

匡金海

客户顾问

jkuang@acs-i.org

如何使用SciFinder获取科技信息

河北师范大学

2019.04.09



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 (MethodsNow Synthesis)
 - 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

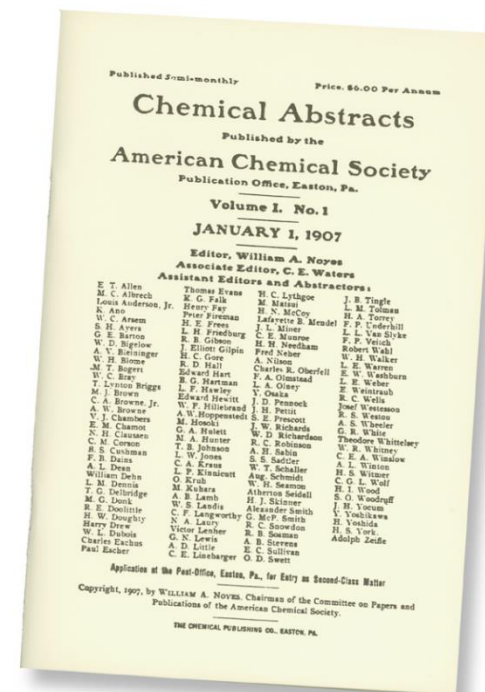


1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯
(William A. Noyes)

- “化学文摘”创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



CAS——构建最高质量的化学数据库



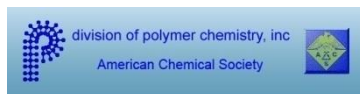
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical
Neuroscience



THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

SCIFINDER[®]
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CAS——构建最高质量的化学数据库



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：

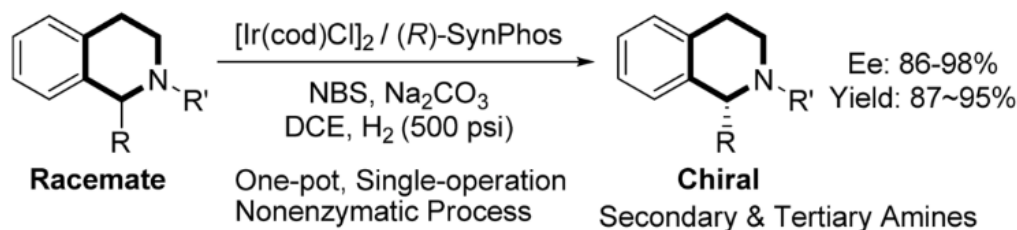
表面化学,催化剂,相平衡,核现象,电化学

CAS数据库最具价值的内容——人工标引

1. Concise Redox Deracemization of Secondary and Tertiary Amines with a Tetrahydroisoquinoline Core via a **Nonenzymatic Process**

By: Ji, Yue; Shi, Lei; Chen, Mu-Wang; Feng, Guang-Shou; Zhou, Yong-Gui

A concise deracemization of racemic secondary and tertiary amines with a tetrahydroisoquinoline core has been successfully realized by orchestrating a redox **process** consisted of N-bromosuccinimide oxidn. and iridium-catalyzed asym. hydrogenation. This compatible redox combination enables one-pot, single-operation deracemization to generate chiral 1-substituted 1,2,3,4-tetrahydroisoquinolines with up to 98% ee in 93% yield, offering a simple and scalable synthetic technique for chiral amines directly from racemic starting materials.



Indexing

Heterocyclic Compounds (One Hetero Atom) (Section27-17)

Concepts

Enantioselective synthesis
Oxidation

Hydrogenation catalysts

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos

stereoselective prepn. of tetrahydroisoquinoline derivs. via iridium-catalyzed deracemization in presence of chiral phosphine ligands

Catalyst use; Uses

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Journal of the American Chemical Society
Volume137
Issue33
Pages10496-10499
Journal; Online Computer File
2015
CODEN:JACSAT
ISSN:0002-7863
DOI:10.1021/jacs.5b06659

COMPANY/ORGANIZATION

State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics
Chinese Academy of Sciences
Dalian, Peop. Rep. China
116023

ACCESSION NUMBER

2015:1340032
CAN163:331216
CAPLUS

PUBLISHER

American Chemical Society

LANGUAGE

English

Tips:

98%以上的文献，都经过人工标引

用Index Term标引文献中的重要技术术语

用CAS RN标引出文献中的重要物质

用CAS Role标引文献中重要物质的研究领域

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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。

CAS最新动向—解决方案

PatentPak™

 **NCI™ Global**
A Solution Powered by CAS

 **METHODSNow™**
A CAS SOLUTION

 **CHEMZENT™**
A CAS SOLUTION

 **SCIFINDER®**
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CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View PATENTPAK

By Beigelman, Le...
From PCT Int. App...

Disclosed he...
phosphate, R...
methods of...
medicament

Patent No.	Kind	Language
WO 2016100441	A1	English

Patent Family

Patent No.	Kind	Language
US 20160176911	A1	English

atkina, Natalia
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R⁴ is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and for a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methylduridine with

12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
23 June 2016 (23.06.2016)

WIPO PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/72 (2006.01)
C07H 19/20 (2006.01) A61K 31/7072 (2006.01)
C07H 19/11 (2006.01) A61K 31/7076 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

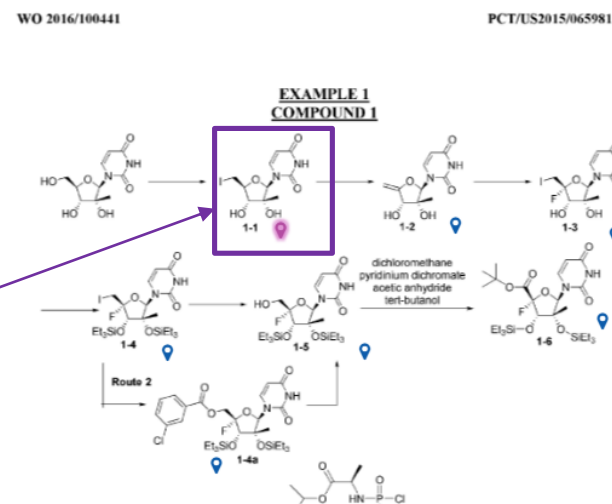
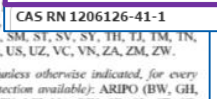
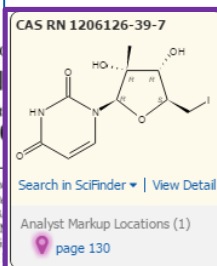
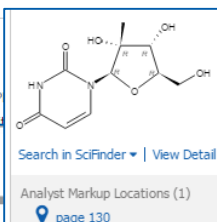
(21) International Application Number:
PCT/US2015/065981

(22) International Filing Date:
16 December 2015 (16.12.2015)

(25) Filing Language:
English

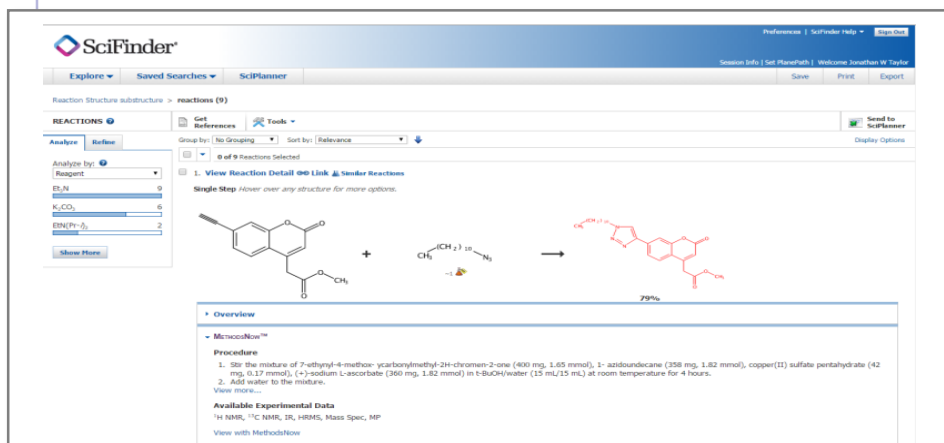
(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BZ, CA, CH, CL, CN, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KZ, LA, LC, LK, LT, LU, LV, MA, MG, MK, MN, MW, MX, MY, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SZ, TZ, UG, ZM, ZW), EPO (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, JP, KR, LK, LT, LU, LV, MA, MG, MK, MN, MW, MX, MY, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).



CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



嵌在SciFinder中的合成模块

CAS Solutions

METHODSNow™

atorvastatin

Results (528)

Sort Relevance

Compare (0/3)

Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography

CAS MN: 1-101-CAS-1389

View Details & Instructions

Add to Compare

Analyte: Atorvastatin

Matrix: Blood plasma

Other Materials: Material: 60 F₂₅₄ silica gel HP TLC plates

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: High-performance thin layer chromatography

Equipment Used: Automatic TLC Sampler 3

Source: HPTLC determination of atorvastatin in plasma

Jamshidi, A.; Nateghi, A. R. Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH

Document Sources

Abstract

单独的分析界面

提纲

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

SciFinder数据库



SciFinder登录网址: <https://scifinder.cas.org/>

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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, there's a header with the SciFinder logo and navigation links like 'Explore', 'Saved Searches', and 'SciPlanner'. A search bar is prominently displayed in the center. On the left, a sidebar lists various search categories: REFERENCES, SUBSTANCES, and REACTIONS. On the right, there's a section for 'SAVED ANSWER SETS' and a 'KEEP ME POSTED' notification. Several callout boxes with Chinese text point to specific features: '检索完，请点击退出' (After searching, please click exit) points to the 'Sign Out' button; '工具栏' (Toolbar) points to the top navigation bar; '检索入口' (Search Entry) points to the search bar; '已保存的结果集' (Saved Results Set) points to the 'SAVED ANSWER SETS' list; and '定题追踪' (Topic Tracking) points to the 'KEEP ME POSTED' section.

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Preferences | SciFinder Help | Sign Out

Welcome Helen Zhu

Explore | Saved Searches | SciPlanner

REFERENCES: RESEARCH TOPIC

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

Search

Advanced Search

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SAVED ANSWER SETS

- CSF1R
- jmc
- EP 19870107847
- Dactatasvir-1
- SUB result
- EX result
- MF result
- polymer1
- polymer1
- structure search
- Autosaved Substance Set

View All | Import

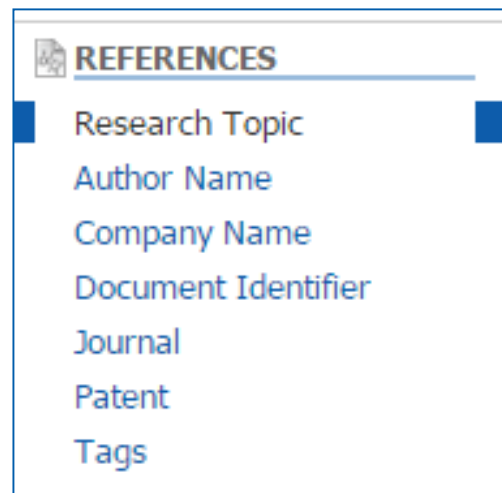
KEEP ME POSTED

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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: 功能分子材料的设计合成

- 检索词: 功能分子材料 设计 合成
- 检索式: synthesis of functional molecular

The screenshot shows the SciFinder web interface. At the top, there's a 'CAS Solutions' dropdown and the SciFinder logo. Below the logo are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The 'Explore' tab is active, showing a breadcrumb trail: 'Research Topic "synthesis of functional molecu..." > references (20601) > refine "design" (2692)'. On the left, a sidebar titled 'REFERENCES' lists various search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. The main content area is titled 'REFERENCES: RESEARCH TOPIC' and contains a search input field with the text 'synthesis of functional molecular'. Below the input field, there are examples of search results: 'Examples: The effect of antibiotic residues on dairy products' and 'Pho...'. A callout box with a purple border points to the search input field, containing the text '关键词之间可用介词连接: in, with, of...'. At the bottom of the main content area is a blue 'Search' button.

主题检索的候选项

Select All Deselect All	
0 of 5 Research Topic Candidates Selected	
	References
<input type="checkbox"/> 5 references were found containing "synthesis of functional molecular" as entered.	5
<input type="checkbox"/> 20601 references were found containing the two concepts "synthesis" and "functional molecular" closely associated with one another.	20601
<input type="checkbox"/> 78675 references were found where the two concepts "synthesis" and "functional molecular" were present anywhere in the reference.	78675
<input type="checkbox"/> 13540914 references were found containing the concept "synthesis".	13540914
<input type="checkbox"/> 476816 references were found containing the concept "functional molecular".	476816
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；

文献检索结果集—Refine

REFERENCES

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Analyze **Refine** Categorize

Sort by: Accession Number

0 of 20601 references Selected Page: 1 of 1031

Refine by:

☒ Research Topic

☐ Author

☐ Company Name

☐ Document Type

☐ Publication Year

☐ Language

☐ Database

Research Topic design

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

☐ 1. **Non-enzymatic glucose sensor based on molecularly imprinted polymer: a theoretical, strategy fabrication and application**
 Quick View Other Sources
By Wu, Haiyan; Tian, Qiong; Zheng, Wei; Jiang, Yan; Xu, Jicheng; Li, Xin; Zhang, Wenchi; Qiu, Fengxian
From Journal of Solid State Electrochemistry (2019), Ahead of Print. | Language: English, Database: CAPLUS
A comprehensive theor. screening of **functional** monomers, structural optimization, interaction energies (ΔE), and Gibbs free energy changes (ΔG) calcns. of the **prepn.** of **molecularly** imprinted polymer (MIP) were performed using d. **functional** theory (DFT) method. Based on the thermodyn. and interaction energy calcns., it is found that acrylamide (AAM) as a **functional** monomer candidate has the potential to interact with glucose more efficiently for the **prepn.** of MIP. In this work, on the basis of the theor. calcns. for the **functional** monomer selection in the MIP **prepn.**, an electrochem. impedance ...

☐ 2. **Molecular recognition and biological application of modified β -cyclodextrins**
 Quick View Other Sources
By Zhang, Ying-Ming; Xu, Qiao-Yan; Liu, Yu
From Science China: Chemistry (2019), Ahead of Print. | Language: English, Database: CAPLUS
The **mol.** recognition based on cyclodextrins (CDs) has become a focus of interest in modern supramol. chem. CDs are known to encapsulate various ions and org./inorg. **mols.** in their hydrophobic cavities and form stable inclusion complexes through cooperative noncovalent interactions. During the past few decades, a large variety of modified CDs have been elaborately designed and **synthesized**, which significantly promotes our **mol.**-level understanding of the structure-**function** relationship in many supramol. systems. Through the accurate anal. on the **mol.** binding behaviors, one can create a librar...

☐ 3. **Preparation and applications of dendronized polymer-enzyme conjugates**
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按被引次数排序— Citing References

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Tools

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Sort by:

Citing References
Accession Number
Author Name
Citing References
Publication Year
Title

Display Options

Page: 1 of 135

1. **... motors and mechanical machines**
By Kay, Euan R.; Leigh, David A.; Zerbetto, Francesco
From Angewandte Chemie, International Edition (2007), 46(1+2), 72-191. | Language: English, Database: CAPLUS
A review with refs. The widespread use of controlled **mol.**-level motion in key natural processes suggests that great rewards could come from bridging the gap between the present generation of **synthetic mol.** systems, which by and large rely upon electronic and chem. effects to carry out their **functions**, and the machines of the macroscopic world, which utilize the synchronized movements of smaller parts to perform specific tasks. This is a scientific area of great contemporary interest and extraordinary recent growth, yet the notion of **mol.**-level machines dates back to a time when the ideas sur... ~17212. **Functional polymers and dendrimers: reactivity, molecular architecture, and interfacial energy**
By Frechet, Jean M. J.
From Science (Washington, DC, United States) (1994), 263(5154), 1710-15. | Language: English, Database: CAPLUS
A review with 57 refs. on the **design** of 3-dimensional **synthetic** polymers and dendrimers to encapsulate reactive sites or provide highly controlled surfaces and interfaces. ~16653. **Metal-Organic Frameworks with Functional Pores for Recognition of Small Molecules**
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Citing Reference: 帮助找到最重要的文献

文献检索结果

文献分析工具

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获取原文

REFERENCES ?

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Analyze Refine Categorize

Sort by: Accession Number

0 of 2692 References Selected

Analyze by: Author Name

Author Name	Count
Feringa Ben L	21
Stoddart J Fraser	16
Li Xin	10
Weiss Paul S	10
Takeuchi Toshifumi	9
Zhang Shuang	9
Hedrick James L	8
Li Jing	8
Sarikaya Mehmet	8

1. **Molecular recognition and biological application of modified β -cyclodextrins**

Quick View Other Sources

By Zhang, Ying-Ming; Xu, Qiao-Yan; Liu, Yu

From Science China: Chemistry (2019), Ahead of Print. | Language: English, Database: CAPLUS

The **mol.** recognition based on cyclodextrins (CDs) has become a focus of interest in modern supramol. chem. CDs are known to encapsulate various ions and org./inorg. **mols.** in their hydrophobic cavities and form stable inclusion complexes through cooperative noncovalent interactions. During the past few decades, a large variety of modified CDs have been elaborately **designed** and **synthesized**, which significantly promotes our **mol.**-level understanding of the structure-**function** relationship in many supramol. systems. Through the accurate anal. on the **mol.** binding behaviors, one can create a librar...

