂N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 13-ethyl-5,6-dihydro-9,10-dimethoxy- (9CI)

4. 86545-10-0

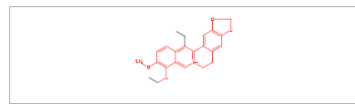
~9



C₂₃H₂₄N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-13-propyl- (9CI)
Spectra

5. 193816-35-2

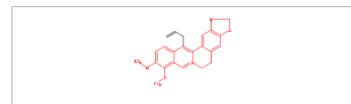
~10



C₂₃H₂₄N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 9-ethoxy-13-ethyl-5,6-dihydro-10-methoxy-

6. 744956-17-0

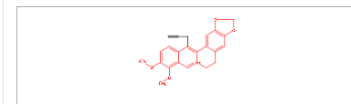
~3



C₂₂H₂₂N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-13-(2-propenyl)- (9CI)

7. 744141-84-2

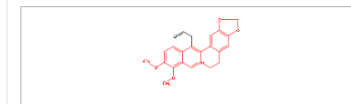
~0



C₂₃H₂₀N₄O₄
Benzo[gh]-1,3-benzodioxolo[5,6-a]quinolinizinium, 5,6-dihydro-9,10-dimethoxy-13-(2-propenyl)- (9CI)

8. 1639859-43-0

~0



C₂₂H₂₀N₄O₅
INDEX NAME NOT YET ASSIGNED

9. 86545-00-7

10. 1024108-35-7

11. 788099-95-6

12. 202193-46-2

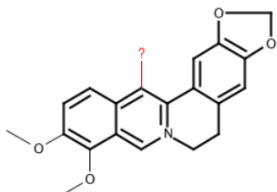


天然产物的结构修饰反应

Refine by Atom Attachment

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	862
<input type="checkbox"/> C	372
<input type="checkbox"/> O	35
<input type="checkbox"/> Br	6
<input type="checkbox"/> N	4
<input type="checkbox"/> I	1
<input type="checkbox"/> Cl	1
<input type="checkbox"/> A - Any (not H)	419
<input checked="" type="checkbox"/> Ak - Alkyl chain	367
<input type="checkbox"/> Q - Any (not C,H)	47
<input type="checkbox"/> X - Halogen	8
<input type="checkbox"/> Gs - Carbons	2

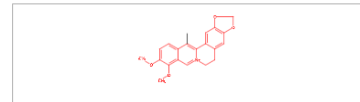
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 367 Substances Selected

1. 38691-92-8

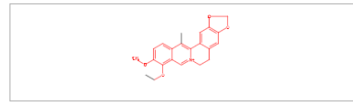
~61



$C_{21}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-methyl-

2. 357213-72-0

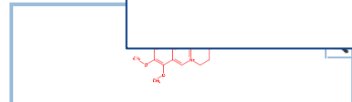
~1



$C_{22}H_{22}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 9-ethoxy-5,6-dihydro-10-methoxy-13-methyl- (9CI)

3. 55582-53

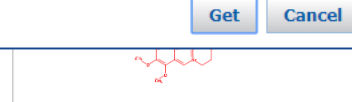
~19



$C_{22}H_{22}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 13-ethyl-5,6-dihydro-9,10-dimethoxy- (9CI)

4. 1639859-43-0

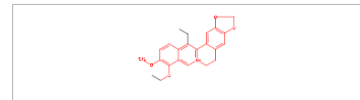
~0



$C_{23}H_{24}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-propyl- (9CI)
Spectra

5. 193816-35-2

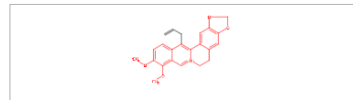
~10



$C_{23}H_{24}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 9-ethoxy-13-ethyl-5,6-dihydro-10-methoxy-

6. 744956-17-0

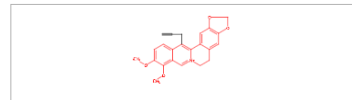
~3



$C_{23}H_{22}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-(2-propenyl)- (9CI)

7. 744141-84-2

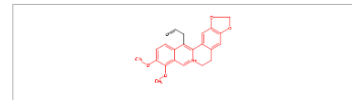
~0



$C_{23}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-(2-propenyl)- (9CI)

