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Application Specialist

cqian@acsi.info

如何使用SciFinder获取科技信息

2016年10月27日

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
 - 反应检索
 - 聚合物检索
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构，愿景：运用化学的力量改善人们的生活
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 全面收集、文摘、标引全球化学相关文献
- 总部位于美国俄亥俄州哥伦布市
- 超过1,400名员工
- 精通50多种语言的科学家



CAS——构建最高质量的化学数据库



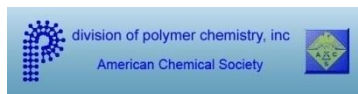
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



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

ACS Chemical
Neuroscience

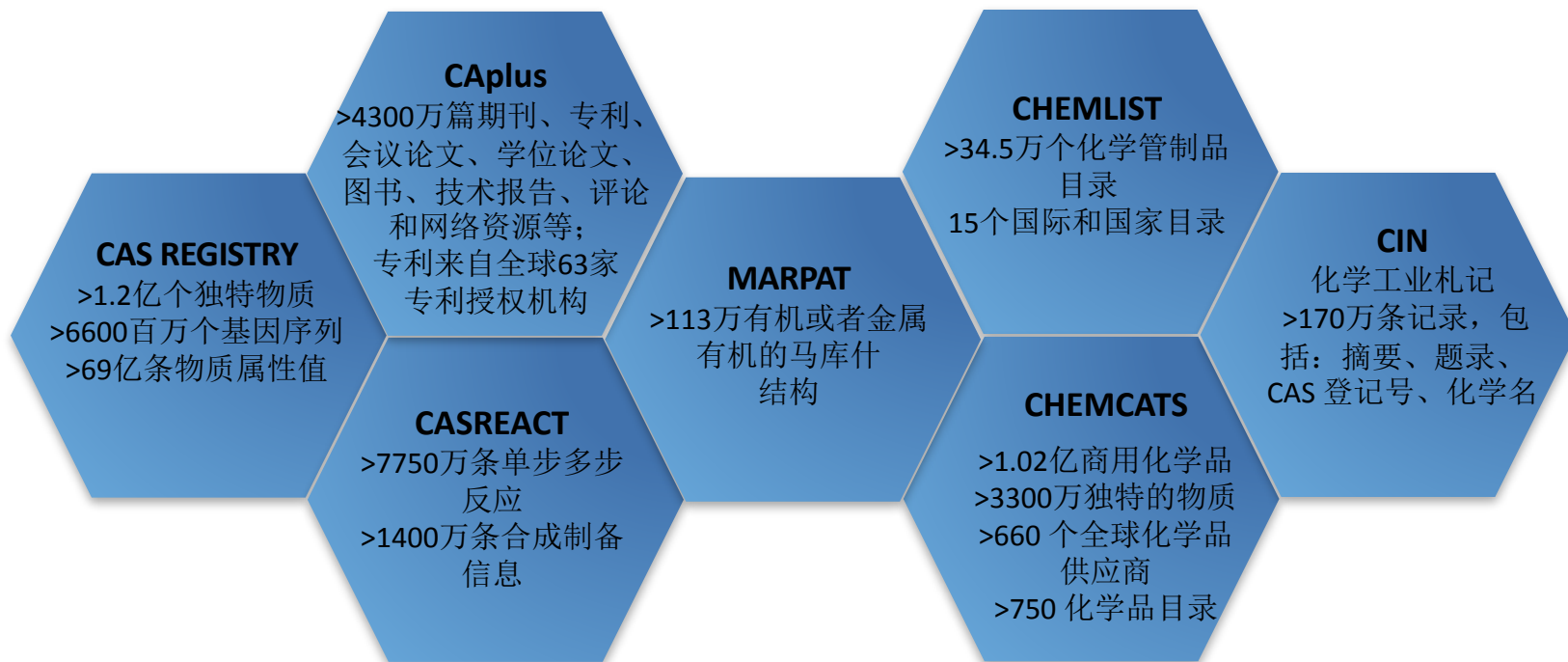


THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters



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CAS——构建最高质量的化学数据库



CAS解决方案——加速科学探索的步伐



CAS数据库——源于化学，超越化学

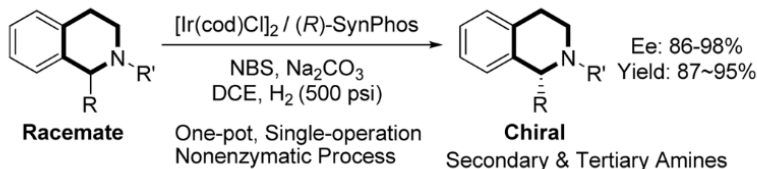
- 生物化学：
 - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- 有机化学各领域：
 - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- 大分子化学各领域：
 - 纤维素、木质素、造纸、涂料、墨水
 - 染料、有机颜料、合成橡胶、纺织品、纤维
- 应用化学各领域：
 - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- 物理、无机、分析化学各领域：
 - 表面化学、催化剂、相平衡、核现象、电化学

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 Hydrogenation catalysts
Oxidation

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

Chiral ligands

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

Catalyst use; Uses

Substances

12112-67-3 Dichlorobis(cyclooctadiene)diiridium
76189-55-4
133545-16-1
445467-61-8
503538-68-9 (S)-SynPhos
503538-69-0

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

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**很好地解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用**SciFinder**中的标引信息（Index Term, CAS RN, CAS Role），提高效率，启发思路。

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - 设计合成路线——SciPlanner使用简介
- SciFinder常见问题及解决

