

匡金海

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jkuang@acs-i.org

如何使用SciFinder获取科技信息

郑州轻工业大学
2018.11.28



提纲

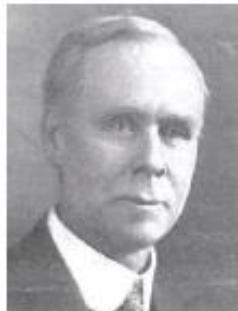
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
- SciFinder常见问题及解决

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

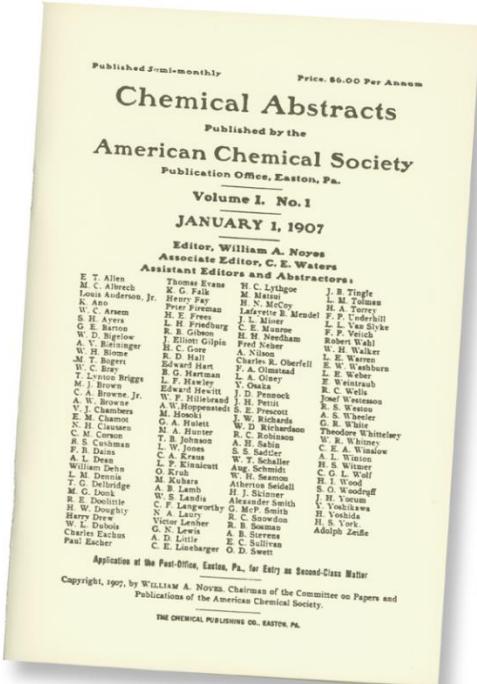


1907年，信息的汇集、管理发生了重大的变化

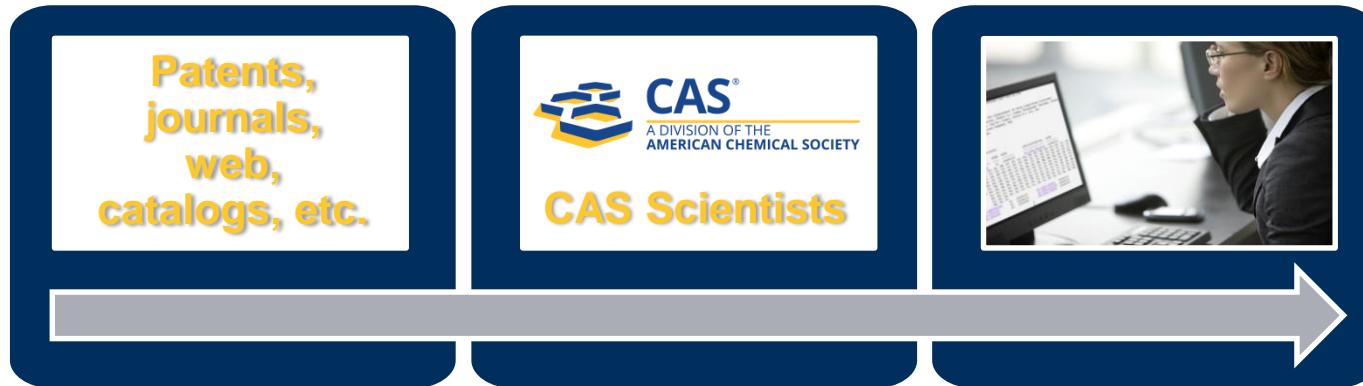


威廉·诺伊斯
(William A. Noyes)

- “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



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ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY

division of polymer chemistry, inc
American Chemical Society

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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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PHYSICAL CHEMISTRY
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CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

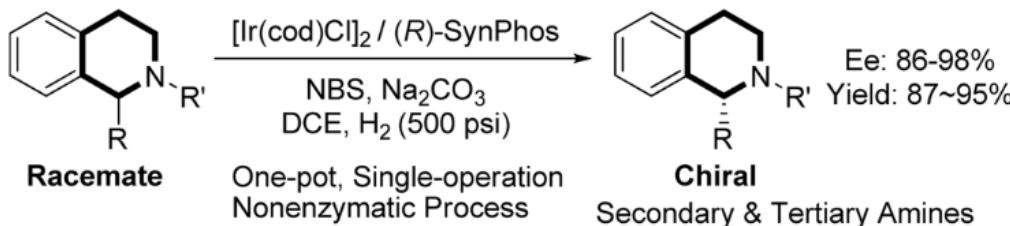


CAS数据库最具价值的内容——人工标引

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
503538-69-0

Chiral ligands

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

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

Catalyst use; Uses

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

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
CPLUS

PUBLISHER

American Chemical Society

LANGUAGE

English



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™



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. WO 2016100441 A1 English

atkina, Natalia Language: English, Database: CAPLUS

Patent Family US 20160176911 A1 English

Disclosed herein phosphate, R¹ methods of t... medicament

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 prep'd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK ▾

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoquo; Lin, Yanfeng From Faming Zuanli Shengqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAP

The propo... method comprising reaction of (1'R)-2'-deoxy-2'-fluoro-2'-methyluridine with

ZOOM DOWNLOAD PDF

8. By From

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT CO... (19) World Intellectual Property Organization International Bureau (43) International Publication Date 23 June 2016 (23.06.2016)

WIPO | PCT (10) Internat... WO 2016100441

(51) International Patent Classification: C07H 19/10 (2006.01) C07H 19/20 (2006.01) C07H 19/11 (2006.01) C07H 19/23 (2006.01) C07H 19/067 (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, CO, DZ, EC, EE, EG, HN, HR, IU, ID, IL, KZ, LA, LC, LK, LM, MK, MN, MW, MX, PA, PE, PG, PH, PL, SD, 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,

Search in SciFinder ▾ | View Detail

Analyst Markup Locations (1) page 130

CAS RN 1206126-39-7

Search in SciFinder ▾ | View Detail

Analyst Markup Locations (1) page 130

CAS RN 1206126-41-1

WO 2016/100441

PCT/US2015/065981

EXAMPLE 1 COMPOUND 1

dichloromethane pyridinium dichromate acetic anhydride tert-butanol

Route 2

Et₂Si-O-Cl Et₂Si-O-SiEt₂-Cl

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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

The screenshot shows the SciFinder interface with a reaction search results page. The search query is "Reactions (9)". The results list a single reaction with a yield of 79%. The reaction scheme shows a substituted chromene reacting with a substituted azide to form a product. The reaction conditions include Et₃N, K₂CO₃, and EIN(Pt)-7. The "MethodsNow" module is highlighted.

嵌在SciFinder中的合成模块

The screenshot shows the MethodsNow interface with a search result for "atorvastatin". The results list a method for "Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography". The method details include the analyte (Atorvastatin), matrix (Blood plasma), and technique (High-performance thin layer chromatography). The source is cited as Chromatographia (2007), 65 (11/12), 763-766. The "MethodsNow" module is also visible here.

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覆盖的数据库



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What is SciFinder?
SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.



News & Updates

Welcome to SciFinder

Did you notice our new look?
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the [CAS Customer Center](#).

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SciFinder主界面

The screenshot shows the SciFinder web interface. A purple speech bubble labeled '检索入口' (Search入口) points to the search bar in the center. Another purple speech bubble labeled '工具栏' (Toolbar) points to the top navigation bar. A third purple speech bubble labeled '已保存的结果集' (Saved Results) points to the 'Saved Searches' sidebar. A fourth purple speech bubble labeled '定题追踪' (Topic Tracking) points to the 'KEEP ME POSTED' section. A fifth purple speech bubble labeled '检索完，请点击退出' (After search, click to exit) points to the 'Sign Out' button in the top right corner.

REFRENCES: RESEARCH TOPIC ?

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

Search

Advanced Search

REFRENCES

- 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
- Daclatasvir-1
- SUB result
- EX result
- MF result
- polymer1
- polymer1
- structure search
- Autosaved Substance Set

View All | Import

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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

主题检索：催化剂的制备及在热分解反应中的应用

关键词：制备、催化剂、热分解反应

检索式： prepare of catalyst

The screenshot shows the SciFinder interface with a blue header bar. On the left, there's a sidebar with a 'REFERENCES' section containing options like 'Research Topic', 'Author Name', 'Company Name', etc. Below it is a 'SUBSTANCES' section. The main area displays the results for the research topic 'prepare of catalyst'. It shows a list of examples such as 'The effect of antibiotic residues on da' and 'Photocyanation of aromatic compound'. A purple box highlights the text '关键词之间用介词连接 : in, with, of...'. At the bottom right, the SciFinder logo is visible.

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Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "prepare of catalyst"

REFERENCES

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

SUBSTANCES

REFRENCES: RESEARCH TOPIC ?

prepare of catalyst

Examples:

The effect of antibiotic residues on da
Photocyanation of aromatic compound

Search

关键词之间用介词连接 : in, with, of...

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主题检索的候选项

Select All Deselect All

0 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 58 references were found containing "prepare of catalyst" as entered.	58
<input type="checkbox"/> 945572 references were found containing the two concepts "prepare" and "catalyst" closely associated with one another.	945572
<input type="checkbox"/> 1540022 references were found where the two concepts "prepare" and "catalyst" were present anywhere in the reference.	1540022
<input type="checkbox"/> 13258959 references were found containing the concept "prepare".	13258959
<input type="checkbox"/> 2928663 references were found containing the concept "catalyst".	2928663

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“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；

文献检索集

REFERENCES ?

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Refine by: ?

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

Research Topic **thermal decomposition** Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

0 of 945572 References Selected Page: 1 of 47279

1. 2-Oxo-1,2,3,4-tetrahydropyrimidines Ethyl Esters as Potent β -Glucuronidase Inhibitors: One-pot Synthesis, In vitro and In silico Studies

By Iqbal, Sarosh; Shaikh, Nimra N.; Khan, Khalid M.; Naz, Sehrish; Ul-Haq, Zaheer; Perveen, Shahnaz; Choudhary, Muhammad I. From Medicinal Chemistry (Sharjah, United Arab Emirates) (2018), Ahead of Print. | Language: English, Database: CAPLUS

Background: Glucuronidation is essential for the metab. and excretion of toxic substances. Glucuronidase enzyme slows down the process of glucuronidation, and thus plays an important role in the on-set of colorectal carcinoma, and many other diseases. Inhibition of glucuronidase activity is thus identified as an important approach for the treatment of several diseases. Objective: Current study was aimed to synthesize a library of 2-oxo-1,2,3,4-tetrahydropyrimidine and to evaluate their glucuronidase inhibitory activity, and their mode of enzyme inhibition. Method: We s...

2. A comparative study on coated and uncoated diesel engine performance and emissions running on dual fuel (LPG - biodiesel) with and without additive

By Mustafa, M. Mohamed From Industrial Crops and Products (2019), 128, 194-198. | Language: English, Database: CAPLUS

The study was conducted on a partially stabilized zirconia coated single cylinder, four stroke, water cooled and direct injection diesel engine and was modified to use the liquefied petroleum gas (LPG) as the primary fuel and pilot spray of biodiesel with and without Di-tert-Bu Peroxide (DTBP) additive as the secondary fuel. The primary fuel was mixed with air in intake manifold,



按被引次数排序— Citing References

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Sort by: Citing References ▾

Accession Number
Author Name
Citing References
Publication Year
Title

1. [Rigid arrays of carbon supporting high dispersions of platinum nanoparticles](#)

By Joo, Sang Hwon; Choi, Seong Jae; Oh, Ilwhan; Kwak, Juhyoun; Liu, Zheng; Terasaki, Osamu; Ryoo, Ryong
From Nature (London, United Kingdom) (2001), 412(6843), 169-172. | Language: English, Database: CAPLUS

Nanostructured carbon materials are potentially of great technol. interest for the development of electronic, **catalytic** and hydrogen-storage systems. Here we describe a general strategy for the **synthesis** of highly ordered, rigid arrays of nanoporous carbon having uniform but tunable diams. (typically 6 nm inside and 9 nm outside). These structures are formed by using ordered mesoporous silicas as templates, the removal of which leaves a partially ordered graphitic framework. The resulting material supports a high dispersion of platinum nanoparticles, exceeding that of other common microporo...

2. [Chemoselective catalytic conversion of glycerol as a biorenewable source to valuable commodity chemicals](#)

Quick View Other Sources

By Zhou, Chun-Hui; Beltramini, Jorge N.; Fan, Yong-Xian; Lu, G. Q.
From Chemical Society Reviews (2008), 37(3), 527-549. | Language: English, Database: CAPLUS

A review. New opportunities for the conversion of glycerol into value-added chems. have emerged in recent years as a result of glycerol unique structure, properties, bioavailability, and renewability. Glycerol is currently produced in large amts. during the transesterification of fatty acids into biodiesel and as such represents a useful byproduct. This paper provides a comprehensive review and crit. anal. on the different reaction pathways for **catalytic** conversion of glycerol into commodity chems., including selective oxidn., selective hydrogenolysis, selective dehydration, **pyrolysis** and g...

Citing Reference: 帮助找到最重要的文献



文献检索结果

创建Alert，追踪最新文献

文献后处理工具

REFERENCES ?

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Substances Reactions Get Related Citations Tools

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Display Options

Sort by: Accession Number ▾

0 of 14733 References Selected

Page: 1 of 737

Analyze by: Publication Year

Publication Year	Count
2017	1182
2015	1146
2016	1144
2014	1105
2013	1000
2012	949
2018	907
2011	874
2010	770

1. A kind of ultra-thin g-c3n4 covering tio2 homogeneous special-shaped array thin film and preparation method thereof [Machine Translation].

Quick View Other Sources

By Wang, Debao; Li, Honghao; Song, Caixia; Geng, Shize; Zhou, Yanhong
From Faming Zhanli Shenqing (2018), CN 108816264 A 20181116. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The invention discloses a kind of ultra-thin g homogeneous shaped cover i, which includes an array of TiO₂ film and preparation method thereof. It is characterized in that, the described film is made up of ultra-thin g i, which includes covering rutile TiO₂ nanorod array with spike shaped rod bundle two homogeneous special-shaped TiO₂ nanostructure are high and low, the described method is taking inorganic titanium sulfate as raw material, under acidic conditions, By one-step hydro-thermal reaction on Fto glass substrate film, and then the precursor is calcined, to obtain...