2. **One kind of barley half dwarf gene ari-e.gp molecular marker and detection method [Machine Translation].**

Quick View Other Sources

By Jia, Qiaojun; Xie, Siyu; Wu, Kangjing; Wang, Feifeng

From Faming Zhuanli Shenqing (2019), CN 109554500 A 20190402. | Language: Chinese, Database: CAPLUS

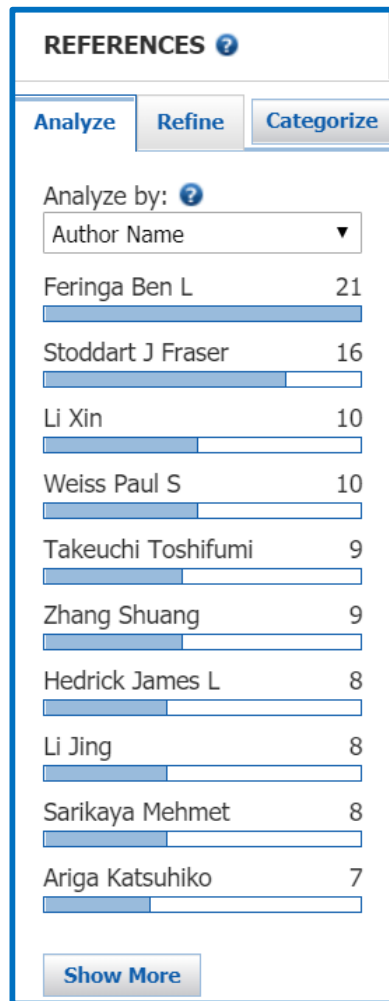
[Machine Translation of Descriptors]. The present invention provides a barley half e.GP Ari dwarf gene **mol.** marker and detection method thereof, which is characterized by that according to a first e.GP dwarf gene Ari-1508 1509 interposed between a base, base, causing the gene **functional** deletion and showed a dwarf insertion site, **designing** and **synthesizing** dCAPS **mol.** marker upstream primer, the nucleotide sequence is shown as SEQIDNO. 5 to downstream primer; the nucleotide sequence as shown by differential; SEQIDNO.6 PCR product by



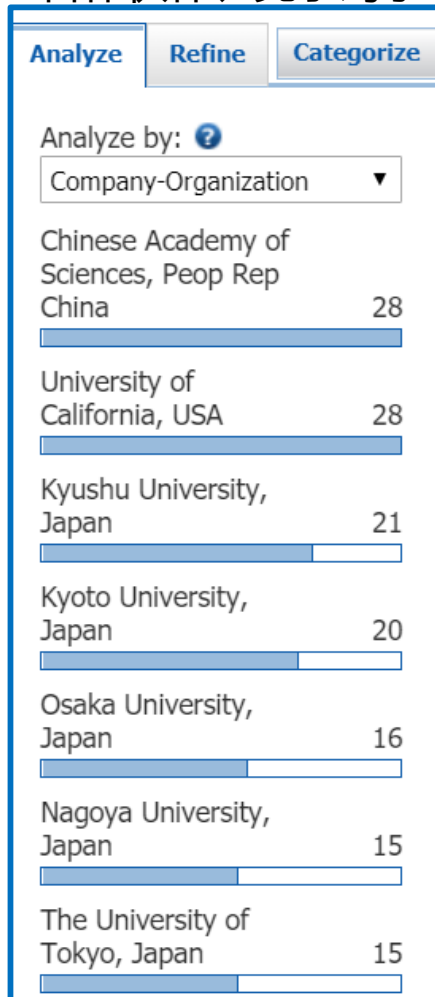
SciFinder提供强大的文献处理工具，帮助处理文献

文献检索结果的Analyze

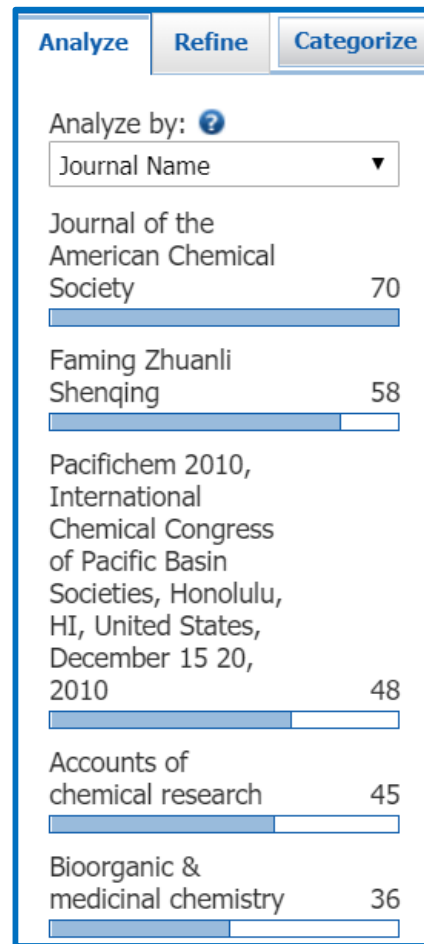
本领域研究人员



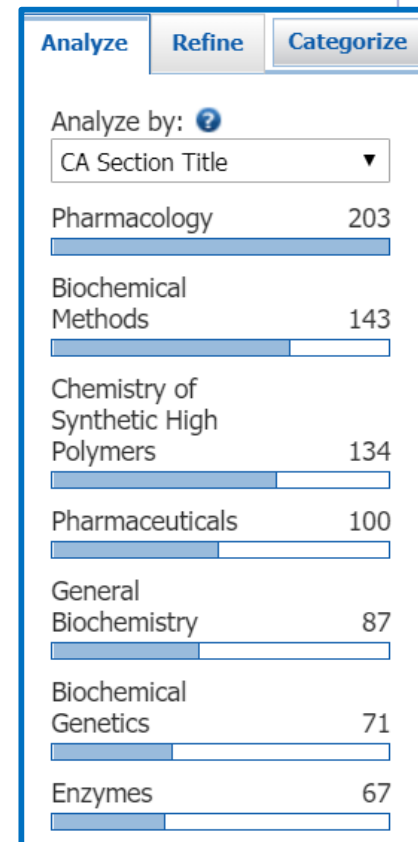
本领域研究机构、 合作伙伴、竞争对手



期刊

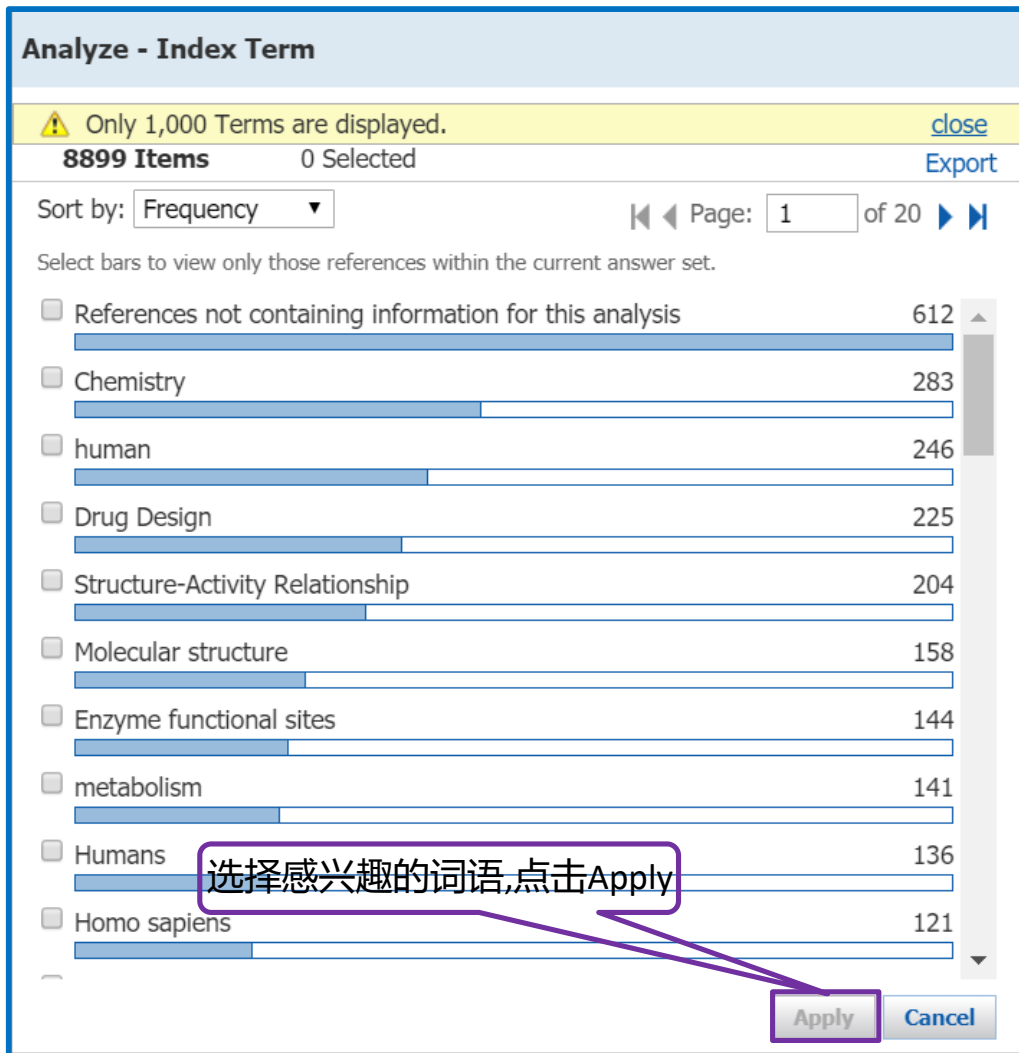
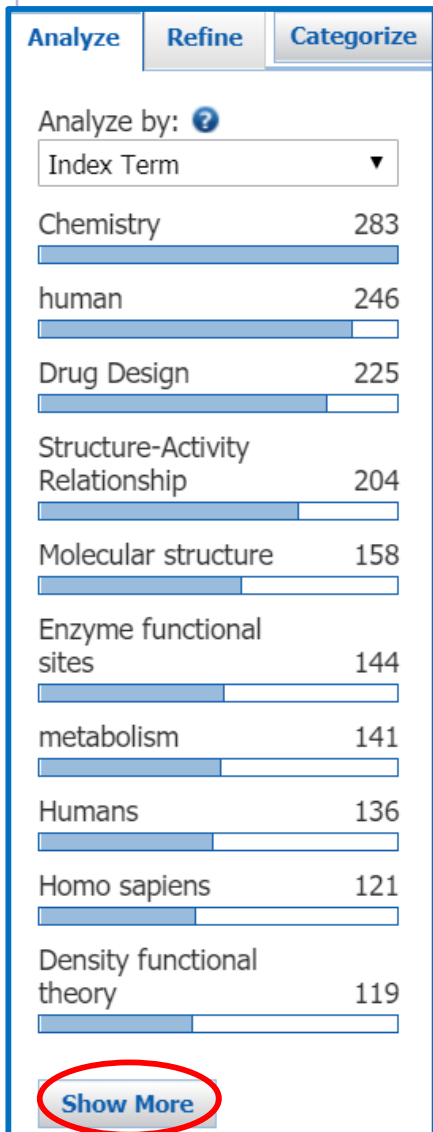


涉及学科领域

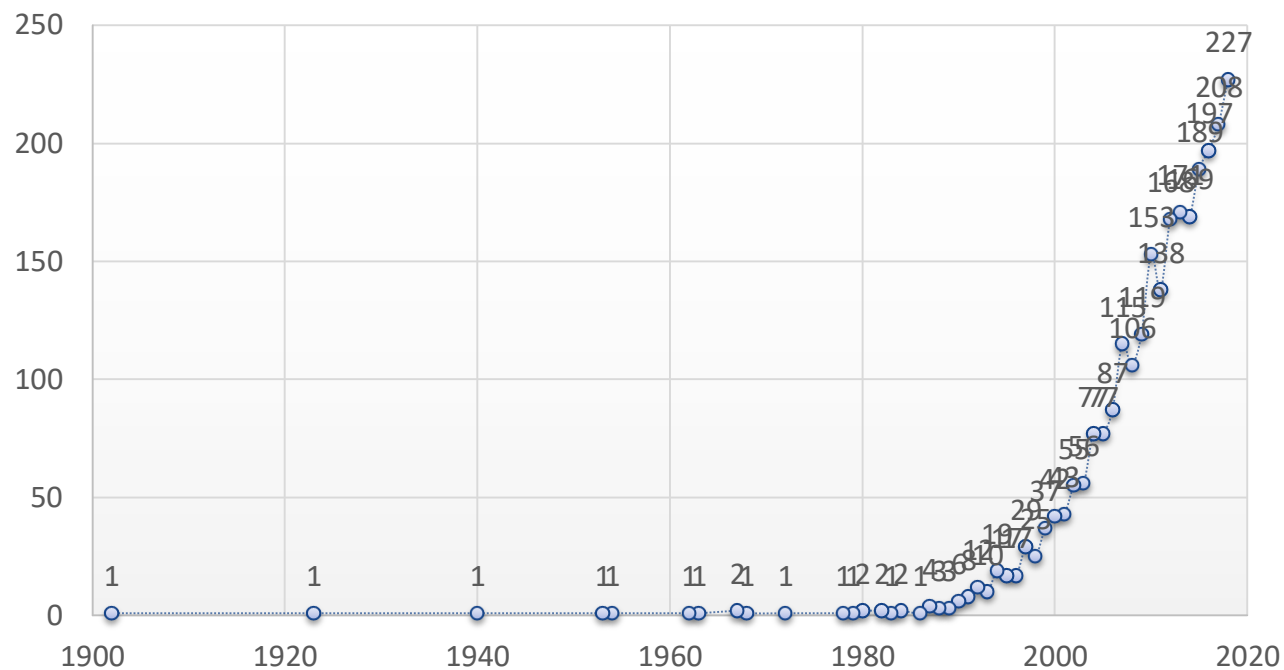
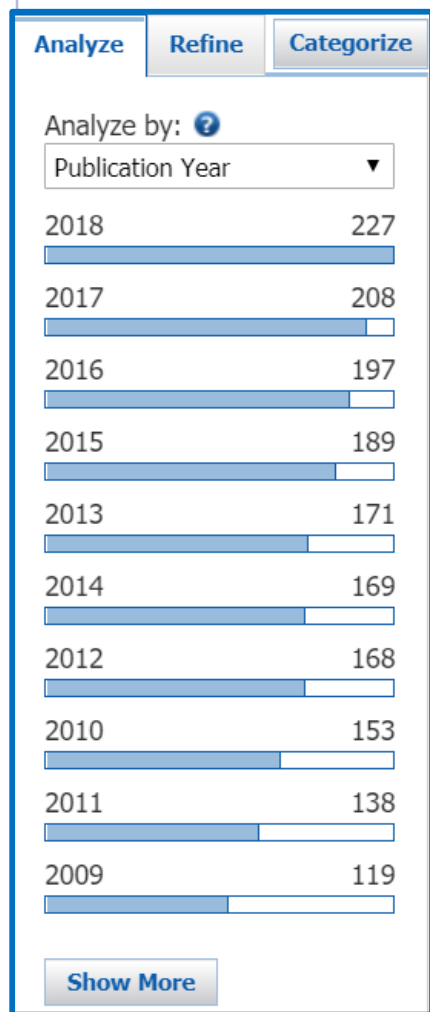


文献检索结果: Analyze

Index Term:帮助用户全景了解本领域涉及的重要技术术语, 精选文献



文献检索结果的Analyze—研究趋势图



Publication Year: 分析领域发展趋势

文献检索结果: Refine

Analyze

Refine

Categorize

Refine by: ?

☐ Research Topic

☐ Author

☐ Company Name

☒ Document Type

☐ Publication Year

☐ Language

☐ Database

Document Type

☐ Biography

☐ Book

☐ Clinical Trial

☐ Commentary

☐ Conference

☐ Dissertation

☐ Editorial

☐ Historical

☐ Journal

☐ Letter

☐ Patent

☐ Preprint

☐ Report

☒ Review

Refine

Get Substances

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Tools

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Sort by: Accession Number

0 of 610 References Selected

Page: 1 of 31

Display Options

☐ 1. **Advances in atom-transfer radical polymerization for drug delivery applications**

Quick View

Other Sources

By Rodrigues, Plinio Ribeiro; Vieira, Ronierik Pioli
From European Polymer Journal (2019), 115, 45-58. | Language: English, Database: CAPLUS

A review. The availability of appropriate materials is the main requisite for the **design** of controlled-release drug delivery systems (DDS), such as nanoparticles, micelles, microparticles, hydrogels and bioconjugates. These delivery platforms must be biocompatible and present appropriate mech., phys., chem. and biol. properties, allowing the desired control over drug loading and release and granting the benefits of this therapeutic administration route. Atom transfer radical polymn. (ATRP) is presently one of the most used methods of controlled polymn., applied to **synthesize** well-defined fu...