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



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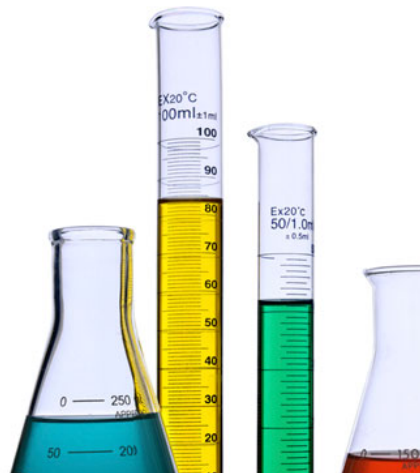
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News & Updates

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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

REFERENCES: RESEARCH TOPIC ?

Examples:

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

Search

Advanced Search

已保存的结果集

SAVED ANSWER SETS ?

S2
S1
importment MNS
for jwkyb
for jwkyb
for wwusq
lung cancer
methodsnow
pincer2
pincer crystal
Autosaved Reference Set
View All | Import

KEEP ME POSTED ?

C-N bond activation
Mar 12, 2016(1)
Mar 05, 2016(2)
Feb 27, 2016(2)

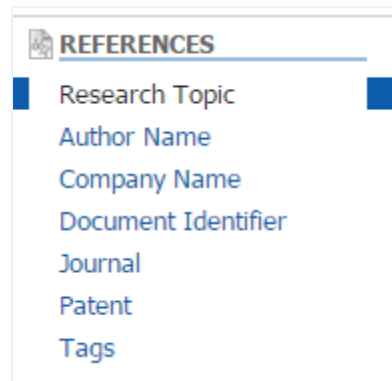
12

检索入口

定题追踪

SciFinder检索——文献检索

- 文献检索方法
 - 主题检索
 - 作者名检索
 - 机构名检索
 - 文献标识符检索
 - 期刊名称和专利信息（公开号，申请号等）
 - 从物质，反应获得文献
- 检索策略推荐
 - 关注某特定领域的文献：主题检索
 - 关注物质有关的文献：先获得物质，再获得文献
 - 关注某科研人员的文献：作者名检索
 - 关注某机构科研进展：机构名检索



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以“OLED发光材料”为例：

- 如何快速了解到领域研究动态
- 如何查找到分析化学的相关文献
- 如何获得光谱学/电子传输的相关文献
- 如何通过**PatentPak**快速获得发光材料的专利信息

文献检索——主题: OLED发光材料

- 检索式: Luminescent materials with OLED

The screenshot displays the SciFinder search interface. On the left is a navigation menu with three main sections: **REFERENCES** (selected), **SUBSTANCES**, and **REACTIONS**. Under **REFERENCES**, options include Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Under **SUBSTANCES**, options include Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. Under **REACTIONS**, the option is Reaction Structure. The main search area is titled 'REFERENCES: RESEARCH TOPIC' and contains a search input field with the text 'Luminescent materials with OLED'. Below the input field are examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button and a link to 'Advanced Search' are also visible.