2. One kind of pine cone shape of zno nano microsphere preparation method, and its application [Machine Translation].

Quick View Other Sources

By Yang, Weijia; He, Xin; Chen, Mei; Liu, Junjie; Liu, Mingquan; Liu, Yanyi; Wang, Nuoyuan; Liu, Junyan; Liang, Ping; Chen, Yizhan
From Faming Zhanli Shenqing (2018), CN 108821327 A 20181116. | Language: Chinese, Database: CAPLUS

[Machine Translation of Descriptors]. The invention provides a kind of echinacea shape of ZnO nano microsphere and its preparation method and application, comprising the following steps: 1), using zinc acetate, porogen, doping agent, prepare precursor mixed solution; (2) the precursor mixed solution, preparation of precursor thin film; 3), by controlling the heating rate is different preparation of echinacea shape ZnO nano microsphere preparation: the invention process is simple, equipment is

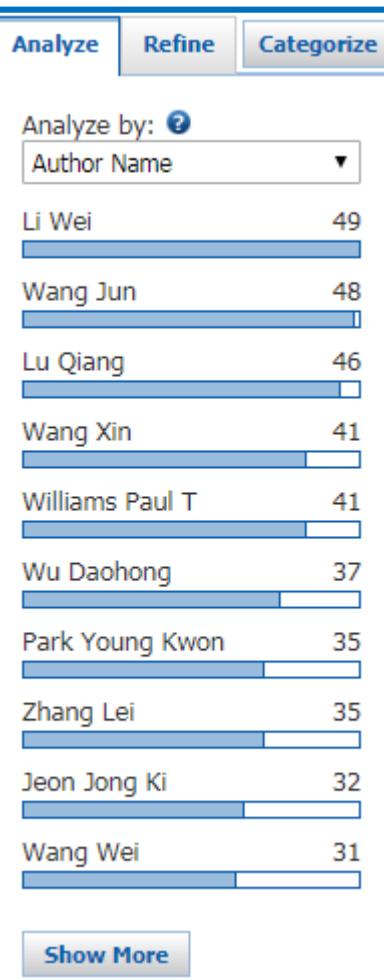
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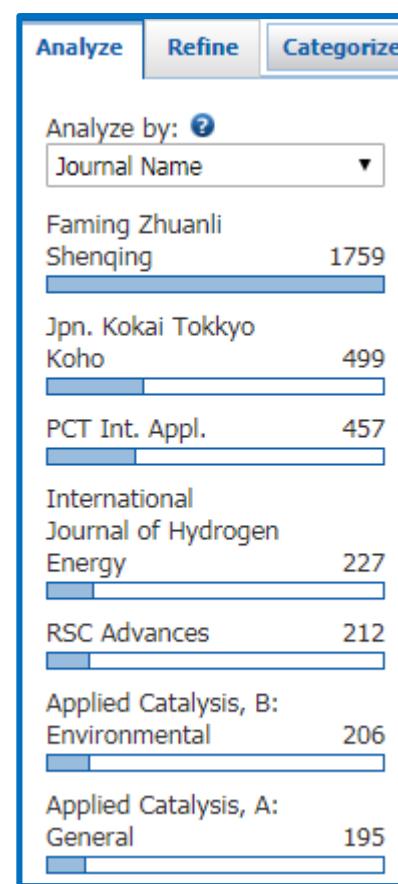
本领域研究人员



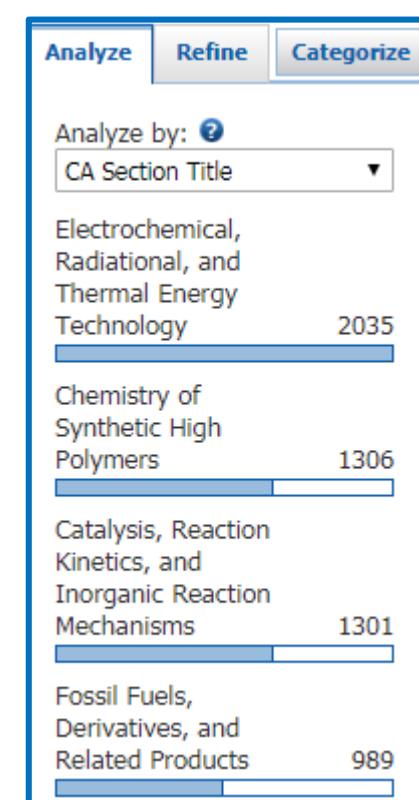
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期刊



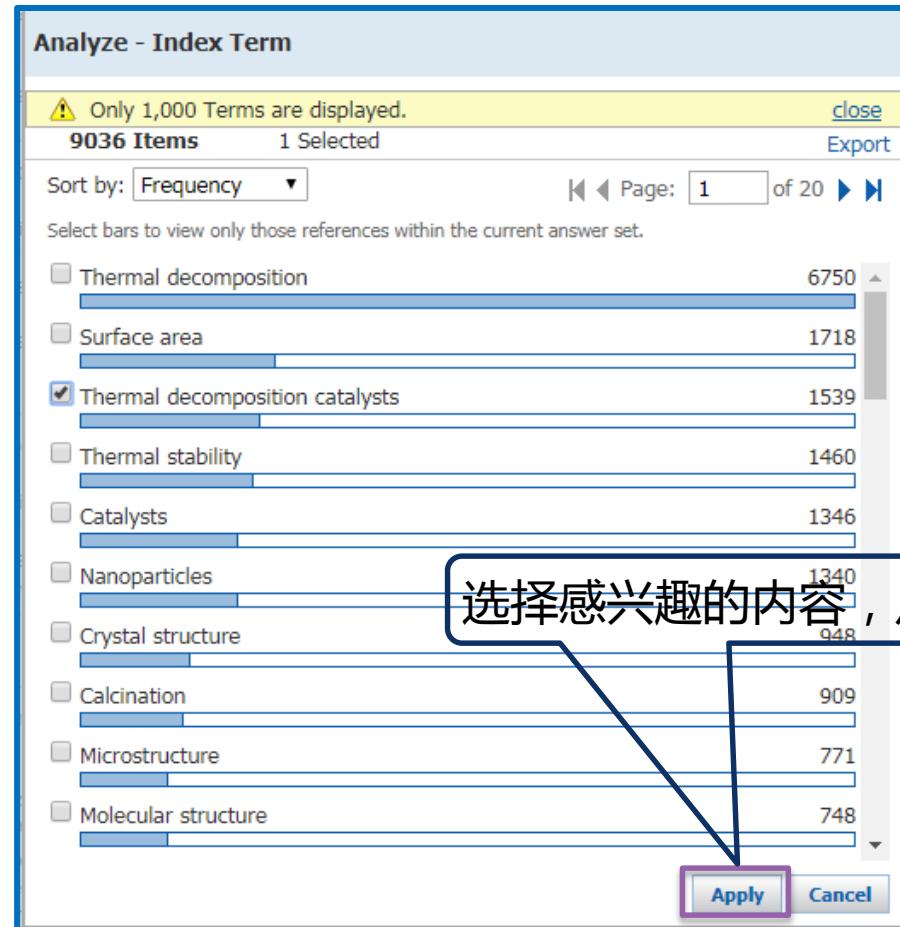
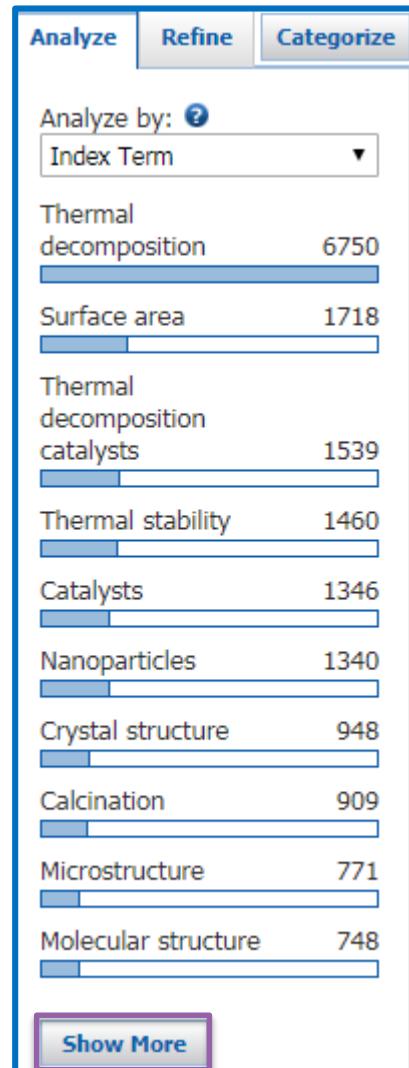
涉及学科领域



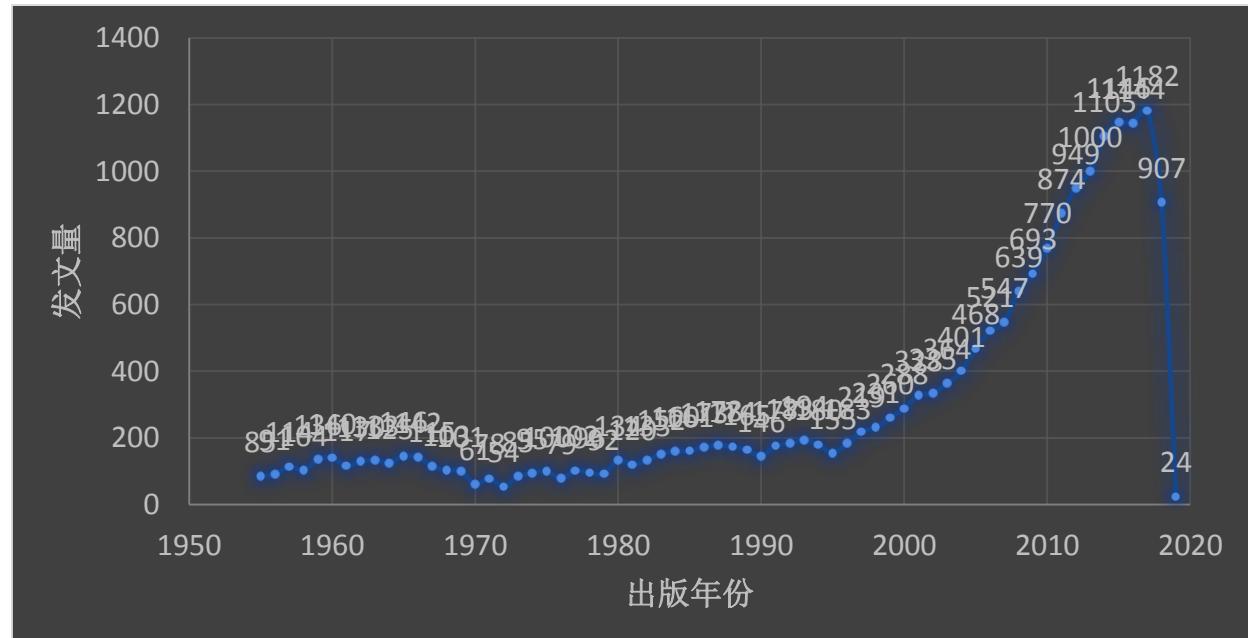
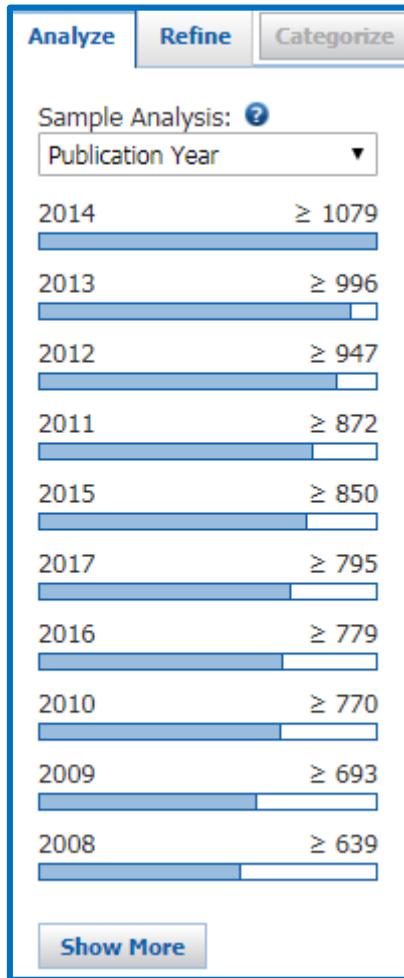
文献检索结果的Analyze

Index Term :

帮助用户了解涉及到的重要技术术语，并修正检索词



文献检索结果的Analyze



Publication Year: 分析领域发展趋势

文献检索结果的Refine

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Refine by: Research Topic Author Company Name Document Type Publication Year Language Database

Document Type(s) Biography Book Clinical Trial Commentary Conference Dissertation Editorial Historical Journal Letter Patent Preprint Report Review

Refine

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0 of 304 References Selected Page: 1 of 16

1. **Research advances in preparation of furfural and its derivatives by selective catalytic conversion of hemicellulose**
By Lu, Yi; Zheng, Zifeng; Huang, Yuanbo; Li, Wenbin
From Linchan Huaxue Yu Gongye (2018), 38(3), 1-16. | Language: Chinese, Database: CAPLUS
The utilization of renewable biomass resources play an important role in solving the energy crisis and reducing environmental pollution. Along this background, the prodn. of furan-based chems. from lignocellulose becomes one of the research focuses in biorefinery. Furfural is the key furan-based building block, which is manufd. from hemicellulose fraction directly, and offers a promising, rich platform for lignocellulosic biofuels and value-added chems. So it is of great practical significance to develop green technologies for the prodn. of furfural and the conversion of furfural to primary...

2. **Recent advances in cleaner hydrogen productions via thermo-catalytic decomposition of methane: Admixture with hydrocarbon**
By Syed Muhammad, Anuar Fauzad; Awad, Ali; Saidur, R.; Masiran, Nurliyana; Salam, Abdus; Abdullah, Bawadi
From International Journal of Hydrogen Energy (2018), 43(41), 18713-18734. | Language: English, Database: CAPLUS
A continuous increase in the greenhouse gases concn. due to combustion of fossil fuels for energy generation in the recent decades has sparked interest among the researchers to find a quick soln. to this problem. One viable soln. is to use hydrogen as a clean and effective source of energy. In this paper, an extensive review was made on the effectiveness of metallic **catalyst** in hydrocarbon reforming for CO_x free hydrogen prodn. via different techniques. Among all metallic **catalyst**, Ni-based materials impregnated with various transition metals as promoters exhibited prolonged stability, high...