☐ 2. **Pharmacological effectors of GRP78 chaperone in cancers**

Quick View

Other Sources

By Bailly, Christian; Waring, Michael J.
From Biochemical Pharmacology (Amsterdam, Netherlands) (2019), 163, 269-278. | Language: English, Database: CAPLUS

A review. The protein chaperone GRP78 is a master regulator of endoplasmic reticulum (ER) **functions** and is frequently over-expressed at the surface of cancer cells where it contributes to chemo-resistance. It represents a well-studied ER stress marker but an under-explored target for new drug development. This review aims to untangle the structural and **functional** diversity of GRP78 modulators, covering over 130 natural products, **synthetic mols.**, specific peptides and monoclonal antibodies that target GRP78. Several approaches to promote or to incapacitate GRP78 are presented, including the...

☐ 3. **A review of theoretical study of graphene chemical vapor deposition synthesis on metals: nucleation, growth, and the role of hydrogen and oxygen**

Quick View

Other Sources

By Habib, Mohammad Rezwani; Liang, Tao; Yu, Xuegong; Pi, Xiaodong; Liu, Yingchun; Xu, Mingsheng
From Reports on Progress in Physics (2018), 81(3), 036501/1-036501/29. | Language: English, Database: CAPLUS

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	Reactants & reagents (9360)
General chemistry	Prepared substances (10940)
Synthetic chemistry	Reactions (322)
Physical chemistry	Bio-prepared substances (346)
Biotechnology	Purified substances (181)
Biology	Manufactured substances (129)
Genetics & protein chemistry	
Technology	
Polymer chemistry	
Analytical chemistry	
Catalysis	
Environmental chemistry	

2. Select index terms of interest.

Index Terms	
Page: 1 of 4	
Select All Deselect All	
<input checked="" type="checkbox"/> Polymerization	43
<input checked="" type="checkbox"/> Reaction kinetics	23
<input type="checkbox"/> Click chemistry	22
<input checked="" type="checkbox"/> Solvent effect	22
<input checked="" type="checkbox"/> Solid phase synthesis	21
<input type="checkbox"/> Electron transfer	18
<input checked="" type="checkbox"/> Crosslinking	17
<input checked="" type="checkbox"/> Reduction	17
<input type="checkbox"/> Synthesis	17
<input checked="" type="checkbox"/> Formation constant	16
<input checked="" type="checkbox"/> Dissociation constant	15
<input type="checkbox"/> Organic synthesis	15
<input type="checkbox"/> Redox reaction	14
<input checked="" type="checkbox"/> Stereochemistry	14
<input type="checkbox"/> Transition state structure	14
<input type="checkbox"/> Oxidation	13
<input type="checkbox"/> Radical atom transfer	13

Selected Terms
Click 'x' to remove the category from 'Selected Terms'
<input checked="" type="checkbox"/> Synthetic chemistry >
<input checked="" type="checkbox"/> 聚合
<input checked="" type="checkbox"/> 反应动力学
<input checked="" type="checkbox"/> 溶剂效应
<input checked="" type="checkbox"/> 固相合成
<input checked="" type="checkbox"/> 交联
<input checked="" type="checkbox"/> 还原
<input checked="" type="checkbox"/> 形成常数
<input checked="" type="checkbox"/> 解离常数
<input checked="" type="checkbox"/> 立体化学

Synthetic chemistry > Reactions > 9 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. 2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (1823)	Page: 1 of 4 Select All Deselect All	分子模拟 the category from
General chemistry	Processes & apparatus (327)	<input checked="" type="checkbox"/> Molecular modeling 104	自组装 by > Processes &
Synthetic chemistry	Materials & products (411)	<input checked="" type="checkbox"/> Self-assembly 100	分子对接
Physical chemistry	Metallurgy (84)	<input checked="" type="checkbox"/> Molecular docking 99	仿真与建模
Biotechnology	Formed, removed, & other substances (174)	<input checked="" type="checkbox"/> Simulation and Modeling 88	分子动力学模拟
Biology	Imaging & recording (48)	<input type="checkbox"/> Adsorption 57	分子开关
Genetics & protein chemistry	Power & fuel topics (22)	<input checked="" type="checkbox"/> Molecular dynamics simulation 42	
Technology	Ceramics (8)	<input type="checkbox"/> Sensors 25	
Polymer chemistry	Construction (9)	<input checked="" type="checkbox"/> Molecular switches 20	
Analytical chemistry		<input type="checkbox"/> Biosensors 19	
Catalysis		<input type="checkbox"/> Nanomachines 18	
Environmental chemistry		<input type="checkbox"/> Surface treatment 17	
		<input type="checkbox"/> Aggregation 14	
		<input type="checkbox"/> Electroluminescent devices 14	
		<input type="checkbox"/> Solid phase extraction 14	

Technology > Processes & apparatus > 6 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	Substances in technology (1823)
General chemistry	Processes & apparatus (327)
Synthetic chemistry	Materials & products (411)
Physical chemistry	Metallurgy (84)
Biotechnology	Formed, removed, & other substances (174)
Biology	Imaging & recording (48)
Genetics & protein chemistry	Power & fuel topics (22)
Technology	Ceramics (8)
Polymer chemistry	Construction (9)
Analytical chemistry	
Catalysis	
Environmental chemistry	

2. Select index terms of interest.

Index Terms	
Page: 1 of 5	
Select All Deselect All	
<input checked="" type="checkbox"/> Fluorescent indicators	30
<input checked="" type="checkbox"/> Antibacterial agents	28
<input type="checkbox"/> Nanostructured materials	19
<input type="checkbox"/> Hydrogen	17
<input type="checkbox"/> Oxygen	17
<input type="checkbox"/> Graphene	15
<input checked="" type="checkbox"/> Antibiotics	14
<input type="checkbox"/> Films	14
<input type="checkbox"/> Fluorescent substances	14
<input type="checkbox"/> Self-assembled monolayers	14
<input checked="" type="checkbox"/> Antioxidants	13
<input type="checkbox"/> Chromophores	13
<input type="checkbox"/> Hybrid organic-inorganic materials	13
<input checked="" type="checkbox"/> Imaging agents	13
<input type="checkbox"/> Semiconductor materials	13

Selected Terms
荧光指示剂
抗菌剂
抗生素
抗氧化剂
显像剂

Technology > Materials & products > 5 Index Term(s) Selected

OK

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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

ational molecu... > references (20601) > refine "design" (2692) > refine by categories > Synthesis and Structural/Funct...

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

Sort by: Accession Number 0 of 30 References Selected Page: 1 of 2

1. **Synthesis and Structural/Functional Characterization of Selective M14 Metallo-carboxypeptidase Inhibitors Based on Phosphinic Pseudopeptide Scaffold: Implications on the Design of Specific Optical Probes**

By Covalada, Giovanni; Gallego, Pablo; Vendrell, Josep; Georgiadis, Dimitris; Lorenzo, Julia; Dive, Vincent; Aviles, Francisco; From Journal of Medicinal Chemistry (2019), 62(4), 1917-1931. | Language: English, Database: CAPLUS

Metallo-carboxypeptidases of the M14 family (MCPs) are found in every tissue or fluid in mammals. These enzymes perform a large variety of physiological functions such as pancreatic diseases, inflammation, fibrinolysis and cancer. Here we describe the **synthesis** and **functional/structural** characterization of a series of reversible tight-binding phosphinic pseudopeptide inhibitors that show high specificity and potency towards these proteases. Characterization of their inhibitory potential against a large variety of MCPs, ...

2. **Chemo- and Regioselective Lysine Modification on Native Proteins**

By Matos, Maria J.; Oliveira, Bruno L.; Martinez-Saez, Nuria; Guerreiro, Ana; Cal, Pedro M. S. D.; Bertoldo, Jean; Maneiro, Maria; Perkins, Elizabeth; Howard, Julie; Deery, Michael J.; et al. From Journal of the American Chemical Society (2018), 140(11), 4004-4017. | Language: English, Database: CAPLUS

文献详细信息

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Export: 导出至本地电脑。

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Export

Export:

☒ All
☐ Selected
☐ Range

Example: 2-20

For:

Citation Manager

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☐ Quoted Format (*.txt)
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Format:

☐ Summary without abstracts
☐ Summary with partial abstracts
☒ Summary with full abstracts
☐ Detail (full record)

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☐ Tags
☐ Comments

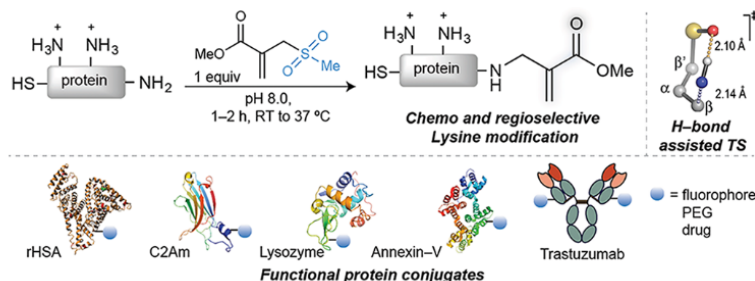
Export Cancel

文献信息—题录、摘要、索引

2. Chemo- and Regioselective Lysine Modification on Native Proteins

By: Matos, Maria J.; Oliveira, Bruno L.; Martinez-Saez, Nuria; Guerreiro, Ana; Cal, Pedro M. S. D.; Bertoldo, Jean; Maneiro, Maria; Perkins, Elizabeth; Howard, Julie; Deery, Michael J.; Chalker, Justin M.; Corzana, Francisco; Jimenez-Oses, Gonzalo; Bernardes, Goncalo J. L.

Site-selective chem. conjugation of **synthetic mols.** to proteins expands their **functional** and therapeutic capacity. Current protein modification methods, based on **synthetic** and **biochem.** technologies, can achieve site selectivity, but these techniques often require extensive sequence engineering or are restricted to the N- or C-terminus. Here we show the computer-assisted **design** of sulfonyl acrylate reagents for the modification of a single lysine residue on native protein sequences. This feature of the **designed** sulfonyl acrylates, together with the innate and subtle reactivity differences conferred by the unique local microenvironment surrounding each lysine, contribute to the **obsd.** regioselectivity of the reaction. Moreover, this site selectivity was predicted computationally, where the lysine with the lowest pK_a was the kinetically favored residue at slightly basic pH. Chemoselectivity was also **obsd.** as the reagent reacted preferentially at lysine, even in those cases when other nucleophilic residues such as cysteine were present. The reaction is fast and proceeds using a single molar equivalent of the sulfonyl acrylate reagent under biocompatible conditions (37°, pH 8.0). This technol. was demonstrated by the quant. and irreversible modification of five different proteins including the clin. used therapeutic antibody Trastuzumab without prior sequence engineering. Importantly, their native secondary structure and **functionality** is retained after the modification. This regioselective lysine modification method allows for further bioconjugation through aza-Michael addn. to the acrylate electrophile that is generated by spontaneous elimination of methanesulfonic acid upon lysine labeling. We showed that a protein-antibody conjugate bearing a site-specifically installed fluorophore at lysine could be used for selective imaging of apoptotic cells and detection of Her2+ cells, resp. This simple, robust method does not require genetic engineering and may be generally used for accessing diverse well-defined protein conjugates for basic biol. and therapeutic studies.



书目信息

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Journal of the American Chemical Society
Volume 140
Issue 11
Pages 4004-4017
Journal; Online Computer File
2018
CODEN: JACSAT
ISSN: 0002-7863
DOI: 10.1021/jacs.7b12874

COMPANY/ORGANIZATION

Department of Chemistry
University of Cambridge
Cambridge, UK

ACCESSION NUMBER

2018:328593
CAN168:490507
CAPLUS

PUBLISHER

American Chemical Society

LANGUAGE

English

Indexing

Biochemical Methods (Section 9-14)

Section cross-reference(s): 63

重要概念

Concepts

Synaptotagmin 1

C2Am domain; chemo- and regioselective lysine reagents

重要物质

Substances

180288-69-1DP Trastuzumab, conjugates with sulfonyl acrylate reagent and crizotinib
877399-52-5DP Crizotinib, conjugates with trastuzumab

chemo- and regioselective lysine modification on native proteins using computer-assisted **designed** sulfonyl acrylate reagents

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

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 根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

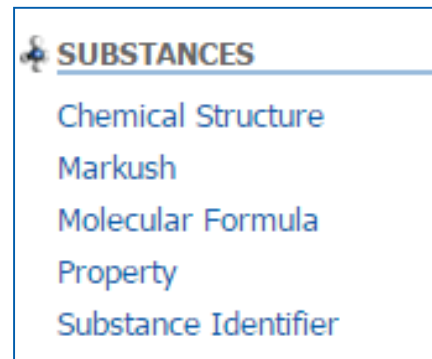
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - 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

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。

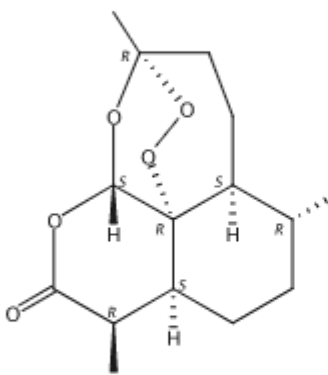
SciFinder中的物质记录

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. 63968-64-9

~5009 ~123



Absolute stereochemistry.

C₁₅ H₂₂ O₅
3,12-Epoxy-12H-pyrano[4,3-f]-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

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SciFinder中的物质记录

SUBSTANCE DETAIL ?

Get References

Get Reactions

Get Commercial Sources

Return

CAS Registry Number 63968-64-9

~5,009 ~123

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...

由物质获得文献，反应，供应商等信息

Absolute stereochemistry.

物质详情

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Get References

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	

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Chinese Annotations:

- 分析化学 (Analytical Chemistry) points to Analytical Study
- 晶体结构 (Crystal Structure) points to Crystal Structure
- 制备 (Preparation) points to Preparation
- 工艺 (Process) points to Process
- 谱图性质性质 (Spectral Properties) points to Spectral Properties

EXPERIMENTAL PROPERTIES

Biological Chemical Density Flow and Diffusion Lipinski Optical and Scattering Structure Related Thermal

Structure Related Properties

Property	Value
Bond Angle	See full text
Bond Length	See full text
Permeability	See full text
X-Ray Diffraction Pattern	See full text

Notes

- (2) Galasso, V.; Chemical Physics 2007, V335(2-3), P141-154 CAPLUS
- (23) Du-Cuny, Lei; Bioorganic & Medicinal Chemistry 2009, V17(19), P
- (25) Sahoo, Nanda Gopal; Journal of Pharmaceutical Sciences 2009, V

实验数据与实验谱图

Note

(2)CAS

(2)CAS

1 of 4

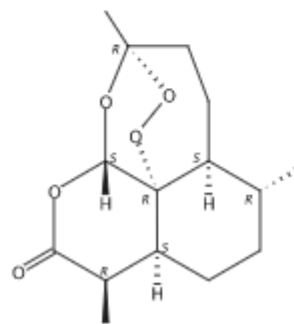
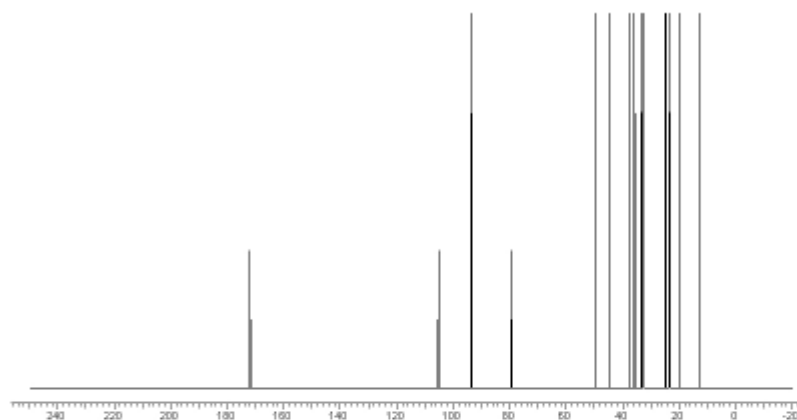
EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman

¹³C NMR Properties

Property	Value
Carbon-13 NMR Spectrum	See spectrum
Carbon-13 NMR Spectrum	See spectrum
Carbon-13 NMR Spectrum	See full text

Carbon-13 NMR Spectrum



Abiraterone chemical structure

FORMULA

C₂₅H₂₂O₅

CAS INDEX NAME

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

NUCLEUS

¹³C

SOURCE

Spectral data were obtained from Advanced Chemistry Development, Inc.

物质检索——理化性质性质检索

SUBSTANCES: PROPERTY ?

☒ Experimental

Select Property... ▼

Select Property...

Boiling Point (°C)

Density (g/cm³)

Electric Conductance (S)

Electric Conductivity (S/cm)

Electric Resistance (ohm)

Electric Resistivity (ohm*cm)

Glass Transition Temp. (°C)

Magnetic Moment (μB)

Median Lethal Dose (LD50) (mg/kg)

Melting Point (°C)

Optical Rotatory Power (degrees)

Refractive Index

Tensile Strength (MPa)

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Explore

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

Select Property... ▼


Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Examples: 44, 25-35, >125

Search

物质检索——理化性质检索：寻找分子量在300—400之间的黄酮类化合物

 **REFERENCES**

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[Journal](#)

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 **SUBSTANCES**


[Chemical Structure](#)

[Markush](#)

[Molecular Formula](#)

[Property](#)

[Substance Identifier](#)

 **REACTIONS**

[Reaction Structure](#)

SUBSTANCES: PROPERTY ?