关键词之间可用介词连接: in, with, of...

文献检索结果

检索结果处理工具

Research Topic "Luminescent materials with

REFERENCES ?

Get Reactions Get Reactions Get Related Citations Tools

Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number

0 of 1117 References Selected

Display Options

Analyze by: Author Name

Wang Ping	99
Zhou Mingjie	99
Chen Jixing	86
Lee Jun Yeob	46
Zhong Tietao	32
Huang Hui	30
Volz Daniel	21
Adachi Chihaya	20

1. **Easy accessible blue luminescent organic light-emitting diodes**

Quick View Other Sources

By Reig, Marta; Gozalvez, Cristian; Bujaldon, ...; Khrystyna; Kostiv, Nataliya; Volyniuk, Dmytro; Grazulevicius, Juozas V.; Velasco, Dolores From Dyes and Pigments (2017), 137, 24-35. | Language: English, Database: CAPLUS

The thermal, optical, electrochem. and charge transport properties of a series of nine straightforward carbazole-based compds. have been analyzed and interpreted according to their mol. structure by means of the X-ray anal. of single crystals. A non-doped **OLED device** with low turn-on voltage and max. luminance up to 1.4×10^4 cd m⁻² was achieved. DFT calcns. have been performed to explain the high efficiency of radiative exciton prodn.

2. **Twist Angle and Rotation Freedom Effects on Luminescent Donor-Acceptor Materials: Crystal Structures, Photophysical Properties, and OLED Application**

Quick View Other Sources

By Jiang, Jianxia; Hu, Dehua; Hanif, Muddasir; Li, Xianglong; Su, Shijian; Xie, Zengqi; Liu, Linlin; Zhang, Shitong; Yang, Bing; Ma, Yuguang From Advanced Optical Materials (2016), Ahead of Print. | Language: English, Database: CAPLUS

The twist angle and rotation freedom between the donor (D) and acceptor (A) in D-A **materials** plays an important role in their photophys. properties. Here, the authors select the asym. acceptor pyridal[2,1,3]thiadiazole (PT) to construct two D-A isomers (p-TPA-PT and d-TPA-PT) with different twist angle and rotation freedom due to the donor triphenylamine (TPA) proximal or distal to N-atom (pyridyl), as well as a sym. bis-triphenylamine-substituted compd. DTPA-PT for their investigation. On the basis of exptl. and theor. anal., the authors have explained how the difference in twist-angle and ...

涉及物质及引文链接

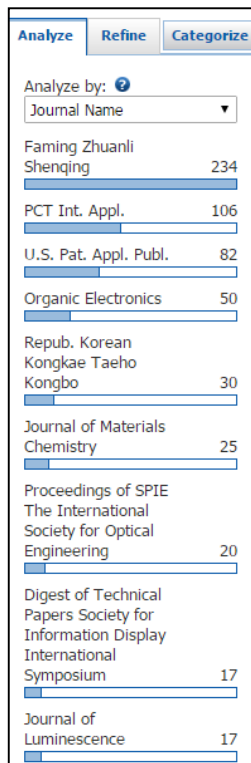
文献检索结果: Analyze

12种文献分析选项

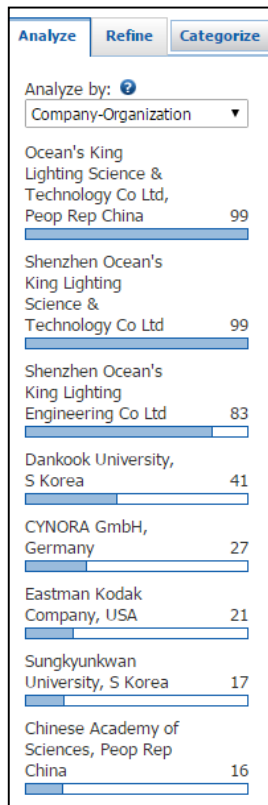
Analyze by: ?