Refine : 帮助用户迅速获得需要的文献



文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Catalysts (7736)
General chemistry	Catalysis (331)
Synthetic chemistry	
Physical chemistry	
Technology	
Catalysis	
Polymer chemistry	
Environmental chemistry	
Genetics & protein chemistry	
Biotechnology	
Analytical chemistry	
Biology	

2. Select index terms of interest.

Index Terms
Zinc oxide 250
Iron oxide (Fe ₂ O ₃) 230
Nickel oxide (NiO) 227
Magnesium oxide 220
Ceria 209
Copper oxide (CuO) 207
Zeolite HZSM-5 189
Zeolite ZSM-5 185
<input checked="" type="checkbox"/> Zeolites, synthetic 168
Cobalt oxide (Co ₃ O ₄) 165
Ruthenium 157
Zirconia 154
Molybdenum 153
Carbon black 128
Zeolite MCM-41 120
Aluminum 110
Thermolysin 110

Selected Terms

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

Catalysis > Catalysts (1 Terms)

Catalysis > Catalysts > 1 Index Term(s) Selected

OK Cancel

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



结果集的保存— Save, Print, Export

The screenshot shows the SciPlanner interface with a search history: "st" > references (945572) > refine "thermal decomposition" (21389) > keep analysis "Document Type" (15554) > refine "1940-" (14834) > refine by categories > Research. The results page displays 168 references. A purple box highlights the title "文献详细信息" (Literature Detailed Information) over the first reference, which is about research advances in furfural preparation. Another arrow points from the "Export" button in the top right to the second reference, which is about H₂ as a pyrolytic agent.

Save : 保存在服务器上，方便以后登陆查看，每次可存1万条记录。

Export : 导出至本地电脑。

Print : 打印成PDF格式

Citation manager: 保存成RIS等格式，可导入EndNote 等文献管理工具

Offline Review : 保存成PDF , RTF等格式，用于脱机浏览

The Export dialog box allows users to choose the type of export, destination, file name, format, and included details. The "For" section includes options for Citation Manager (RIS, Bibtex), Offline review (PDF, RTF, Answer Keys), and Saving locally (eXchange). The "Details" section requires a file name and provides options for including Task History, Tags, and Comments. The "Format" section offers choices for Summary without abstracts, Summary with partial abstracts, Summary with full abstracts, and Detail (full record).



文献信息一题录、摘要、索引

2. Effect of H₂ as Pyrolytic Agent on the Product Distribution during Catalytic Fast Pyrolysis of Biomass Using Zeolites

By: Wang, Shule; Persson, Henry; Yang, Weihong; Joensson, Paer Goeran

Bio-oil generated from catalytic fast pyrolysis or hydrotreating processes represents one of the most promising alternatives to liq. fossil fuels. The use of H₂ as carrier gas in the pyrolysis of biomass requires further research to study the catalytic fast pyrolysis reactions in the case of using reactive atm. In this work, pyrolysis expts. with lignocellulosic biomass have been performed in a fixed bed reactor in H₂ and N₂ atmospheres with/without HZSM-5 addns. to investigate the influence of the pyrolytic agents during fast pyrolysis of biomass and upgrading of pyrolytic vapors over a zeolitic catalyst. It was found that in a H₂ atmosphere, H₂ was consumed in both the catalytic pyrolysis processes, resp. Higher yields of nonaq. liqs. and permanent gases are obtained in a H₂ atmosphere compared to a N₂ atmosphere. A ca. 书目信息 process using HZSM-5 in a H₂ atmosphere increased the prodn. of polymer arom. hydrocarbons and suppressed the prodn. of monomer arom. hydrocarbons compared to similar tests performed in a N₂ atmosphere. The results show an overall increased activity of HZSM-5 in the reactive H₂ atmosphere compared to a N₂ atmosphere.

Indexing

Electrochemical, Radiational, and Thermal Energy Technology (Section52-1)

Concepts

重要概念

Ashes(residues)
Catalysts
Fixed-bed reactors

Biomass
Chars
Thermal decomposition

effect of H₂ as pyrolytic agent on product distribution during catalytic fast pyrolysis of biomass using zeolites

Carbohydrates

Polymer

effect of H₂ as pyrolytic agent on product distribution during catalytic fast pyrolysis of biomass using zeolites

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

Substances

重要物质

64-19-7 Acetic acid, analysis
71-43-2 Benzene, analysis
85-01-8 Phenanthrene, analysis
86-73-7 Fluorene
90-05-1
90-12-0
91-20-3 Naphthalene, analysis
91-57-6
1-6 Creosol
8-7 analysis
3-6

QUICK LINKS

0 Tags, 0 Comments

SOURCE

Energy & Fuels
Volume32
Issue8
Pages8530-8536
Journal; Online Computer File
2018
CODEN:ENFUEM
ISSN:0887-0624
DOI:10.1021/acs.energyfuels.8b01779

COMPANY/ORGANIZATION

Royal Institute Of Technology, Department of Materials Science and Engineering
School of Industrial Engineering and Management
Stockholm, Swed. 114 28

ACCESSION NUMBER



文献检索小结

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

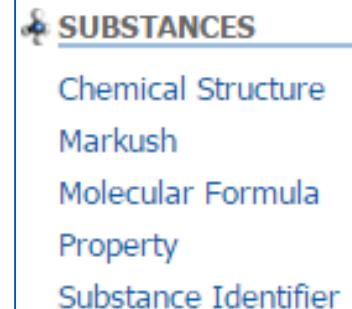
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (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

The screenshot shows the SciFinder software interface. At the top, there are three navigation tabs: 'Explore ▾', 'Saved Searches ▾', and 'SciPlanner'. Below these, a breadcrumb trail indicates the search path: 'Substance Identifier "artemisinin" > substances (1) > 63968-64-9'. On the left, there is a sidebar with sections for 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush, Molecular Formula). The main right panel is titled 'SUBSTANCES: SUBSTANCE IDENTIFIER ?' and contains a text input field with the word 'artemisinin' entered. Below the input field, instructions say 'Enter one per line.' and 'Examples: 50-00-0, 999815, Acetam...'. A callout box with a purple border and white text provides two tips:

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

SciFinder中的物质记录

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

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

CAS Registry Number: 63968-64-9

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

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

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

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

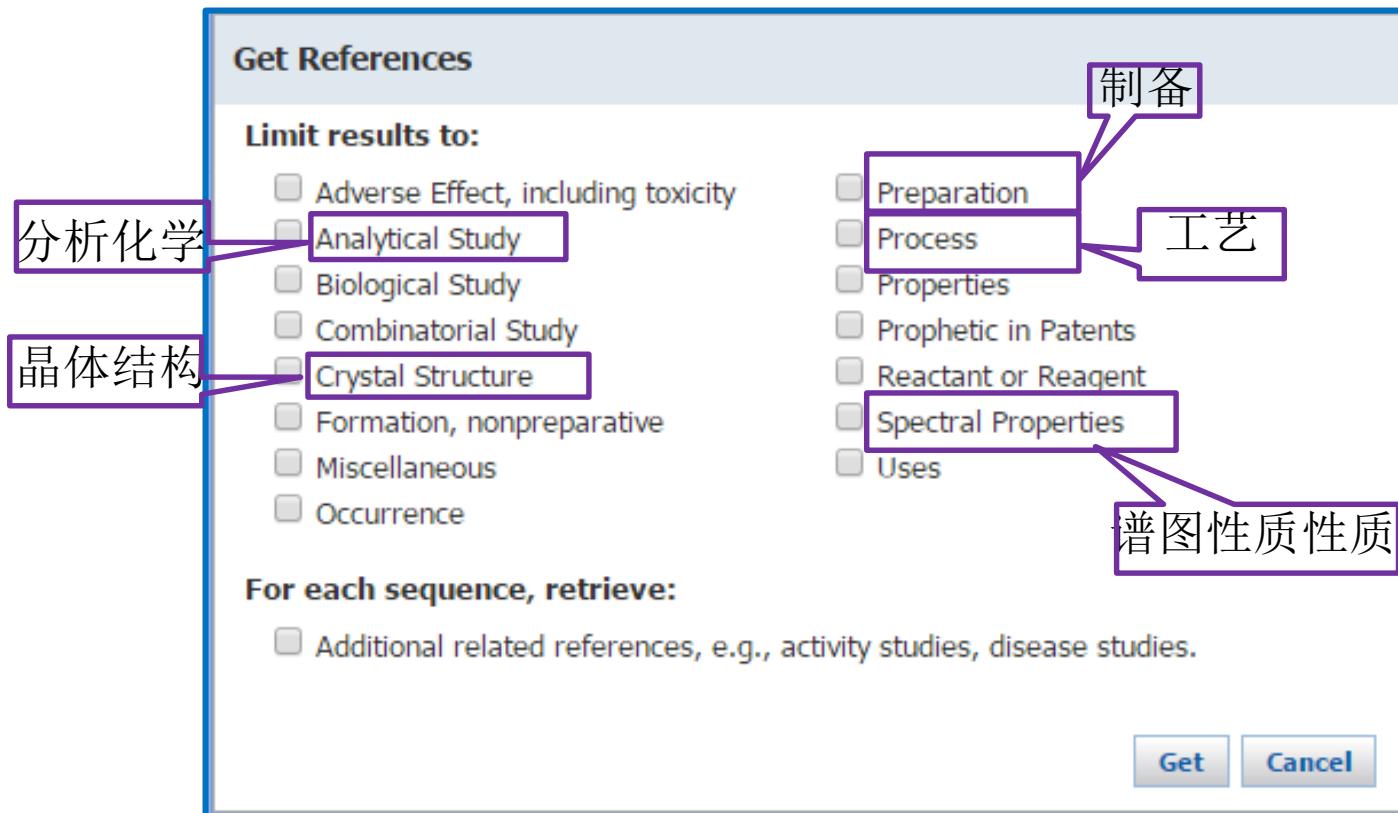
Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*J*]-1,2-benzodioxepin-10(3*H*)-one,
octahydro-3,6,9-trimethyl-, [3*R*-(3*a*,5a*B*,6*B*,8a*B*,9*O*,12*B*,12a*R*^{*})]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-
12*H*-pyrano[4,3-*J*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-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

通过物质获得文献



EXPERIMENTAL PROPERTIES

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

Structure Related Properties

	Value	Note
Bond Angle	See full text	(2)CAS
Bond Length	See full text	(2)CAS
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

EXPERIMENTAL SPECTRA

¹H NMR ¹³C NMR Hetero NMR IR Mass Raman

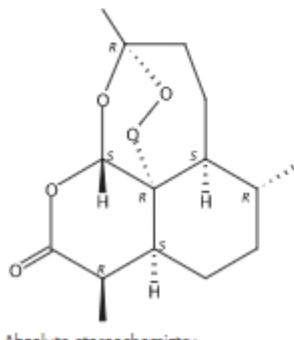
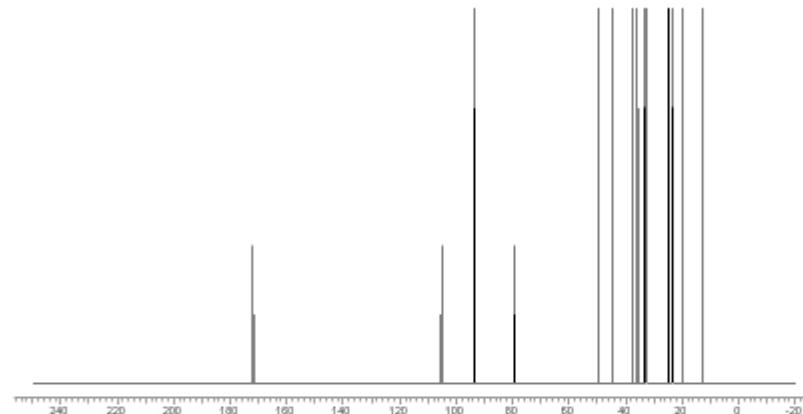
¹³C NMR Properties

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

实验数据与实验谱图

1 of 4

Carbon-13 NMR Spectrum



Absolute stereochemistry

FORMULA
 $C_{15} H_{22} O_5$

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

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... Examples: 44, 25-35, >125

Select Property... Examples: 44, 25-35, >125

- 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 (μ B)
- Median Lethal Dose (LD50) (mg/kg)
- Melting Point (°C)
- Optical Rotatory Power (degrees)
- Refractive Index
- Tensile Strength (MPa)

Explore Select Property...
v.ip138.com—IP Ho

Searches ▾

SUBSTANCES ▾

Search

Select Property... Examples: 44, 25-35, >125

Select Property... Examples: 44, 25-35, >125

- 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



物质检索——理化性质检索：寻找旋光值为-15°的物质

The screenshot shows the SciFinder interface. In the top navigation bar, the 'Explore' button is selected. On the left sidebar, under the 'SUBSTANCES' section, the 'Property' option is chosen. The main search area is titled 'SUBSTANCES: PROPERTY'. A dropdown menu lists various properties, with 'Optical Rotatory Power (degrees)' selected. To its right, the value '-15' is entered into a search field, with examples like '44, 25-35, >125' listed below. Other properties visible in the dropdown include 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), Refractive Index, and Tensile Strength (MPa).

SciFinder物质检索结果

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine

Sort by: CAS Registry Number ▾

Display Options

Analyze by: Substance Role

Preparation 1081

Reactant or Reagent 658

Properties 362

Biological Study 361

Uses 237

Occurrence 140

Process 140

Analytical Study 132

Formation, Nonpreparative 92

Prophetic in Patents 39

0 of 1193 Substances Selected

1. 1433200-70-4

CC(C)C(=O)N[C@@H](C(=O)NCCc1ccncc1)C(=O)N[C@@H](C(=O)O)C(C)C

Absolute stereochemistry.

C₁₅H₂₁N₃O₄
L-Leucine, N-[2-oxo-2-[(4-pyridinylmethyl)amino]acetyl]-, methyl ester

Key Physical Properties
Experimental Properties

2. 1433200-67-9

CC(C)C(=O)N[C@@H](C(=O)NCCc1ccncc1)C(=O)N[C@@H](C(=O)O)C(C)C

Absolute stereochemistry.

C₁₅H₂₁N₃O₄
L-Leucine, N-[2-oxo-2-[(3-pyridinylmethyl)amino]acetyl]-, methyl ester

Key Physical Properties
Experimental Properties

3. 1346255-54-6

CCOC(=O)C=C1[C@H]2[C@H]1C(=O)c3ccccc3[C@H]2C(=O)N(C)Cc4ccccc4

Double bond geometry as shown., Relative stereochemistry.