8. 1639859-43-0

~0



$C_{22}H_{20}NO_5$
INDEX NAME NOT YET ASSIGNED

9. 86545-00-7

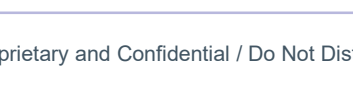
~0



$C_{21}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-methyl- (9CI)

10. 1024108-35-7

~0



$C_{21}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-methyl- (9CI)

11. 788000-05-6

~0



$C_{21}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-methyl- (9CI)

12. 202103-46-2

~0



$C_{21}H_{20}NO_4$
Benzo[g]-1,3-benzodioxolo[5,6-a]quinolinium, 5,6-dihydro-9,10-dimethoxy-13-methyl- (9CI)

Get Reactions

Retrieve reactions for:

- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get

Cancel

天然产物的结构修饰反应

Group by: No Grouping Sort by: Accession Number

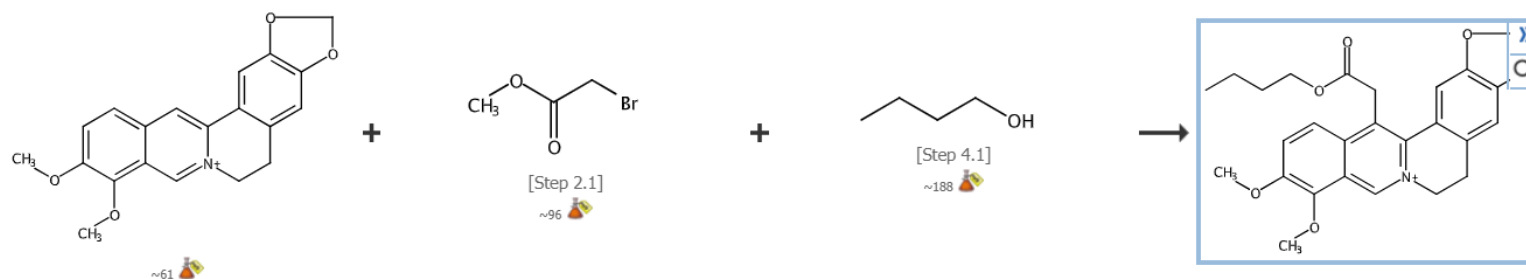
Display Options

0 of 102 Reactions Selected

Page: 1 of 3

1. View Reaction Detail Link

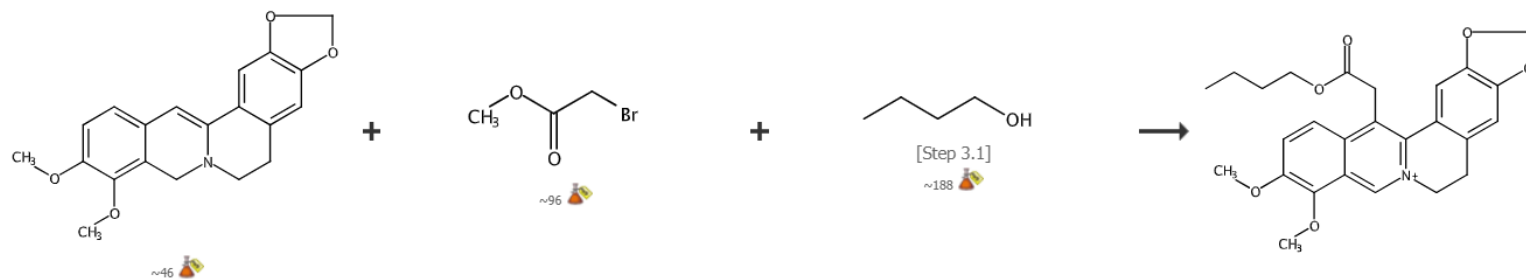
4 Steps Hover over any structure for more options.