- Author Name
- CAS Registry Number
- CA Section Title
- Company-Organization
- Database
- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

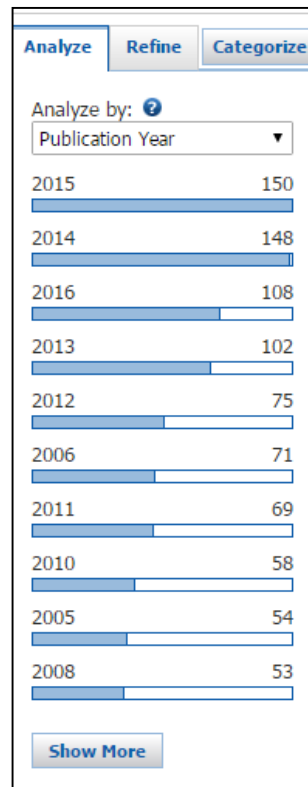
成果披露媒介



主要研究机构,
合作伙伴, 竞争对手

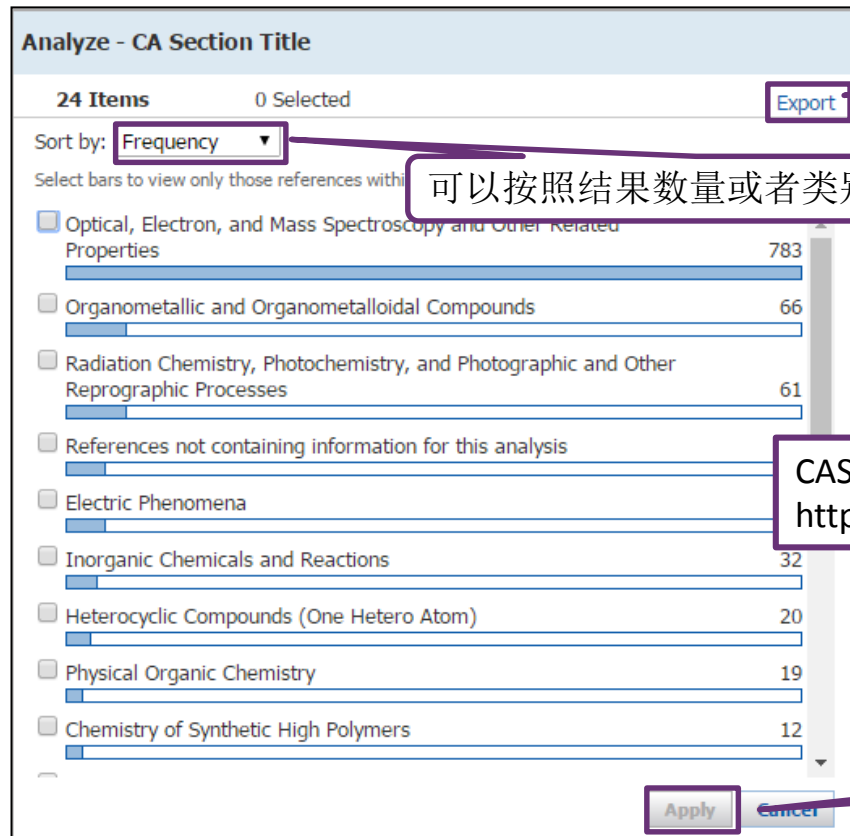
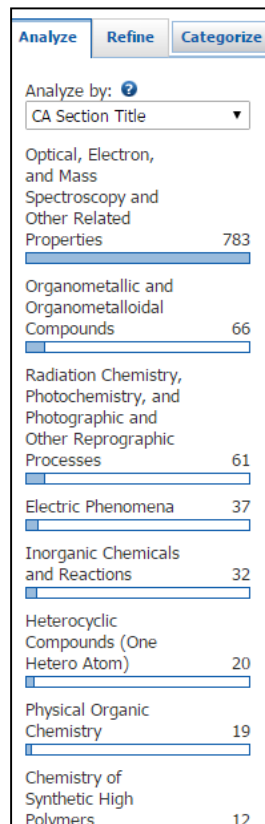