C₁₈H₂₀I₁N₁O₄
2-Propenoic acid, 3-[(6R,6aR,10aS)-1,2,4,5,6,6a,7,8-octahydro-3-iodo-1-methyl-2,8-dioxobenz[*h*]indol-6-yl]-, ethyl ester, (2*E*)-rel

Key Physical Properties
Experimental Properties

分子式检索

The screenshot shows the SciFinder interface with a blue header bar. The header includes the "CAS Solutions" dropdown, the SciFinder logo with "A CAS SOLUTION" below it, and navigation tabs: "Explore ▾", "Saved Searches ▾", and "SciPlanner".

The main content area has a light gray background. On the left, there is a sidebar with three sections: "REFERENCES", "SUBSTANCES", and "REACTIONS".

- REFERENCES:**
 - Research Topic
 - Author Name
 - Company Name
 - Document Identifier
 - Journal
 - Patent
 - Tags
- SUBSTANCES:**
 - Chemical Structure
 - Markush
 - Molecular Formula** (highlighted)
 - Property
 - Substance Identifier
- REACTIONS:**
 - Reaction Structure

The main search area is titled "SUBSTANCES: MOLECULAR FORMULA ?". It features a search input field with placeholder text "Examples: H4SiO4, (C3H6O.C2H4O)x", a "Search" button, and a help icon (?) above the input field.



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。

合金的检索——钴铁锰合金

Screenshot of the SciFinder interface showing search results for substances with molecular formula "Co . Fe . Mn".

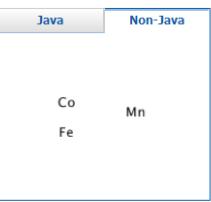
The search results page displays 257 substances. The results are listed in a grid format, each row representing a substance with its CAS Registry Number, component ratios, and a brief description.

Rank	CAS Registry Number	Component	Component Ratio / Percent	Description
1	2222373-78-4	Co	7.5	Co . Fe . Mn Cobalt, compd. with iron and manganese (7.5:2.5:2.5)
2	2222373-77-3	Co	5	Co . Fe . Mn Cobalt, compd. with iron and manganese (5:5:2.5)
3	2222373-76-2	Co	2.5	Co . Fe . Mn Cobalt, compd. with iron and manganese (2.5:7.5:2.5)
4	2192220-92-9	Fe	0 - 79	Co . Fe . Mn Iron alloy, base, Fe 0-79, Co 21-62, Mn 0-39
5	2170121-60-3	Fe	82	Co . Fe . Mn Iron alloy, base, Fe 82, Mn 13, Co 5
6	2159146-09-3	Mn	13	Co . Fe . Mn Iron alloy, base, Fe 65, Mn 20, Co 15
7	2159146-06-0	Co	5	Co . Fe . Mn Iron alloy, base, Fe 0-79, Co 21-62, Mn 0-39
8	2159146-00-4			
9	1632299-36-5			



合金的检索——掺杂钴铁锰的合金

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:
 Java Non-Java

 Click image to change structure or view detail.
 Import CXF

Search Type:
 Exact Structure Substructure Similarity
 Show precision analysis

Advanced Search Always Show

Characteristics
 Single component
 Commercially available
 Included in references

Classes
 Alloys
 Coordination compounds
 Incompletely defined
 Mixtures
 Polymers
 Organics, and others not listed

Studies
 Analytical
 Biological

SUBSTANCES ?

Analyze Refine Sort by: CAS Registry Number ↴

Sample Analysis: Substance Role
 Uses ≥ 15150
 Properties ≥ 8744
 Process ≥ 6775
 Preparation ≥ 2075
 Biological Study ≥ 330
 Analytical Study ≥ 128
 Reactant or Reagent ≥ 100
 Miscellaneous ≥ 80
 Formation, Nonpreparative ≥ 23
 Occurrence ≥ 9

Get References Get Reactions Get Commercial Sources Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Display Options Page: 1 of 2156

0 of 32331 Substances Selected

1. 2247891-60-5 

Component	Component Percent
Fe	50 - 76
Co	20 - 40
Zr	2 - 4
V	1 - 2.5
B	0.2 - 1.5
Ni	0.2 - 1
Mn	0.1 - 0.2
Cu	0 - 0.2
Si	0 - 0.2

B . Co . Cu . Fe . Mn . Ni . Si . V . Zr
INDEX NAME NOT YET ASSIGNED

2. 2247888-96-4 

Component	Component Percent
Al	1.4 - 17
Mg	1.4 - 17
Mn	1.4 - 17
Co	14
Cr	14
Fe	14
Ti	14

Al . Co . Cr . Fe . Mg . Mn . Ti
INDEX NAME NOT YET ASSIGNED

3. 2247811-26-1 

Component	Component Percent
Fe	33 - 74
Ni	25 - 40
V	0.5 - 3
Co	0 - 3
Cr	0 - 3
Si	0.1 - 2
Mn	0 - 2
Mo	0.4 - 1.9
Al	0 - 1.5
Cu	0 - 1.5
Hf	0 - 1.5
Nb	0 - 1.5
Ta	0 - 1.5
Ti	0 - 1.5
W	0 - 1.5
Zr	0 - 1.5
C	0.1 - 0.4

C . Al . Co . Cr . Cu . Fe . Hf . Mn . Mo . Nb . Ni . Si . Ta . Ti . V . W . Zr
INDEX NAME NOT YET ASSIGNED



物质检索——结构

SUBSTANCES: CHEMICAL STRUCTURE [?](#)

Structure Editor:

Java **Non-Java**

Click to Edit

Import CXF

Search

Advanced Search Always Show

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

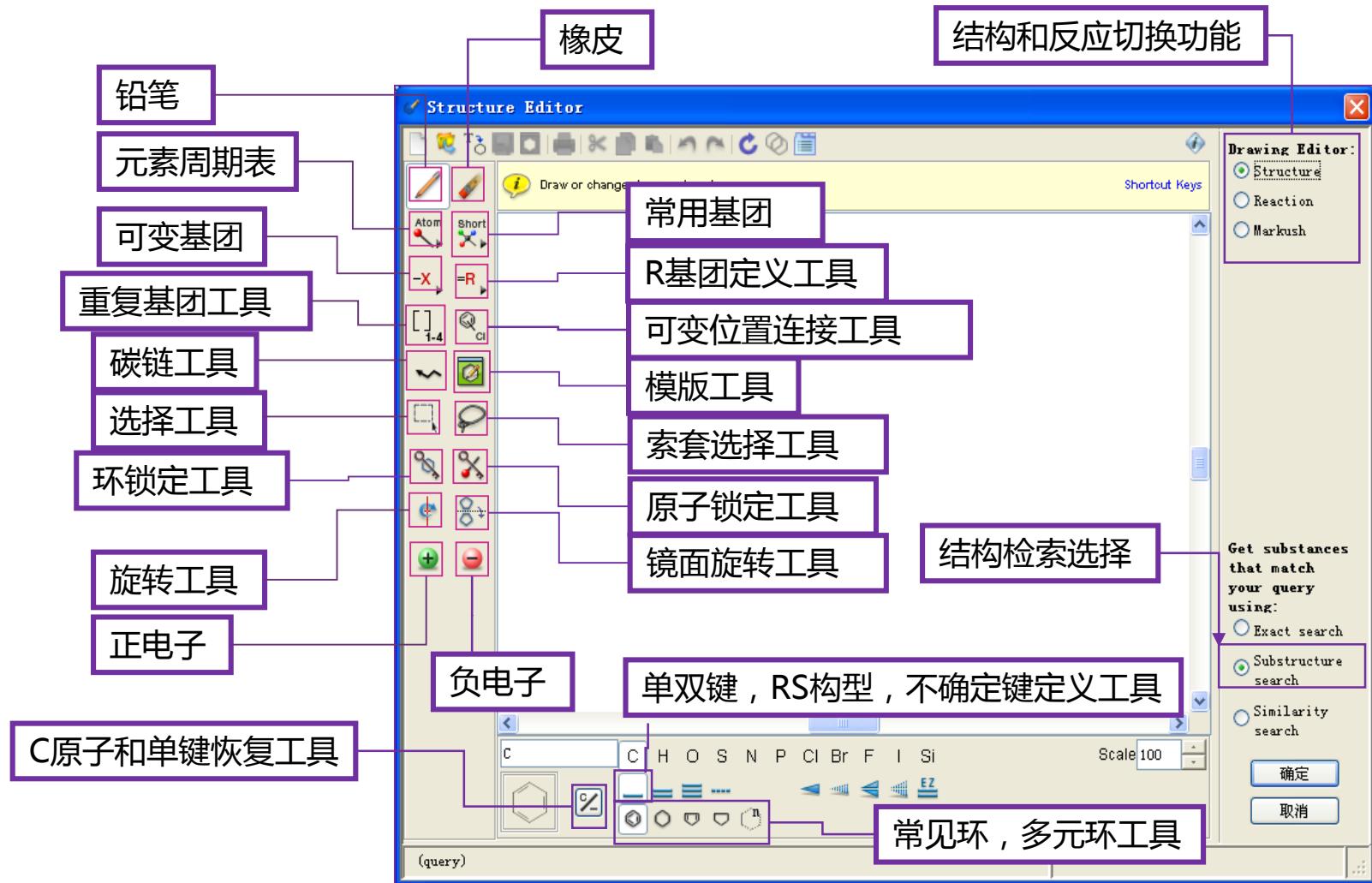
Search Type:

- Exact Structure
- Substructure
- Similarity

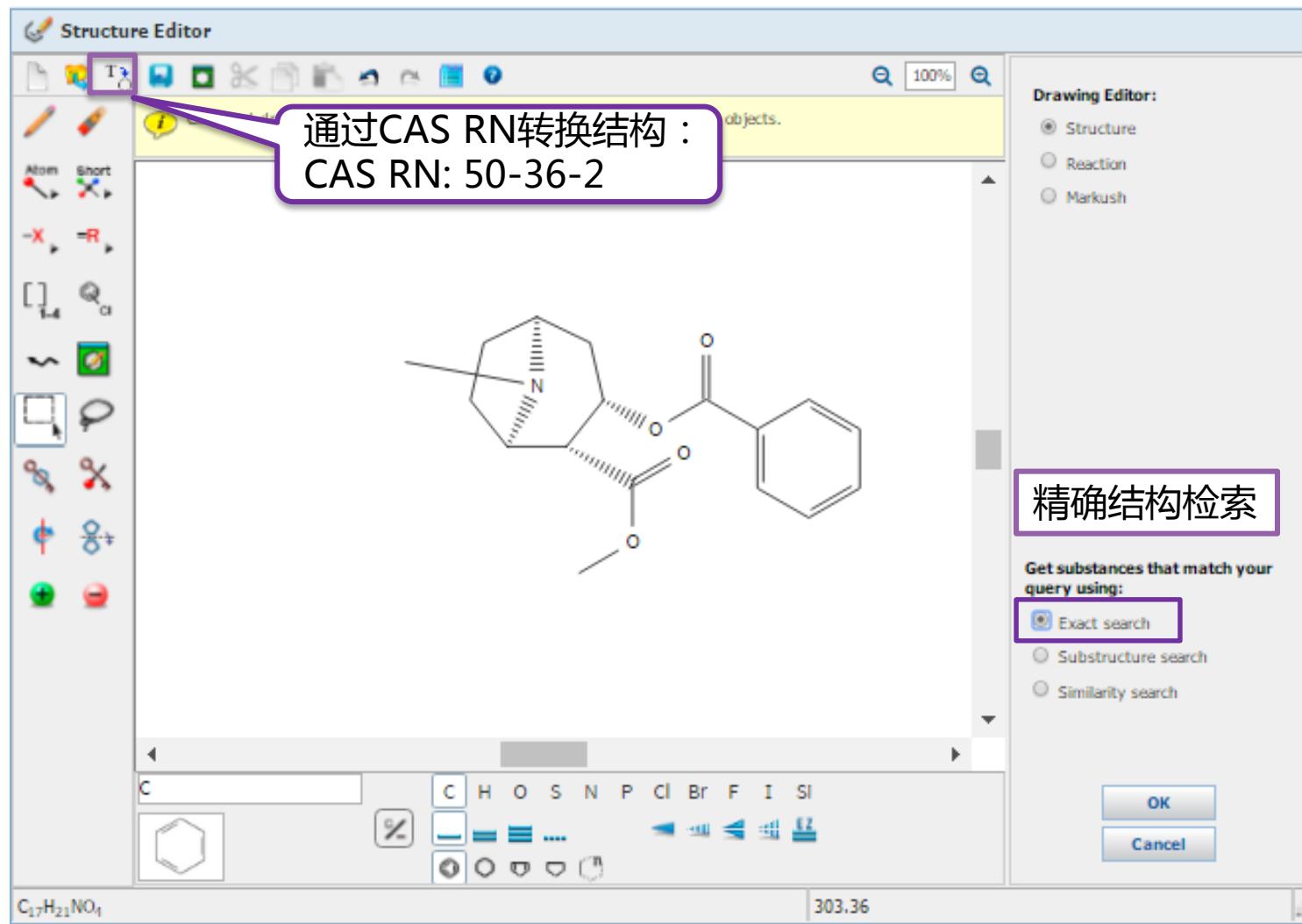
Show precision analysis

 **ChemDraw®**
Launch a SciFinder substance or reaction search

物质检索——结构



物质检索——精确结构检索

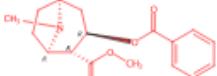


精确结构检索结果

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

Sort by: Relevance ▾

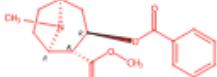
0 of 6 Substances Selected

1. 668-19-9 
Absolute stereochemistry.

CN1[C@H](C[C@H]1C(=O)OC(=O)c2ccccc2)C(=O)OC
 $\text{C}_{17}\ \text{H}_{21}\ \text{N}\ \text{O}_4$
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (*1R,2R,3R,5S*)-

Key Physical Properties
Spectra

可卡因

2. 114599-38-1 
Absolute stereochemistry.

CN1[C@H](C[C@H]1C(=O)OC(=O)c2ccccc2)C(=O)OC
 $\text{C}_{17}\ \text{H}_{21}\ \text{N}\ \text{O}_4$
668-19-9

3. 109496-04-0 
Absolute stereochemistry.

