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2021.6



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- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果排序、筛选和详情
- 物质相关信息的获取策略
 - 常见的物质检索方法
 - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果排序、筛选和详情



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Revealing unseen relationships that spark ideas and speed
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确定加速增长的趋势和新机遇

CAS具有最全面的学科连接内容合集



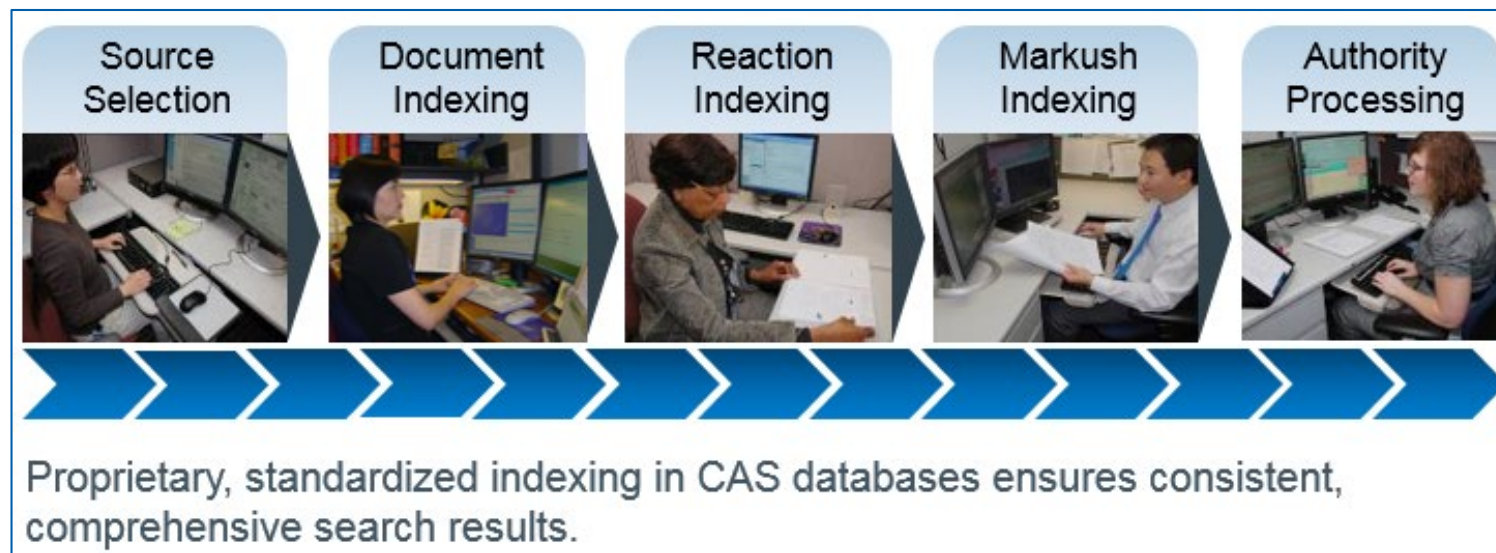
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and documents

Over
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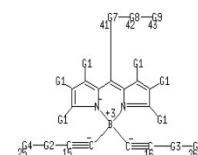
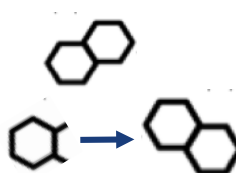
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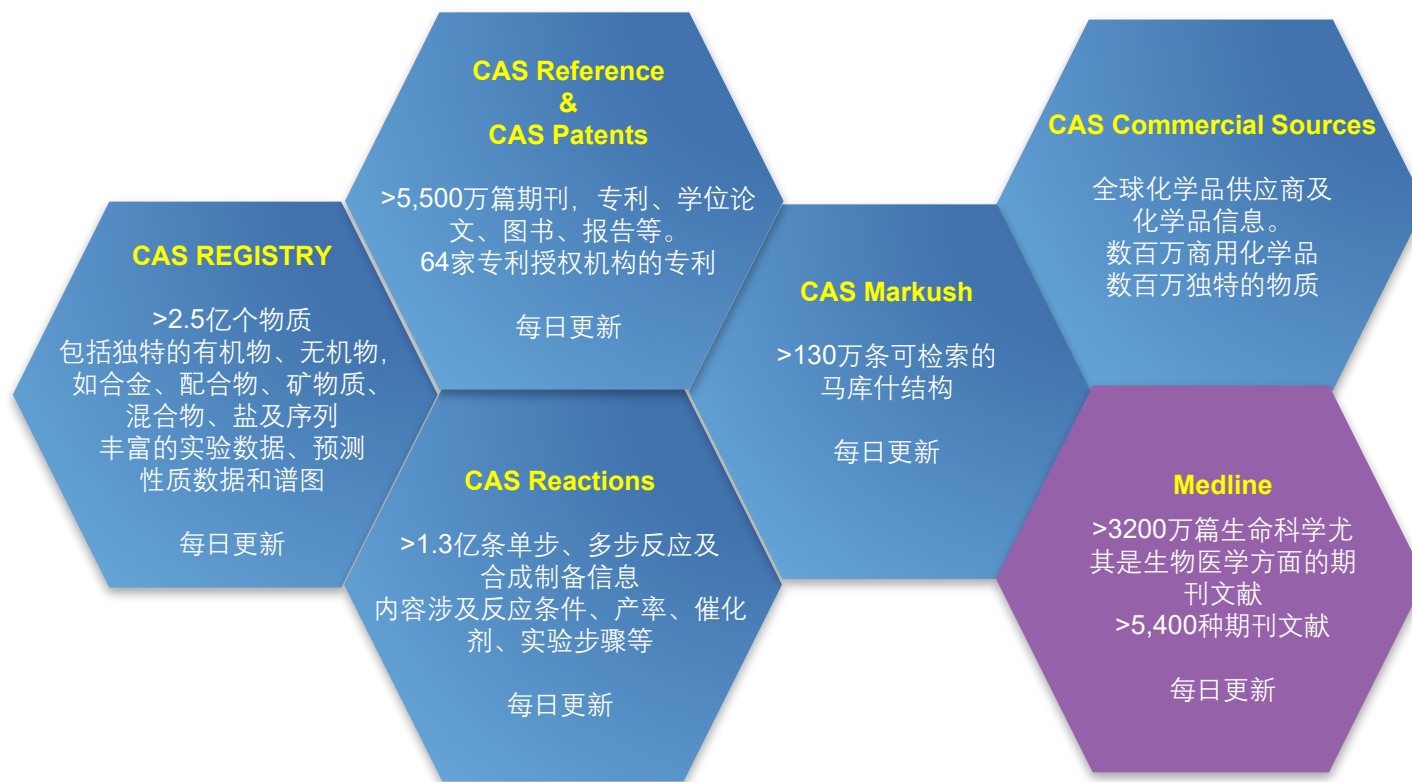
1990
Smith, M.
anthracene



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17β)-

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The screenshot displays the CAS SciFinder main interface. At the top, the 'CAS Solutions' logo and 'SciFinder A CAS SOLUTION' are visible. The navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The left sidebar is divided into three sections: 'REFERENCES' (with options like Research Topic, Author Name, etc.), 'SUBSTANCES' (with options like Chemical Structure, Markush, etc.), and 'REACTIONS' (with Reaction Structure). The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field with examples, a 'Search' button, and a link to 'Advanced Search'. On the right, a 'SAVED ANSWER SETS' panel lists various saved searches and results. A 'KEEP ME POSTED' section at the bottom right indicates no profiles are currently set.

工具栏

文献检索

物质检索

反应检索

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定题追踪

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- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果排序、筛选和详情
- 物质相关信息的获取策略
 - 常见的物质检索方法
 - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果排序、筛选和详情



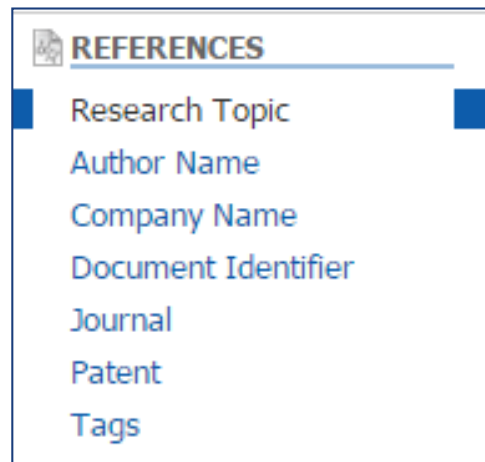
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■ 文献检索方法

- 主题检索
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- 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）
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文献检索--主题

主题检索：中药在咽炎治疗中的应用

检索式：Chinese Medicine **in** treatment **of** pharyngitis

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Research Topic "Chinese Medicine in treatment ..."

REFERENCES

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

SUBSTANCES

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

REFERENCES: RESEARCH TOPIC

Chinese Medicine in treatment of pharyngitis

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

Search

Advanced Search

关键词之间用介词连接：in, with, of...

主题检索的候选项

Select All Deselect All	
1 of 12 Research Topic Candidates Selected	
	References
☐ 18 references were found containing "Chinese Medicine in treatment of pharyngitis" as entered.	18
☒ 1798 references were found containing all of the concepts "Chinese Medicine", "treatment" and "pharyngitis" closely associated with one another.	1798
☐ 2685 references were found where all of the concepts "Chinese Medicine", "treatment" and "pharyngitis" were present anywhere in the reference.	2685
☐ 163407 references were found containing the two concepts "Chinese Medicine" and "treatment" closely associated with one another.	163407
☐ 209931 references were found where the two concepts "Chinese Medicine" and "treatment" were present anywhere in the reference.	209931
☐ 2313 references were found containing the two concepts "Chinese Medicine" and "pharyngitis" closely associated with one another.	2313
☐ 3199 references were found where the two concepts "Chinese Medicine" and "pharyngitis" were present anywhere in the reference.	3199
☐ 6680 references were found containing the two concepts "treatment" and "pharyngitis" closely associated with one another.	6680
☐ 12341 references were found where the two concepts "treatment" and "pharyngitis" were present anywhere in the reference.	12341
☐ 355768 references were found containing the concept "Chinese Medicine".	355768
☐ 14586866 references were found containing the concept "treatment".	14586866
☐ 25948 references were found containing the concept "pharyngitis".	25948
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；



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文献结果集的排序--Citing Reference

Explore ▼ Saved Searches ▼ SciPlanner Save Print Export

Research Topic "Chinese Medicine in treatment ..." > 文献筛选工具

REFERENCES

Analyze Refine Categorize

Analyze by: Author Name

Name Not Translated 26

Xu Jun 15

Wang Yajun 10

Zhang Jianjun 10

Chen Zhijin 9

Jiang Guochao 8

Qu Yunzhi 7

Shen Juanyan 7

Wang Wei 7

Yang Gaolin 7

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Display Options Page: 1 of 89

1. **Isolation and characterization of flavonoids and organic acid from *Trollius chinensis* Bunge**

Quick View Other Sources

By Li, Yao-Lan; Ma, Shuang-Cheng; Yang, Yi-Ting; Ye, Shao-Ming; But, Paul Pui-Hay

From Journal of Ethnopharmacology (2002), 79(3), 365-368. | Language: English, Database: CAPLUS

The flower of *Trollius chinensis* Bunge is used for treating pharyngitis, tonsillitis, and bronchitis in Chinese folk medicine. The antiviral activities of the crude ext., total flavonoids, orientin, vitexin and proglobeflowery acid isolated from the flowers of *T. chinensis* were investigated. The results showed that the crude ext. and total flavonoids exhibited a weak antiviral activity against Para 3. Proglobeflowery acid showed w...

2. **Suppression of Inflammatory Responses by Dihydromyricetin, a Flavonoid from *Ampelopsis grossedentata*, via Inhibiting the Activation of NF- κ B and MAPK Signaling Pathways**

Quick View Other Sources

By Hou, X. L.; Tong, Q.; Wang, W. Q.; Shi, C. Y.; Xiong, W.; Chen, J.; Liu, X.; Fang, J. G.

From Journal of Natural Products (2015), 78(7), 1689-1696. | Language: English, Database: CAPLUS

 **Ampelopsis grossedentata**, an indigenous plant in southern China, has been used for treating pharyngitis in traditional Chinese medicine for hundreds of years. In this study, the authors explored the anti-inflammatory activity of dihydromyricetin, its major bioactive component, and the underlying mechanism of this action. The authors demonstrated that dihydromyricetin suppressed the levels of pro-inflammatory cytokines such as tumor necrosis factor- α (TNF- α), interleukin-1 β (IL-1 β), and interleukin-6 (IL-6) as well as increased the level of the anti-inflammatory cytokine interleukin-10 (IL-10)...