年度发表数量



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文献检索结果: Analyze



可以将分析结果导出xls文件

可以按照结果数量或者类别字母顺序排序

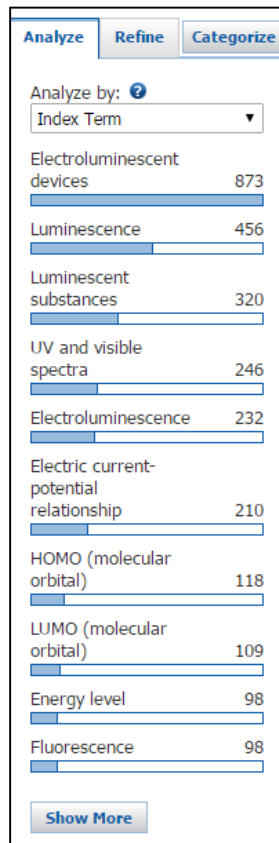
CAS把收录的信息分为5个大类80个小类:
<http://www.cas.org/content/ca-sections>

选择感兴趣的词语,点击Apply

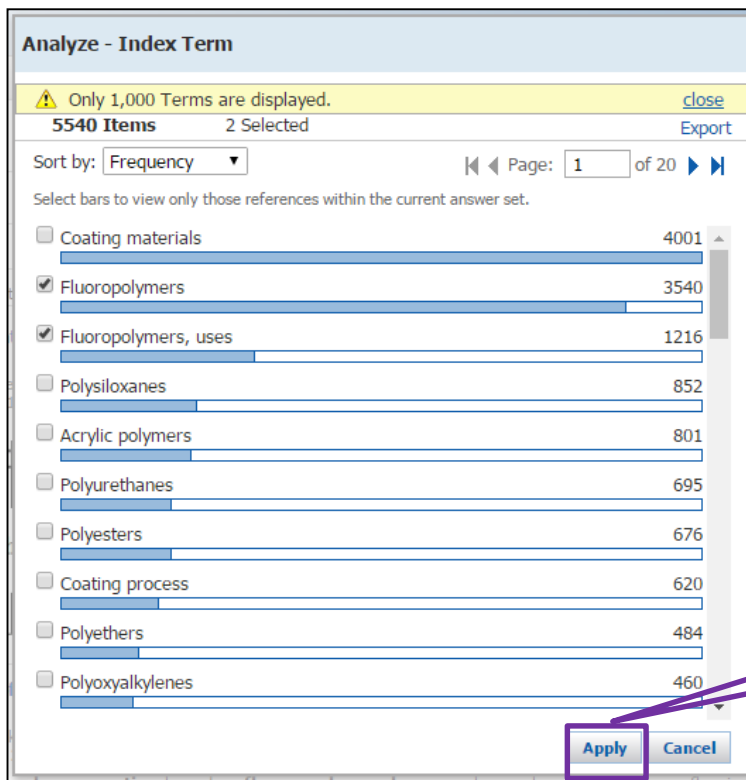


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文献检索结果: Analyze



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



选择感兴趣的词语, 点击Apply



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文献检索结果: Refine

- 七种限定选项, 包括主题词、作者姓名、机构名称、出版年代、语言、所属数据库

Research Topic "luminescent material with OLED" > references (1115) > refine "white" (97)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▾

Analyze Refine Categorize

Sort by: Accession Number ▾

0 of 97 References Selected

Refine by: ⓘ

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

Research Topic

white

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

1. Solution processable white organic light-emitting diodes using new blue host material including substituent group

Quick View Other Sources

By Lee, Jaehyun; Shin, Hwangyu; Park, Jongwook

From Journal of Nanoscience and Nanotechnology (2016), 16(2), 2101-2104. | Language: English, Database: CAPLUS

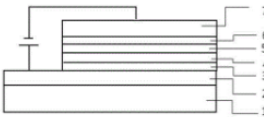
New host material of T-TATa isomer substituted t-Bu group was investigated in soln. process WOLED device comp N,N-diphenylaniline [TATa]. A two-color WOLED of a co-host system using soln. process method was demonstrated. The emitting layer (50 nm)/TPBi (20 nm)/LiF (1 nm)/Al. The emitting layer consisted of TATa or T-TATa isomer, NPB was used as not only blue host but also helping hole carrier transport. The device using T-TATa c...