☐ Experimental

Select Property...

▼

Examples: 44, 25-35, >125

☒ Predicted

Molecular Weight

▼

300-400

Examples: 44, 25-35, >125

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SUBSTANCES

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0 36450079 Substances Selected Page: 1 of 2430006

Refine by:

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

Structure Editor:

Java Non-Java

Search type: **Exact Structure**

Only retrieve substances that:

1. **2276697-80-2**

C₂₂H₃₄O₃Si
1-Cyclohexene-1-carboxaldehyde, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-5-[(4-methylphenyl)methoxy]-, (3*R*,5*R*)-

[Key Physical Properties](#)

2. **2276697-79-9**

C₂₁H₃₁F O₃ Si
1-Cyclohexene-1-carboxaldehyde, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-[(4-fluorophenyl)methoxy]-2-methyl-, (3*R*,5*R*)-

[Key Physical Properties](#)

3. **2276697-78-8**

C₂₂H₃₃N O₂ Si
1-Cyclohexene-1-carbonitrile, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-5-[(4-methylphenyl)methoxy]-, (3*R*,5*R*)-

[Key Physical Properties](#)

4. **2276697-77-7**

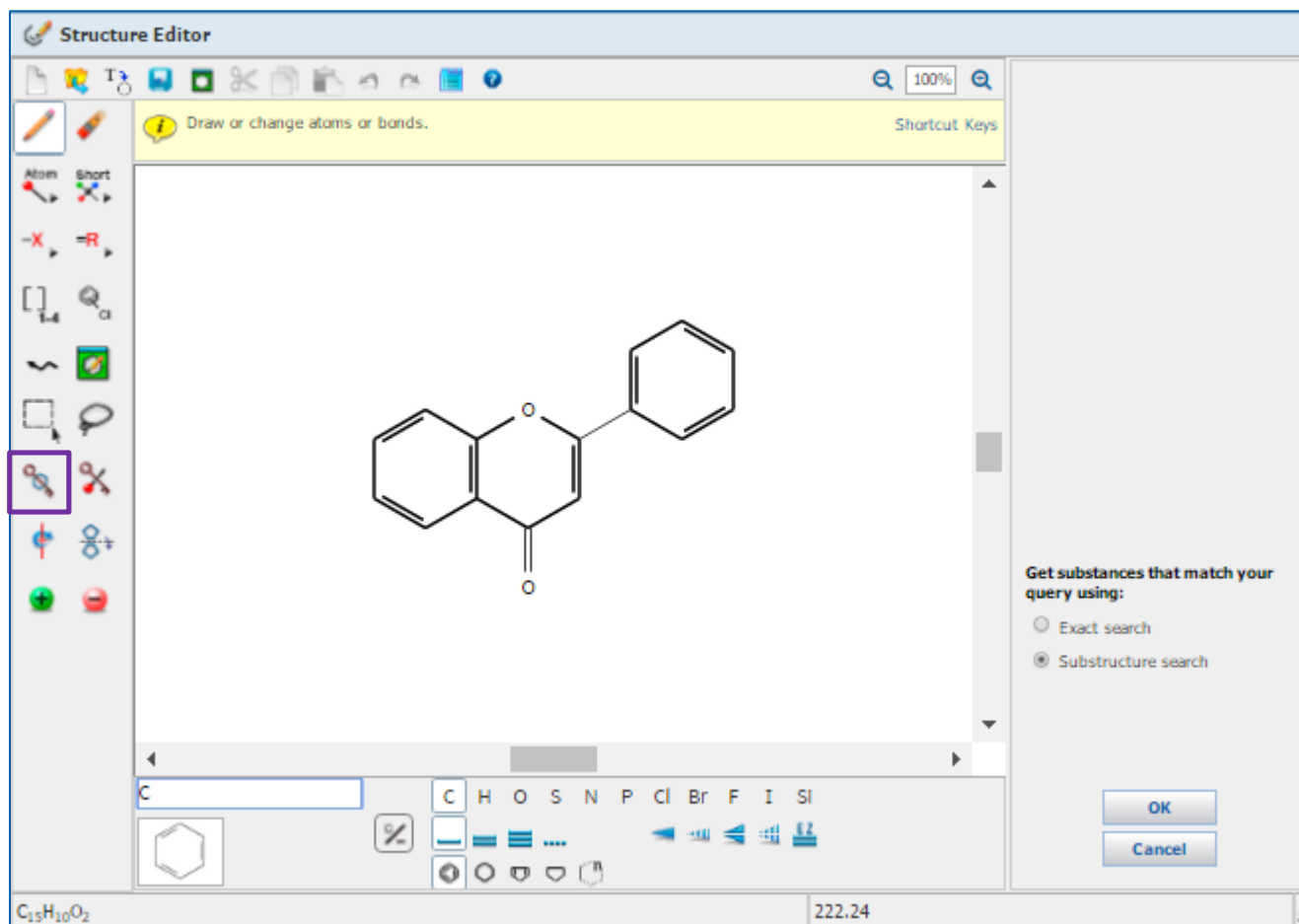
C₂₀H₃₉N O₂ Si₂

5. **2276697-74-4**

6. **2276697-53-9**

3600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

SUBSTANCES ?

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

物质检索结果集

SUBSTANCES ?

Get ReferencesGet ReactionsGet Commercial SourcesTools

AnalyzeRefine

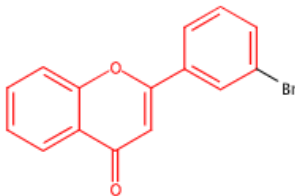
Analyze by: ?
Substance Role

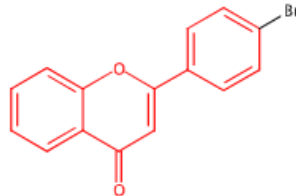
Preparation7670
Biological Study6066
Uses4109
Reactant or Reagent3432
Properties2751
Analytical Study784
Occurrence678
Process337
Formation, Nonpreparative153
Prophetic in Patents75

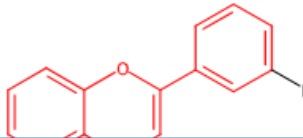
Show More

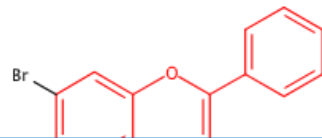
Sort by: Relevance

0 of 15312 Substances Selected

1. 3754-53-8
~34

C₁₅ H₉ Br O₂
4/1-benzopyran-4-one, 2-(3-bromophenyl)-
Key Physical Properties
Experimental Properties

2. 20525-20-6
~100

C₁₅ H₉ Br O₂
4/1-benzopyran-4-one, 2-(4-bromophenyl)-
Key Physical Properties
Spectra
Experimental Properties


4. 1026-41-1
~12

C₁₅ H₉ I O₂
4/1-benzopyran-4-one, 2-(3-iodophenyl)-
Key Physical Properties
Experimental Properties

5. 1148-47-6
~38

C₁₅ H₉ Br O₂
4/1-benzopyran-4-one, 2-(4-bromophenyl)-
Key Physical Properties
Spectra
Experimental Properties

从3600多万个结构中
筛选出15312个黄酮类物质

分子式检索


CAS Solutions ▾

 **SciFINDER®**
A CAS SOLUTION

Explore ▾

Saved Searches ▾

SciPlanner

 **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

分子式书写规则—Hill 规则

- 单一组分物质：
 - 对于不含C的物质，按照字母顺序排序
 - 对于含C的物质，C、H写在前面，其他的按照字母顺序排列
 - 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
 - 区分大小写
- 多组分物质：
 - 每一组分必须遵照单一组分物质的分子式来书写。
 - 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。**用点将不同的组分分开**
 - 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

盐的检索——十二烷基磺酸钠

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction

SUBSTANCES: MOLECULAR FORMULA ?

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

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

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

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

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

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

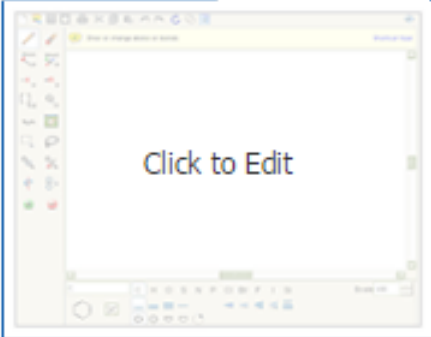
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:


Java Non-Java



Search Type:


- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

 **ChemDraw**
Launch a SciFinder substance or reaction

Import CXF

Search

 Advanced Search ☒ Always Show

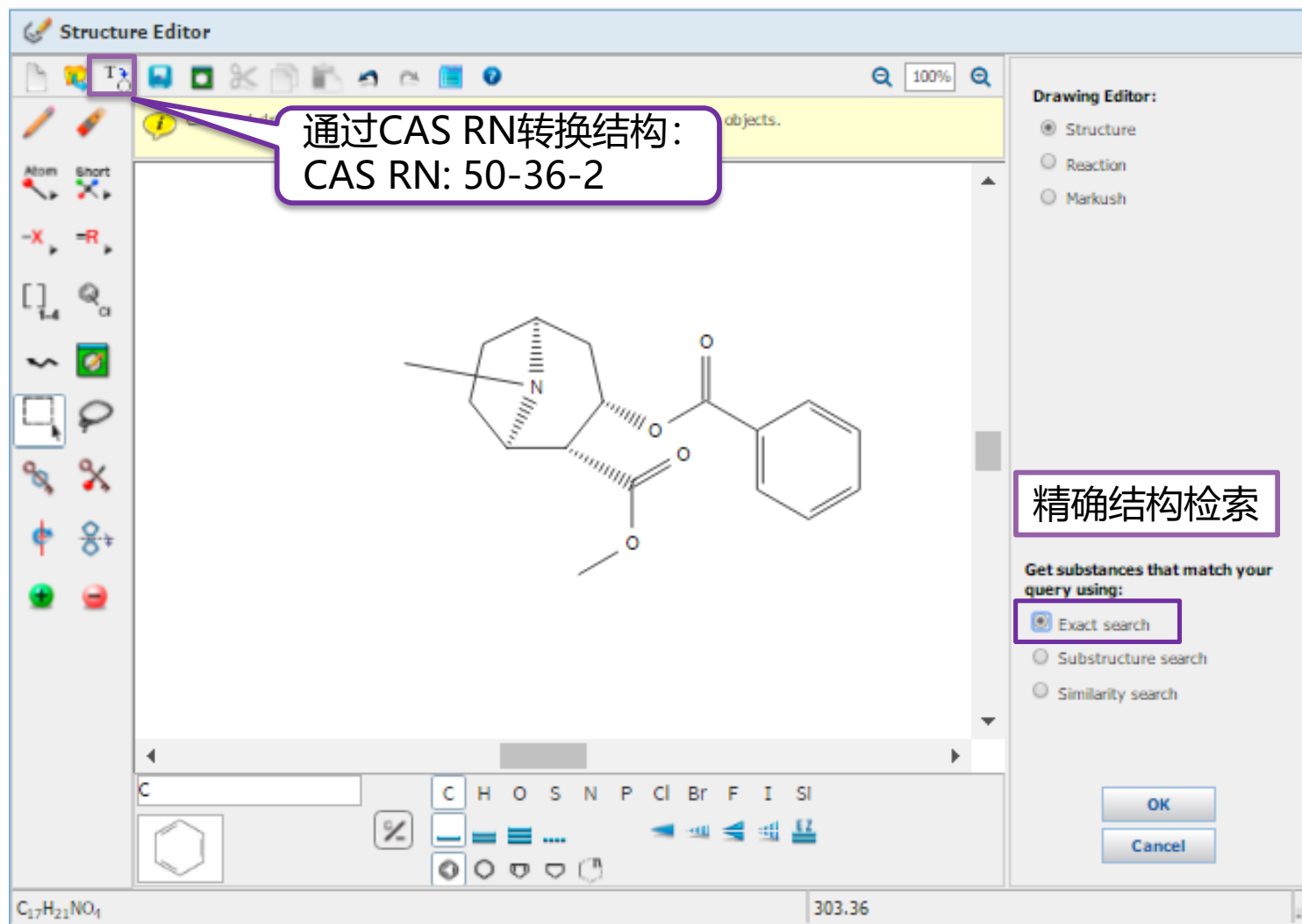
物质检索——结构

The image shows the SciFinder Structure Editor interface with various tool labels in Chinese. The labels are connected to specific tools or functions in the software:

- 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)
- 负电子 (Electron)
- 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 (Loop Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Ring, Polycyclic Ring Tool)
- 结构检索选择 (Structure Search Selection)

The interface includes a toolbar with icons for drawing and editing, a central workspace for the chemical structure, and a right-hand panel for search options (Exact search, Substructure search, Similarity search) and buttons for '确定' (OK) and '取消' (Cancel).

物质检索——精确结构检索



精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**

~18 ~1

Absolute stereochemistry.

$C_{17}H_{21}NO_4$
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**

~5

可卡因组合物

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

Absolute stereochemistry.

88-89-1
 $C_6H_3N_3O_7$

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

3. **109496-04-0**

(Component: 668-19-9)

~1

* HCl

Absolute stereochemistry.

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

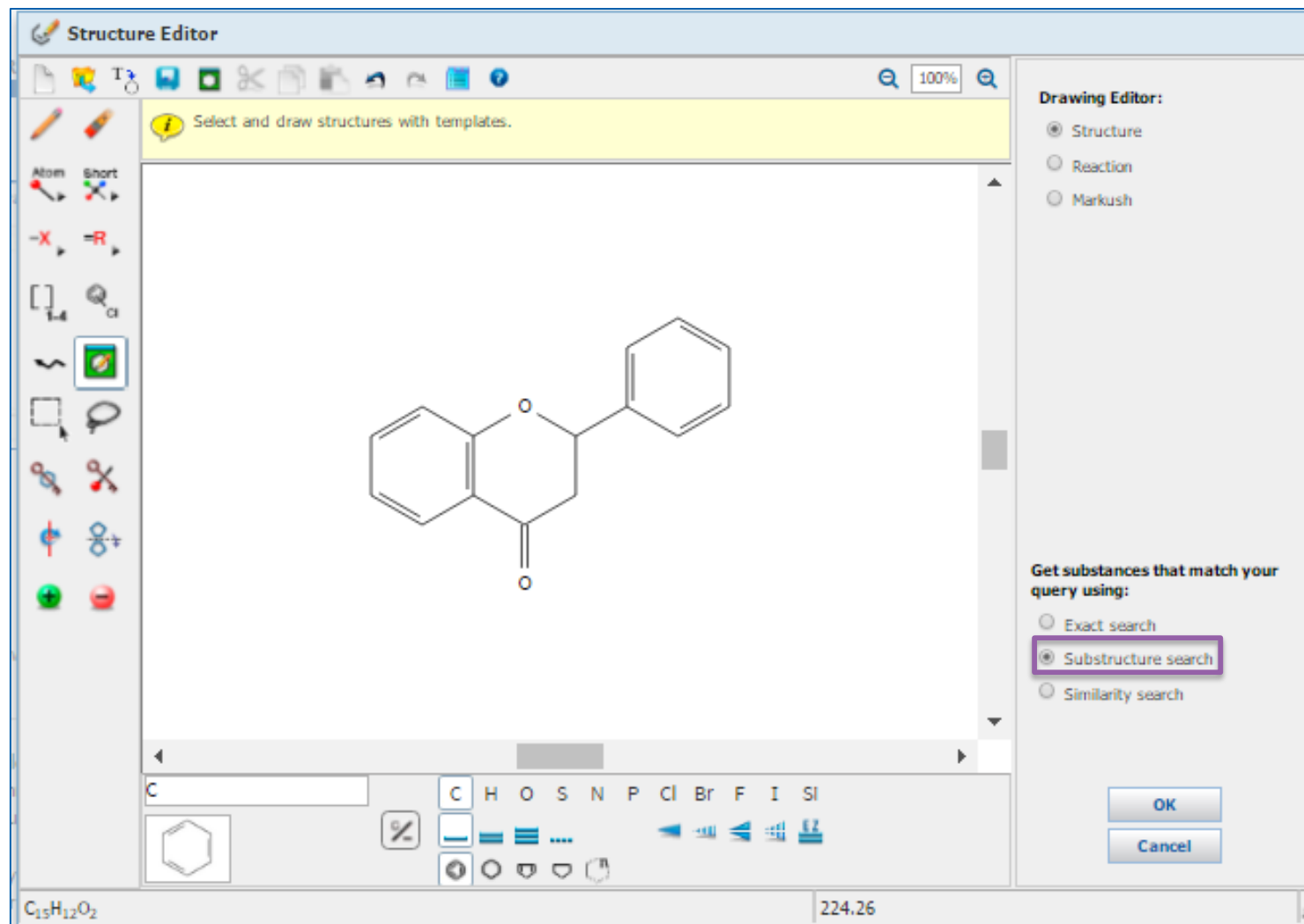
盐酸可卡因

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

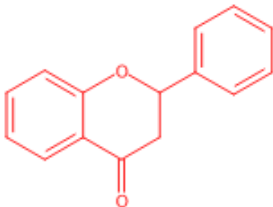


物质检索——亚结构检索

0 of 23824 Substances Selected

1. **487-26-3**

~2093

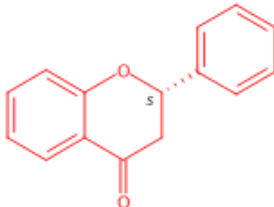


C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. **17002-31-2**

~244



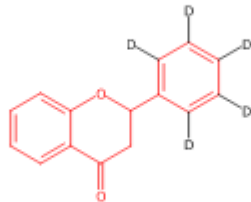
Absolute stereochemistry...Rotation (-).