3. **Physalin A induces apoptosis via p53-Noxa-mediated ROS generation, and autophagy plays a protective role against apoptosis through p38-NF- κ B survival pathway in A375-S2 cells**

Quick View Other Sources

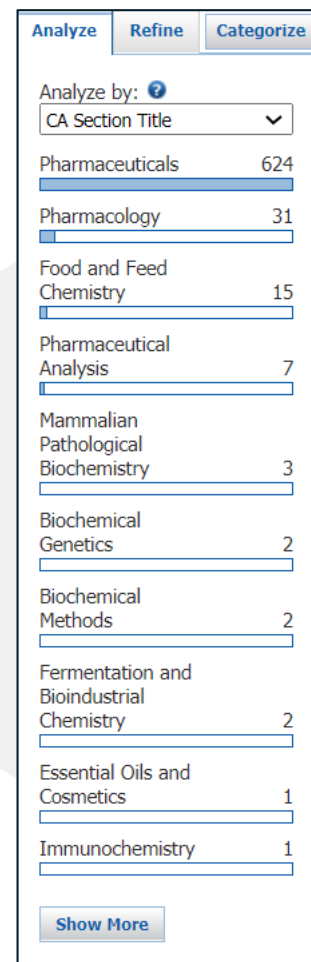
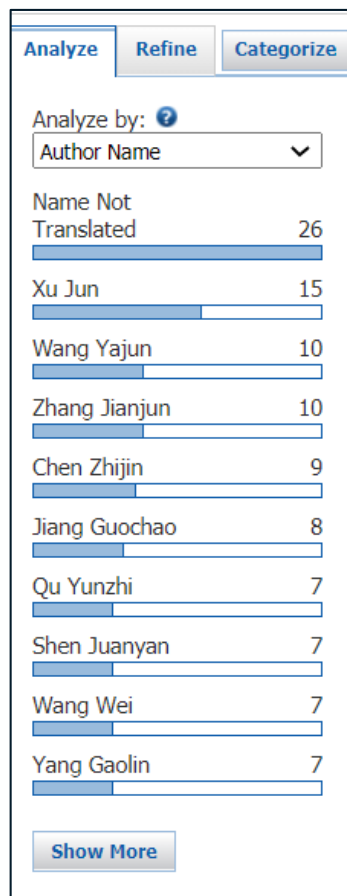
By He, Hao; Zang, Ling-He; Feng, Yong-Sheng; Chen, Li-Xia; Kang, Ning; Tashiro, Shin-ichi; Onodera, Satoshi; Qiu, Feng; Ikejima, Takashi

From Journal of Ethnopharmacology (2013), 148(2), 544-555. | Language: English, Database: CAPLUS

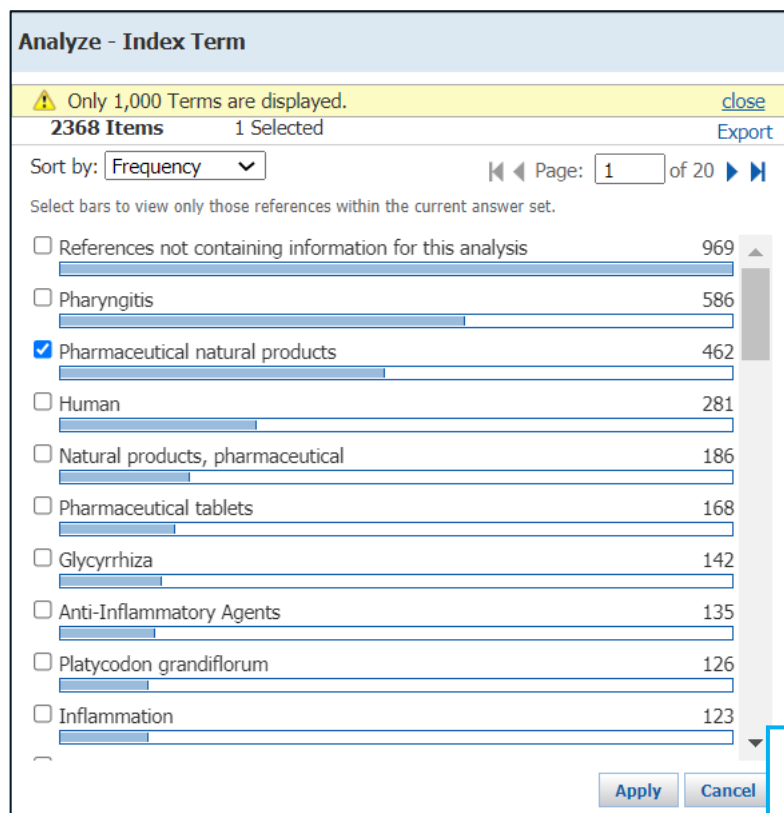
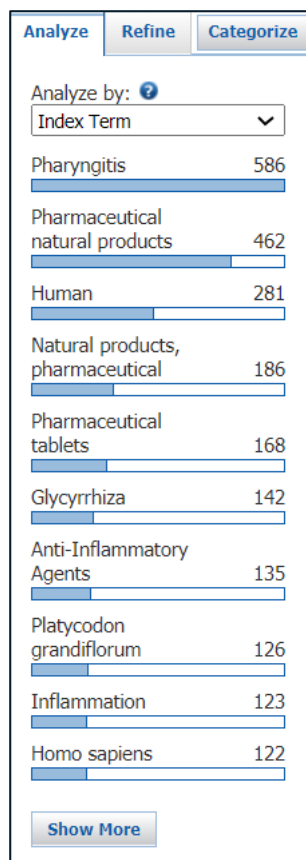
Physalin A is a bioactive withanolide isolated from natural plant *Physalis alkekengi* L. var. *franchetii* (Mast.) Makino, a traditional Chinese herbal medicine named Jindenglong which has long been used for the treatment of cough, sore throat, hepatitis, eczema, dysuria and tumors in China. Based on the previous study that physalin A induced cytotoxic effect in human melanoma A375-S2 cells, this study was designed to further illustrate the mol. mechanisms...

Citing Reference: 帮助找到最重要的文献

文献结果集的筛选--Analyze



文献结果集的筛选--Analyze



Index Term:

帮助用户了解涉及到的重要技术术语，并修正检索词

文献结果集的筛选--Refine

AnalyzeRefineCategorize

Refine by: ⓘ

- ☐ Research Topic
- ☐ Author
- ☐ 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

Sort by: Citing References ↓

Display Options

0 of 6 References Selected

☐

1. Chinese medicinal herbs for sore throat

Quick ViewOther Sources

By Huang Yushan; Wu Taixiang; Zeng Linmiao; Li Sheng
From The Cochrane database of systematic reviews (2012), (3), CD004877. | Language: English, Database: MEDLINE

BACKGROUND: Chinese herbal medicines are commonly used to treat sore throat in China and are used worldwide by practitioners of traditional Chinese medicine (TCM). Their efficacy in treating sore throat has not previously been systematically reviewed. OBJECTIVES: To assess the efficacy and safety of Chinese herbal medicines for patients with sore throat. SEARCH METHODS: We searched CENTRAL (The Cochrane Library Issue 4, 2011) which contains the Cochrane Acute Respiratory Infections Group's Specialised Register; MEDLINE (1966 to week 3, November 2011); EMBASE (1980 to December 2011); AMED...

~10

☐

2. Marsdenia tenacissima: A Review of Traditional Uses, Phytochemistry and Pharmacology

Quick ViewOther Sources

By Wang, Pelle; Yang, Jing; Zhu, Zhenfeng; Zhang, Xiaojian
From American Journal of Chinese Medicine (2018), 46(7), 1449-1480. | Language: English, Database: CAPLUS

A review. The stems and roots of Marsdenia tenacissima (Roxb.) Wight et Arn., a traditional Chinese medicine and Dai herbal medicine, have been widely used for the treatment of asthma, trachitis, tonsillitis, pharyngitis, cystitis, pneumonia and drug or food poisoning. Nowadays, the ext. of Marsdenia tenacissima, under the trademark of "Xiao-ai-ping", is widely used in clinic for the treatment of different cancers in China. To date, approx. 196 chem. ingredients covering steroids, triterpenes and org. acids have been identified from different parts of this plant. Steroids are the major cha...

~8

☐

3. Chinese medicinal herbs for sore throat

Quick ViewOther Sources

By Shi Y; Gu R; Liu C; Ni J; Wu T
From The Cochrane database of systematic reviews (2007), (3), CD004877. | Language: English, Database: MEDLINE

BACKGROUND: Chinese herbal medicines are commonly used to treat sore throat in China and among Chinese people worldwide. Their efficacy in treating sore throat has not previously been systematically reviewed. OBJECTIVES: To assess the efficacy and safety of Chinese herbal medicines for patients with sore throat. SEARCH STRATEGY: We searched the Cochrane Central Register of Controlled Trials (CENTRAL) (The Cochrane Library, Issue 3, 2006) which contains the Acute Respiratory Infections Group's specialised register; MEDLINE (1966 to August 2006); EMBASE (1980 to August 2006); AMED (1985 to...

~6

☐

4. The phytochemistry, pharmacology and applications of Melicope pteleifolia: A review

Quick ViewOther Sources

By Yao, Qi; Gao, Ying; Lai, Chencen; Wu, Chong; Zhao, Chen-Liang; Wu, Jin-Lin; Tang, Dong-Xin
From Journal of Ethnopharmacology (2020), 251, 112546. | Language: English, Database: CAPLUS

A review. The leaves, stems and roots of Melicope pteleifolia (Champ. ex Benth.) T. Hartley (MP; Rutaceae, called sanyaku in Chinese; syn.: Euodia leptia), have been used traditionally for the treatment of sore throat, rheumatism, eczema, dermatitis, bruises, and insect, rat, snake bites based on traditional Chinese medicine concepts. Aim of this study: This paper aims to provide a comprehensive and crit. anal. of studies on MP and focusing on potential relationships between traditional uses and pharmacol. effects, assessing the therapeutic potential as a medicine. Relevant data on MP were ...

~3

☐

5. Andrographis paniculata (Burm.f.) Nees and its major constituent andrographolide as potential antiviral agents

Quick ViewOther Sources

By Jiang, Maoyuan; Sheng, Feiya; Zhang, Zhen; Ma, Xiao; Gao, Tianhui; Fu, Chaomei; Li, Peng
From Journal of Ethnopharmacology (2021), 272, 113954. | Language: English, Database: CAPLUS

A review. Andrographis paniculata (Burm.f.) Nees is widely used all over the world, esp. in subtropical regions such as India, Thailand, Vietnam, and China. As a traditional folk Chinese medicine, A. paniculata has been extensively utilized for the treatment of cold, fever, sore throat, cough, carbuncle, and sores, and it is commonly employed for clearing heat and resolving toxicity. Typical symptoms of 'heat and toxicity include swollen, painful gums, assoc. with virus-related diseases to a great extent. In vivo and in vitro expts. have demonstrated the potential antiviral properties of...

~0

Refine: 帮助用户迅速获得需要的文献

文献结果集的筛选--Categorize

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Medicine (195)
General chemistry	Substances in medicine (522)
Genetics & protein chemistry	Food (114)
Physical chemistry	Agriculture (15)
Polymer chemistry	Substances in food chemistry (79)
Biotechnology	Substances in biological uses (30)
Biology	Toxicology & forensics (12)
Technology	Substances in adverse effects (23)
Analytical chemistry	
Environmental chemistry	
Synthetic chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms		Selected Terms
Page: 1 of 2		Click 'x' to remove the category from 'Selected Terms' ✕ Biotechnology > Medicine (5 Terms)
Select All Deselect All		
☒ Pharmaceutical tablets	170	
☐ Anti-inflammatory agents	133	
☐ Ethanol	119	
☒ Pharmaceutical granules	118	
☒ Pharmaceutical capsules	111	
☐ Chinese medicine	87	
☒ Pharmaceutical powders	79	
☒ Pharmaceutical decoctions	68	
☐ Analgesics	47	
☐ Antitussives	46	
☐ Antinvertics	43	

Biotechnology > Medicine > 5 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。

文献结果集的保存

SciPlanner

Save Print Export

in treatment ..." > references (1775) > refine by categories > Development and validation of ...

Get Substances Get Reactions Get Related Citations Tools

Sort by: Citing References

0 of 326 References Selected

1. Development and validation of a UPLC-DAD-MS method for characterization and quantification of alkaloids in Menisperm Rhizoma and its preparations

Quick View Other Sources

By Liu, Yanan; Song, Xiao; Yan, Ruiqing; Li, Tianxiang; Chai, Xin; Ai, Ai; Wang, Yuefei; Jiang, Zhenzuo

From Journal of Food and Drug Analysis (2013), 21(2), 206-218. | Language: English, Database: CAPLUS

Menisperm Rhizoma (MR), a well known traditional Chinese medicine, is widely used to prevent and treat sore throat, enteritis, dysentery, and rheumatoid arthralgia clin. However, many rhizomes of Chinese herbal medicines are mistaken as MR due to their similar appearance, which could affect MR quality and cause serious consequences for patients. To guarantee the quality of MR products, an ultra-high-performance liq. chromatog.-diode array detector-tandem mass spectrometry (UPLC-DAD-MS) method was established for the characterization of major active ingredients in MR and its preps. By comp...

2. A metabolic profiling analysis of the acute toxicological effects of the realgar (As2S2) combined with other herbs in Niu Huang Jie Du Tablet using 1H NMR spectroscopy

Quick View Other Sources

By Xu Wenfeng; Wang Haifeng; Chen Gang; Zhang Xiaoli; Li Wen; Xiang Rongwu; Pei Yuehu

From Journal of ethnopharmacology (2014), 153(3), 771-81. | Language: English, Database: MEDLINE

ETHNOPHARMACOLOGICAL RELEVANCE: Niu Huang Jie Du Tablet (NJT), composed of Realgar (As2S2), Bovis Calculus Artificialis, Bombylium Synthetica, Cuscuta Fibrosa, Dipsacis Radix et Rhizoma (DR), Scutellaria Radix (SR), Platycodonis Radix (PR) and Glycyrrhizae Radix et Rhizoma (GR), is an effective formula of traditional Chinese medicine (TCM) used in the level of realgar (As2S2) as a potentially toxic element is contained. In our previous experiments, NJT was significantly less toxic than realgar.

3. Simultaneous determination of eight constituents in rat plasma by HPLC-MS/MS and its application to a pharmacokinetic study after oral administration of Shejin-liyan Granule (SJLY)

Quick View Other Sources

By Li, Ling; Zhang, Xiuwen; Bu, Fengjiao; Chen, Nianzu; Zhang, Hongmei; Gu, Jifeng

From Biomedical Chromatography (2019), 33(11), e4648. | Language: English, Database: CAPLUS

Shejin-liyan Granule (SJLY) is an effective traditional Chinese prescription medicine for the treatment of acute pharyngitis. In the simultaneous detn. of the following eight constituents in the plasma: galuteolin, tectoridin, tectorigenin, iridin, irigenin, irisflorelin, arctiin and anal. was carried out on a C18 column using a gradient elution at a flow rate of 0.3 mL/min. The concn. of these analytes was qua...