2. White organic light emitting device of exciplex and its preparation method

Quick View PATENTPAK ▾

By Zhang, Zhiyong; Zhao, Qingshan; Liu, Xing; Zhao, Wei

From Faming Zhuanli Shenqing (2016), CN 105789460 A 20160720. | Language: Chinese, Database: CAPLUS



3. White organic light emitting device using iridium complexes and its fabrication method

Quick View PATENTPAK ▾

文献检索结果: Categorize

学科主分类

学科副分类

学科副分类涉及的重要技术术语/物质

Categorize ?

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

Category Heading	Category	Index Terms	Selected Terms
All	Analysis (17)	Select All Deselect All	Click 'X' to remove the category from 'Selected Terms'
General chemistry	Reagents & other substances (16)	<input type="checkbox"/> Cyclic voltammetry 61	<input checked="" type="checkbox"/> Physical chemistry > Spectra & spectroscopy (3 Terms)
Technology		<input type="checkbox"/> Thermal analysis 42	
Polymer chemistry	Analytes & matrixes (4)	<input type="checkbox"/> Differential scanning calorimetry 11	
Synthetic chemistry		<input type="checkbox"/> Thermogravimetric analysis 8	
Physical chemistry		<input type="checkbox"/> Elemental analysis 5	
Biotechnology		<input type="checkbox"/> Liquid chromatography 3	
Genetics & protein chemistry		<input type="checkbox"/> Photoelectron spectroscopy 2	
Catalysis		<input type="checkbox"/> Atomic force microscopy 1	
Analytical chemistry		<input type="checkbox"/> Chromatography 1	
Environmental chemistry		<input type="checkbox"/> Colorimetry 1	
Biology		<input type="checkbox"/> Electrospray ionization mass spectrometry 1	
		<input type="checkbox"/> Ellipsometry 1	
Analytical chemistry > Analysis			OK Cancel

与分析化学相关的文献

基于学科对文献进行自动分类，
帮助用户精准定位所关注的学科和技术术语

文献检索结果: Categorize

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in property studies (4318)
General chemistry	Substances in processes (2406)
Technology	Spectra & spectroscopy (122)
Polymer chemistry	Electric & magnetic phenomena (73)
Synthetic chemistry	Gas, liquid, & solid phenomena (132)
Physical chemistry	Quantum mechanics (54)
Biotechnology	Thermodynamics (32)
Genetics & protein chemistry	Miscellaneous substances (74)
Catalysis	Surface phenomena (22)
Analytical chemistry	Mechanics (31)
Environmental chemistry	
Biology	

2. Select index terms of interest.

Index Terms	
Page: 1 of 2	
Select All Deselect All	
<input checked="" type="checkbox"/> Blue luminescence	11
<input type="checkbox"/> Delayed fluorescence	10
<input type="checkbox"/> Light	9
<input type="checkbox"/> Luminescence decay	9
<input type="checkbox"/> IR spectra	8
<input type="checkbox"/> Optical properties	8
<input type="checkbox"/> Charge transfer transition	7
<input type="checkbox"/> Fluorescence decay	7
<input type="checkbox"/> Raman spectra	7
<input type="checkbox"/> UV-visible absorption	7
<input type="checkbox"/> Emission spectra	6
<input checked="" type="checkbox"/> Light, red	6
<input type="checkbox"/> Mass spectra	6
<input checked="" type="checkbox"/> White light	6
<input type="checkbox"/> Dipole moment	5

Selected Terms

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

Physical chemistry > Spectra & spectroscopy (3 Terms)

e.g.:光谱学相关的文献

文献检索结果: Categorize

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in property studies (4318)
General chemistry	Substances in processes (2406)
Technology	Spectra & spectroscopy (122)
Polymer chemistry	Physical chemistry
Synthetic chemistry	Electric & magnetic phenomena (73)
Biotechnology	Gas, liquid, & solid phenomena (132)
Genetics & protein chemistry	Quantum mechanics (54)
Catalysis	Thermodynamics (32)
Analytical chemistry	Miscellaneous substances (74)
Environmental chemistry	Surface phenomena (22)
Biology	Mechanics (31)