CN1[C@H](C[C@H]1C(=O)OC(=O)c2ccccc2)C(=O)OC
 $\text{C}_{17}\ \text{H}_{21}\ \text{N}\ \text{O}_4 \cdot \text{Cl}\ \text{H}$
(Component: 668-19-9)
Allococaine, hydrochloride (6CI)

可卡因组合物

盐酸可卡因

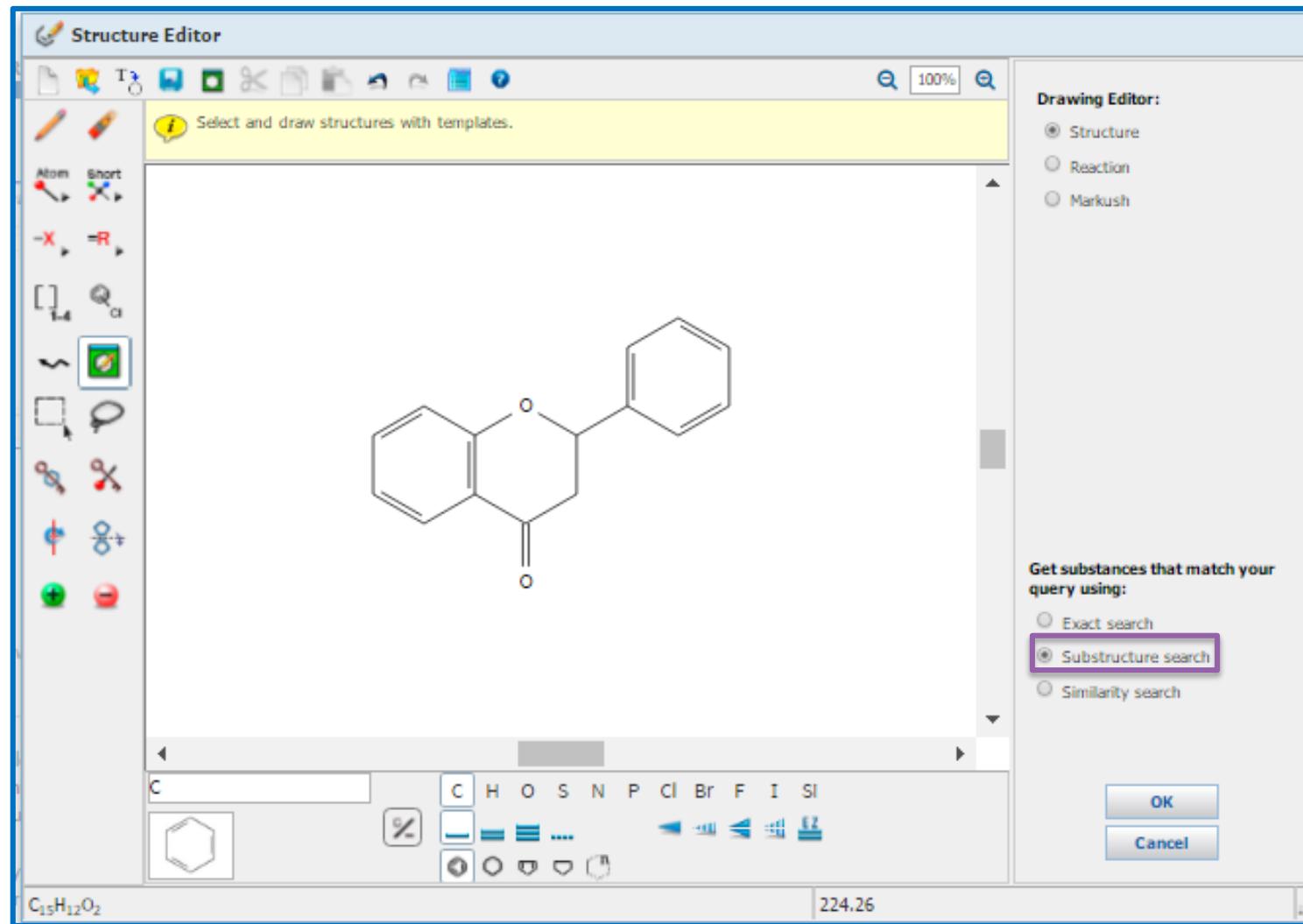
物质检索——精确结构检索

- 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 ~69

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

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244 ~4

Absolute stereochemistry: Rotation (-)

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

Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5

C₁₅H₇D₅O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-(phenyl-d₃)- (9CI)
Spectra

同位素

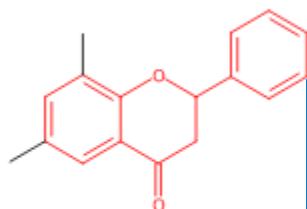
亚结构检索结果

281. 123251-10-5

~3



取代物



C₁₇H₁₆O₂

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

► Key Physical Properties

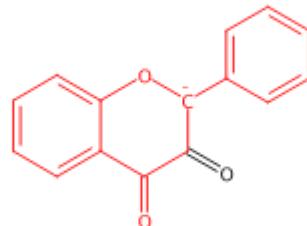
Experimental Properties

~0

295. 780723-19-5

~0

离子



C₁₅H₉O₃

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

亚结构检索结果的限定

Analysis Refine

Refine by:

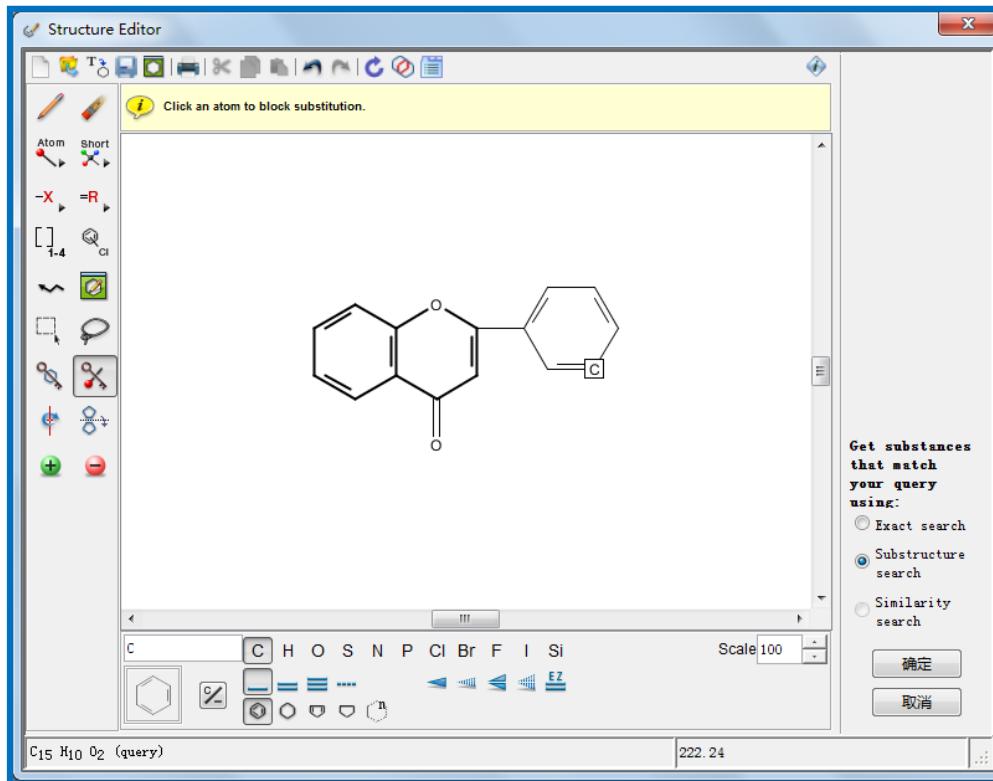
- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

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:

Java **Non-Java**

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

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

Refine

Get References Get Reactions Get Commercial Sources Tools ▾

Sort by: Relevance

0 of 17496 Substances Selected

1. 487-26-3

~2374 ~71

C₁₅ H₁₂ O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~265 ~7

Absolute stereochemistry.,Rotation (-).

C₁₅ H₁₂ O₂
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-
Key Physical Properties
Experimental Properties

4. 104550-32-5

5. 75524-43-5

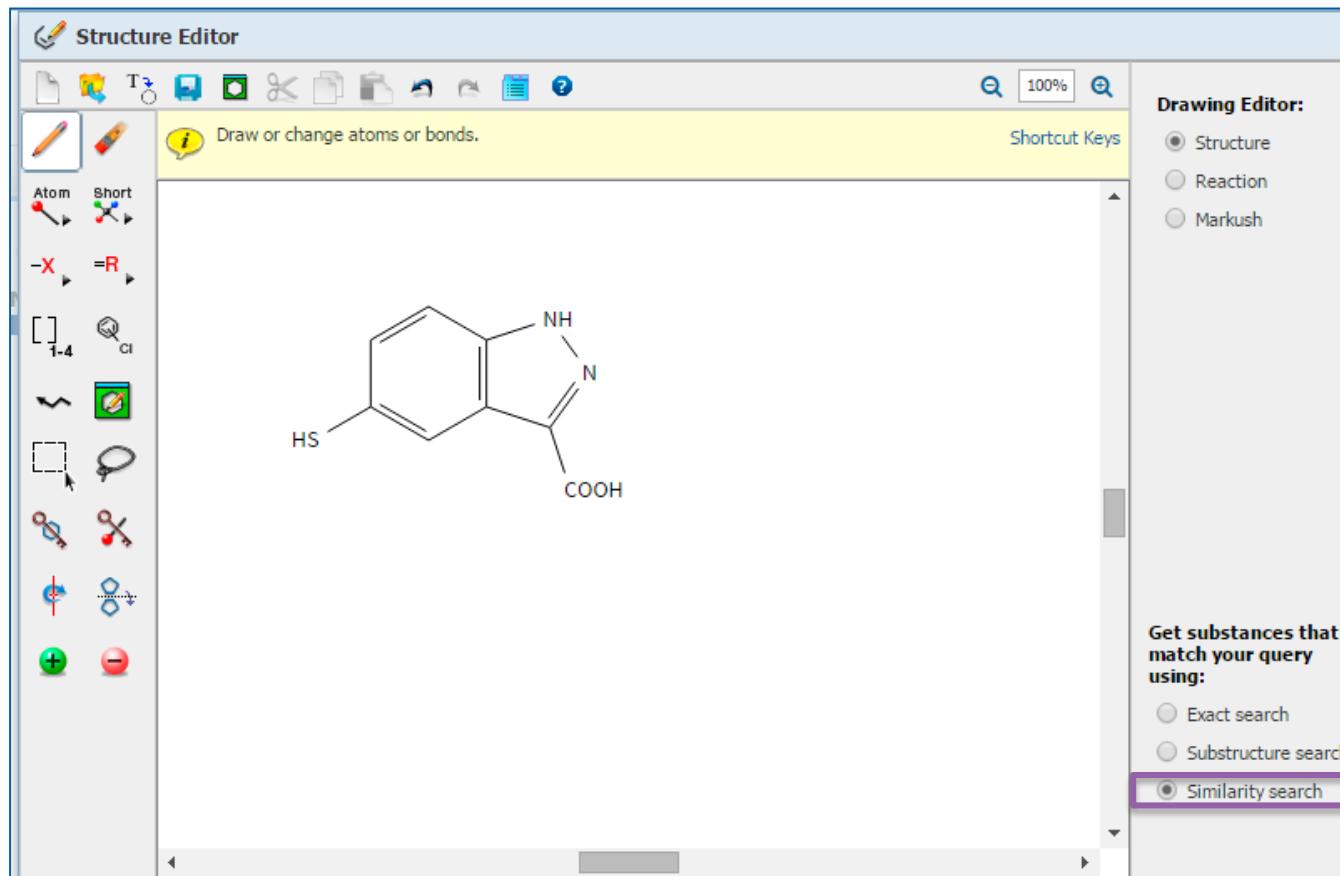
物质检索——亚结构检索

- 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 checked="" 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

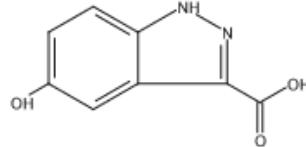
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5



~35



C₈H₆N₂O₃

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

► Key Physical Properties

取代基变化

Score: 86

5. 858227-12-0

取代基位置变化



~7

~41

~41



C₉H₈N₂O₂

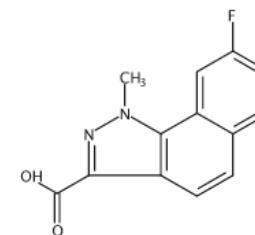
1*H*-Indazole-3-carboxylic acid, 6-methyl-

► Key Physical Properties

Score: 65

541. 1100422-

母体结构变化



C₁₃H₉FN₂O₂

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

► Key Physical Properties



SCI-FINDER®
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

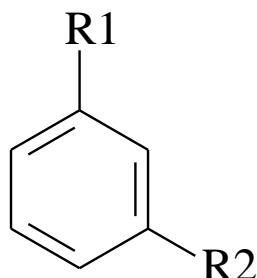
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

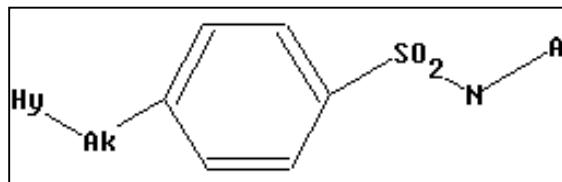
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
- SciFinder常见问题及解决

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



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

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Get Markush patents where the structure(s) are:

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

OK Cancel

A C H O S N P Cl Br F I Si

Hy - Ak - SO₂ - NH - A



Markush检索



Welcome Helen Zhu

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

REFERENCES ? [Get Substances](#) [Get Reactions](#) [Get Related Citations](#) [Tools](#) [Create Keep Me Posted Alert](#) [Send to SciPlanner](#)

Analyze Refine Categorize Sort by: Accession Number ▾

Analyze by: Document Type

Patent 1969

Journal 1

Show More

0 of 1969 References Selected Page: 1 of 99

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



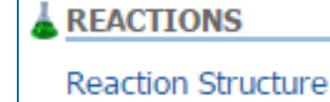
提纲

- 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——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