4. Traditional Chinese medicinal composition for treating pharyngitis

Quick View PATENTPAK

By Liang, Zhenhui

From Faming Zhuanli Shengqing (2007), CN 1927313 A 20070314. | Language: Chinese, Database: CAPLUS

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文献结果详情--题录、摘要、索引

1. Development and validation of a UPLC-DAD-MS method for characterization and quantification of alkaloids in Menisperm Rhizoma and its preparations

By: Liu, Yanan; Song, Xiao; Yan, Ruiqing; Li, Tianxiang; Chai, Xin; Qi, Aidi; Wang, Yuefei; Jiang, Zhenzuo

Menisperm Rhizoma (MR), a well known traditional Chinese medicine, is widely used to prevent and treat sore throat, enteritis, dysentery, and rheumatoid arthralgia clin. However, many rhizomes of Chinese herbal medicines are mistaken as MR due to their similar appearance, which could affect MR quality and cause serious consequences for patients. To guarantee the quality of MR products, an ultra-high-performance liq. chromatog.-diode array detector-tandem mass spectrometry (UPLC-DAD-MS) method was established for the characterization of major active ingredients in MR and its preps. By comparing their retention times and characteristic fragmentations with those of authentic compds., 9 alkaloids in MR were unequivocally identified as acutumidine, acutumine, magnoflorine, menisperine, dauricine, menisporphine, N-demethyl-N-formyldehydronuciferine, 6-O-demethylmenisporphine, and dauriporphine. Quant. anal. of the 9 alkaloids in MR and its preps. was accomplished by UPLC-DAD. A UPLC C18 column was employed for the chromatog. sepn. which was effected by a gradient elution with acetonitrile and 0.1% aq. formic acid soln. contg. 5 mM ammonium acetate at a flow rate of 0.3 mL/min. This quant. method was validated with good linearity ($R^2 \geq 0.9991$), desirable intra- and inter-day precisions ($RSD \leq 3.32\%$), and acceptable recoveries (97.90-106.8%). The method was also successfully applied to quantify 9 alkaloids in 8 batches of MR, 6 batches of MR capsules and 2 batches of MR pills. A counterfeit MR sample from Henan province was identified by the validated method, followed by further verification by appearance and microscopic identification. The developed UPLC-DAD-MS method overcame the shortcomings of other quality control methods, such as scant chem. marker, long anal. time, consumption of large amts. of org. solvents and limitation to MR or its single dosage form.

Indexing

Pharmaceutical Analysis (Section64-2)	
Section cross:	重要概念
Concepts	
Pharmaceutical natural products	
Menisperm Rhizoma; RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menisperm Rhizoma	
Mass spectrometry	
RP-UPLC, combined with; RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menisperm Rhizoma	
Counterfeiting Pharmaceutical capsules Quality control	Menispermum dauricum Pharmaceutical tablets
RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menisperm Rhizoma	
Alkaloids	
RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menisperm Rhizoma	
Analyte; Analytical study	

Substances 重要物质

111017-06-2
RP-UPLC-DAD-MS method for characterization and detn. of alkaloids in Menisperm Rhizoma
Analyte; Natural product occurrence; Properties; Analytical study; Biological study; Occurrence
524-17-4 Dauricine
2141-09-5 Magnoflorine
17088-50-5 Acutumine
18145-26-1 Acutumidine
25342-82-9 Menisperine
83287-02-9 Menisporphine
83287-03-0 6-O-Demethylmenisporphine
88142-60-3 Dauriporphine
RP-UPLC-DAD-MS method for characterization and detn.
Analyte; Properties; Analytical study

QUICK LINKS

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SOURCE

Journal of Food and Drug Analysis
Volume21
Issue2
Pages206-218
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CODEN:JFDAAF
ISSN:1021-9498
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COMPANY/ORGANIZATION

Tianjin State Key Laboratory of Modern Chinese Medicine
Tianjin University of Traditional Chinese Medicine
Tianjin, Peop. Rep. China

ACCESSION NUMBER

2014:154544
CAN163:592365
CAPLUS

PUBLISHER

Elsevier B.V.

LANGUAGE

English

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



ACS
International



CAS PatentPak--专利工作流程解决方案

6. Traditional Chinese medicine oral preparation containing maackiain for treating nasopharyngeal carcinoma and identification method and application thereof

Quick View PATENTPAK

By Miao, Jianhua; From Faming Zhu

Patent No. CN 111317741

PatentPak Options PDF | PDF+ | Viewer

Kind A

Language Chinese

ing, Xiaomei; Ou, Chunli; Tang, Binglan; Mo, Shandan; et al

Database: CAPLUS

The present trifolirhizin and sophoranochromene as active ingredients, where the content of maackiain is greater than or equals to 0.59 mg/g, and/or the total content of maackiain, trifolirhizin and sophoranochromene is greater than or equal to 2.00 mg/g. The oral prepn. has good antitumor activity, small toxic and side effects and good application prospect, and can be used for prepg. medicaments for treating respiratory tract cancers and/or respiratory tract inf

PATENTPAK
A CAS SOLUTION

Key Substances in Patent

CAS RN 2035-15-6

Oc1ccc2c(c1)oc3cc4c(c2)oc5ccccc5c4c3

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 2

CAS RN 23057-59-2

Oc1ccc2c(c1)oc3cc4c(c2)oc5ccccc5c4c3

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 2

CAS RN 6807-83-6

Oc1ccc2c(c1)oc3cc4c(c2)oc5ccccc5c4c3

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 2

CAS RN 485-72-3

Oc1ccc2c(c1)oc3cc4c(c2)oc5ccccc5c4c3

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 2

PAGE 2 / 25

ZOOM - +

DOWNLOAD PDF

CN 111317741 A

权利要求书

1/1 页

1. 用于治疗鼻咽癌的中药口服制剂,其特征在于,其有效活性成分包括高丽槐素、红车轴草苷和环广豆根素,且高丽槐素的含量大于等于0.59mg/g,和/或高丽槐素、红车轴草苷和环广豆根素的总含量大于等于2.00mg/g。

2. 如权利要求1所述的用于治疗鼻咽癌的中药口服制剂,其特征在于,其标准指纹图谱中包含12个特征峰,其中,按出峰顺序以第8个特征峰为参照物峰,第1个特征峰的相对保留时间为0.331,对应的化合物为芒柄花苷,第2个特征峰的相对保留时间为0.446,对应的化合物为红车轴草苷,第3个特征峰的相对保留时间为0.497,第4个特征峰的相对保留时间为0.599,对应的化合物为染料木苷,第5个特征峰的相对保留时间为0.653,对应的化合物为染料木黄酮,第6个特征峰的相对保留时间为0.709,对应的化合物为乙酰红车轴草苷,第7个特征峰的相对保留时间为0.764,第8个特征峰对应的化合物为高丽槐素,第9个特征峰的相对保留时间为1.067,对应的化合物为2-(2',4'-二羟基苯基)-5,6-二氧亚甲基苯并呋喃,第10个特征峰的相对保留时间为1.734,对应的化合物为4',7-二羟基-6,8-二异戊烯基黄酮,第11个特征峰的相对保留时间为1.908,第12个特征峰的相对保留时间为2.004,对应的化合物为环广豆根素。

3. 如权利要求1所述的用于治疗鼻咽癌的中药口服制剂,其特征在于,其剂型包括片剂、颗粒剂、胶囊剂、丸剂、散剂、膏剂、口服液和合剂。

4. 如权利要求1-3任一所述的用于治疗鼻咽癌的中药口服制剂的鉴别方法,其特征在于,包括,

采用薄层色谱法对待测中药口服制剂中的高丽槐素和红车轴草苷进行定性检测;

采用高效液相色谱法对待测中药口服制剂中的高丽槐素进行定量检测;

采用薄层色谱法对待测中药口服制剂中的高丽槐素和红车轴草苷进行定性检测,且高丽槐素的含量大于等于0.59mg/g,和/或高丽槐素、红车轴草苷和环广豆根素的总含量大于等于2.00mg/g。

跳转回SciFinder
开启新检索

在PatentPak浏览器中点击物质下面的紫色灯泡,快速定位到PDF文件中的物质信息。也可从PDF文件中与PatentPak进行互动

文献检索小结

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

大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果排序、筛选和详情
- 物质相关信息的获取策略
 - 常见的物质检索方法
 - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果排序、筛选及详情



CAS SciFinder检索--物质检索

■ 物质检索方法

- 结构式检索
- 分子式检索
- 理化性质（物质属性）检索
- 物质标识符检索：化学名称、CAS RN
- 从文献或反应结果获得

■ 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



SUBSTANCES

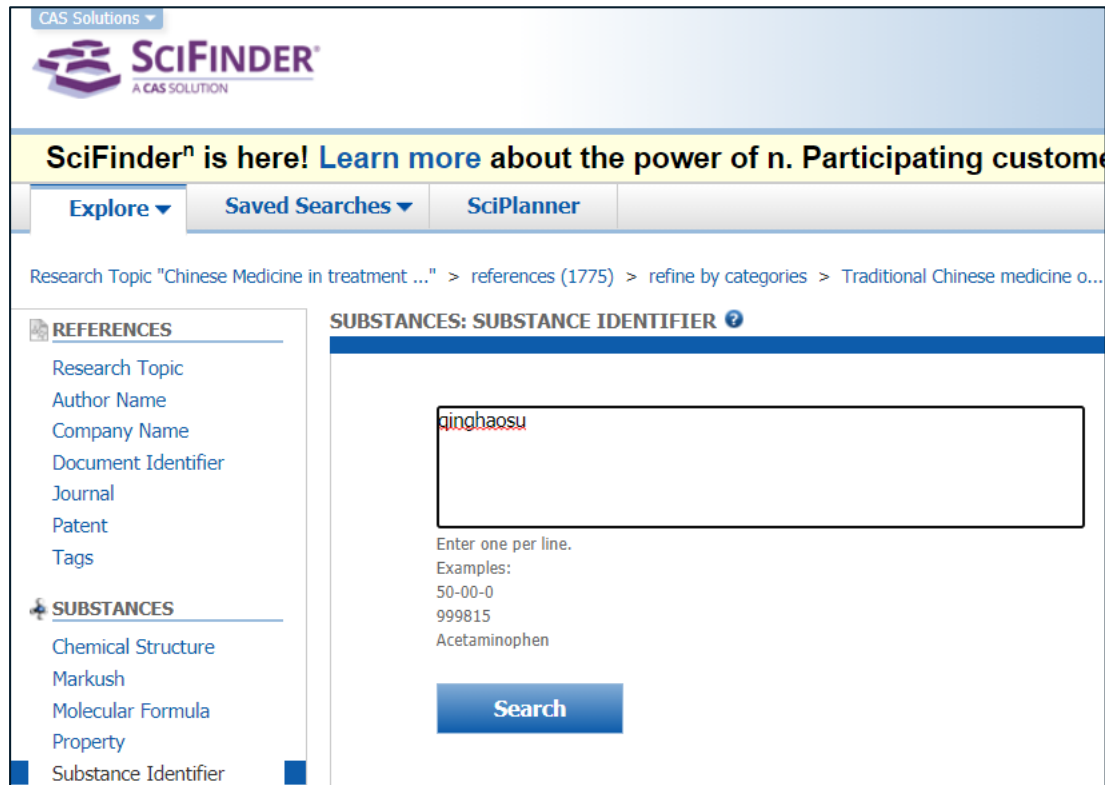
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier



ACS
International



物质检索--标识符检索



The screenshot shows the SciFinder web interface. At the top, there's a navigation bar with 'CAS Solutions' and the SciFinder logo. Below this, a banner reads 'SciFinderⁿ is here! Learn more about the power of n. Participating customers'. The main navigation tabs are 'Explore', 'Saved Searches', and 'SciPlanner'. The current page is 'Explore', showing a breadcrumb trail: 'Research Topic "Chinese Medicine in treatment ..." > references (1775) > refine by categories > Traditional Chinese medicine o...'. On the left, there's a sidebar with two main sections: 'REFERENCES' and 'SUBSTANCES'. Under 'REFERENCES', there are links for Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under 'SUBSTANCES', there are links for Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The 'SUBSTANCES: SUBSTANCE IDENTIFIER' section is active, showing a large text input box with 'qinghaosu' entered. Below the input box, it says 'Enter one per line. Examples: 50-00-0, 999815, Acetaminophen'. A blue 'Search' button is at the bottom of this section.

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。

物质结果集

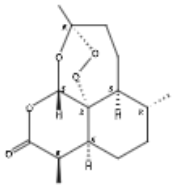
点击CAS RN 获得物质详细信息

0 of 1 Substance Selected

1. 63968-64-9

~6284

~126



Absolute stereochemistry.

C₁₅H₂₂O₅
3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-
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

Export as Image

Export as molfile

Send to SciPlanner

在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

物质结果详情

SUBSTANCE DETAIL

Get References Get Reactions Get Commercial Sources

[Return](#)

CAS Registry Number 63968-64-9

~6,284 ~126

C₁₅ H₂₂ O₅
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*aS*,6*R*,8*aS*,9*R*,12*S*,12*aR*)-

Molecular Weight
282.33

Melting Point (Experimental)
Value: 156-157 °C

Boiling Point (Predicted)
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.300 g/cm3

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5*aβ*,6*β*,8*aβ*,9*a*,12*β*,12*aR*)]-(3*R*,5*aS*,6*R*,8*aS*,9*R*,12*S*,12*aR*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
[View more...](#)

Absolute stereochemistry.

Get References

Limit results to:

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

For each sequence, retrieve:

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

Get

Cancel



ACS
International



EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

¹H NMR

¹³C NMR

Hetero NMR

IR

Mass

Raman

UV and Visible

Additional Spectra

¹³C NMR Properties

Carbon-13 NMR Spectrum

Carbon-13 NMR Spectrum

Carbon-13 NMR Spectrum

Notes

(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.