Overview

2. View Reaction Detail Link

3 Steps Hover over any structure for more options.



Overview

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
 - 案例分析
- SciFinder常见问题及解决

SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

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

点击Send to SciPlanner

Overview

Steps/Stages

- 1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF
- 2.1 R: NaH, S: THF
- 3.1 R: POCl₃, reflux

Notes

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

References

Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

SciPlanner SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

- New
- Open
- Save
- Duplicate
- Import
- Export
- Print
- Close

Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile

1 2 3

打开中间产物的标准菜单
选择Synthesize this

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

2 Steps Hover over any structure for more options.

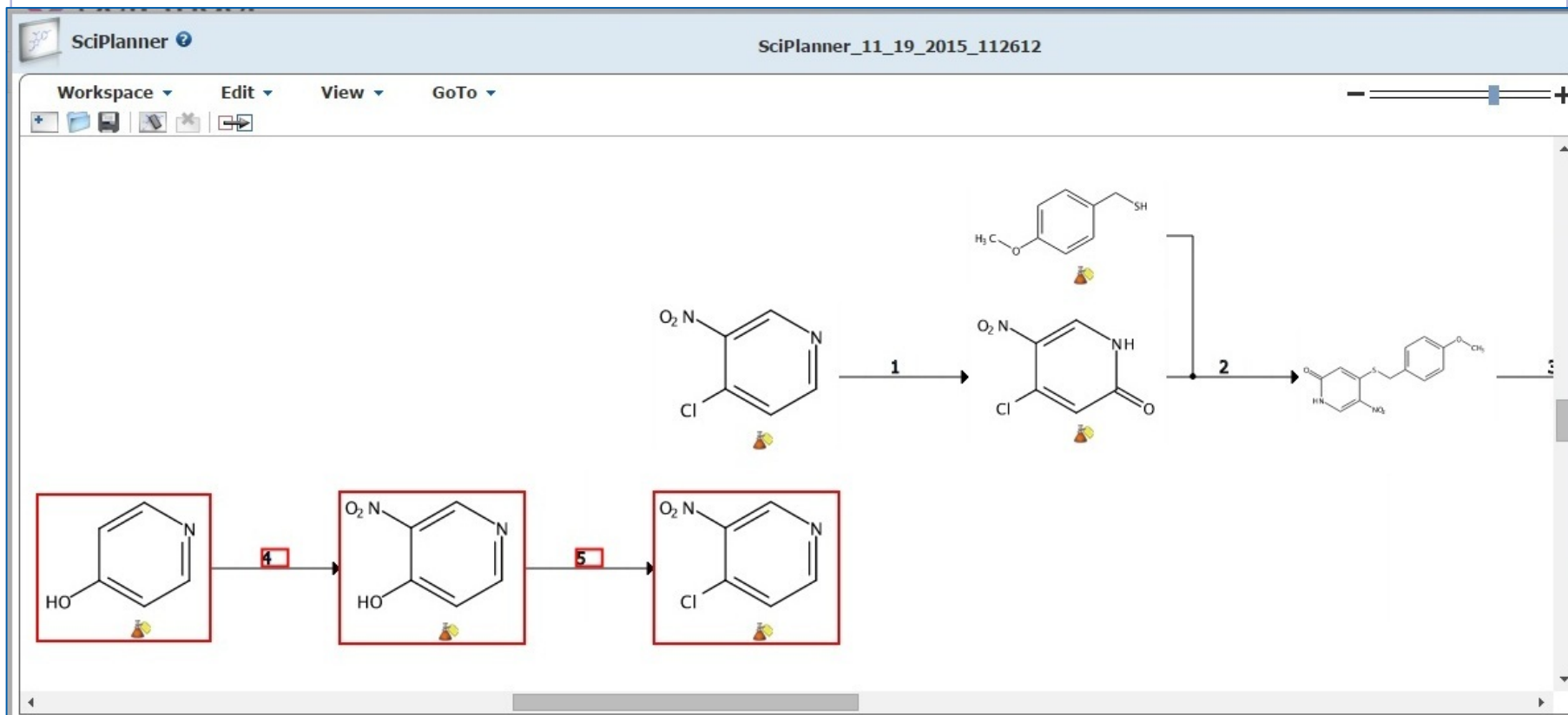
在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