2. Select index terms of interest.

Index Terms	
Select All	Deselect All
<input type="checkbox"/>	Current efficiency 42
<input type="checkbox"/>	NMR (nuclear magnetic resonance) 40
<input type="checkbox"/>	Current density 28
<input type="checkbox"/>	Hole mobility 24
<input type="checkbox"/>	Doping 23
<input type="checkbox"/>	Electric potential 23
<input type="checkbox"/>	Electron mobility 21
<input type="checkbox"/>	Electron transfer 20
<input type="checkbox"/>	Oxidation potential 19
<input type="checkbox"/>	Electric current carriers 17
<input type="checkbox"/>	Ionization potential 15
<input type="checkbox"/>	Hole (electron) 13
<input type="checkbox"/>	Redox potential 13
<input type="checkbox"/>	Electron acceptors 10
<input type="checkbox"/>	Electron donors 10

Selected Terms

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

✱ Physical chemistry > Spectra & spectroscopy (3 Terms)

Physical chemistry > Electric & magnetic phenomena

OK

Cancel

e.g.: 电子传输/空穴传输相关的文献



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以“OLED发光材料”为例：

- 如何快速了解到领域研究动态
- 如何查找到分析化学的相关文献
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- 如何通过**PatentPak**快速获得发光材料的专利信息

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- 在**CAS**专利族文献中找到你所熟悉语言的专利

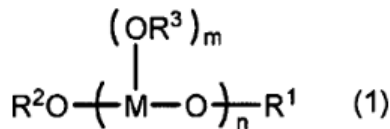
点击PatentPak, 一键获得专利pdf文件, 快速定位到关键物质

17. Compound, desiccant, sealing structure and organic electroluminescent element

Quick View **PATENTPAK**

By Hoshina, Yusuke; Takakura, Yoshie

From Ger. Offen. (2015), DE 102015209342 A1 20151126. | Language: German, Database: CAPLUS



A compd. represented by the formula $\text{R}^2\text{O}(\text{M}(\text{OR}^3)_m\text{O})_n\text{R}^1$ (wherein M represents an aluminum atom, a titanium atom, a silicon atom or a boron atom; m represents 1 or 2; n is a pos. integer; R^1 , R^2 and R^3 each independently represent a C_{1-16} alkyl group which is optionally substituted with one or more fluorine atoms, or a C_{2-17} acyl group which is optionally substituted with one or more fluorine atoms, represent, and when a plurality of R^3 are present, the plurality of R^3 may be the same or different from each other) is described for uses as a desiccant in top-emission type org. electroluminescent el...

18. Organic compounds and composition, and organic optoelectronic compounds as electroluminescent hosts

Quick View **PATENTPAK**

By Lee, Han-Il; S

From Eur. Pat. Ap

Patent No.	Kind	Language
EP 2947071	A1	English
Patent Family		
KR 2015133566	A	Korean
US 20150340626	A1	English
JP 2015218165	A	Japanese
CN 105085412	A	Chinese

点击PatentPak, 获取PatentPak Viewer

istics employing the

lin, Soo-Hyun; Jo, Eun-Sung; Jung, Ho-Kuk
age: English, Database: CAPLUS

d are org. compd. represented by Formula (I), where X, L^{1-6} , R^{1-22} , and n1-4 are described in the detailed description; a for an org. optoelec. device including the org. compd., an org. optoelec. device including the org. compd. or the compn., and y device including the org. optoelec. device. Thus, org. electroluminescent devices with remarkably improves luminous y and life-span characteristics were fabricated using the org. compds. as electroluminescent hosts.

19. Condensed cyclic compounds with excellent elec. characteristics and thermal stability, and organic light-emitting devices including the compounds in emitting or electron-transporting layer

Quick View **PATENTPAK**



SCIFINDER®
A CAS SOLUTION

点击PatentPak，一键获得专利pdf文件，快速定位到关键物质

PatentPak浏览器

下载包含物质位置等信息的专利PDF文件

下载PDF文件

在PatentPak Viewer中点击物质下面的灯泡，快速定位到PDF文件中的物质信息

The screenshot displays the PatentPak browser interface. On the left sidebar, under 'Key Substances in Patent', two entries are listed: 'CAS RN 1830362-23-6' and 'CAS RN 1830362-24-7', each accompanied by a chemical structure. The main viewing area shows a patent document page 33 of 65. It features a chemical reaction scheme where intermediate I-1 reacts with 4-bromobenzimidamide hydrochloride and sodium hydroxide in ethanol to form intermediate I-2. The text of the patent is visible, including a paragraph [0093] describing the reaction conditions and yield. A sidebar on the right shows 'Analyst Markup Locations (1)' with a 'page 33' marker. Annotations include a callout for the 'Download PDF' button in the top toolbar, a callout for the 'Download PDF' button in the sidebar, and a callout for the 'lightbulb' icon below the chemical structures, which is used to quickly locate the substance information in the PDF file.