(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS

(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

Value

See spectrum

See spectrum

See full text

Condition

Carbon-13 NMR Spectrum

SPECTRUM ID

7MED36_38.C

CAS REGISTRY NUMBER

63968-64-9

FORMULA

C₁₅H₂₂O₅

CAS INDEX NAME

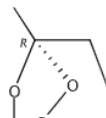
3,12-Epoxy-12H-pyrano[4,3-*f*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5*S*,6*R*,8*S*,9*R*,12*S*,12*aR*)-

NUCLEUS

¹³C

SOURCE

Spectral data were obtained from Advanced Chemistry Development, Inc.



物质检索--Property Explorer

https://scifinder.cas

CAS Solutions

SciFINDER[®]
A CAS SOLUTION

Explore Saved Searches

REFERENCES

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

SUBSTANCES

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

Select Property...

- Bioconcentration Factor
- Boiling Point (°C)
- Density (g/cm³)
- Enthalpy of Vaporization (kJ/mol)
- Flash Point (°C)
- Freely Rotatable Bonds
- H Donor/Acceptor sum
- H Acceptors
- H Donors
- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molar Volume (cm³/mol)
- Molecular Weight**
- pKa
- Molecular Weight

Examples: 44, 25-35, >125

250-400

Examples: 44, 25-35, >125

Search

寻找分子量在250-400之间的物质

物质结果集的筛选--Refine

Property "Predicted - Molecular Weight, ..." > substances (78557824)

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze **Refine**

Sort by: CAS Registry Number

0 of 78557824 Substances Selected

Display Options

Page: 1 of 1571157

Refine by:

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

Structure Editor:

Java **Non-Java**

Click to Edit

Search type: **Exact Structure**

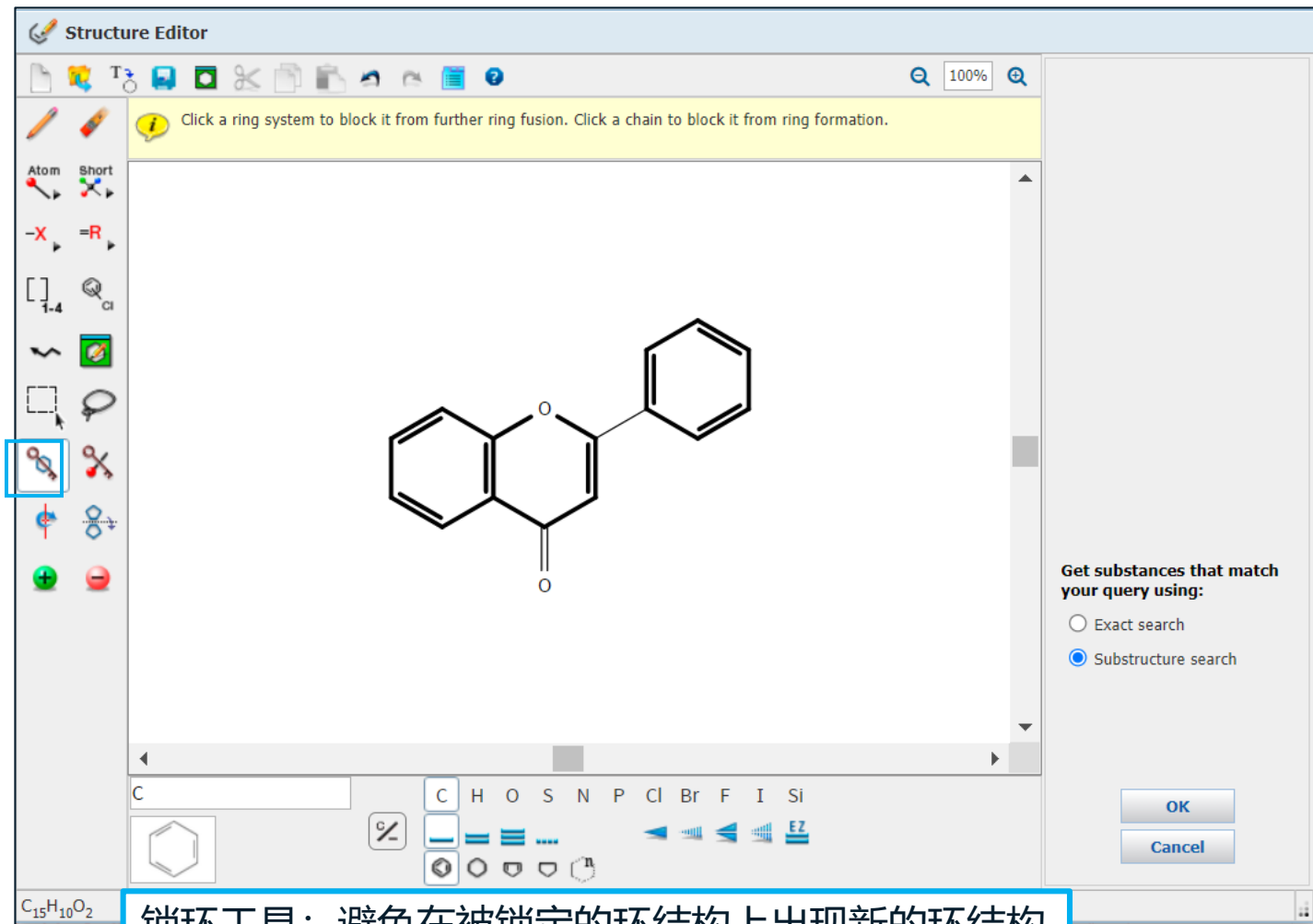
Only retrieve substances that:

- ☐ Have references
- ☐ Are commercially available
- ☐ Are a single component
- ☐ Are in specific substance classes
- ☐ Are in specific ty

☐ 1. 2640164-31-2 C₂₆H₁₈O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 2. 2640164-29-8 C₁₄H₂₀O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 3. 2640164-28-7 C₁₈H₂₂O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 4. 2640164-27-6 C₂₁H₃₀O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties
☐ 5. 2640164-26-5 C₁₅H₂₆O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 6. 2640164-25-4 C₁₅H₂₆O₄ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 7. 2640164-20-9 Relative stereochemistry. C₁₃H₂₁NO₆ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties	☐ 8. 2640164-19-6 Relative stereochemistry. C₁₃H₂₁NO₆ INDEX NAME NOT YET ASSIGNED ▶ Key Physical Properties
☐ 9. 2640164-18-5 	☐ 10. 2640164-17-4 	☐ 11. 2640164-15-2 	☐ 12. 2640164-14-1

4500多万个结构,
如何筛选黄酮类物质?

物质结果集的筛选--Refine



锁环工具：避免在被锁定的环结构上出现新的环结构

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

物质结果集的筛选--Refine

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Analyze by: Substance Role

Preparation 9220

Biological Study 7994

Uses 5377

Reactant or Reagent 4842

Properties 3778

Analytical Study 1168

Occurrence 865

Process 579

Formation, Nonpreparative 251

Prophetic in Patents 114

Show More

Sort by: Relevance

0 of 19423 Substances Selected

Page: 1 of 389

1. 1373355-19-1

Cc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{17}H_{14}O_2$
4#1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-

Key Physical Properties

2. 912915-64-1

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{15}H_{10}O_4$
4#1-Benzopyran-4-one, 2-(3,5-dihydroxyphenyl)-

Key Physical Properties

3. 1174710-12-3

CCc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{17}H_{14}O_2$
4#1-Benzopyran-4-one, 2-(4-ethylphenyl)-

Key Physical Properties

4. 6665-68-5

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{15}H_{10}O_4$
4#1-Benzopyran-4-one, 5-hydroxy-2-(3-hydroxyphenyl)-

Key Physical Properties
Spectra
Experimental Properties

5. 22395-22-8

COc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{16}H_{12}O_3$
4#1-Benzopyran-4-one, 7-methoxy-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

6. 108238-40-0

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{15}H_{10}O_4$
4#1-Benzopyran-4-one, 7-hydroxy-2-(3-hydroxyphenyl)-

Key Physical Properties
Spectra
Experimental Properties

7. 58996-67-1

O=Cc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{15}H_{10}O_3$
Benzaldehyde, 4-(4-oxo-4#1-benzopyran-2-yl)-

Key Physical Properties
Experimental Properties

8. 40052-90-2

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

$C_{16}H_{12}O_3$
4#1-Benzopyran-4-one, 7-(hydroxymethyl)-2-phenyl-

Key Physical Properties

9. 700843-44-3

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

10. 480-40-0

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

11. 4143-74-2

CCc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

12. 53906-83-5

Oc1ccc(cc1)-c2cc3c(cc2)c(=O)c4ccccc43

从7855多万个结构中
筛选出19423个黄酮类物质

物质检索--分子式检索

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: MOLECULAR FORMULA ?

Examples:
H4SiO4
(C3H6O.C2H4O)x
Search

分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前; 如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

无机金属盐: 金属离子和阴离子间用点 (.) 分开

40. **151-21-3**

(Component: 151-41-7)

~79363 ~283

• Na

C₁₂ H₂₆ O₄ S . Na
Sulfuric acid monododecyl ester sodium salt (1:1)

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

物质检索--结构式检索

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:

JavaNon-Java

Click to Edit

Search Type:
☐ Exact Structure
☒ Substructure
☐ Similarity
☐ Show precision analysis

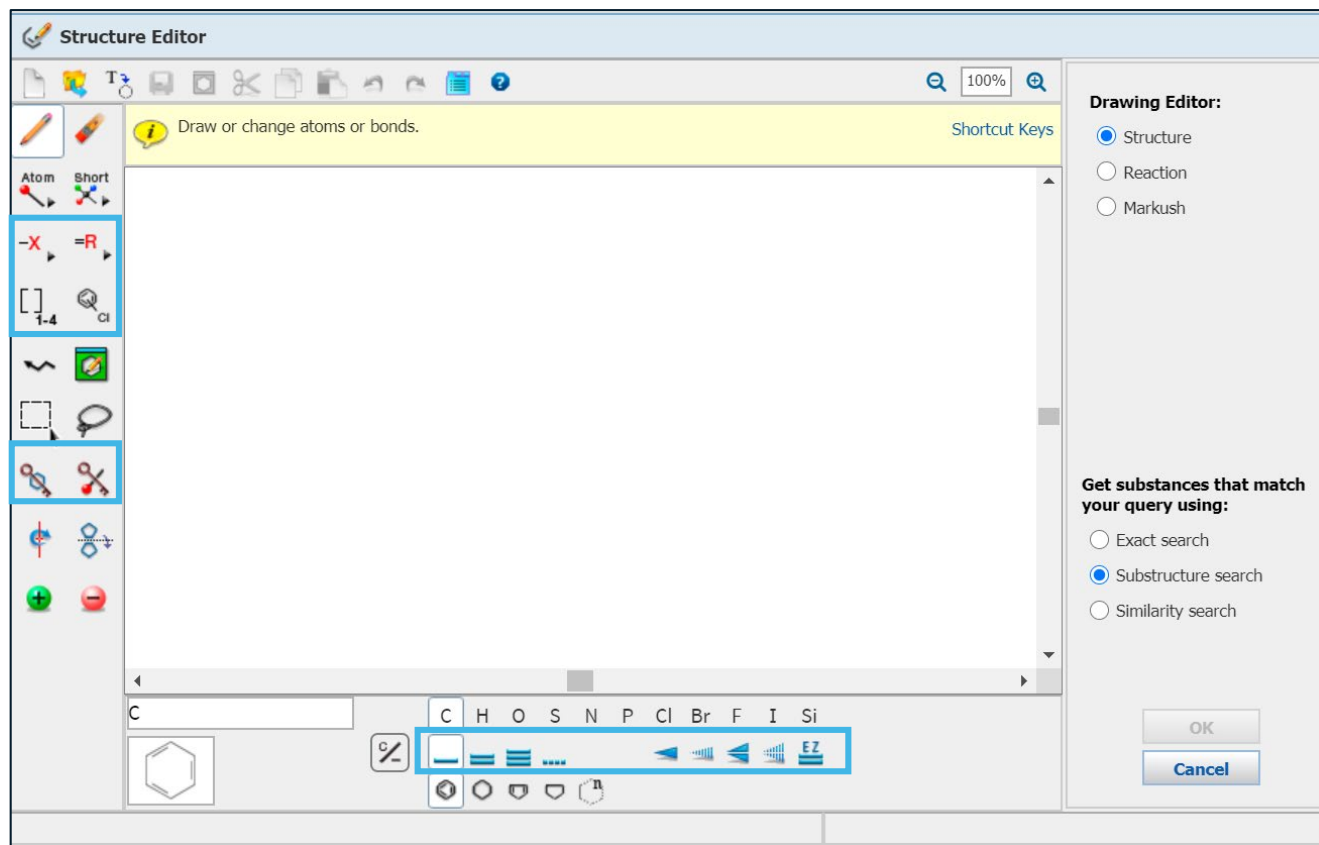
Import CXF

Search

Advanced Search ☒ Always Show

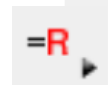
ChemDraw
Launch a SciFinder substance or reaction