C₁₅H₁₂O₂
4-phenyl-4H-benzopyran-4-one, 2,3-dihydro-

▶ **Key Physical Properties**
Experimental Properties

10. **146196-91-0**

~1 ~5



C₁₅H₇D₅O₂
4-(2,3,4,5-tetradeuteriophenyl)-4H-benzopyran-4-one, 2,3-dihydro- (9CI)

Spectra

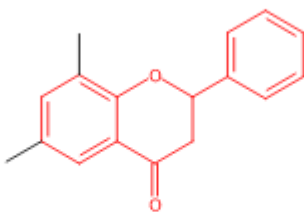
同位素

亚结构检索结果

281. 123251-10-5

~3 ~1

取代物



$C_{17}H_{16}O_2$

4H-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

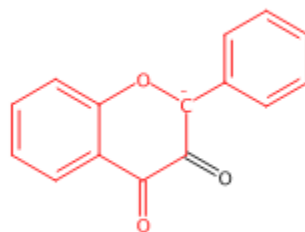
► Key Physical Properties

Experimental Properties

295. 780723-19-5

~0

离子



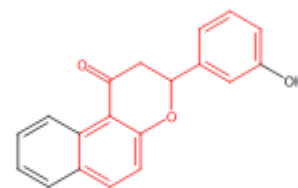
$C_{15}H_9O_3$

2H-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

~2

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



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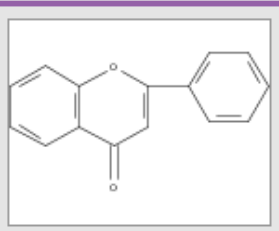
亚结构检索结果的限定

Analysis Refine

Refine by:

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

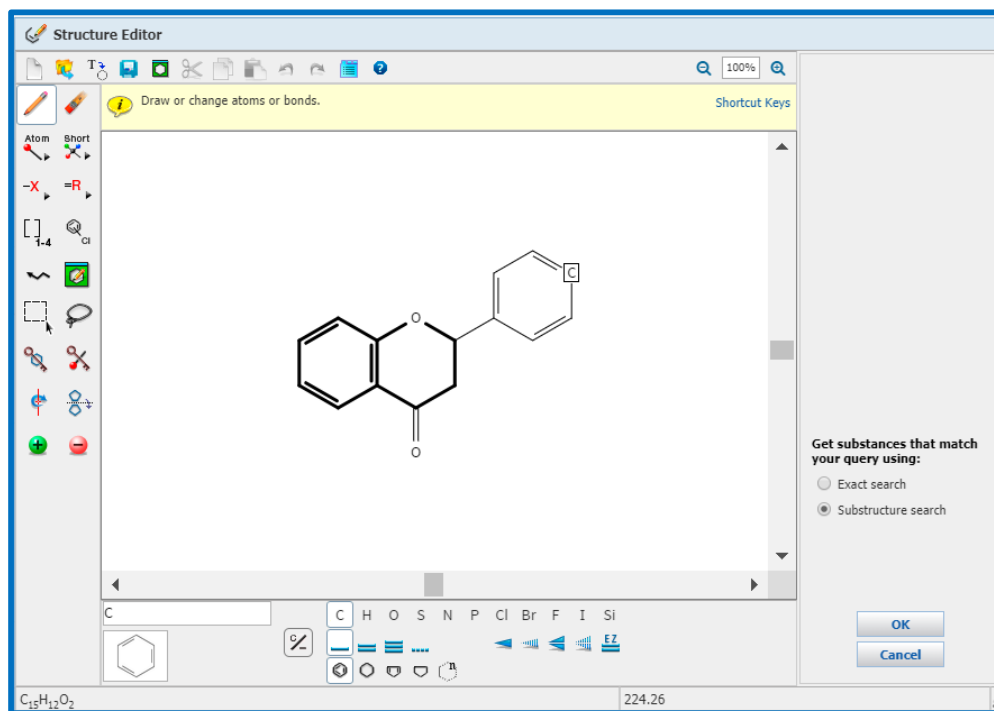
Chemical Structure:



Click image to change structure or view detail

Search type: **Substructure**

化学结构的再次限定



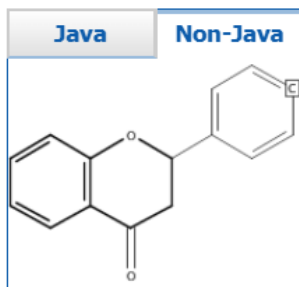
环锁定



原子锁定

亚结构检索结果的限定

Structure Editor:



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

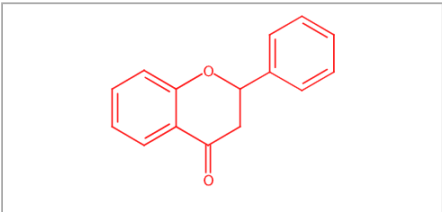
Sort by: Relevance

0 of 4459 Substances Selected

Page: 1 of 298

1. **487-26-3**

~2455 ~83

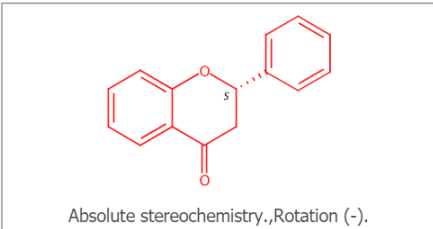


C₁₅H₁₂O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

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

2. **17002-31-2**

~269 ~10



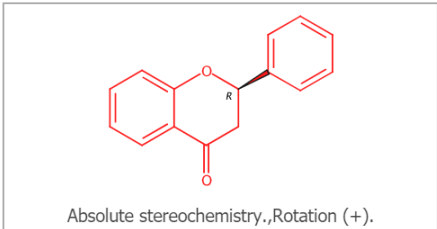
Absolute stereochemistry.,Rotation (-).

C₁₅H₁₂O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

► **Key Physical Properties**
Experimental Properties

3. **27439-12-9**

~238 ~8



Absolute stereochemistry.,Rotation (+).

C₁₅H₁₂O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*R*)-

► **Key Physical Properties**
Experimental Properties

4. **104550-32-5**

~3

5. **75524-43-5**

~2

6. **146196-89-6**

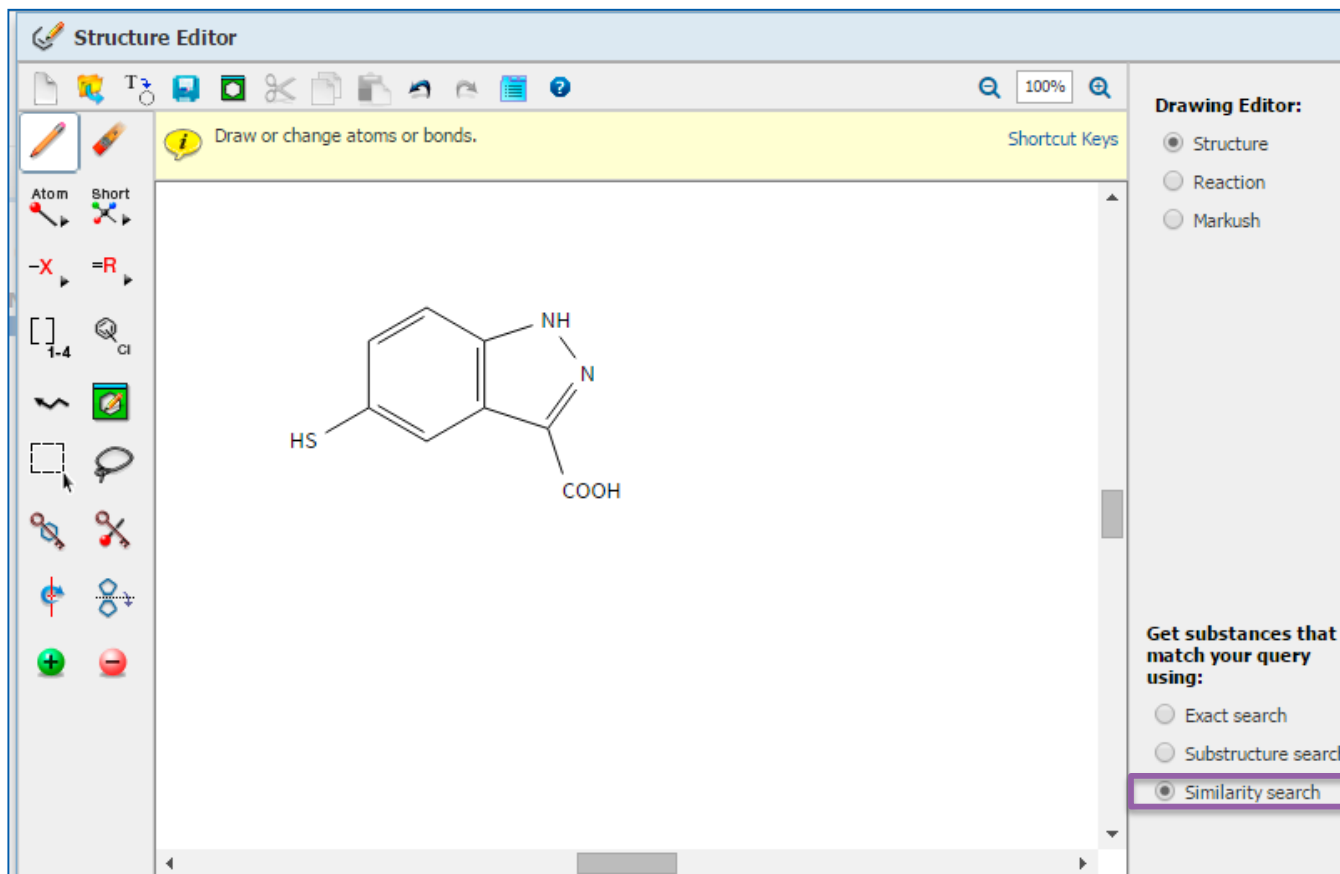
~2

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

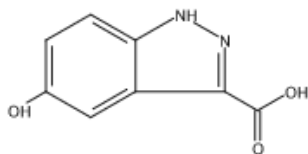
评分越高，相似度越高，结构越相似

Score: 88

☐ 1. 885518-94-5

取代基变化

~1 ~35



$C_8 H_6 N_2 O_3$

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

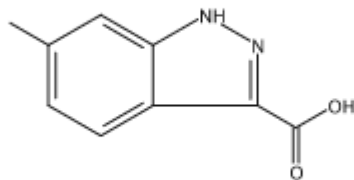
► Key Physical Properties

Score: 86

☐ 5. 858227-12-0

取代基位置变化

~7 ~41



$C_9 H_8 N_2 O_2$

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

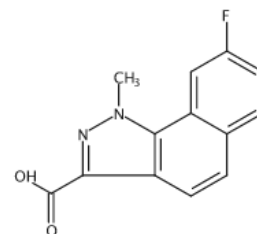
► Key Physical Properties

Score: 65

☐ 541. 1100422-

母体结构变化

~1



$C_{13} H_9 F N_2 O_2$

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

► Key Physical Properties



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A CAS SOLUTION

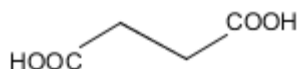
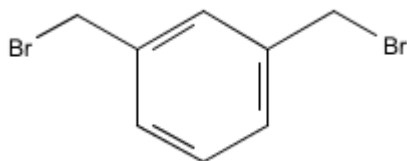
物质检索——相似结构检索

- 相似结构检索：

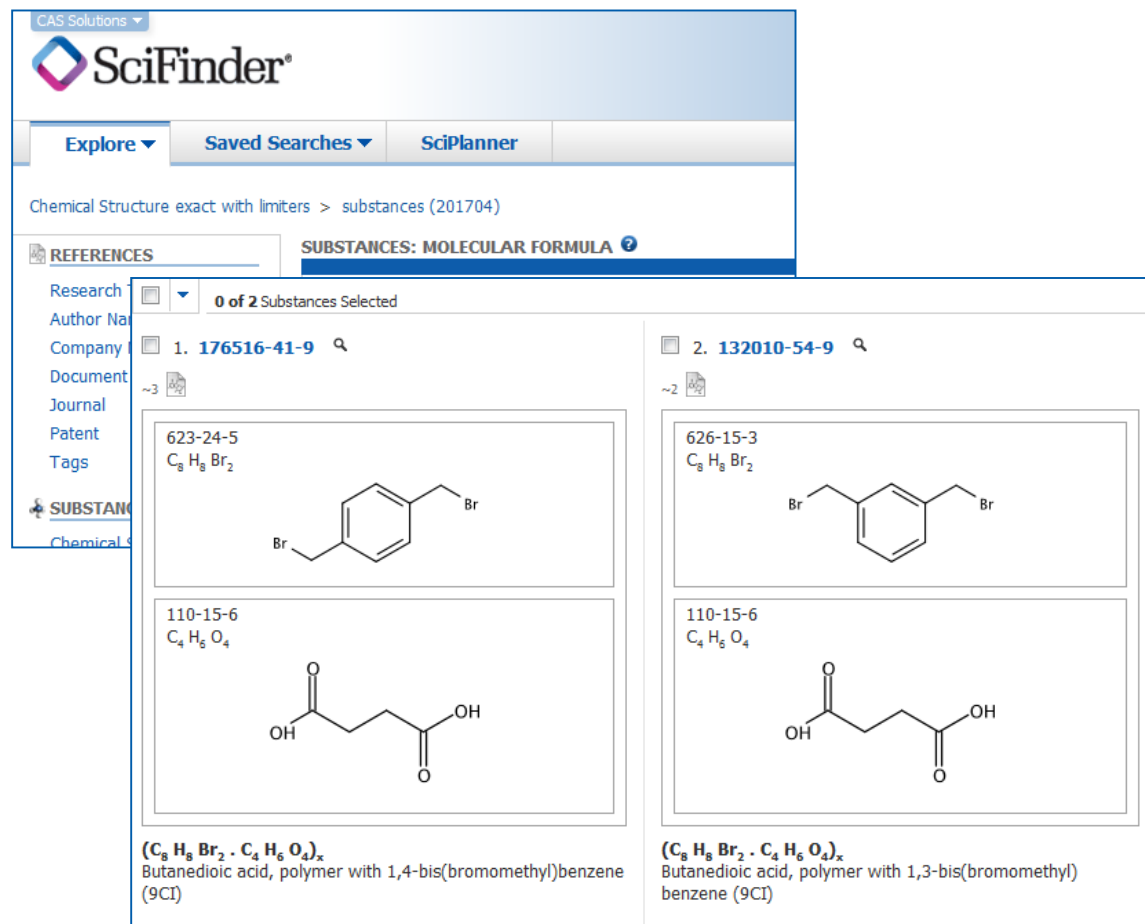
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

聚合物的检索

已知起始原料的聚合物



$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$



Chemical Structure exact with limiters > substances (201704)

REFERENCES

0 of 2 Substances Selected

1. 176516-41-9

2. 132010-54-9

623-24-5
 $C_8H_8Br_2$

626-15-3
 $C_8H_8Br_2$

110-15-6
 $C_4H_6O_4$

110-15-6
 $C_4H_6O_4$

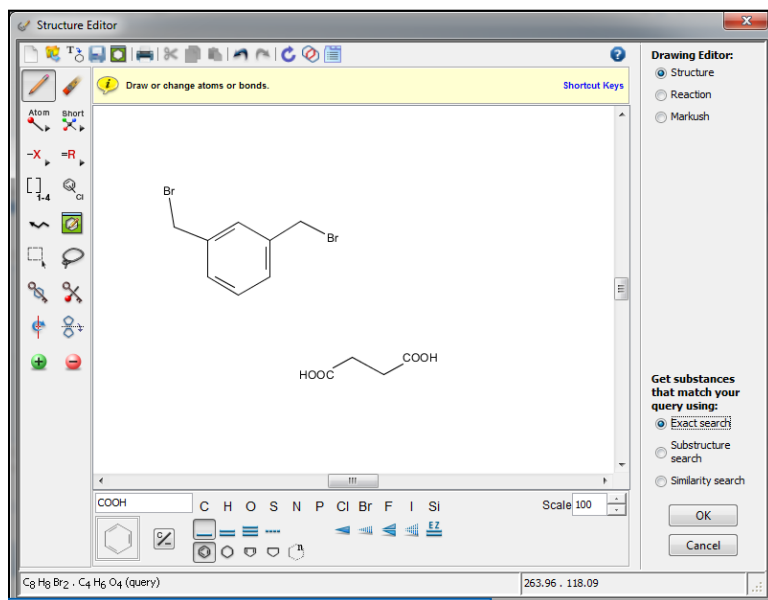
$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,4-bis(bromomethyl)benzene (9CI)

$(C_8H_8Br_2 \cdot C_4H_6O_4)_x$
Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

分子式检索后会得到同分异构体



聚合物的检索



- | | |
|-----------------|--|
| Characteristics | <input checked="" type="checkbox"/> Single component
<input type="checkbox"/> Commercially available
<input type="checkbox"/> Included in references |
| Classes | <input type="checkbox"/> Alloys
<input type="checkbox"/> Coordination compounds
<input type="checkbox"/> Incompletely defined
<input type="checkbox"/> Mixtures
<input checked="" type="checkbox"/> Polymers
<input type="checkbox"/> Organics, and others not listed |
| Studies | <input type="checkbox"/> Analytical
<input type="checkbox"/> Biological
<input type="checkbox"/> Preparation
<input type="checkbox"/> Reactant or reagent |

单一组分

聚合物

0 of 1 Substance Selected

1. **132010-54-9** 🔍

~2

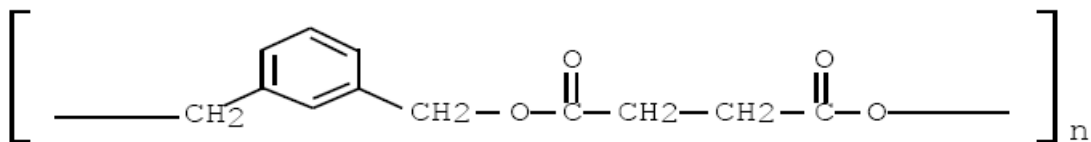
626-15-3
C₈ H₈ Br₂

110-15-6
C₄ H₆ O₄

(C₈ H₈ Br₂ . C₄ H₆ O₄)_x
 Butanedioic acid, polymer with 1,3-bis(bromomethyl)benzene (9CI)

聚合物的检索

已知重复单元的聚合物



(C₁₂ H₁₂ O₄)_n

SciFinder[®] interface showing search results for the molecular formula (C₁₂ H₁₂ O₄)_n. The results list includes:

- 1. 1801551-81-4
- 2. 1637772-98-5
- 3. 1421756-46-8
- 4. 1392419-56-5
- 5. 1353713-96-8
- 6. 1341223-97-9

Substance 3 (1421756-46-8) is highlighted, showing the chemical structure and the formula (C₁₂ H₁₂ O₄)_n. A message indicates: "Substance Image Cannot Be Displayed 1421756-46-8".