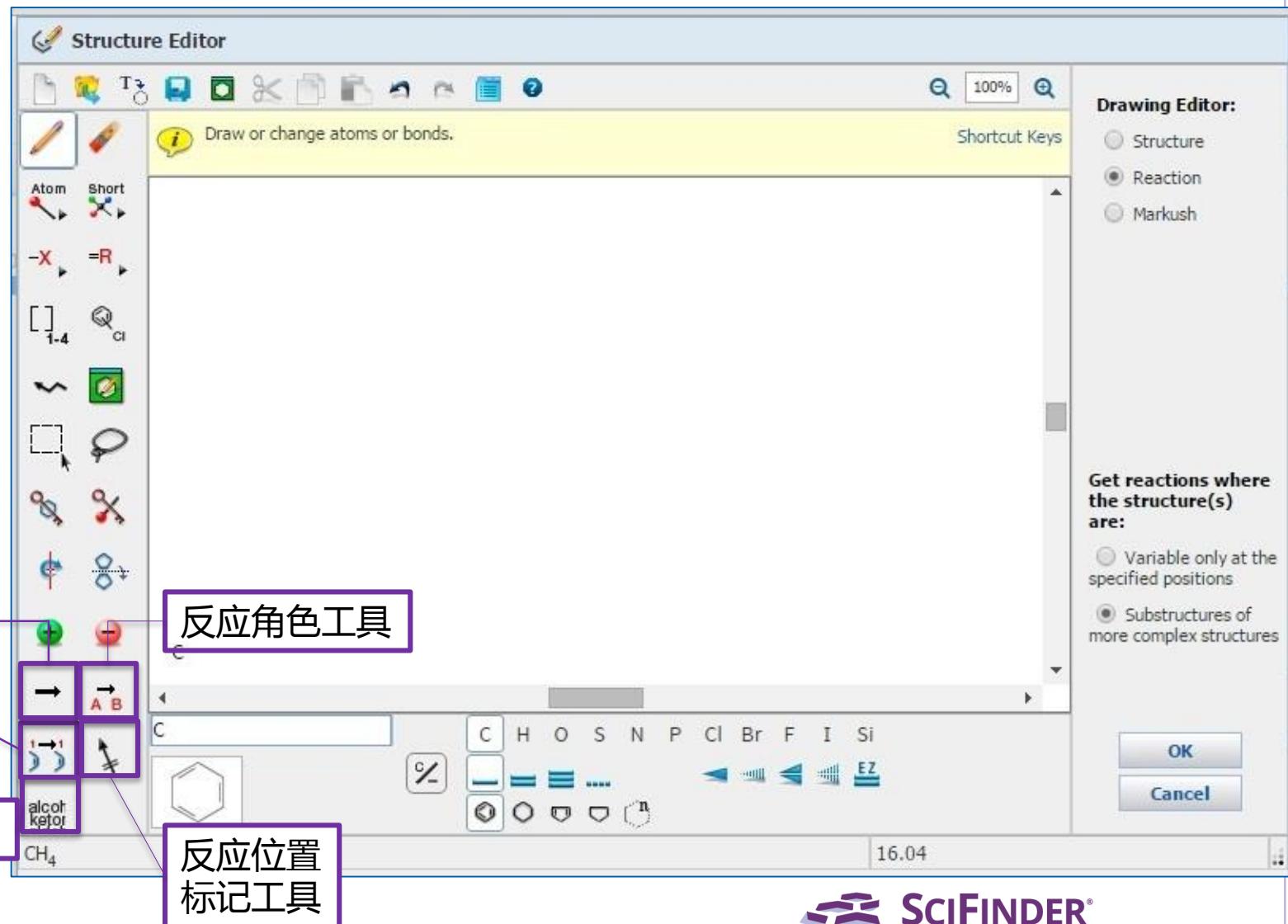
- 精确结构反应检索

- 亚结构反应检索

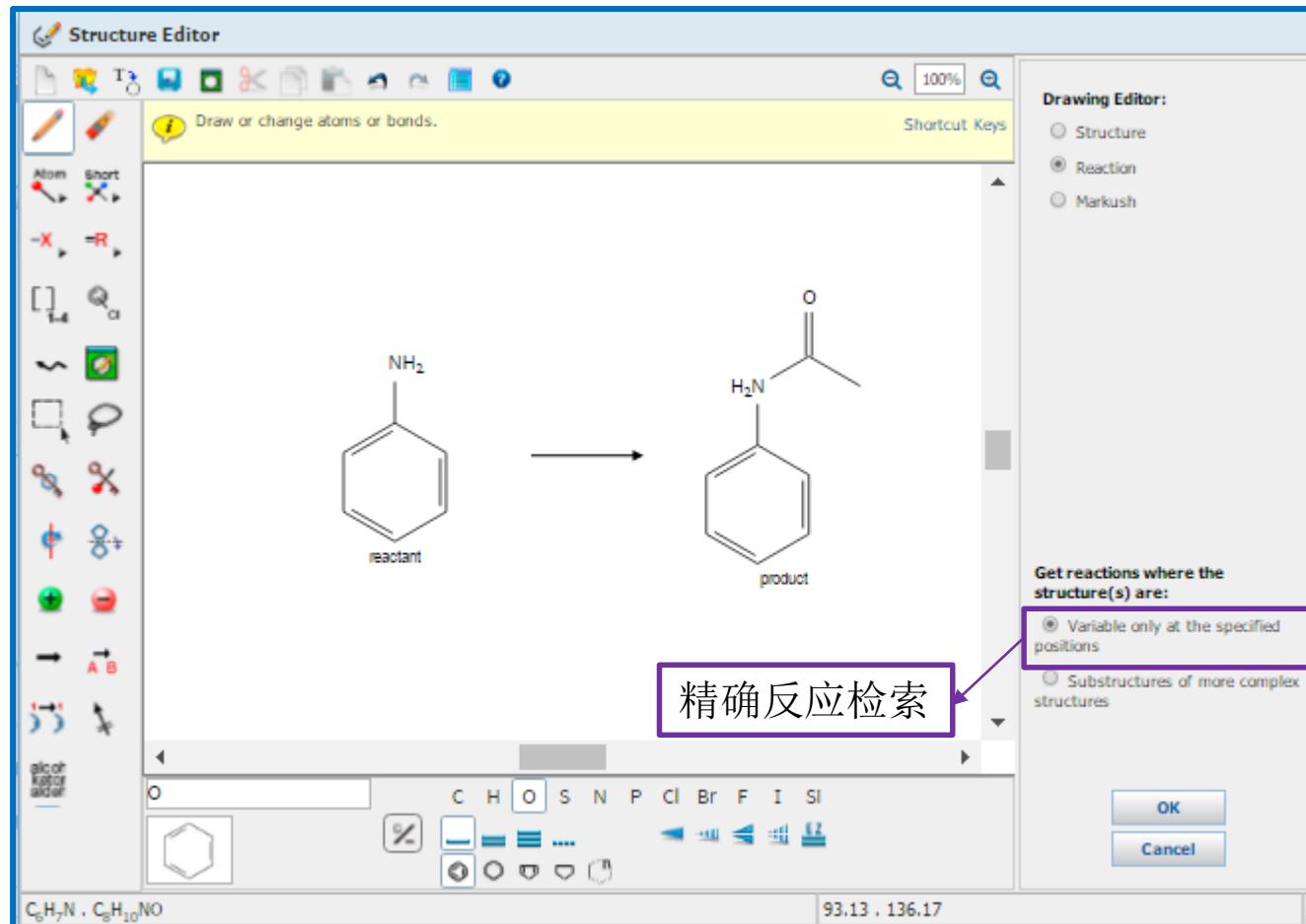
Get reactions where
the structure(s)
are:

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

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 ▾ Sort by: Relevance ▾

No Grouping
Document Selected
Transformation

1. View Reaction Detail Similar Reactions

Single Step Hover over any structure for more options.

Reaction scheme:

+
→
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：

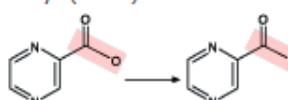
- Broad : 仅反应中心相似
- Miedum : 反应中心及附属原子和键
- Narrow : 反应中心及扩展的原子和键

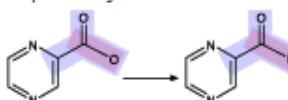
Get Similar Reactions ?

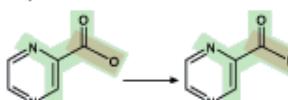
Retrieve similar reactions from:

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

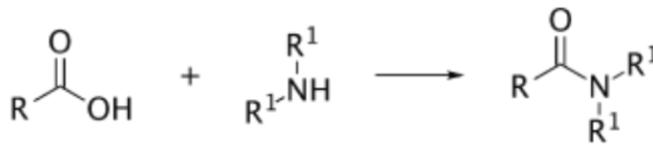
Group by: Transformation ▼ Sort by: Frequency ▼

0 of 605 Reactions Selected

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

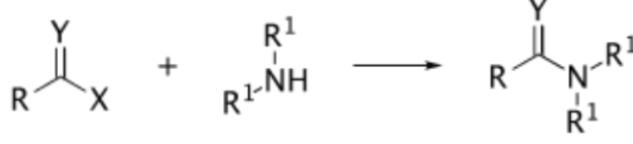


2. Acylation of Nitrogen Nucleophiles by Carboxylic Acids
81 Reactions



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



$Y = O, S, NR'$

反应检索结果的筛选

Analyze Refine

Group by: No Grouping Sort by: Relevance ↴

Analyze by: Solvent

H ₂ O	99
CH ₂ Cl ₂	65
MeCN	55
THF	27
PhMe	26
AcOH	25
CHCl ₃	22
DMF	15
DMSO	15
Me ₂ CO	15

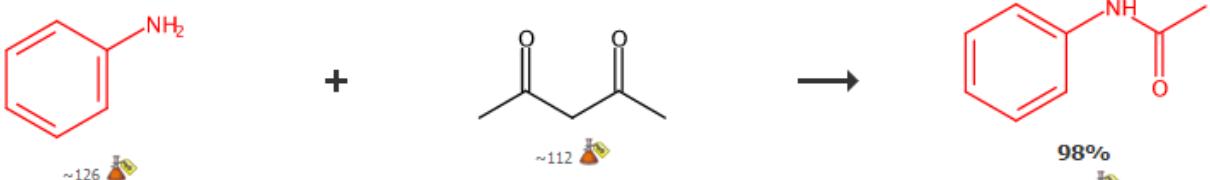
Show More

0 of 606 Reactions Selected

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

Single Step Hover over any structure for more options.

筛选用水作溶剂的反应



Overview

Steps/Stages

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

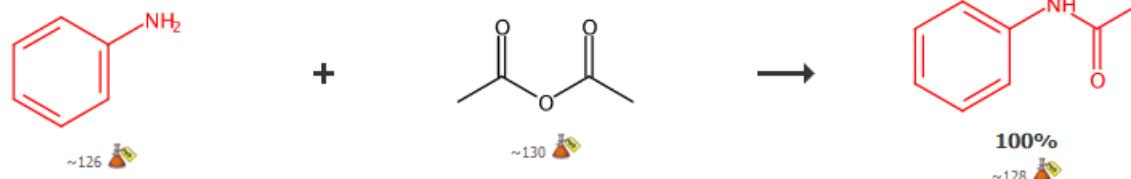
Notes

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

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

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

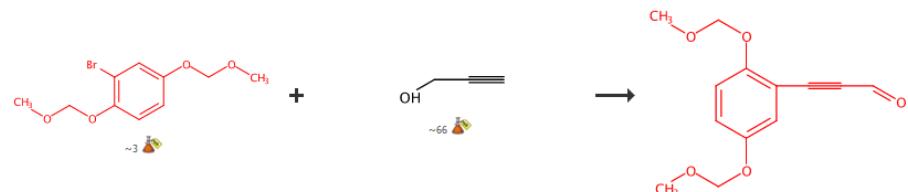


Representative procedure for the preparation of acetanilides: Aniline (10.1 mL, 109.7 mmol, 1 eq) was added to a round-bottom flask via syringe and fitted with a rubber septum. The flask was purged with argon and dry DCM (300 mL, 0.4 M) was added. Acetic anhydride (12.5 mL, 132.2 mmol, 1.2 eq) was added 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.



Overview

Steps/Stages

- 1.1 C:Pd(PPh_3)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
- 2.4 R:LiCl, P:BuNH₂Cl, 20 min, rt

Notes

- 1) key step, alternate catalyst concentration, catalyst (CuI) and temperature yield, Sonogashira coupling, 2) key intermediate, Swern oxidation, scale method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, Stoichiometry: 1, Time: 1, Temperature: 1, Yield: 1, Product: 1
Most stages in any one step: 4

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。

Experimental Procedure

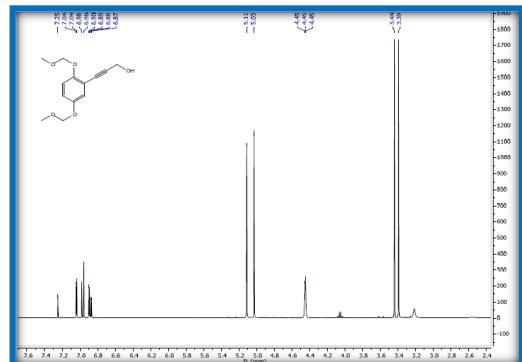
NATURAL PRODUCTS

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(Ph_3)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%). β -[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol⁴² (**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. β -[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal⁴³ (**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

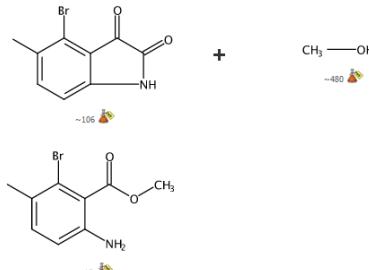
MethodsNow

A New Method for Synthesis of Nolatrexed Dihydrochloride

By Zhao, Xueqing; Li, Fei; Zhang, 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



1 →

Products	Benzolic acid, 6-amino-2-bromo-3-methyl-, methyl ester, 84%, CAS RN: 147149-88-0
Reactants	1H-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">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).Add $K_2S_2O_8$ (1.90 kg, 7.03 mol) to the mixture in parts 10°C with an ice-water bath.After addition the reactant mixture turns yellow, continue the stirring for 1 hour at room temperature.Adjust the reaction mixture to pH 8-9 with aqueous 36% HCl (1.24 L) 15 °C.Destroy the excessive $K_2S_2O_8$ by aqueous 5% $Na_2S_2O_3$ solution (450 mL).After rotary evaporation under a reduced pressure at 55 °C, Leave a brown liquid.Mix the mixture with CH_2Cl_2 (6 L) and H_2O (4 L).Separate the organic phase.Extract the aqueous phase with CH_2Cl_2 (4 L).Dry the combined organic phases over Na_2SO_4.Concentrate the combined organic phases with a rotavapor.Distill the resulted brown liquid under high vacuum.
Scale	milligram
1H NMR	$CDCl_3$: δ 2.28 (s, 3 H, Ar- CH_2), 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	$KBr cm^{-1}$: ν 3472, 3382, 2953, 2924, 1716, 1622, 1480, 1277, 816.