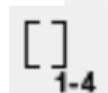
物质检索--结构编辑器



重要绘制工具注释

 选择可变基团

 自定义R基团

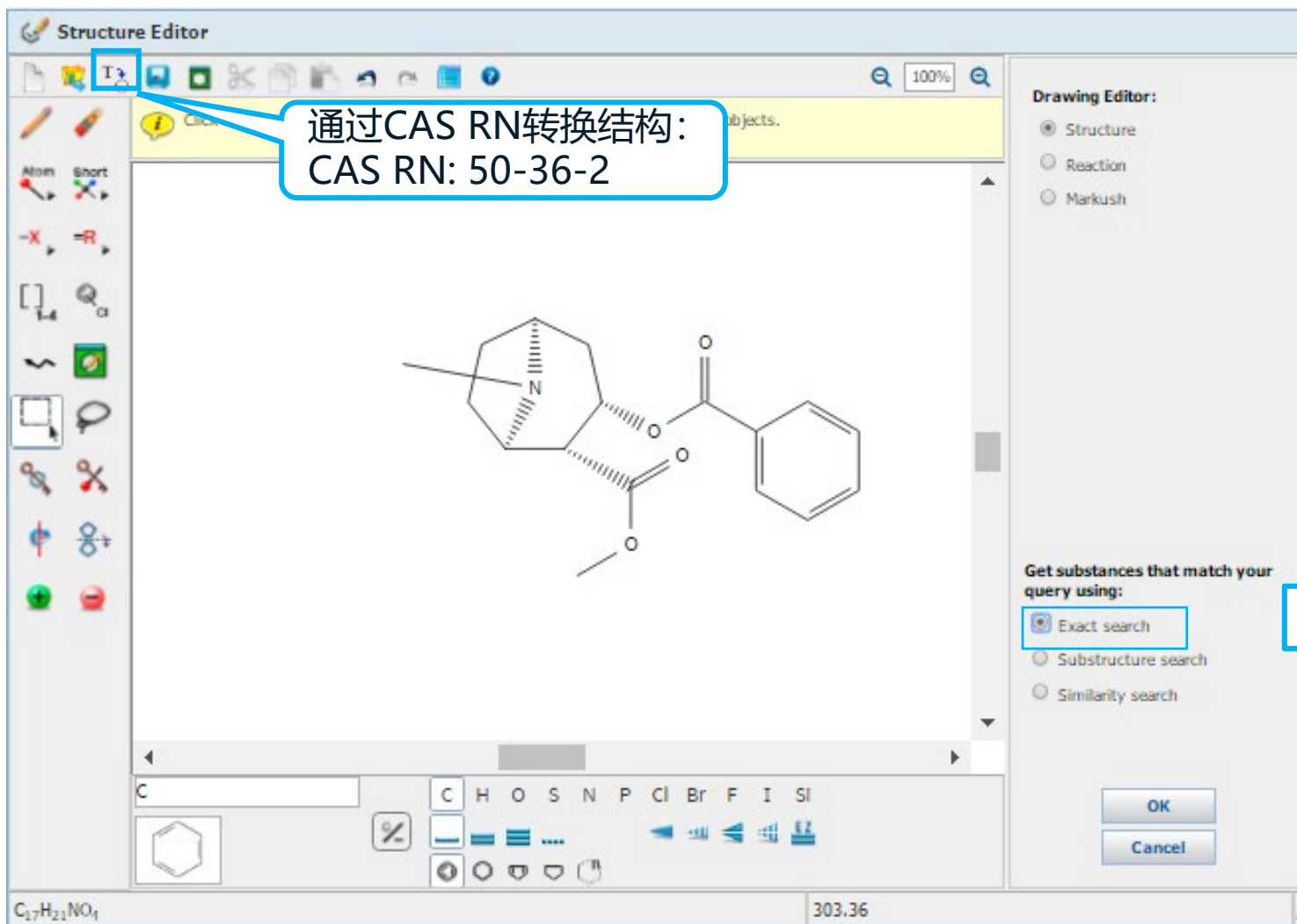
 重复工具

 取代位置可变

 锁环工具

 锁原子工具

物质检索--精确结构检索



精确结构检索

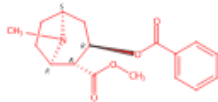
物质检索--精确结构检索

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

Sort by: Relevance

0 of 6 Substances Selected

1. 668-19-9



Absolute stereochemistry.

$C_{17}H_{21}NO_4$
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1R,2R,3R,5S)-

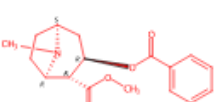
Key Physical Properties
Spectra

可卡因

2. 114599-38-1

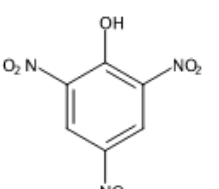
可卡因组合物

668-19-9
 $C_{17}H_{21}NO_4$



Absolute stereochemistry.

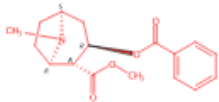
88-89-1
 $C_6H_3N_3O_7$



$C_{17}H_{21}NO_4 \cdot C_6H_3N_3O_7$
Alcocaine, picrate (6CI)

3. 109496-04-0

(Component: 668-19-9)



Absolute stereochemistry.

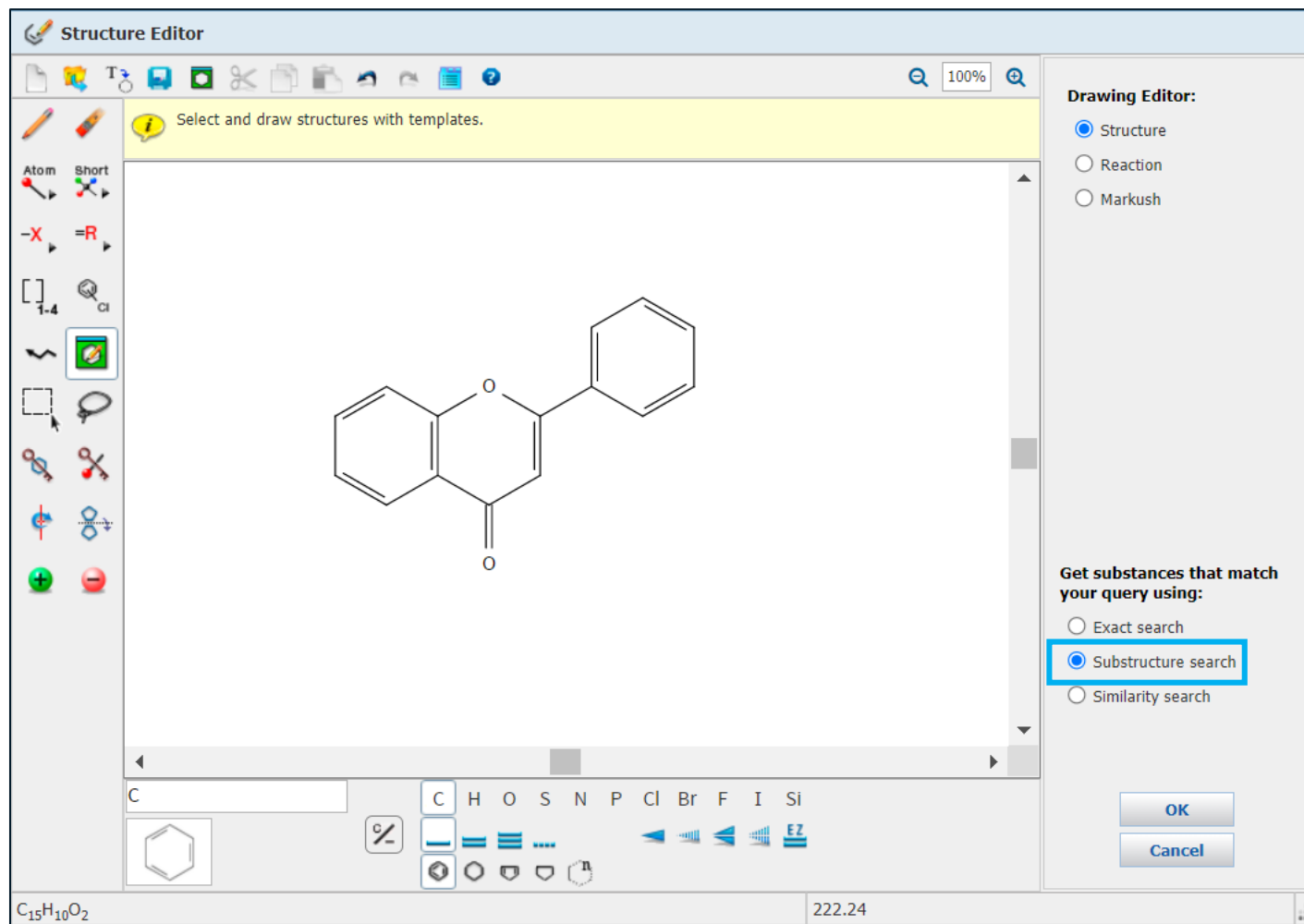
$C_{17}H_{21}NO_4 \cdot ClH$
Alcocaine, hydrochloride (6CI)

盐酸可卡因

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



物质检索--亚结构检索结果集

0 of 23824 Substances Selected

1. 487-26-3

c1ccc(cc1)C2=CC(=C(C=C2)OC3=CC=CC=C3)C4=CC=CC=C4

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-di-
▶ **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

10. 146196-91-0

c1ccc(cc1)C2=CC(=C(C=C2)OC3=CC(=C(C=C3)O)O)C4=CC=CC=C4

同位素

281. 123251-10-5

Cc1cc(C)cc2c1oc(cc2C3=CC=CC=C3)C4=CC=CC=C4

取代物

$C_{17}H_{16}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-2-
▶ **Key Physical Properties**
Experimental Properties

295. 780723-19-5

c1ccc(cc1)C2=CC(=C(C=C2)OC3=CC=CC=C3)C4=CC(=O)C(=O)C4

离子

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

284. 136116-23-9

Oc1ccc(cc1)C2=CC(=C(C=C2)OC3=CC4=CC=CC=C4C(=O)C3C4)C5=CC=CC=C5

稠环物质

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

物质检索--亚结构检索结果集的限定

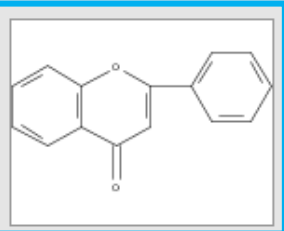
化学结构的再次限定

Analysis Refine

Refine by:

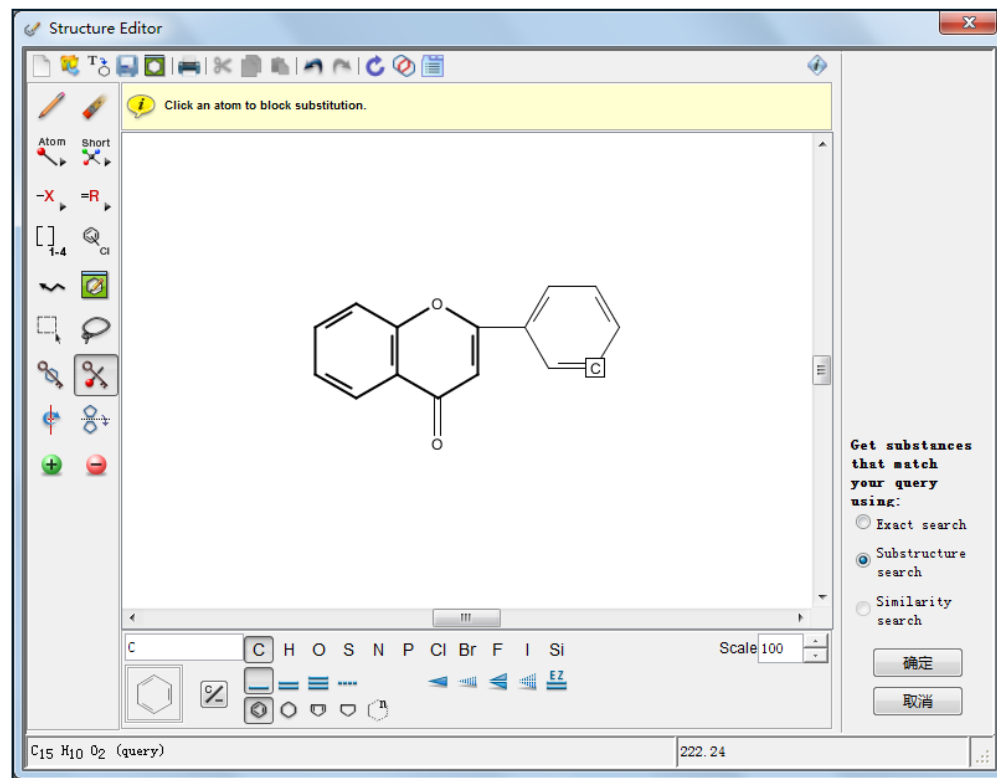
- ☒ Chemical Structure
- ☐ Isotope-Containing
- ☐ Metal-Containing
- ☐ Commercial Availability
- ☐ Property Availability
- ☐ Property Value
- ☐ Reference Availability
- ☐ Atom Attachment

Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**



环锁定

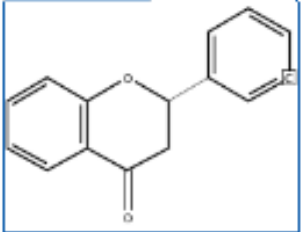


原子锁定

物质检索--亚结构检索结果集的限定

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

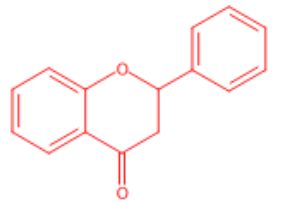
Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

1. 487-26-3

~2093

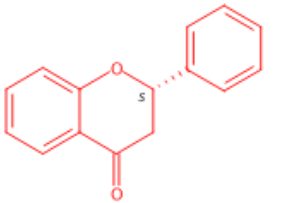


$C_{15}H_{12}O_2$
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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-benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-