聚合物的检索

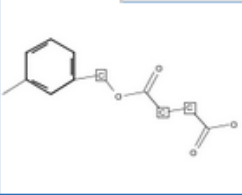
Analyze Refine

Refine by: ?

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

Structure Editor:

Java Non-Java

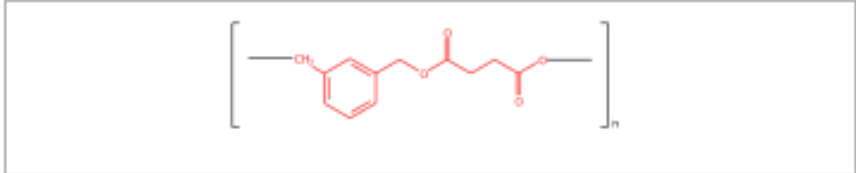


Click image to change structure or view detail.
Search type: **Substructure**

0 of 1 Substance Selected

1. 132010-11-8

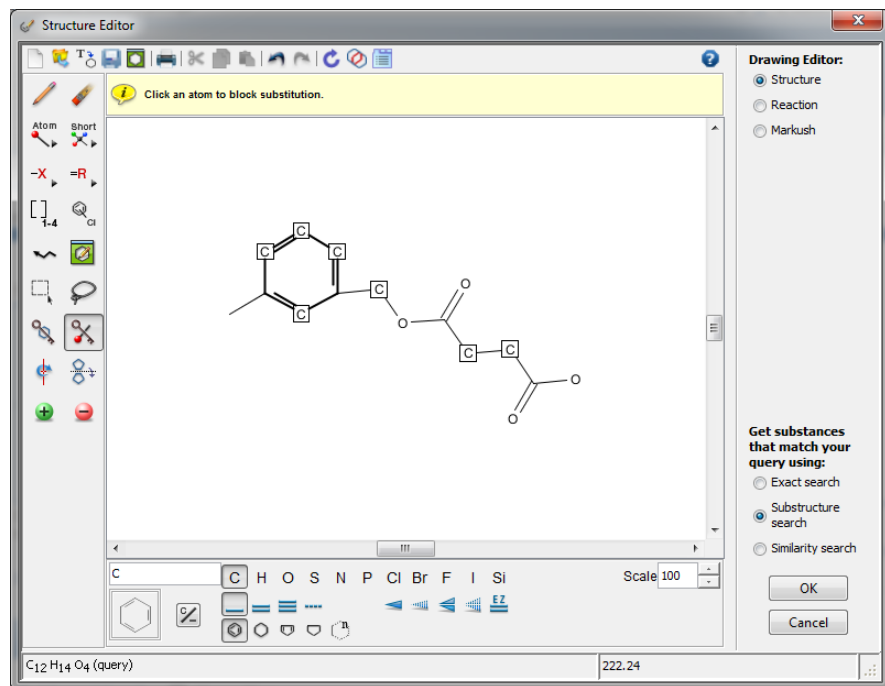
~2



$(C_{12}H_{12}O_4)_n$
Poly[oxy(1,4-dioxo-1,4-butanediyl)oxymethylene-1,3-phenylenemethylene] (9CI)

利用结构特征进行Refine，迅速查找需要的物质

聚合物检索



绘制好SRU后用亚结构检索
因为两段为开放状态

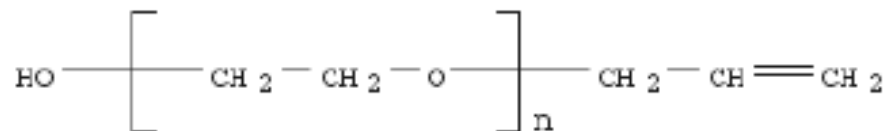
- | | |
|-----------------|--|
| Characteristics | <input checked="" type="checkbox"/> Single component
<input type="checkbox"/> Commercially available
<input type="checkbox"/> Included in references |
| Classes | <input type="checkbox"/> Alloys
<input type="checkbox"/> Coordination compounds
<input type="checkbox"/> Incompletely defined
<input type="checkbox"/> Mixtures
<input checked="" type="checkbox"/> Polymers
<input type="checkbox"/> Organics, and others not listed |
| Studies | <input type="checkbox"/> Analytical
<input type="checkbox"/> Biological
<input type="checkbox"/> Preparation
<input type="checkbox"/> Reactant or reagent |

单一组分

聚合物

聚合物的检索

含端基和SRUs的聚合物



Explore ▾ Saved Searches ▾ SciPlanner

REFERENCES

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

SUBSTANCES: MOLECULAR FORMULA ?

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

SUBSTANCES



↑
SRU部分

↑
两端部分

0 of 4 Substances Selected

1. 1500029-22-0

~3

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-(1-methylethenyl)-ω-hydroxy-

2. 191403-44-8

~5

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-1-propen-1-yl-ω-hydroxy-

3. 50856-25-2

~57

$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-ethenyl-ω-methoxy-

4. 27274-31-3

~1115 ~15

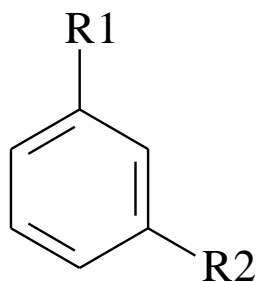
$(\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_3 \text{ H}_6 \text{ O}$
Poly(oxy-1,2-ethanediyl), α-2-propen-1-yl-ω-hydroxy-
Regulatory Information

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 (MethodsNow Synthesis)
 - SciPlanner
- SciFinder常见问题及解决

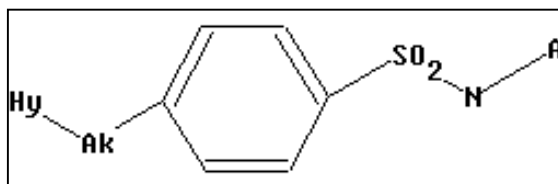
Markush检索

- 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(CH₃)—halogen,



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

Markush检索



[Explore](#)
[Saved Searches](#)
[SciPlanner](#)
[Save](#)
[Print](#)
[Export](#)

Welcome Helen Zhu

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

REFERENCES

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[Get Reactions](#)
[Get Related Citations](#)
[Tools](#)

[Create Keep Me Posted Alert](#)
[Send to SciPlanner](#)

[Analyze](#)
[Refine](#)
[Categorize](#)

Sort by: [Accession Number](#)

0 of 1969 References Selected

Page: 1 of 99

Analyze by:

Document Type

Patent	1969
Journal	1

[Show More](#)

1. **Compounds and methods for anticoagulation therapy**

[Quick View](#)
[PATENTPAK](#)

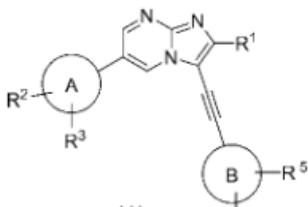
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

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)**


[Quick View](#)
[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^aR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

全部是专利



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A CAS SOLUTION

ACS / Proprietary and Confidential / Do Not Distribute

71

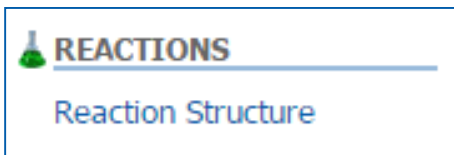
提纲

- 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 (MethodsNow Synthesis)
 - 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



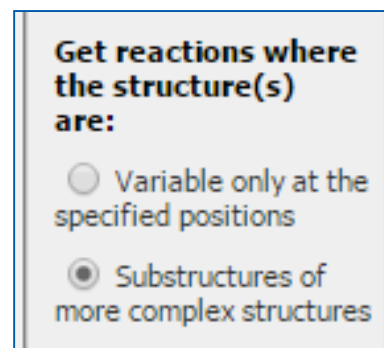
- 常用获取方法

已知物质：由物质获取反应

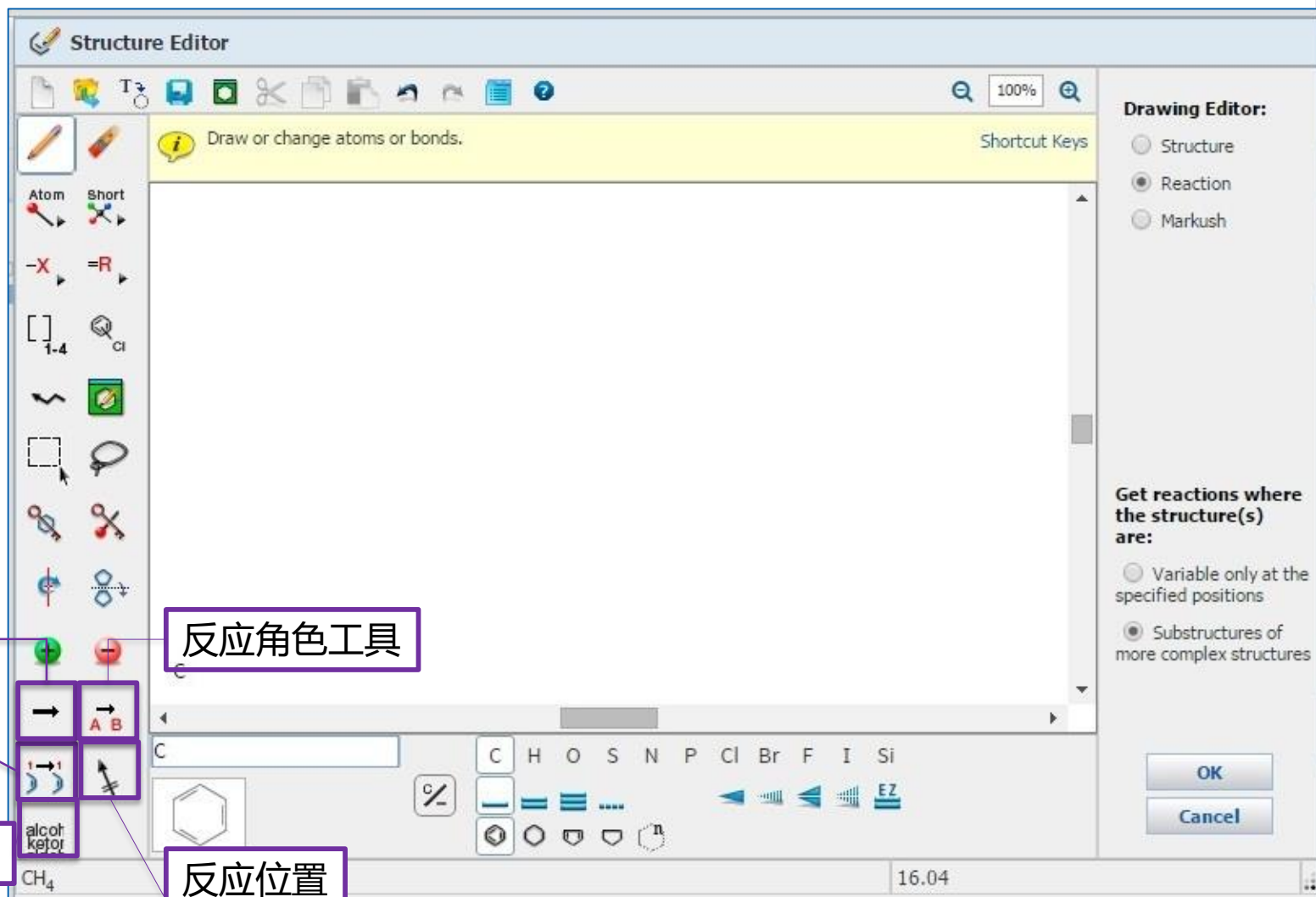
已知文献：从文献中获取反应

精确结构反应检索

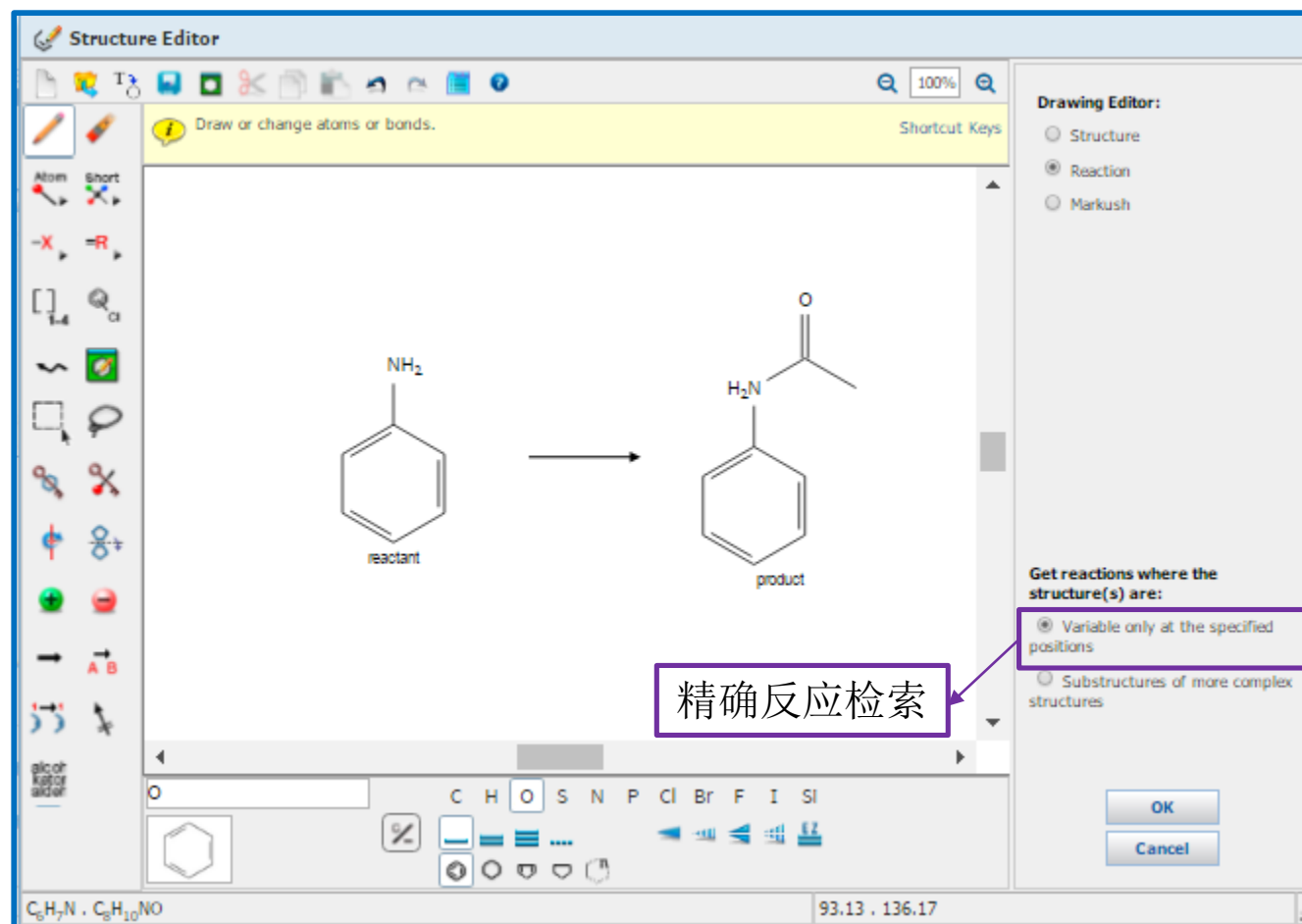
亚结构反应检索



反应绘制工具



SciFinder反应检索——精确反应检索



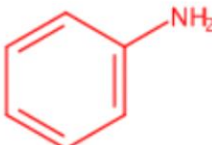
反应检索结果


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

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

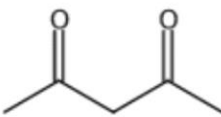
☐ 1. **View Reaction Detail** [Link](#) [Similar Reactions](#)


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



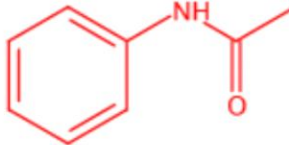
~126 


+



~112 

→



98%
~128 

▼ **Overview**

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm

Notes

green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

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

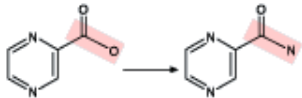
Get Similar Reactions ?