物质信息

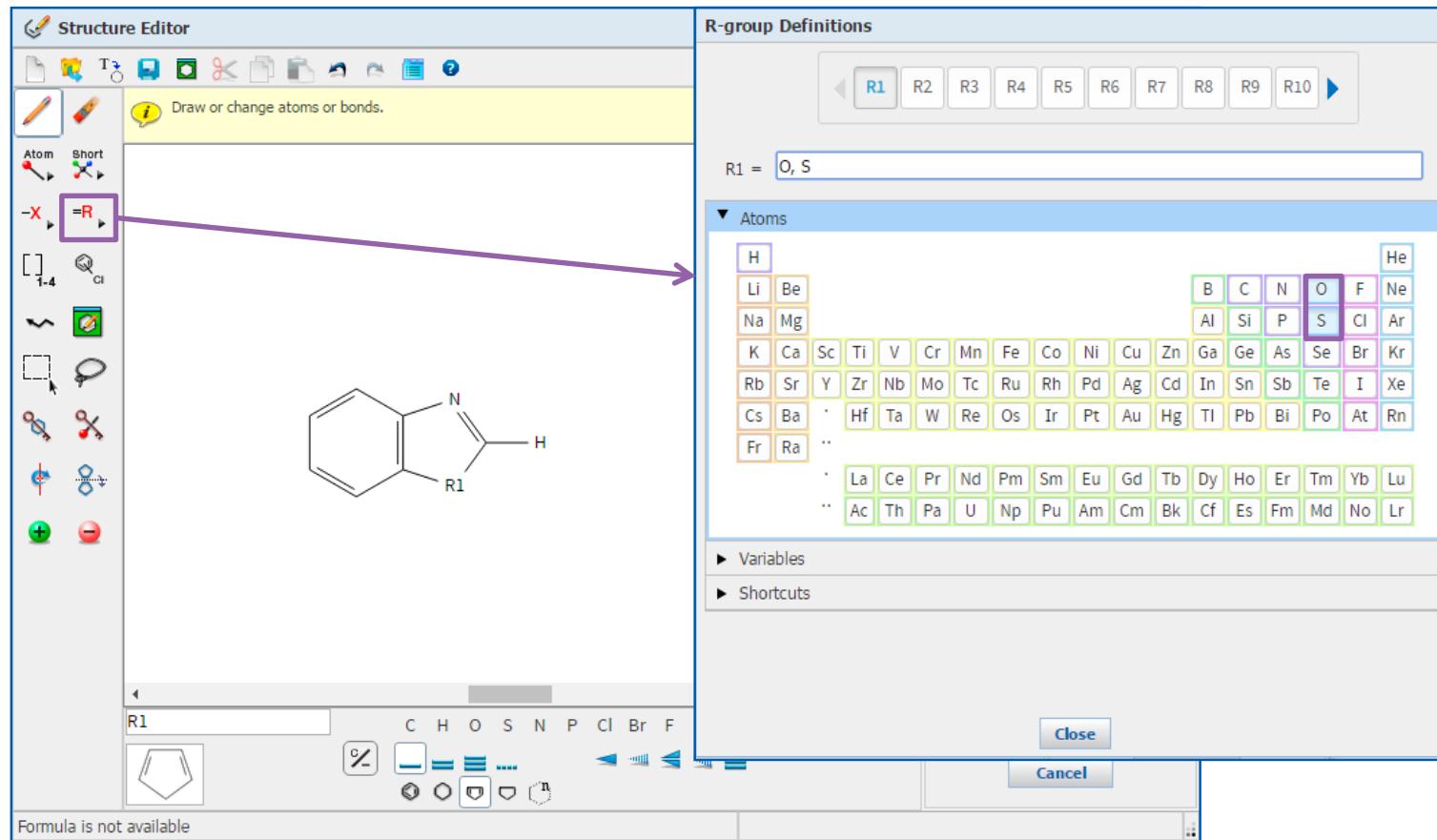
实验过程

图谱信息

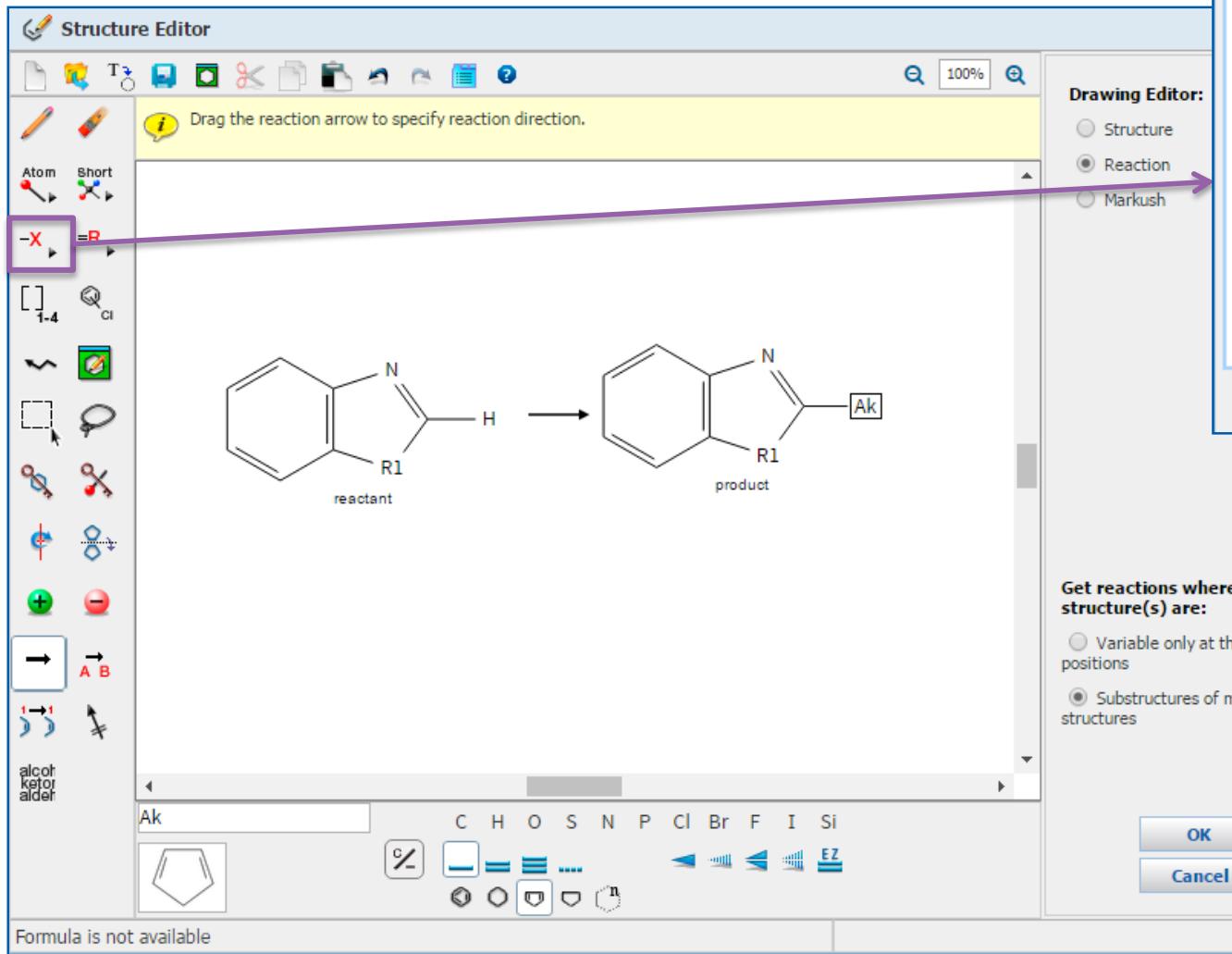
SCI-FINDER®
A CAS SOLUTION

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



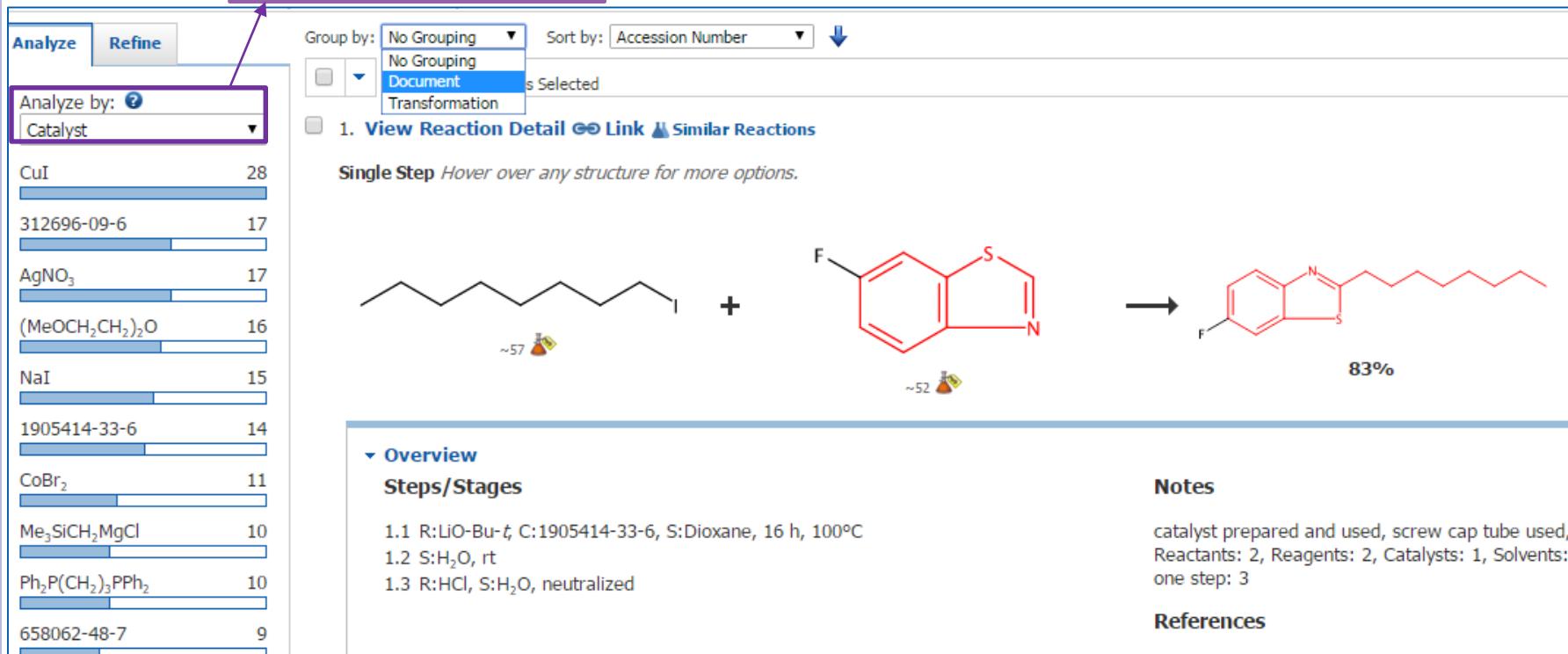
Variables

- 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

Close

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

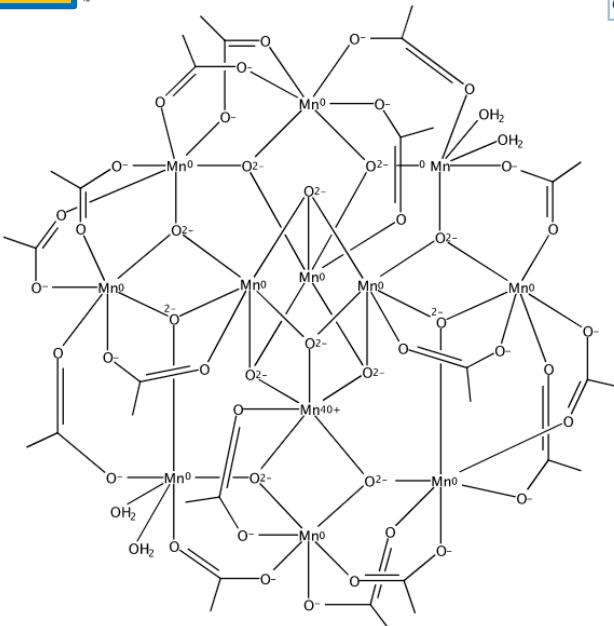


ACS / Proprietary and Confidential / Do Not Distribute

案例一：查找多氧族金属的反应信息

CAS Registry Number 76210-25-8
~612 Mn₁₂ O₄₈
C32H56Mn12O48
Manganese, hexadecakis[μ-(acetato-*O*,*O'*)]tetraquadodeca-μ₃-oxododeca-, compd. with acetic acid, hydrate (1:2:4)
Other Names
Manganese, hexadecakis[μ-(acetato-*O*,*O'*)]tetraquadodeca-μ₃-oxododeca-, compd. with acetic acid (1:2), tetrahydrate (9CI)
Hexadecaacetatotetraquadodecaoxododecamanganese-acetic acid tetrahydrate (1:2)
Mn₁₂
Mn₁₂ acetate
View more...

也可以获得反应信息



64-19-7
C2H4O3


CAS Registry Number: 76125-82-1
View Substance Detail
Explore by Structure
Synthesize this...
Get Reactions where Substance is a ▾
Product
Reactant
Reagent
Reactant/Reagent
Get Commercial Sources
Get Regulatory Information
Get References
Export as Image
Export as molfile
Send to SciPlanner

Reagent
Catalyst
Solvent
Any Role

查看反应信息详情

Analyze Refine Group by: No Grouping Sort by: Accession Number Display Options

0 of 12 Reactions Selected

1. View Reaction Detail [Link](#)

Single Step Hover over any structure for more options.