Key Physical Properties
Experimental Properties

4. 104550-32-5

~3

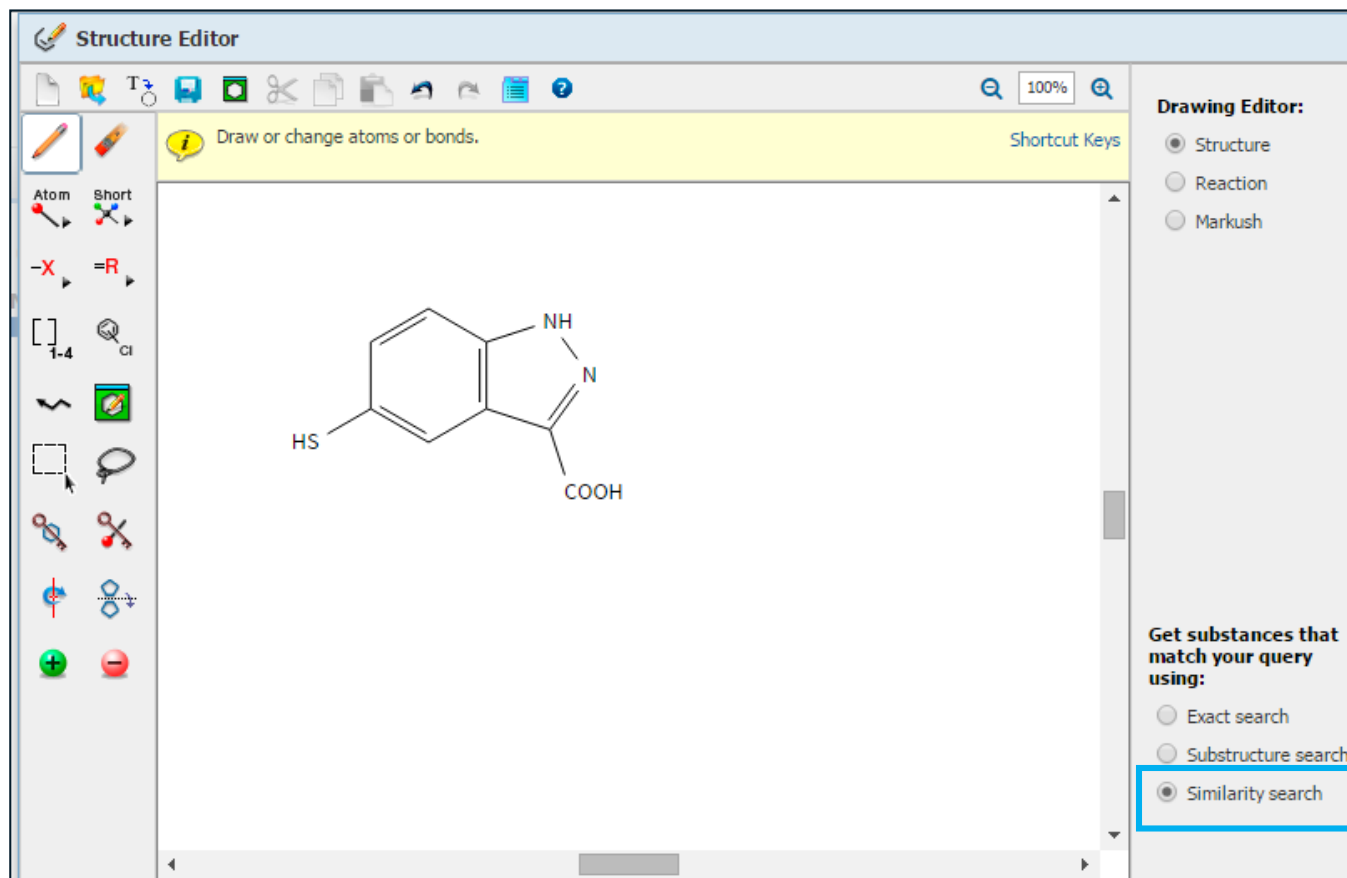
5. 75524-43-5

~2

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



物质检索--相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

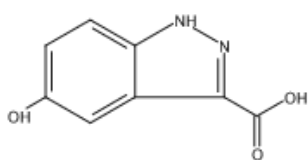
Similarity Range	Substances
☐ ≥ 99 (most similar)	0
☐ 95-98	0
☐ 90-94	0
☐ 85-89	11
☐ 80-84	34
☐ 75-79	84
☐ 70-74	267
	696
	1818

相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化



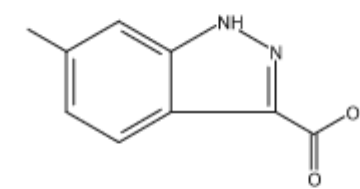
C₈H₆N₂O₃
1H-Indazole-3-carboxylic acid, 5-hydroxy-

► Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化



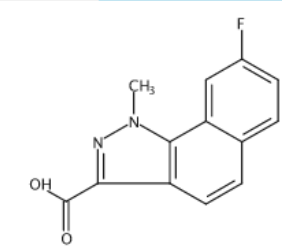
C₉H₈N₂O₂
1H-Indazole-3-carboxylic acid, 6-methyl-

► Key Physical Properties

Score: 65

541. 1100422-

母体结构变化



C₁₃H₉FN₂O₂
1H-Benz[g]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

► Key Physical Properties

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

CAS Markush检索

(19) 中华人民共和国国家知识产权局



(12) 发明专利申请

(10) 申请公布号 CN 104945470 A

(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4

(22) 申请日 2014.03.30

(71) 申请人 浙江大学

地址 浙江省杭州市西湖区浙大路38号

申请人 中国科学院上海药物研究所

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代理人 张法高 赵杭丽

(51) Int. Cl.
C07K 5/087(2006.01)
C07K 5/083(2006.01)

权利要求书3页 说明书24页 附图4页

(54) 发明名称

杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要

本发明提供一种杂环构建的三肽环氧酮类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶抑制活性及细胞增殖抑制活性,是有前景的蛋白酶抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式 I 的结构通式:

CAS Markush检索

预测性物质[Prophetic Substance]:

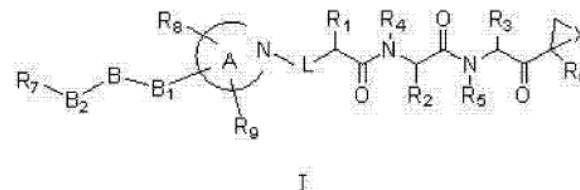
- 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过结构检索检不到的专利

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



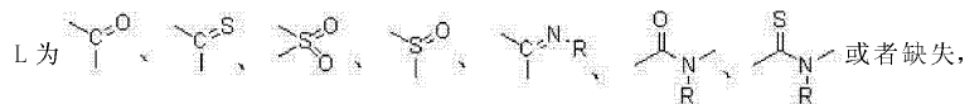
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 N(R_a) (R_b) 或缺失， R_a, R_b 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、C(O)O- C_{1-6} 烷基、C(O)NH- C_{1-6} 烷基、芳烷基；

X 为 O、S、NH、N- C_{1-6} 烷基或 N- 卤代的 C_{1-6} 烷基；

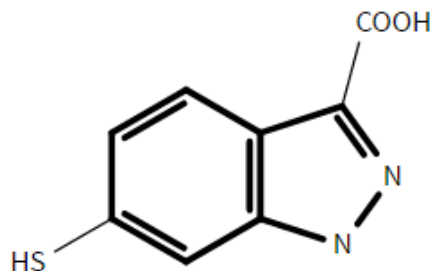


其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基 -D、芳基、杂环芳基、环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

CAS Markush检索



Explore ▼	Saved Searches ▼	SciPlanner
⚠ Explore Substances resulted in 0 substances Return		
Chemical Structure substructure with limiters > substances (0)		
SUBSTANCES		
Analyze	Refine	
Analyze by: <i>No substances available</i>		

Substance检索结果为0!

CAS Markush检索

Markush substructure > references (69)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

0 of 69 References Selected

Analyze by: Author Name

Boga Sobhana Babu 3

Deng Yongqi 3

Nan Yang 3

Paliwal Sunil 3

Shih Neng Yang 3

Shipp Gerald W Jr 3

Tsui Hon Chung 3

Alhassan Abdul Basit 2

Beier Norbert 2

Bulawa Christine Ellen 2

Show More

1. Preparation of ethynylheterocycles as rho-associated coiled-coil kinase (ROCK) inhibitors for the treatment of diseases

Quick View PATENTPAK

By Li, An-Hu; Sakilam, Satish Kumar; Gadhiya, Satish Kumar; Lim, Dong Sung; Zong, Yao; Ponnala, Shashikanth; Zhang, Ying; Jung, Dawoon; Oehlen, Lambertus J. W. M.
From PCT Int. Appl. (2021), WO 2021016256 A2 20210128. | Language: English, Database: CAPLUS

The invention relates to prepn. of ethynylheterocycles of formula (I): and pharmaceutically acceptable salts thereof, wherein Cy¹, Cy², Cy³ each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl; R, R¹, R², and R³ each independently represents an aryl, heteroaryl, or heterocyclic, which is optionally fused with a 3-8 membered cycloalkyl, 3-8 membered heterocycloalkyl, 6-membered aryl, or 5-6 membered heteroaryl, and pharmaceutical compns. thereof, ...

2. Indazoles and azaindazoles as LRRK2 inhibitors in the treatment of CNS disorders and their preparation

Quick View PATENTPAK

By Garofalo, Albert W.; De Lombaert, Stephane; Schwarz, Jacob Bradley; Andreotti, Daniele; Sabbatini, Fabio Maria; Serra, Elena; Bernardi, Silvia; Migliore, Marco; Budassi, Federica; Beato, Claudia
From PCT Int. Appl. (2021), WO 2021007477 A1 20210114. | Language: English, Database: CAPLUS

The invention relates compds. of formula I, their prepn. and their use as inhibitors of LRRK2 in the treatment of CNS disorders. Compd. I, wherein A is halo, (un)substituted C₁₋₆ alkyl, (un)substituted C₂₋₆ alkenyl, etc.; ring B is Ph and 5- to 10-membered heteroaryl wherein said 5- to 10-membered heteroaryl comprises 1, 2 and 3 ring-forming heteroatoms independently selected from N, O and S; X² is N and CR²; X³ is N and CR³; X⁴ is N and CR⁴; no more than two of X², X³ and X⁴ are simultaneously N; R¹ is independently H, halo, C₁₋₆ alkyl, etc.; R² and R⁴ are independently H, halo, C₂₋₆ alke...

3. Organic electroluminescent materials and devices

Quick View PATENTPAK

By Ji, Zhiqiang; Boudreault, Pierre-Luc T.; Shih, Wei-Chun
From U.S. Pat. Appl. Publ. (2020), US 20200358008 A1 20201112. | Language: English, Database: CAPLUS

Provided are organometallic compds. comprising novel ligands represented by a general chem. formula I (Y = R, OR, SR etc.; Z = O, S, NRⁿ; X¹⁻⁵ = C, N; R^A, R^B = substitution; R, Rⁿ = alkyl, cycloalkyl heteroalkyl etc.) as OLED materials for OLED.

Formula 1

Formula 2

为了尽可能全面地获得公开的结构信息， 需要同时进行Substance和Markush结构检索

物质检索小结

1. 选择合适的检索方式
2. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
3. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
4. 正确理解Exact、Substructure、Similarity检索结果集的意义和范围
5. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
6. 利用CAS Markush检索尽可能全面的获得结构的公开信息

大纲

- CAS及CAS SciFinder介绍
- 文献相关信息的获取策略
 - 文献检索方法
 - 文献结果排序、筛选和详情
- 物质相关信息的获取策略
 - 常见的物质检索方法
 - 物质结果排序、筛选和详情
- 反应相关信息的获取策略
 - 反应的获取方法
 - 反应结果排序、筛选及详情



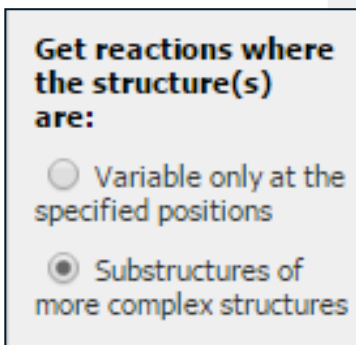
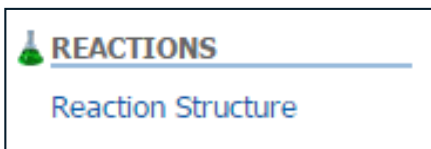
CAS SciFinder检索--反应检索