Oc1cccnc1 → O=[N+]([O-])c1ccc(Cl)cn1

~161 ~192

SciPlanner使用简介

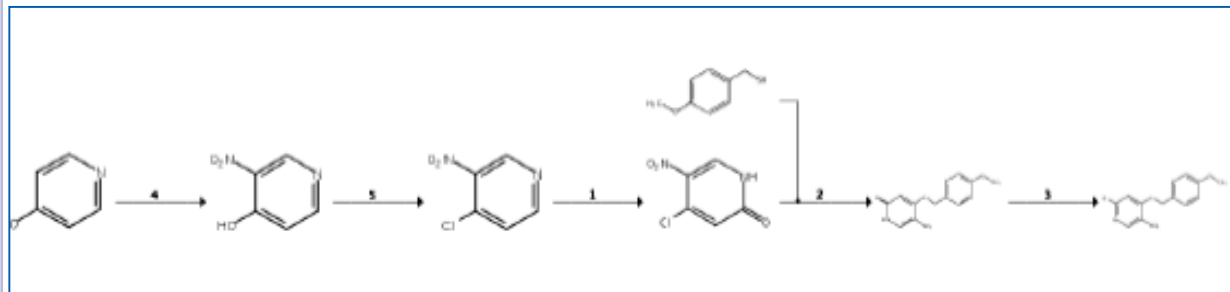


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar are menu options: "Workspace", "Edit", "View", and "GoTo". A "Workspace" dropdown menu is open on the left, listing "New", "Open", "Save", "Duplicate", "Import", "Export", "Print", and "Close". The "Export" option is highlighted in blue. In the center, a chemical reaction sequence is shown: a starting material (a pyridine ring with a nitro group and a hydroxyl group) reacts (step 4) to form a product (a pyridine ring with a nitro group and a chlorine atom). This product then reacts (step 5) to form another product (a pyridine ring with a nitro group and a chlorine atom). Finally, this product reacts (step 1) to form a final product (a pyridine ring with a nitro group and a chlorine atom). A pink callout box points to the "Export" menu item with the text: "点击 Workspace, 选择 Export 导出结果". Another pink callout box points to the second product structure with the text: "用鼠标将两个同样的结构拖至重叠, 两条反应合并". A third pink callout box points to the "Export" dialog box with the text: "选择适当的输出格式, 输出结果". The "Export" dialog box is open on the right, showing options for "For:" (Offline Review: Portable Document Format (*.pdf), Citations (*.ris), Image (*.png)), "Saving Locally" (SciPlanner eXchange (*.pkx)), "Details:" (File Name: SciPlanner_11_19_2015_112612, Title:), and "Include:" (SciPlanner Image, Reaction Details, Substance Details, Reference Details). The "Export" and "Cancel" buttons are at the bottom right of the dialog box.

SciPlanner导出结果



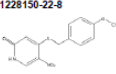
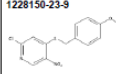
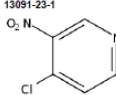
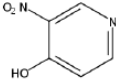
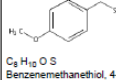
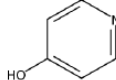
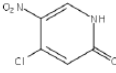
Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information		
<p>1228150-22-8</p>  <p>C₁₃H₁₂N₂O₄S 2-(1H)-Pyridinone, 4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p>  <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p>  <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 301 References Reactions ~ 100 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p>  <p>C₆H₄N₂O₃ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p>  <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p>  <p>C₅H₅N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p>  <p>C₆H₃ClN₂O₃ 2-(1H)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner
- SciFinder常见问题及解决

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号

The screenshot displays the SciFinder registration form, divided into three main sections:

- CONTACT INFORMATION--**: Includes fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (dropdown menu), and Job Title (dropdown menu).
- USERNAME AND PASSWORD--**: Includes fields for Username (with a *Tips* link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a Security Question (dropdown menu) and an Answer field (with a *Why?* link).

At the bottom of the form, there are two buttons: "Register>>" and "Clear All".

请注意：

1. 必须输入**真实姓名**和**学校邮箱**。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

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

例：abc@123

4. 从下拉列表中选择一个密码提示问题并给出答案。
单击 Register (注册) 。

如何获取SciFinder账号

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=B8CB6727-86F3-F014-11E6-D312D80AC094>

This link is valid for only one use and will expire within 48 hours.