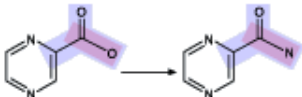
Retrieve similar reactions from:

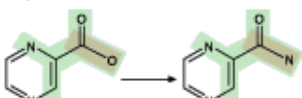
- ☒ All reactions
- ☐ Current answer set

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)



Get Reactions

Cancel

按照反应类型排序

Group by: Transformation Sort by: Frequency

0 of 605 Reactions Selected

1. Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarboxates
188 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{O}-\text{C}(=\text{O})-\text{R}^2 + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2 + \text{R}^2-\text{C}(=\text{O})-\text{OH}$$

2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions

$$\text{R}-\text{C}(=\text{O})-\text{OH} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{O})-\text{N}(\text{R}^1)_2$$

更精确的查找需要的反应

3. Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
55 Reactions

$$\text{R}-\text{C}(=\text{Y})-\text{X} + \text{R}^1-\text{NH}-\text{R}^1 \longrightarrow \text{R}-\text{C}(=\text{Y})-\text{N}(\text{R}^1)_2$$

Y = O, S, NR'

反应检索结果的筛选

Analyze Refine

Analyze by: ?
Solvent

H₂O 99

CH₂Cl₂ 65

MeCN 55

THF 27

PhMe 26

AcOH 25

CHCl₃ 22

DMF 15

DMSO 15

Me₂CO 15

Show More

Group by: No Grouping Sort by: Relevance

0 of 606 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Nc1ccccc1
~126

+

CC(=O)CC(=O)C
~112

→

CC(=O)Nc1ccccc1
98%
~128

Overview

Steps/Stages

1.1 R:H₂O, R:O₂, C:SiO₂ (sulfuric acid), C:H₂SO₄ (silica), 2 h, 120°C, 1 atm


Notes

green chemistry-reagent, silica supported and used, no solvent, aerobic, optimization optimized on temperature, Reactants: 2, Most stages in any one step: 1

References

Silica sulfuric acid mediated acylation of a

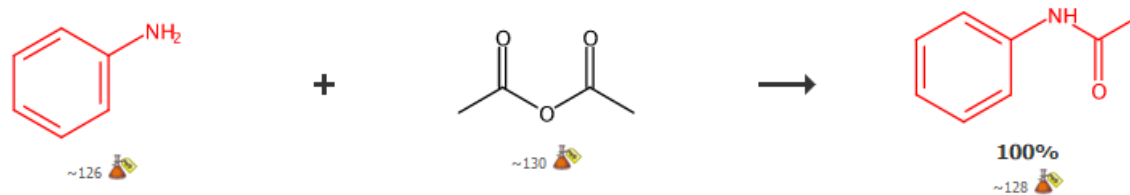
筛选用水作溶剂的反应

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79

SciFinder囊括最大的反应实验过程合集



▼ Overview

Steps/Stages

1.1 S:CH₂Cl₂, 20-120 min, rt

Notes

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

References

Indole Synthesis via Rhodium Catalyzed Oxidative Coupling of Acetanilides and Internal Alkynes

Q Quick View Other Sources

By Stuart, David R. et al

From Journal of the American Chemical Society, 130(49), 16474-16475; 2008

不用阅读全文，直接获得包含
实验过程的反应记录

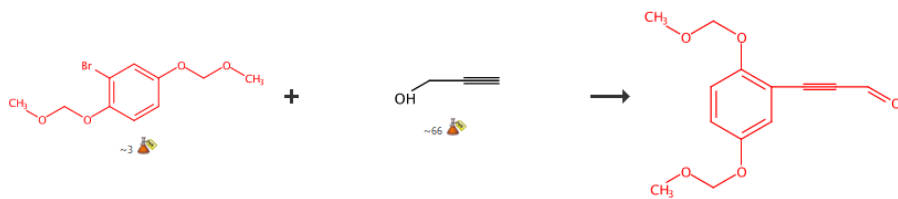
▼ Experimental Procedure



Representative procedure for the preparation of acetanilides: Aniline (10.1 mL, 109.7 mmol, 1 eq) was added to a round-bottom flask via syringe and fitted with a rubber septum. The flask was purged with argon and dry DCM (300 mL, 0.4 M) was added. Acetic anhydride (12.5 mL, 132.2 mmol, 1.2 eq) was added and the reaction was stirred at room temperature and monitored by TLC. Upon completion (generally a couple of hours, but as short as 20 minutes) the reaction mixture was washed with a saturated solution of sodium carbonate, the organic layers dried with MgSO₄ and the solvent removed under reduced pressure. The product was obtained in quantitative yield (14.8 g). In most cases analytically pure acetanilides can be obtained after extraction however if necessary purification by flash chromatography with ethyl acetate/pet. ether was used (see below for specific conditions). **Acetanilide (1a):** The above procedure was followed to afford the product in quantitative yield. This compound can also be purchased from commercial sources (CAS: 103-84-4). ¹H NMR (400 MHz, CDCl₃, 293 K): δ 7.50 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 2H), 7.10 (t, J = 7.4 Hz, 1H), 2.17 (s, 3H). The signal for the exchangeable NH does not appear in the spectrum.

SciFinder囊括最大的反应实验过程合集

2 Steps Hover over any structure for more options.



Experimental Procedure: 我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 去免费的Supporting Information查? 可能只有图谱。

Overview

Steps/Stages

- 1.1 C: Pd(PPh₃)₄; S: BuNH₂; 21 h, 100°C
- 2.1 R: DMSO, R: Cl(O=)CC(=O)Cl, S: CH₂Cl₂, 15 min, -78°C
- 2.2 S: CH₂Cl₂, -78°C; 2 h, -78°C
- 2.3 R: Et₃N, 30 min, -78°C; -78°C → rt
- 3.4 R: H₂O, R: NH₄Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, scale method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, Stages in any one step: 4

Experimental Procedure

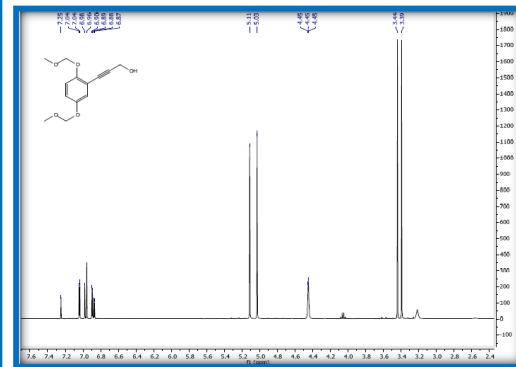
NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and Pd(Ph₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10–50%). 3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol² (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); ¹³C NMR (CDCl₃, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]⁺ (calcd for C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH₂Cl₂ (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH₂Cl₂ (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et₃N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. 3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



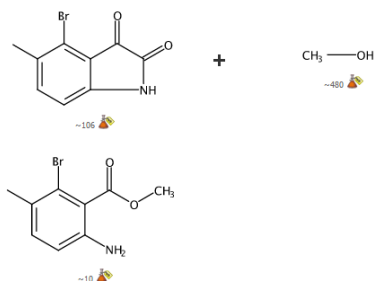
MethodsNow Synthesis

MethodsNow

A New Method for Synthesis of Nolatrexed Dihydrochloride

By Zhao, Xueqing; Li, Fei; Zhuang, Weiping; Xue, Xiaowen; Lian, Yuanyang; Fan, Jianhui; Fang, Dongsheng
From Organic Process Research & Development, 14(2), 346-350; 2010
Published by American Chemical Society

Reaction Steps **1** 2 3



Products	Benzoic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1-Indole-2,3-dione, 4-bromo-5-methyl-, CAS RN: 147149-84-6 Methanol, CAS RN: 67-56-1
Reagents	Potassium persulfate, CAS RN: 7727-21-1 Sodium methoxide, CAS RN: 124-41-4 Hydrochloric acid, CAS RN: 7647-01-0 Sodium dithionite, CAS RN: 7775-14-6
Solvents	Methanol, CAS RN: 67-56-1 Water, CAS RN: 7732-18-5
Procedure	<ol style="list-style-type: none"> 1. Add sodium methoxide (22.6%, 4.80 kg, 20.1 mol) to a mixture of 4-bromo-5-methylisatin (6.67 mol) and anhydrous methanol (6.70 L). 2. Add K₂S₂O₈ (1.90 kg, 7.03 mol) to the mixture in parts 10°C with an ice-water bath. 3. After addition the reactant mixture turns yellow, continue the stirring for 1 hour at room temperature. 4. Adjust the reaction mixture to pH 8-9 with aqueous 36% HCl (1.24 L) 15 °C. 5. Destroy the excessive K₂S₂O₈ by aqueous 5% Na₂S₂O₄ solution (450 mL). 6. After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid. 7. Mix the mixture with CH₂Cl₂ (6 L) and H₂O (4 L). 8. Separate the organic phase. 9. Extract the aqueous phase with CH₂Cl₂ (4 L). 10. Dry the combined organic phases over Na₂SO₄. 11. Concentrate the combined organic phases with a rotavapor. 12. Distill the resulted brown liquid under high vacuum.
Scale	milligram
¹H NMR	CDCl ₃ : δ 2.28 (s, 3 H, Ar-CH ₃), 3.91 (s, 3 H, -OCH ₃), 4.26 (br s, 2 H, NH ₂), 6.54 (d, J = 8.2 Hz, 1 H, Ar-H), 7.00 (d, J = 8.2 Hz, 1 H, Ar-H).
IR	KBr cm ⁻¹ : 3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

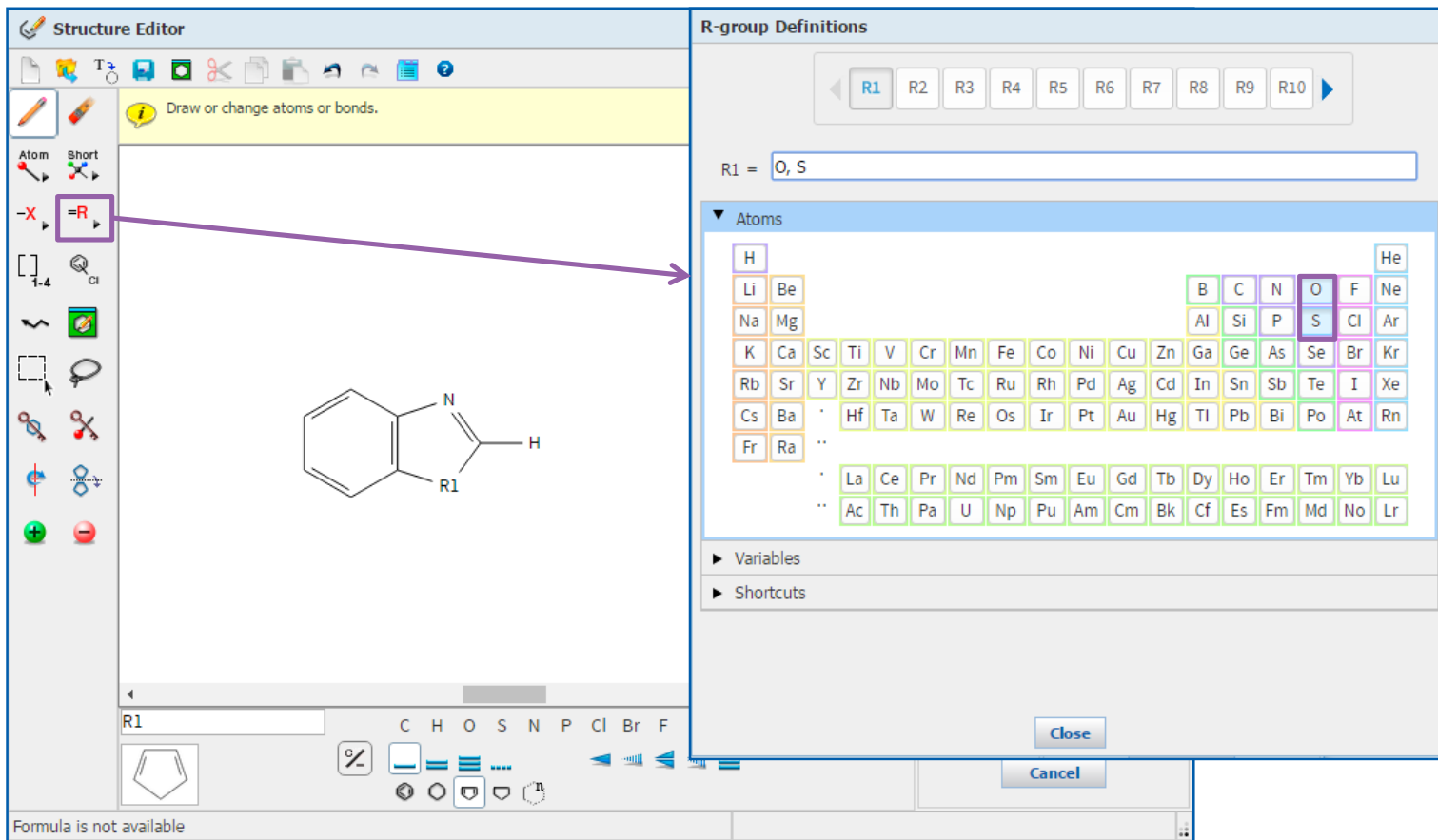
物质信息

实验过程

图谱信息

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索

Structure Editor

Drag the reaction arrow to specify reaction direction.

Drawing Editor:

- ☐ Structure
- ☒ Reaction
- ☐ Markush

Variables

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

Get reactions where the structure(s) are:

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

Chemical Reaction:

Reactant: A benzimidazole derivative with a substituent R1 and a hydrogen atom at the 2-position.

Product: A benzimidazole derivative with a substituent R1 and a substituent Ak at the 2-position.

Formulas:

Reactant: C1=NC2=CC=CC=C2N1C(R1)=C

Product: C1=NC2=CC=CC=C2N1C(R1)=C(Ak)

Formula is not available

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze **Refine**

Analyze by: Catalyst

CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping Sort by: Accession Number

☐ No Grouping
☒ Document
☐ Transformation

1. **View Reaction Detail** **Link** **Similar Reactions**

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

Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t* C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

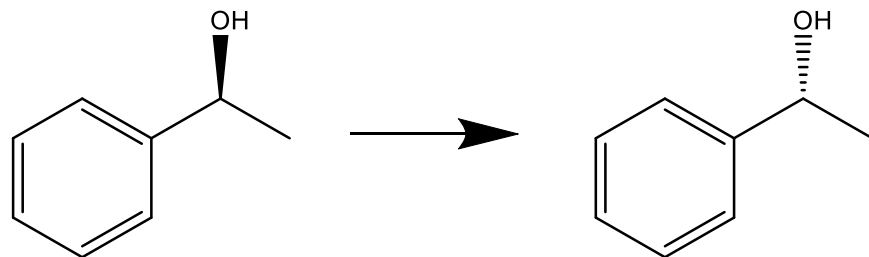
Notes

catalyst prepared and used, screw cap tube used,
Reactants: 2, Reagents: 2, Catalysts: 1, Solvents:
one step: 3

References

ACS / Proprietary and Confidential / Do Not Distribute

案例：如何获取手性翻转反应



1. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



6. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



4. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.



94. View Reaction Detail [Link](#)

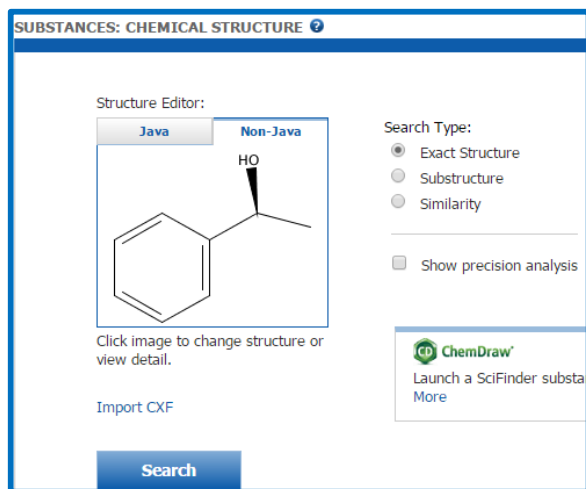
Single Step Hover over any structure for more options.



案例：如何获取手性翻转反应

检索思路：

- 1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。
- 2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。
- 3). 两个结果集取交集。



1 of 52 Substances Selected

1. 1445-91-6

~3499

~90

Absolute stereochemistry, Rotation (-).