■ 反应检索方法

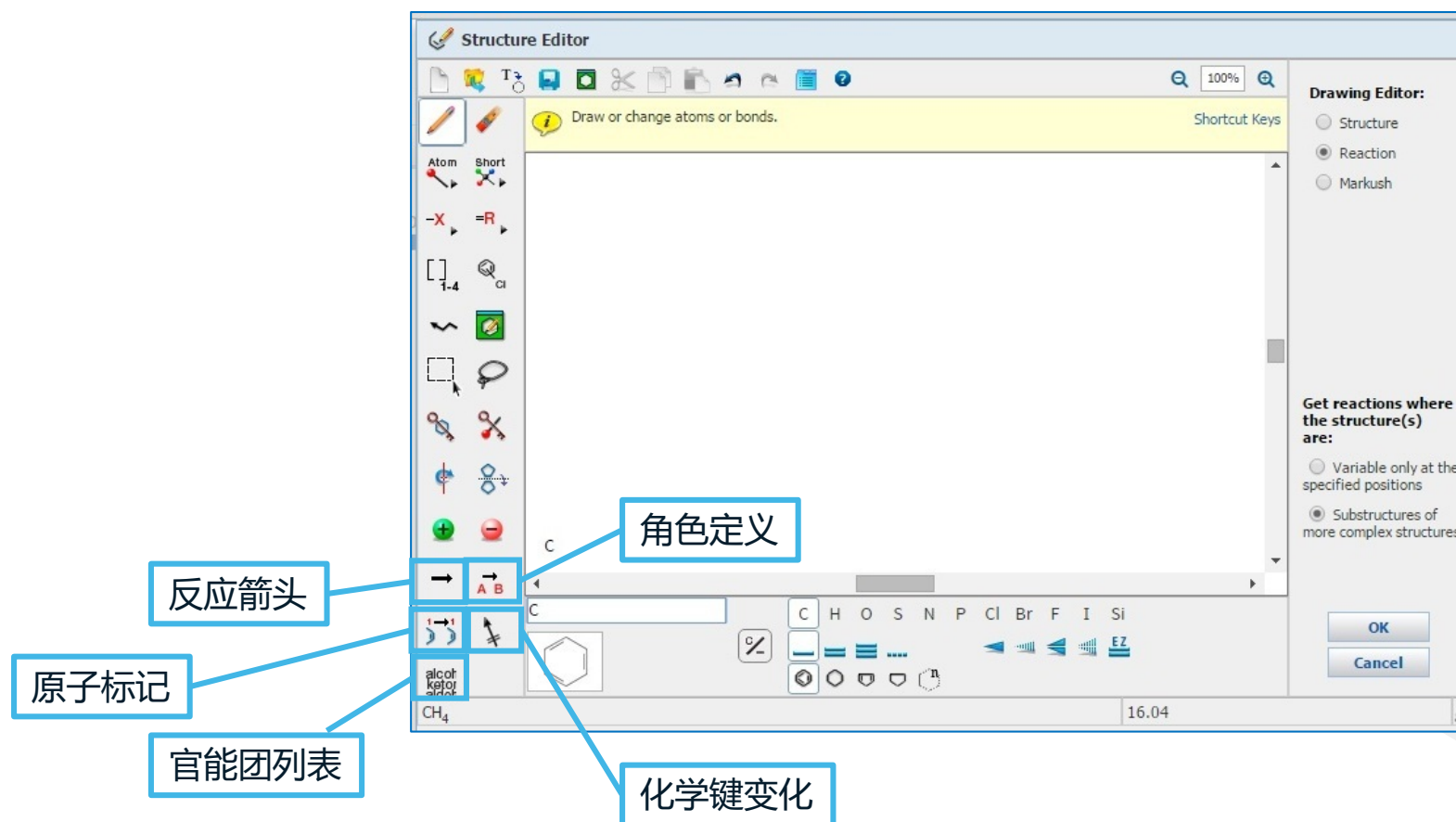
- 结构式

■ 常用获取方法

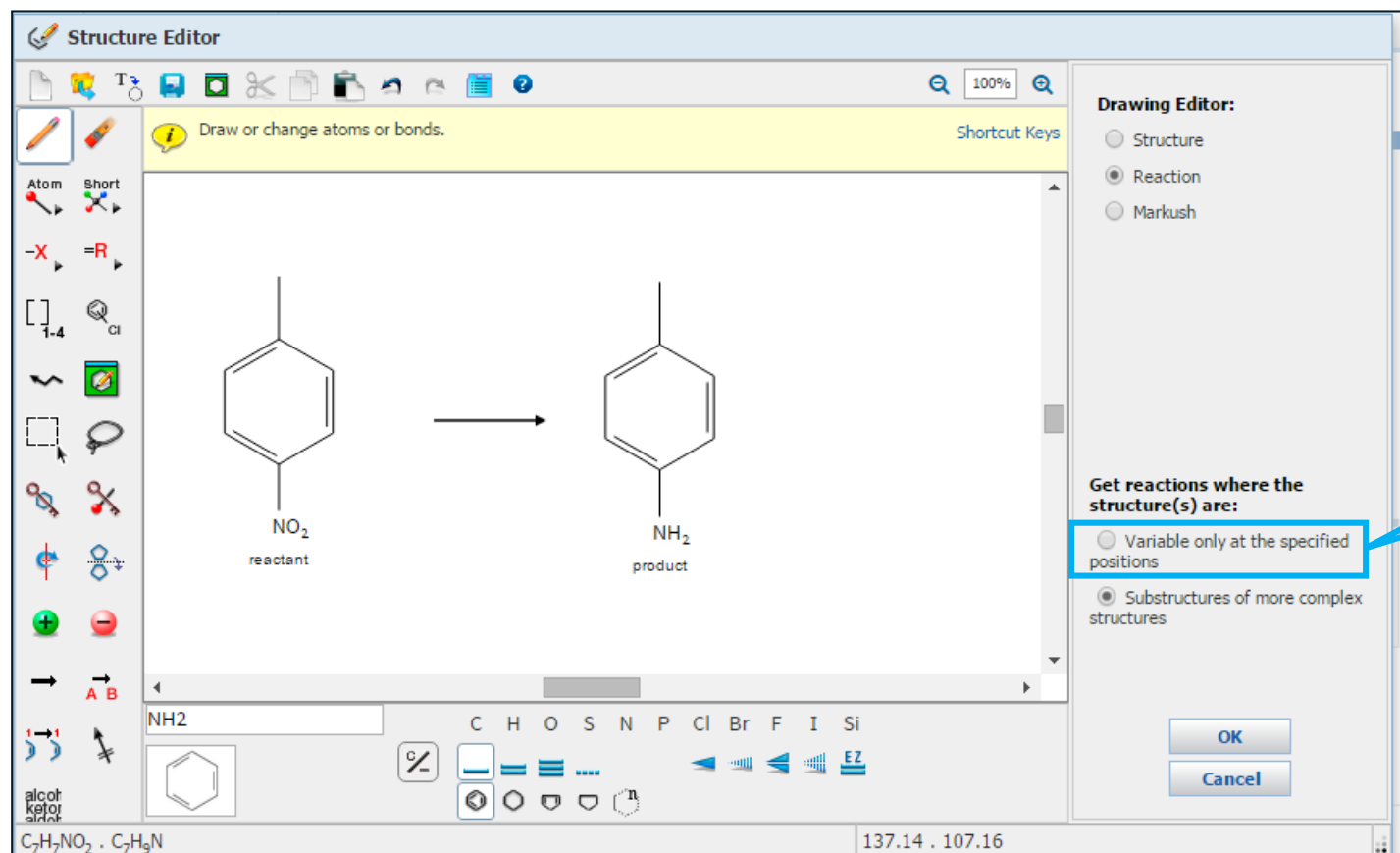
- 已知物质：由物质获取反应
- 已知文献：从文献中获取反应
- 精确结构反应检索
- 亚结构反应检索



结构编辑器--绘制反应工具



反应检索--精确反应检索



精确反应检索

反应检索结果集--排序

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

Get References Tools

Group by: No Grouping No Grouping Document Transformation Sort by: Relevance

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

Single Step Hover over any structure for more options.



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

扩展反应检索--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

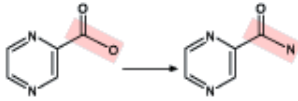
Get Similar Reactions ?

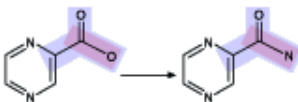
Retrieve similar reactions from:

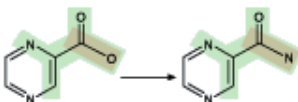
- ☒ All reactions
- ☐ Current answer set

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



反应检索结果集--筛选

获得特定物质做还原剂的反应

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

H₂ 148

NaBH₄ 51

N₂H₄·H₂O 43

KOH 17

CO 16

HCO₂H 16

NH₄⁺·HCO₂⁻ 16

H₂O 14

N₂H₄ 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

Overview

Steps/Stages

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

Notes

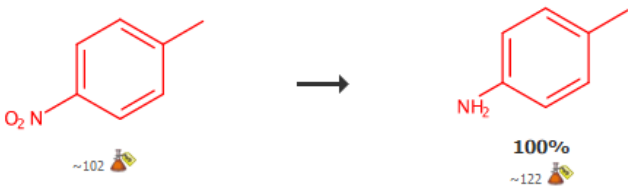
solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

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

反应检索结果--Experimental Procedure

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

反应检索结果--MethodsNow

REACTIONS

Get References Tools

Analyze Refine

Analyze by: MethodsNow

MethodsNow Not Available 1890

MethodsNow Available 1029

Show More

Group by: No Grouping Sort by: Relevance

0 of 2919 Reactions Selected

20. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Overview

METHODSNow™

Procedure

1. Place Pd@Hal-CCD catalyst (1 wt%) and nitroarene (1 mmol) in deionized water
2. Purge hydrogen (1 bar) as reducing agent into the stirring reaction mixture at room temperature for 1.5 h.

View more...

View with MethodsNow

MethodsNow中的实验详情不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容

MethodsNow

Pd stabilized on nanocomposite of halloysite and β -cyclodextrin derived carbon: An efficient catalyst for hydrogenation of nitroarene

By Sadjadi, Samahe; Ghoreyshi Kahangi, Fatemeh; Heravi, Majid M.
From Polyhedron, 175, 114210; 2020
Published by Elsevier Ltd.

物质信息

名称、角色

Products	Aniline, 100%, CAS RN: 62-53-3
Reactants	Nitrobenzene, CAS RN: 98-95-3
Reagents	Hydrogen, CAS RN: 1333-74-0
Catalysts	Palladium, CAS RN: 7440-05-3
Solvents	Water, CAS RN: 7732-18-5
Procedure	1. Place Pd@Hal-CCD catalyst (1 wt%) and nitroarene (1 mmol) in deionized water as solvent (2 mL) in the reaction vessel. 2. Purge hydrogen (1 bar) as reducing agent into the stirring reaction mixture at room temperature for 1.5 h. 3. Hold the reaction and separate Pd@Hal-CCD from the reaction mixture. 4. Isolate the aniline by evaporation of water. 5. Recycle Pd@Hal-CCD and wash the recovered catalyst with water and EtOH several times. 6. Dry in oven at 80°C for 8 h.
Transformation	Reduction of Nitro Compounds to Amines
CAS Method Number	3-522-CAS-21010612

实验过程

反应类型

Print/Export Close

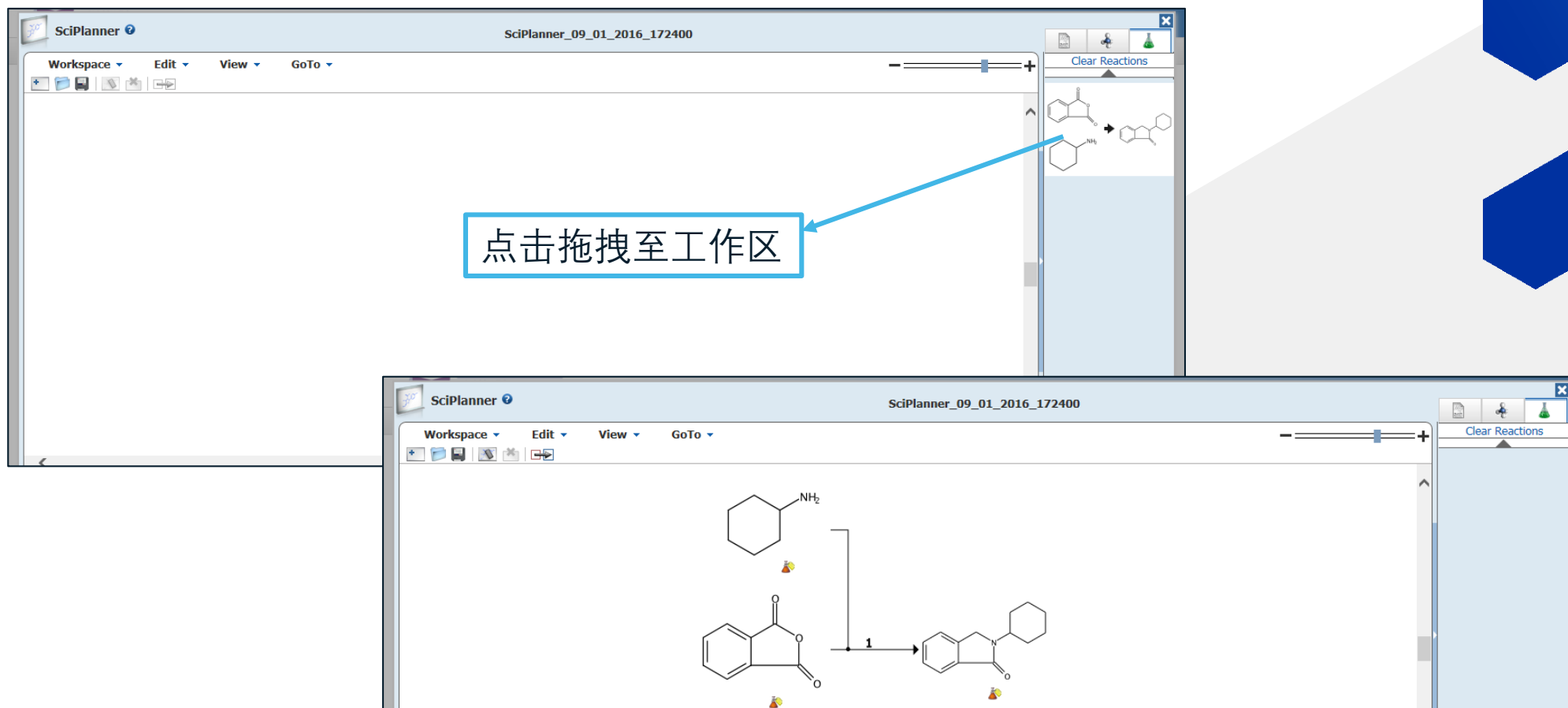
SciPlanner--设计合成反应路线

点击打开SciPlanner工作界面

The screenshot shows the SciPlanner web interface. At the top, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. Below the tabs, the breadcrumb navigation reads 'Reaction Structure substructure > reactions (1208) > refine "Catalyzed" (535)'. The main content area is titled 'REACTIONS' and includes a 'Get References' button and a 'Tools' dropdown. On the left, there are 'Analyze' and 'Refine' tabs, with 'Analyze by: Catalyst' selected. The main list shows '1 of 535 Reactions Selected'. A callout box points to a 'Send to SciPlanner' button in the top right of the reaction list. Below the list, a chemical reaction scheme is displayed: a benzofuranone derivative (labeled ~136) reacts with cyclohexylamine (labeled ~95) to form a bicyclic amide (labeled 87% yield, ~1).