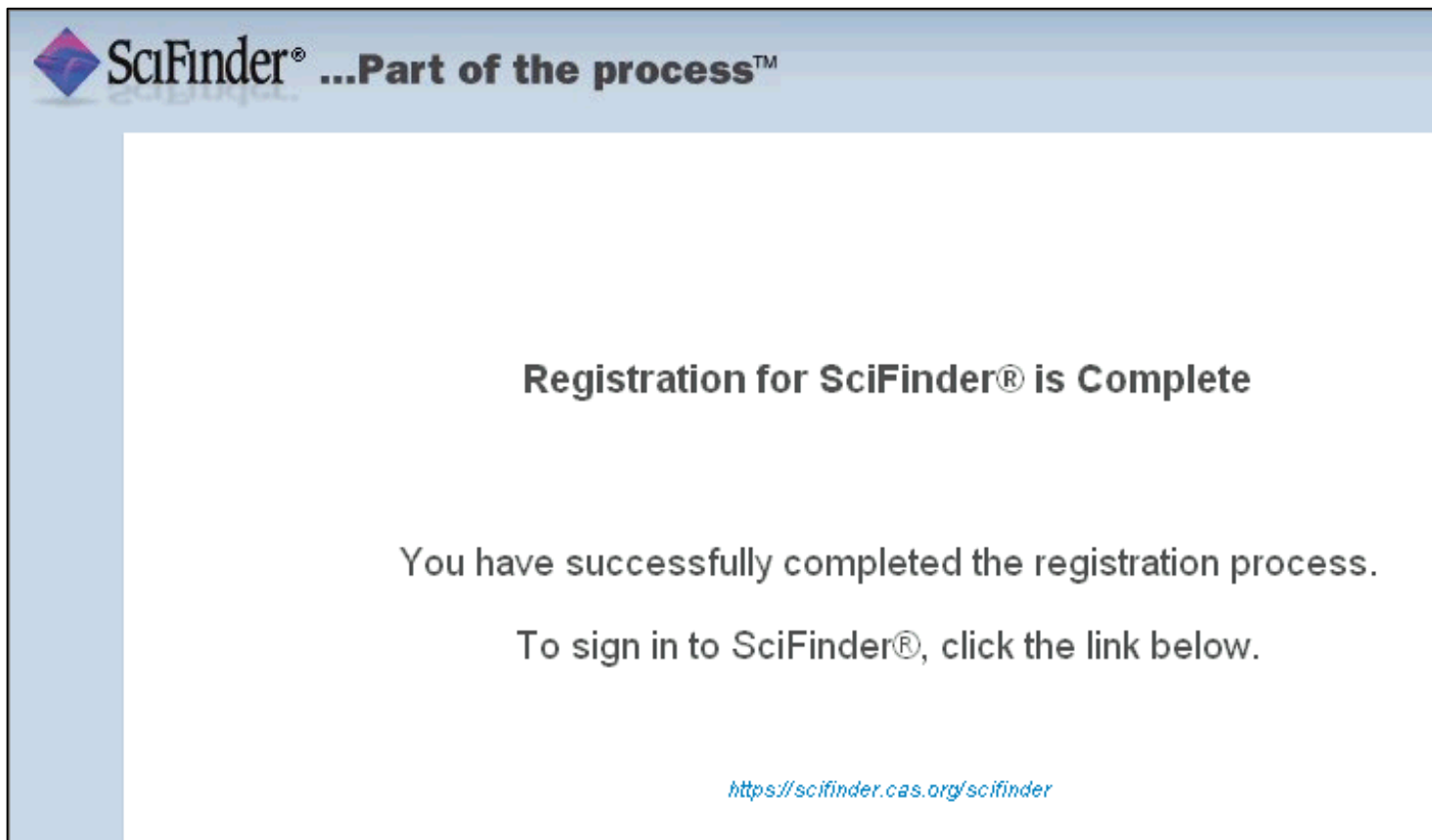
If you need assistance at any time, consult the key contact at your organization.

打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件



如何获取SciFinder账号



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

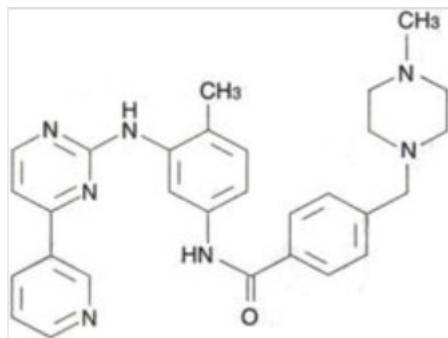
更多培训资料请访问

<http://www.cas-china.org/index.php?c=list&cs=scifinder-train>



上机练习

- 检索“中药在帕金森病（Parkinson's disease）治疗中的应用”的文献。被引次数最高的文献来自哪份期刊？发文最多的研究机构是哪家？该研究领域专利多还是期刊多？
- 找出分析黄芩素（baicalein）的相关文献？用TLC方法做分析的文献？
- 检索格列卫（Gleevec）的合成制备方法



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