Analyze by: Reagent

Reagent	Count
KMnO ₄	6
TEA chloride	2
110743-42-5	1
Ce(NH ₄) ₂ (NO ₃) ₆	1
H ₂ O	1
Mn(OAc) ₂	1

Show More

complex with picoline

▼ Overview

Steps/Stages

1.1 R:Ce(NH₄)₂(NO₃)₆, S:MeCN, rt; 15 min, rt

Notes

crystals formed after 3 days at room temperature, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Manganese/Cerium Clusters Spanning a Range of Oxidation Levels and CeMn₈, Ce₂Mn₄, and Ce₆Mn₄ Nuclearities: Structural, Magnetic, and EPR Properties
Q Quick View [Other Sources](#)
By Lampropoulos, Christos et al.
From Inorganic Chemistry, 53(13), 6805-6816; 2014

▼ Experimental Procedure

Inorganic Chemistry General/Typical Procedure: **Method B.** To a stirred solution of [Mn₁₂O₁₂(O₂CMe)₁₆(H₂O)₄] (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and pyridine (10 mL) was slowly added solid (NH₄)₂[Ce(NO₃)₆] (0.28 g, 0.50 mmol). The resulting solution was stirred for 15 min, during which time the color changed slightly from dark brown to reddish brown. The solution was filtered and left undisturbed for a period of 3 d, during which time black needles of 1·2py·6MeCN grew. They were isolated as for Method A; the yield was based on Ce. The identity of the product was confirmed by elemental analysis, IR spectral comparison, and unit cell determination to be identical to material from Method A. The picoline version [Ce₆Mn₁₂(O₂CMe)₁₆(NO₃)₄(pic)₄] (1') can be obtained in comparable yield by the same method using picoline instead of pyridine. Anal. Calcd (Found) for 1'·2H₂O: C, 21.14 (21.25); H, 2.50 (2.75); N, 4.48 (4.26)%.

▼ METHODSNow™

Procedure

- Slowly add solid (NH₄)₂[Ce(NO₃)₆] (0.28 g, 0.50 mmol) to a stirred solution of [Mn₁₂O₁₂(O₂CMe)₁₆(H₂O)₄] (0.50 g, 0.25 mmol) in a solvent mixture comprising MeCN (15 mL) and picoline (10 mL).

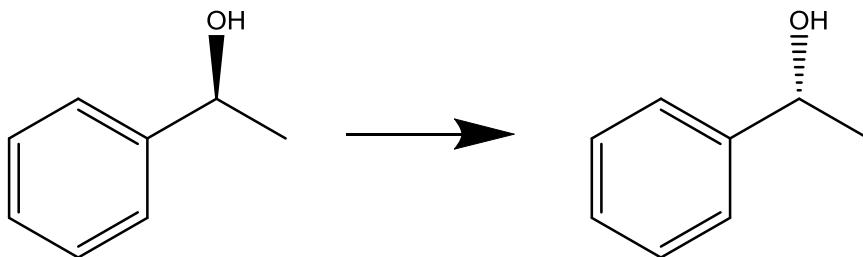
View more...

Available Experimental Data

Elemental Analysis

[View with MethodsNow](#)

案例二：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.



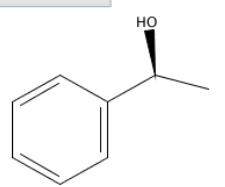
案例：如何获取手性翻转反应

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。

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

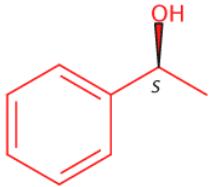
Show precision analysis

ChemDraw® Launch a SciFinder substance search

1 of 52 Substances Selected

1. 1445-91-6

~3499 ~90



Absolute stereochemistry, Rotation (-).

C₈H₁₀O
Benzinemethanol, 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 search

1 of 54 Substances Selected

1. 1517-69-7

~3531 ~94

Absolute stereochemistry,,Rotation (+).

C₈H₁₀O
Benzinemethanol, α-methyl-, (αR)-

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

Reactions (52) > get reactions (7938)

Get References Tools ▾ Find Additional Reactions Combine Answer Sets

Group by: No Group 0 of 79. Display Options Page: 1 of 530

1. View Reaction Details

4 Steps Hover over any structure for more options.

Chemical structures shown: NC=CC(=O)C, CC, CC(=O)C, CC(C)(N)C, C=C[C@H](CS)O.

Combine Answer Sets

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

<input checked="" type="checkbox"/>	Combine	Include all reactions from both sets
<input checked="" type="checkbox"/>	Intersect	Include only reactions that appear in both sets
<input type="checkbox"/>	Exclude	Include only answers from 2 that are not in 1
<input type="checkbox"/>	Exclude	Include only answers from 1 that are not in 2

Combine Answer Sets **Cancel**

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)

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.



100%
~100

Overview

Steps/Stages

1.1 S:H₂O, 5:Me,  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 (PatentPak)
 - 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

勾选想要的反应

3 Steps Hover over any structure for more options.

Send to SciPlanner Display Options

进入SciPlanner 新建文件

将刚推送过来的反应拖至编辑面板

The screenshot shows the SciPlanner software interface. At the top, there's a reaction scheme with two reactants and one product. The first reactant is 4-nitro-2-chloropyridine (~192). The second reactant is 4-methoxybenzenethiol (~72) labeled as [Step 2.1]. The product is 4-(4-methoxybenzylthio)-2-chloro-6-nitropyridine. Below the reaction scheme, there's an 'Overview' section with 'Steps/Stages' and 'Notes'. The 'Steps/Stages' section lists three steps: 1.1 R:NH₃, R:*t*-BuOK, R:*t*-BuOOH, S:THF; 2.1 R:Nah, S:THF; 3.1 R:*t*-BuOCl₃, reflux. The 'Notes' section mentions Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1. In the bottom left, there's a 'Workspace' menu with options like New, Open, Save, Duplicate, Import, Export, Print, and Close. The workspace itself is empty, with a message saying 'Your Workspace is empty.' and instructions to drag items from the reference, substance, and reaction libraries. On the right side, there's a preview area showing the reaction scheme.



SciPlanner使用简介

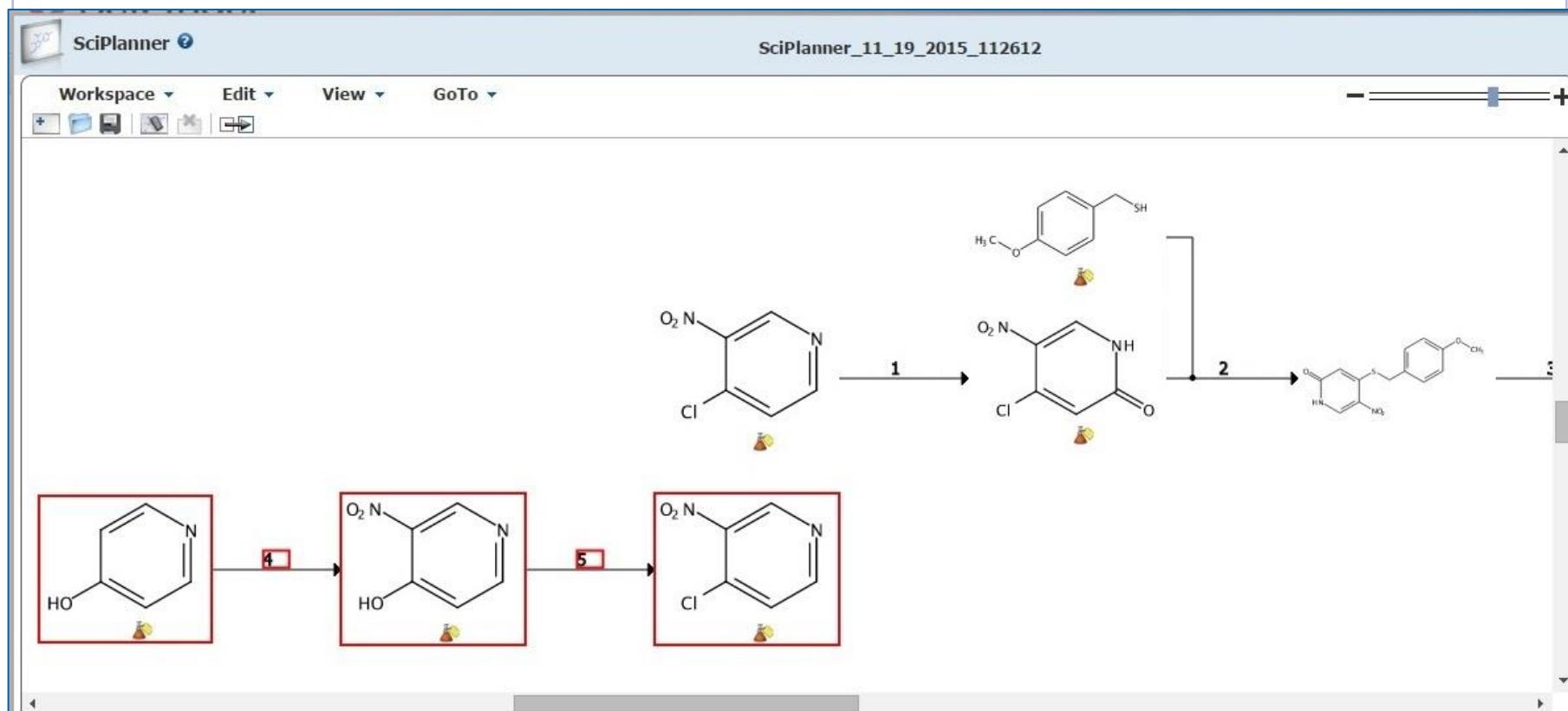
The screenshot shows the SciPlanner software interface. At the top, there is a menu bar with options like Workspace, Edit, View, GoTo, and a CAS Registry Number field (13091-23-1). A context menu is open over a chemical structure, with the option "Synthesize this..." highlighted. Below the menu, a synthesis route is displayed with three steps. Step 1 shows the conversion of 4-nitrochlorobiphenyl to 4-chloro-2-(2,4-dichlorophenyl)butan-2-one. Step 2 shows the reaction of this intermediate with 2-(4-methoxyphenyl)thiophene to form 2-(4-chlorophenyl)-4-(4-methoxyphenyl)-2-thiophenylmethane. Step 3 shows the final product being converted to a derivative with a nitro group. In the bottom left, a reaction detail for the first step is shown, comparing 4-hydroxypyridine and 4-nitro-4-chloropyridine. The bottom right features the SciPlanner logo and the text "Send selected records to SciPlanner".

打开中间产物的标准菜单
选择Synthesis 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 ?

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

Chemical reaction scheme:

- Reaction 4: A nitrile (R₁-C≡N) reacts with 4-hydroxy-2-nitropyridine to form 4-(R₁-methylsulfonyl)-2-nitropyridine.
- Reaction 5: 4-hydroxy-2-nitropyridine reacts with 3-chloropyridine to form 3,4-dichloro-2-nitropyridine.
- Reaction 1: 3,4-dichloro-2-nitropyridine reacts with 4-hydroxy-2-nitropyridine to form 3,4-dichloro-2,2'-bipyridine.

Export

For: Offline Review

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

Saving Locally

- SciPlanner eXchange (*.pkx)

Details:

* Required

File Name: *
SciPlanner_11_19_2015_112612

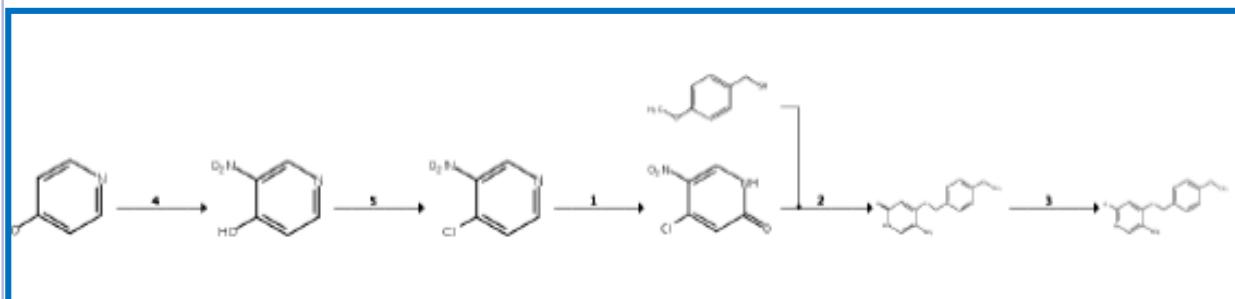
Title

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 1.2 R:K ₂ CO ₃ , S:H ₂ O, cooled, pH 10	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2 Transformation: 1. Formation of Alkyl Halides from Alcohols	90%
		References High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes By Poloeck, Anurach et al From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014	

Substance Information		
1228150-22-8 C ₁₃ H ₁₂ N ₂ O ₄ S 2(1H)-Pyridone, 4-[(4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions	1228150-23-9 C ₁₃ H ₁₁ ClN ₂ O ₄ S Pyridine, 2-chloro-4-[(4-methoxyphenyl)methyl]thio]-5-nitro- Related Info: ~ 2 References Reactions	13091-23-1 C ₆ H ₃ ClN ₂ O ₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 301 References Reactions ~ 180 Commercial Sources Regulatory Information
5435-54-1 C ₆ H ₄ N ₂ O ₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information	6258-60-2 C ₈ H ₁₀ OS Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	626-64-2 C ₆ H ₅ N ₂ O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information
850663-54-6 C ₆ H ₃ ClN ₂ O ₃ 2(1H)-Pyridone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources		

提纲

- 美国化学文摘社简介
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 - 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 screenshot shows the registration process for SciFinder. It consists of three main sections:

- Contact Information:** Fields for First Name, Last Name, Email, Confirm Email, Phone Number, Fax Number, Area of Research (dropdown), and Job Title (dropdown).
- Username and Password:** Fields for Username, Password, and Re-enter Password. There are "Tips" links next to the Password and Re-enter Password fields.
- Security Information:** Fields for Security Question (dropdown) and Answer. There are "Why?" links next to the Security Question and Answer fields.

At the bottom left are "Register>>" and "Clear All" buttons.

请注意：

- 必须输入真实姓名和学校域名邮箱。
- 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)
- 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 @、#、%、&、*）
- 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96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



The screenshot shows a registration confirmation page for SciFinder. At the top left is the SciFinder logo with the tagline "...Part of the process™". The main message in the center reads "Registration for SciFinder® is Complete". Below it, a success message states "You have successfully completed the registration process." and provides instructions to "To sign in to SciFinder®, click the link below." followed by a blue hyperlink: <https://scifinder.cas.org/scifinder>.

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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