选择感兴趣的反应，点击send to SciPlanner

SciPlanner--工作界面



SciPlanner--工作界面

SciPlanner 09_01_2016_172400

Workspace Edit View GoTo

CAS Registry Number: 85-44-9

- 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

点击物质右上角的双箭头，检索其合成方法

Get References Tools

Group by: No Grouping Sort by: Accession Number

1 of 382 Reactions Selected

4. View Reaction Detail Link Similar Reactions

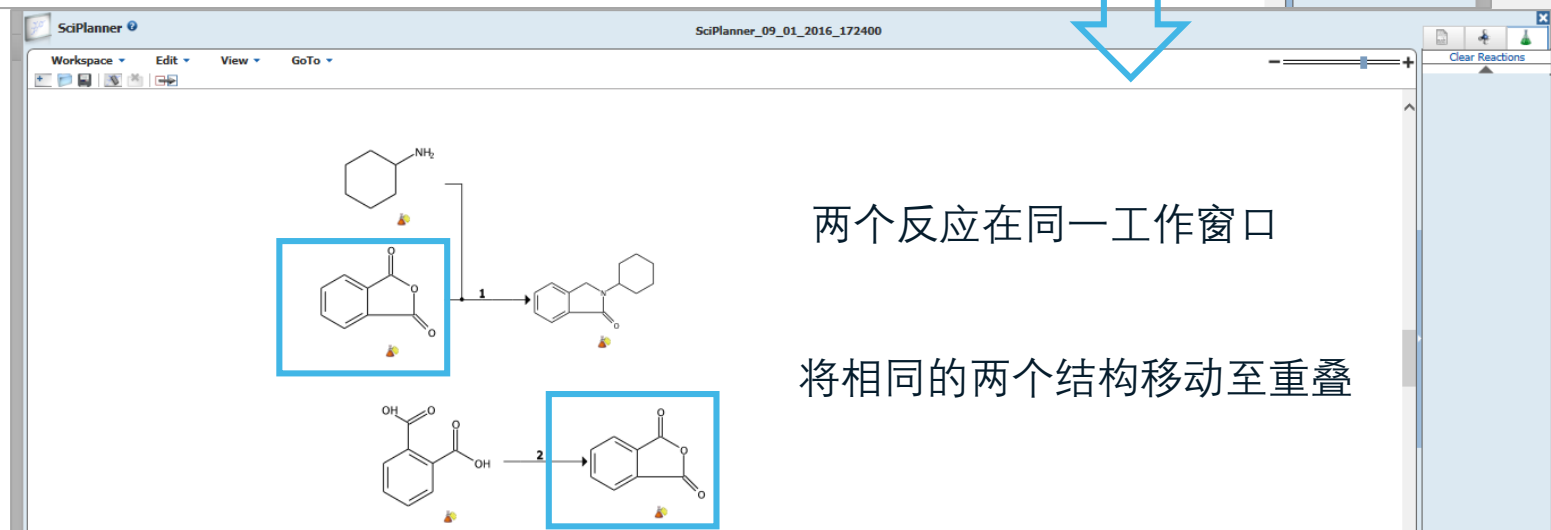
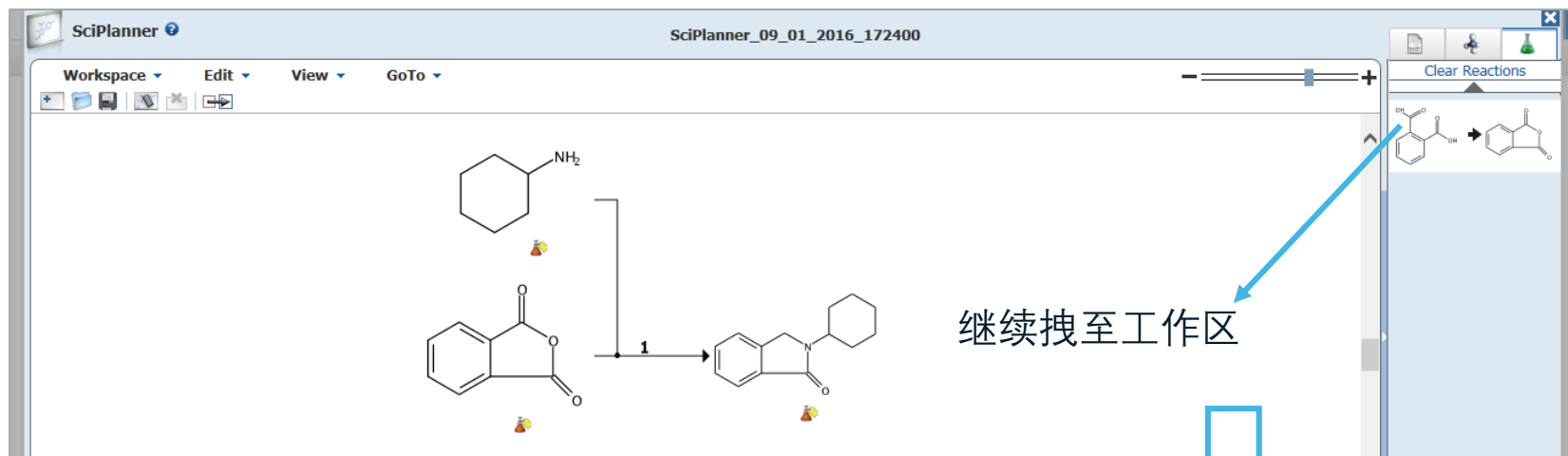
Single Step Hover over any structure for more options.

Reaction scheme showing the synthesis of phthalic anhydride from phthalic acid (97% yield).

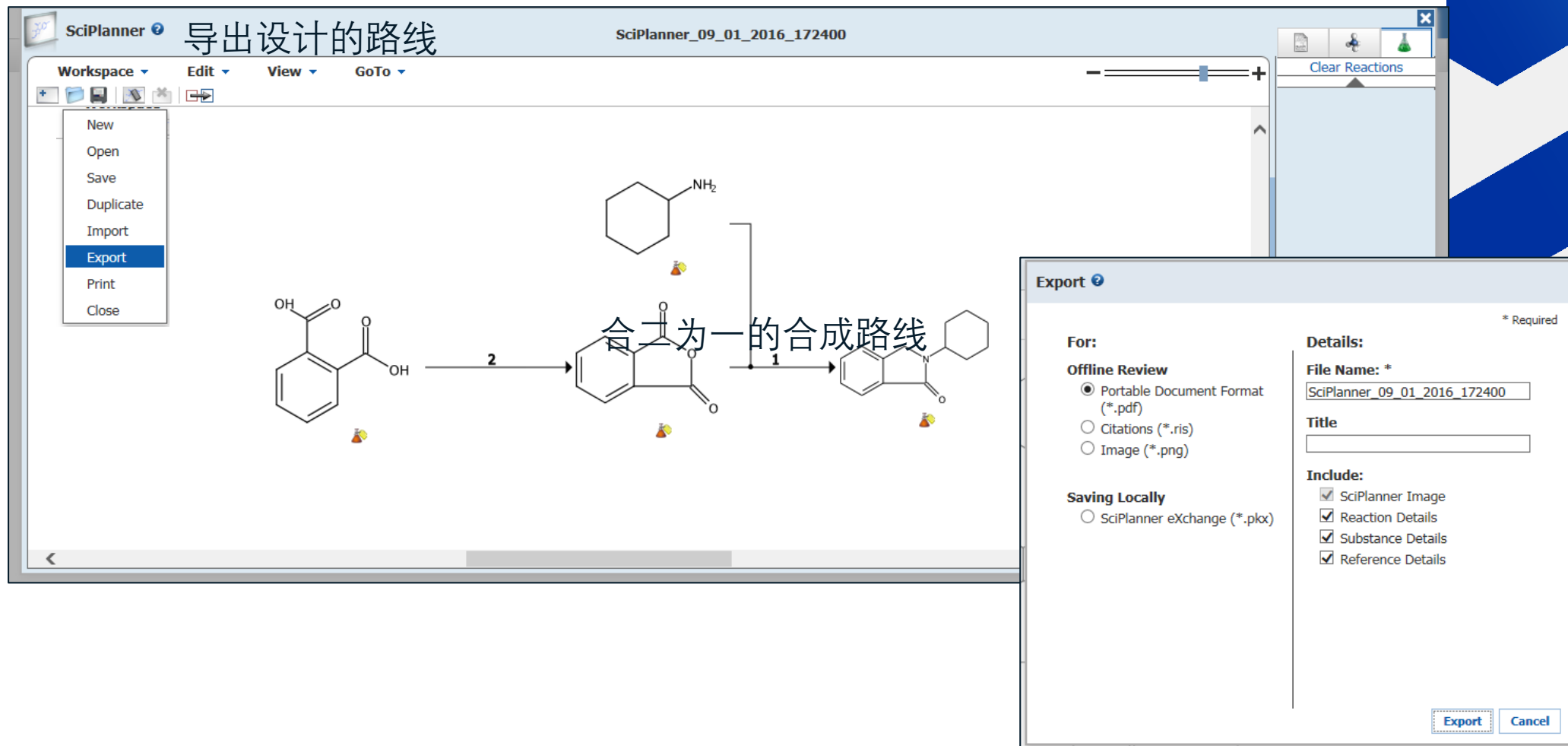
Send to SciPlanner

从结果中选择感兴趣的反应，继续推送至SciPlanner

SciPlanner--工作界面



SciPlanner--设计拟合成的反应路线



反应检索小结

1. 反应检索方法汇总与区分
2. 反应绘制工具的灵活使用
3. 反应结果排序: Group by Transformation/Document
4. 反应结果的快速纵览及筛选, 例如non-participating functional group;
5. 相似反应的获取获得更多启发
6. MethodsNow获取反应详情
7. SciPlanner工具助于自定义设计拟合成反应路线

浏览器选择建议

- Windows 7以上用户建议升级IE到10以上，不支持IE7、IE8
- 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CAS SciFinder账号

填写注册申请表（如下）、提交证件照片（学生证的个人信息页和学籍注册页或是工作证的个人信息页照片，放在附件中），用申请注册的邮箱发送至 china@acs-i.org

SciFinder 注册信息确认	
个人信息(Personal Information)	
学校名称(University):	
院系(College):	
专业(Major):	
中文名(Name):	
电话(Tel):	
身份 (Identity) : ☐ 教师	
☐ 博士 年级(Grade):	
☐ 硕士 年级(Grade):	
☐ 本科 年级(Grade):	
联系信息(Contact Information)	
院系办公室联系电话 (School/Dept. Contact Tel) :	
院系办公室联系人 (School/Dept. Contact Person) :	
Email Address:	



如何获取CAS SciFinder账号

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Last Name':

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Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username': [Tips](#)

Password':

Re-enter Password':

--SECURITY INFORMATION--

Security Question':

Answer': [Why?](#)

请注意：

1.必须输入真实姓名和邮箱。
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：

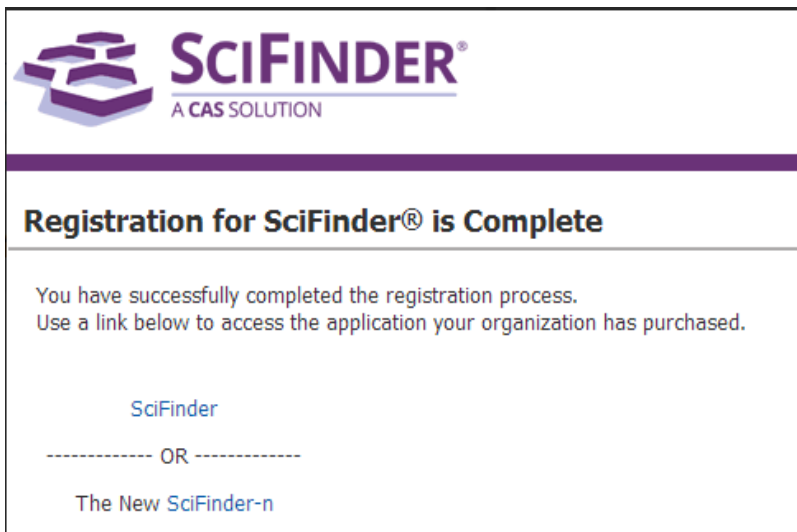
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

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CAS SciFinder账号



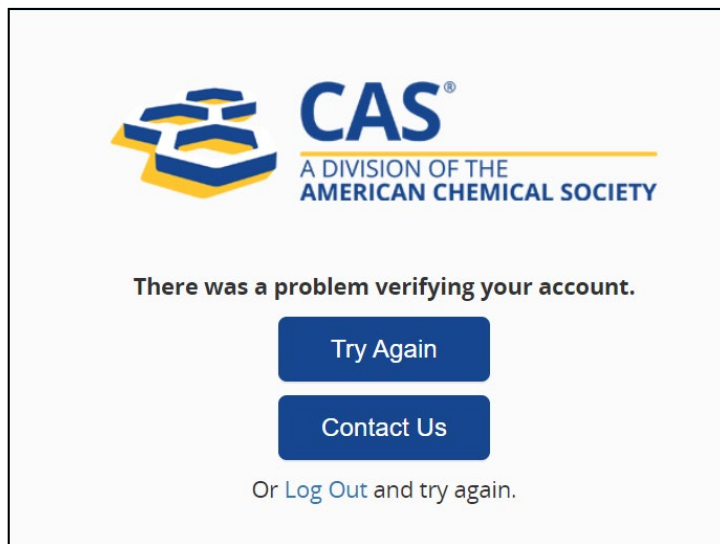
所有信息提交后注册成功。

之后直接点击<https://SciFinder.cas.org>即可访问SciFinder数据库

使用注意事项

- 一人注册一个帐号
- 实名注册， 请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（以电子形式存储不超过5,000条记录）
- 不得账号分享
- 不得将账号用于非学术研究

常见问题



- 确认账号密码是否正确

- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

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