C₈ H₁₀ O
Benzenemethanol, α-methyl-, (αS)-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

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

案例：如何获取手性翻转反应

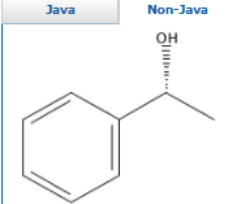
检索思路：

- 1). 先获取反应物物质，然后再获取其作为反应物的反应，得到检索结果集1。
- 2). 先获取产物物质，然后再获取其作为产物的反应，得到检索结果集2。
- 3). 两个结果集取交集。

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF

Search

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

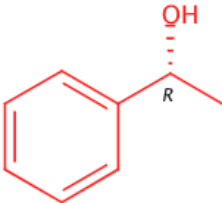
ChemDraw

Launch a SciFinder substance

1 of 54 Substances Selected

1. 1517-69-7

~3531 ~94



Absolute stereochemistry, Rotation (+).

C₈H₁₀O
Benzenemethanol, α -methyl-, (R)-

Key Physical Properties

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

案例：如何获取手性翻转反应

ances (52) > get reactions (7938)

Get References **Tools** Send to SciPlanner

Group by: No Group

0 of 79

1. View Reaction Detail

4 Steps Hover over any structure for more options.





Chemical structures: NC(=O)C, CC(=O)C, CC1(C)CC1, NC1(C)CC1, C/C=C/C(O)C

Combine Answer Sets

2 of 50 Reaction A

- ☒ 2 (4185)
产物
Chemical Structure e
- ☒ 1 (7938)
反应物
Chemical Structure e
- ☐ 2 (3888)
Chemical Structure e
- ☐ 1 (9519)
Chemical Structure e
- ☐ 手性2 (172)

Select an option for combining the two selected saved answer sets:

-  **Combine** Include all reactions from both sets
-  **Intersect** Include only reactions that appear in both sets
-  **Exclude** Include only answers from 2 that are not in 1
-  **Exclude** Include only answers from 1 that are not in 2

Combine Answer Sets Cancel

反应检索结果集

Get References

Tools ▾

Send to SciPlanner

Group by: No Grouping ▾ Sort by: Accession Number ▾

Display Options

0 of 27 Reactions Selected

Page: 1 of 2

1. View Reaction Detail Link

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



Overview

Steps/Stages

1.1 S:H₂O, S:M , 360 h, 30°C



Notes

biotransformation, ee=92%, resting cells of the yeast *C. albicans* used, stereoselective, Reactants: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Deracemization of 1-phenylethanol via tandem biocatalytic oxidation and reduction

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 (MethodsNow Synthesis)
 - SciPlanner
- 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

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

Send to SciPlanner

Display Options

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
Quick View Other
By Huang, Yuhua et al

SciPlanner

SciPlanner_11_19_2015_112612

Workspace **Edit** **View** **GoTo**

New
Open
Save
Duplicate
Import
Export
Print
Close

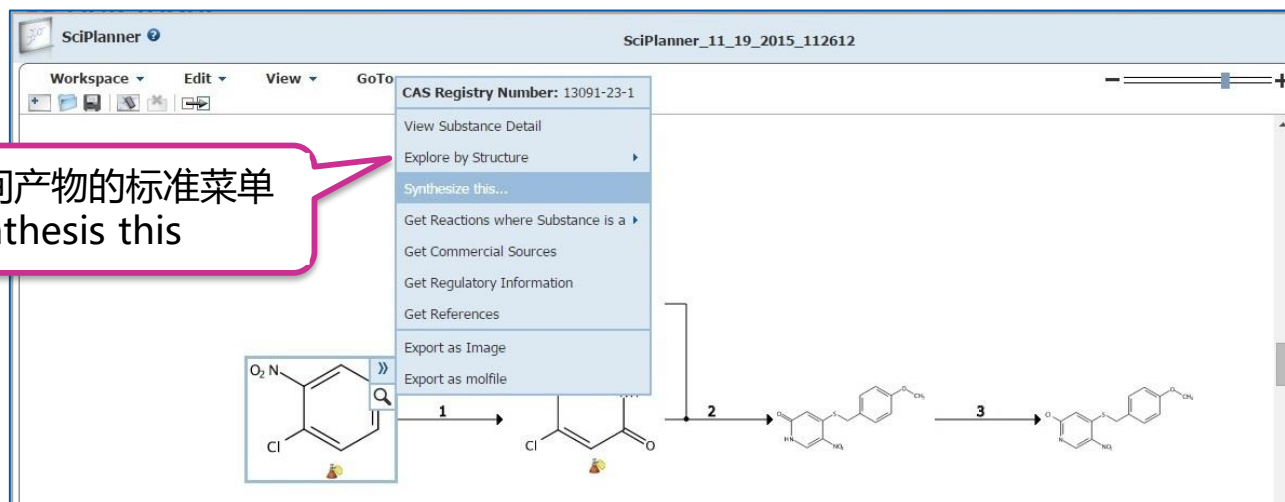
Your Workspace is empty.

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

Clear Reactions

SciPlanner使用简介

打开中间产物的标准菜单
选择Synthesize this

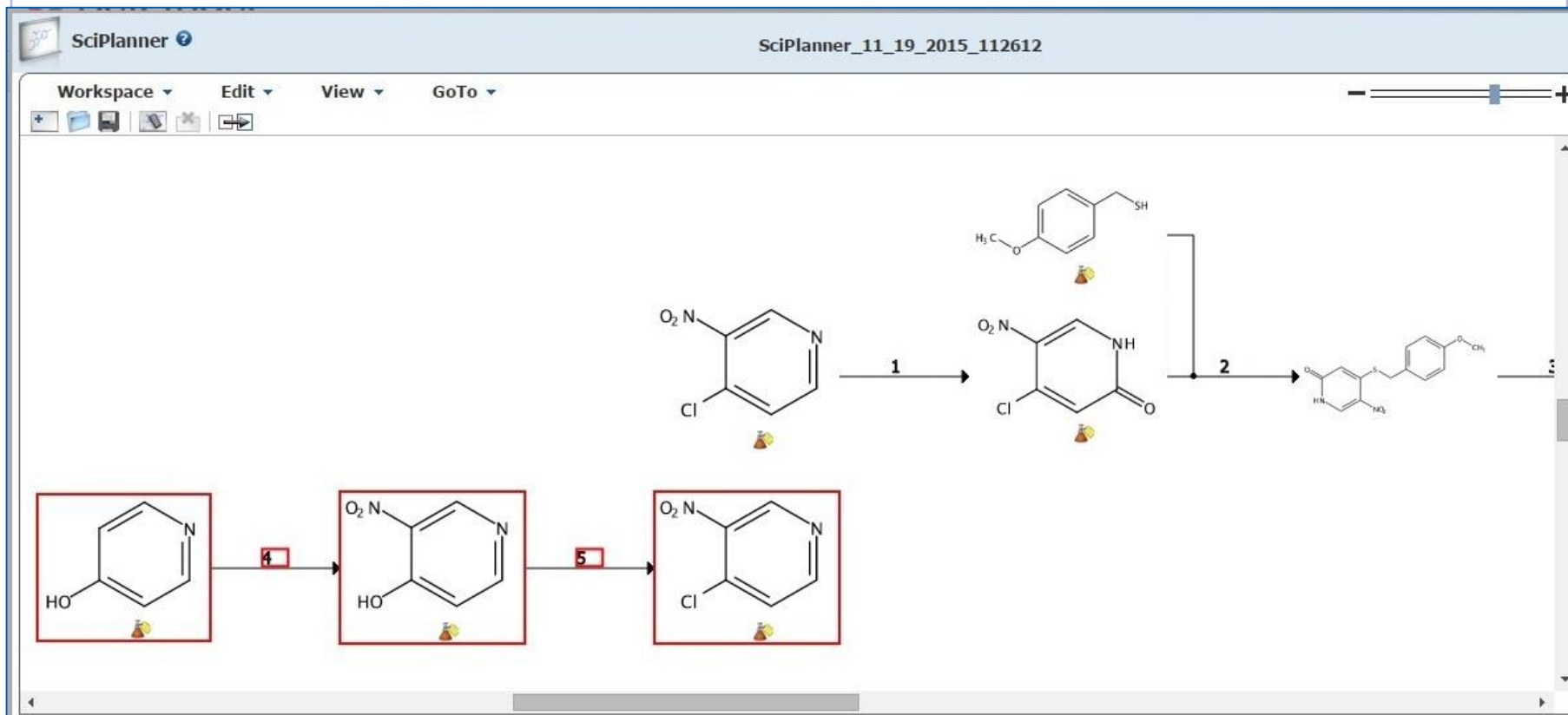


在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner



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

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

New
Open
Save
Duplicate
Import
Export
Print
Close

点击 Workspace, 选择 Export 导出结果

用鼠标将两个同样的结构拖至重叠, 两条反应合并

选择适当的输出格式, 输出结果

Export

For:

Offline Review

- ☒ Portable Document Format (*.pdf)
- ☐ Citations (*.ris)
- ☐ Image (*.png)

Saving Locally

- ☐ SciPlanner eXchange (*.pkx)

Details:

File Name: *

SciPlanner_11_19_2015_112612

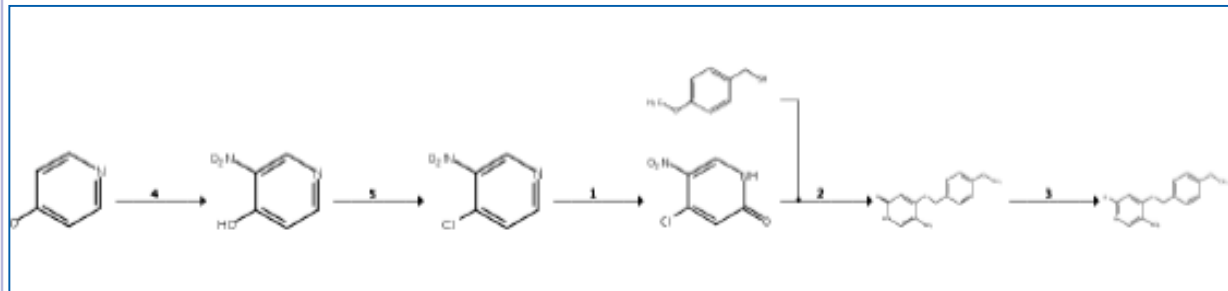
Title

Include:

- ☒ SciPlanner Image
- ☒ Reaction Details
- ☒ Substance Details
- ☒ Reference Details

Export **Cancel**

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	1.1 R:POCl ₃ , S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Transformation: 1. Formation of Alkyl Halides from Alcohols	

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-2H-pyridine, 2-chloro-4-[[4-methoxyphenyl(methyl)thio]]-5-nitro-2H-pyridine</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₄S Pyridine, 2-chloro-4-[[4-methoxyphenyl(methyl)thio]]-5-nitro-2H-pyridine</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 ~ 190 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>C₈H₃ClN₂O₃ 2-(1H-Pyridinone, 4-chloro-5-nitro-2H-pyridine, 2-chloro-4-[[4-methoxyphenyl(methyl)thio]]-5-nitro-2H-pyridine</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

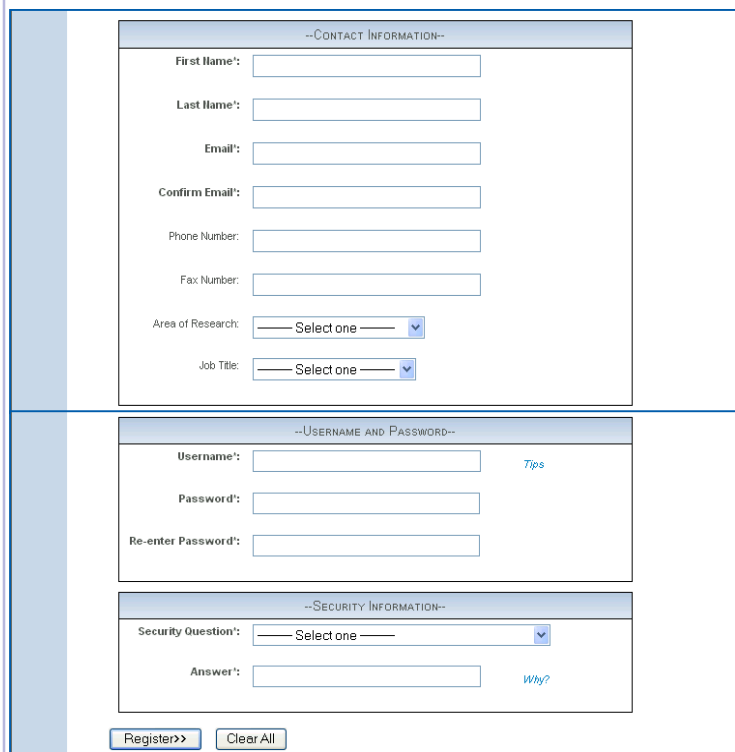
提纲

- 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 (MethodsNow Synthesis)
 - 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 registration form is divided into three main sections: Contact Information, Username and Password, and Security Information. The Contact Information section includes fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (a dropdown menu), and Job Title (a dropdown menu). The Username and Password section includes fields for Username, Password, and Re-enter Password, with a 'Tips' link next to the Password field. The Security Information section includes a Security Question (a dropdown menu) and an Answer field, with a 'Why?' link next to the Answer field. At the bottom of the form are two buttons: 'Register>>' and 'Clear All'.

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username:

Password: [Tips](#)

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

请注意：

1.必须输入真实姓名和学校域名邮箱。
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>

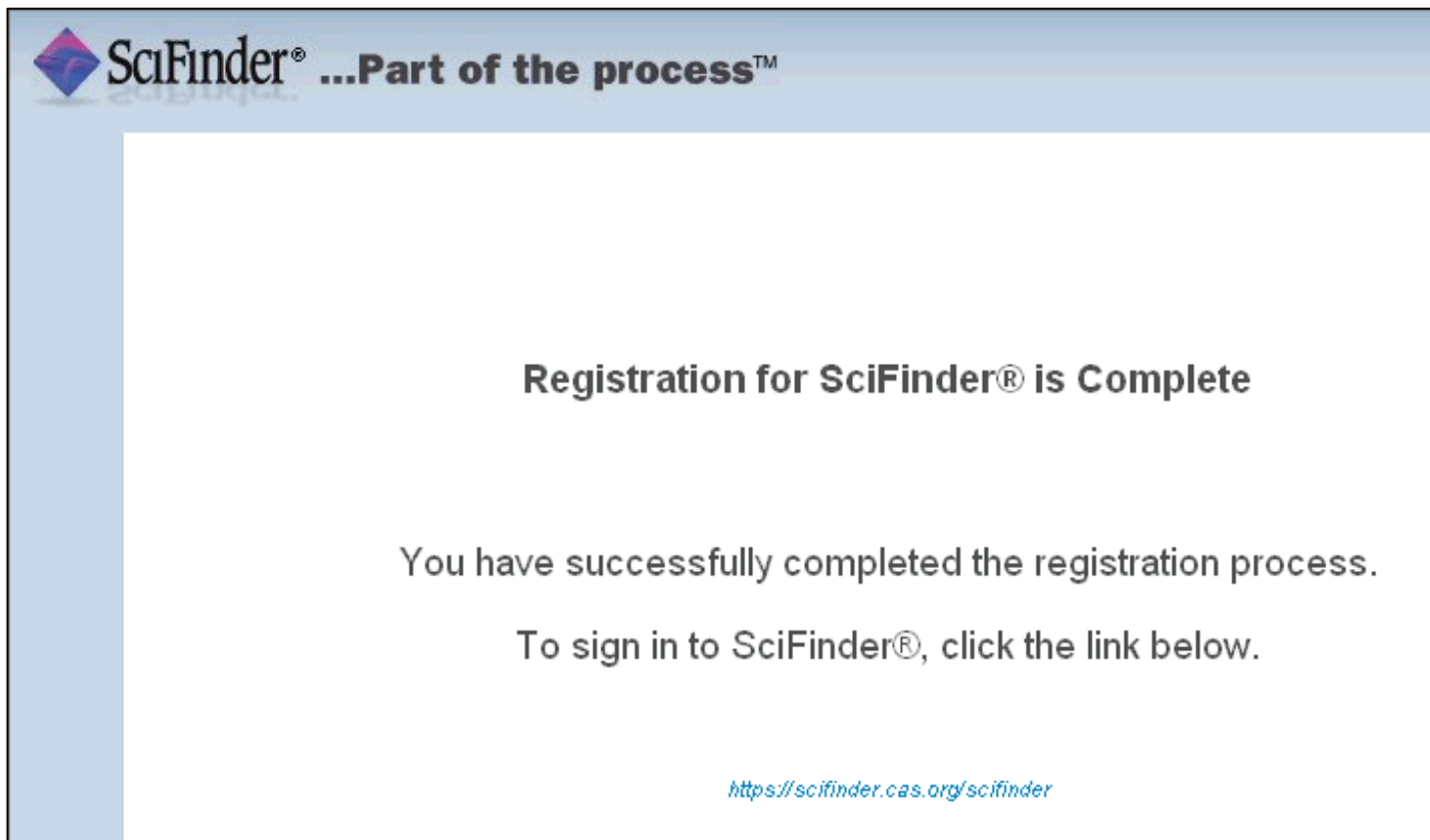
This link is valid for only one use and will expire within 48 hours.

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

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china@acs-i.org