PatentPak——专利工作流程解决方案

The screenshot displays the PatentPak interface, a tool for patent analysis. The top navigation bar includes the PatentPak logo, a page indicator (PAGE 45 / 65), zoom controls, and a download PDF button. The left sidebar, titled 'Key Substances in Patent', lists 'Search in SciFinder' and 'View Detail' for two analyst markup locations (page 44 and page 45). Below this, a chemical structure is shown for 'CAS RN 2085-33-8'. The main content area displays patent text with line numbers 45, 50, and 55. The text describes the formation of an emission layer and the structure of an organic light emitting diode. A purple line highlights a specific chemical structure within the text, which is linked to the 'View Detail' button in the sidebar. A callout box points to this structure, stating: '可在PatentPak Viewer中直接返回SciFinder进行结构、马库什和反应检索' (Can directly return to SciFinder in PatentPak Viewer for structure, Markush, and reaction searches). Another callout box points to the top right corner of the interface, stating: '也可实现PDF文件与PatentPak Viewer互动' (Can also achieve interaction between PDF files and PatentPak Viewer).

PATENTPAK[™]
A CAS SOLUTION

PAGE 45 / 65 ZOOM DOWNLOAD PDF

Key Substances in Patent

Search in SciFinder | View Detail

Analyst Markup Locations (2)

- page 44
- page 45

CAS RN 2085-33-8

Search in SciFinder | View Detail

Analyst Markup Locations (2)

- page 44
- page 45

45 phosphorescent dopant based on 100 wt% of the total amount of the emission layer.

45 [0199] On the emission layer, a 50 Å-thick hole blocking layer was formed by depositing bis (2-methyl-8-quinolinolate)-4-(phenylphenolato)aluminium (BALq) under the same vacuum deposition condition. Subsequently, a 250 Å-thick electron transport layer (ETL) was formed by depositing tris (8-hydroxyquinolino)aluminium (Alq3) under the same vacuum deposition condition. LiF and Al were sequentially deposited to form a cathode on the electron transport layer (ETL), manufacturing an organic light emitting diode.

50 [0200] The organic light emitting diode has a structure of ITO/BNTPD 60nm/HT-1 30 nm/EML (a compound 1 (93 wt%) + Ir(pq)2acac (7 wt%), 30nm)/Balq (5 nm)/Alq3 25 nm/LiF (1 nm)/Al (100 nm).

Example 2

55 [0201] An organic light emitting diode was manufactured according to the same method as Example 1 except for using the compound 2 according to Synthesis Example 22 instead of the compound 1 according to Synthesis Example 21.

44

也可实现PDF文件与PatentPak Viewer互动

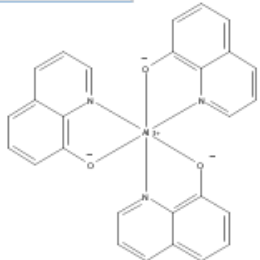
可在PatentPak Viewer中直接返回SciFinder进行结构、马库什和反应检索

PatentPak——专利工作流程解决方案

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java **Non-Java**



Click image to change structure or view detail.

Import CXF


Search

Advanced Search

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

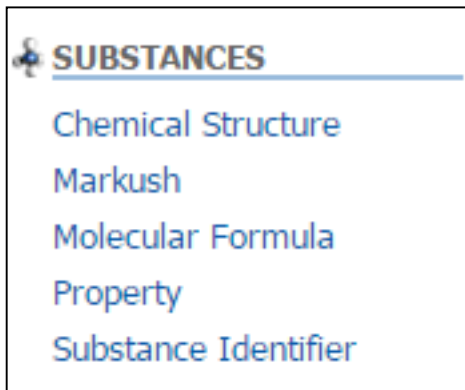
☐ Show precision analysis

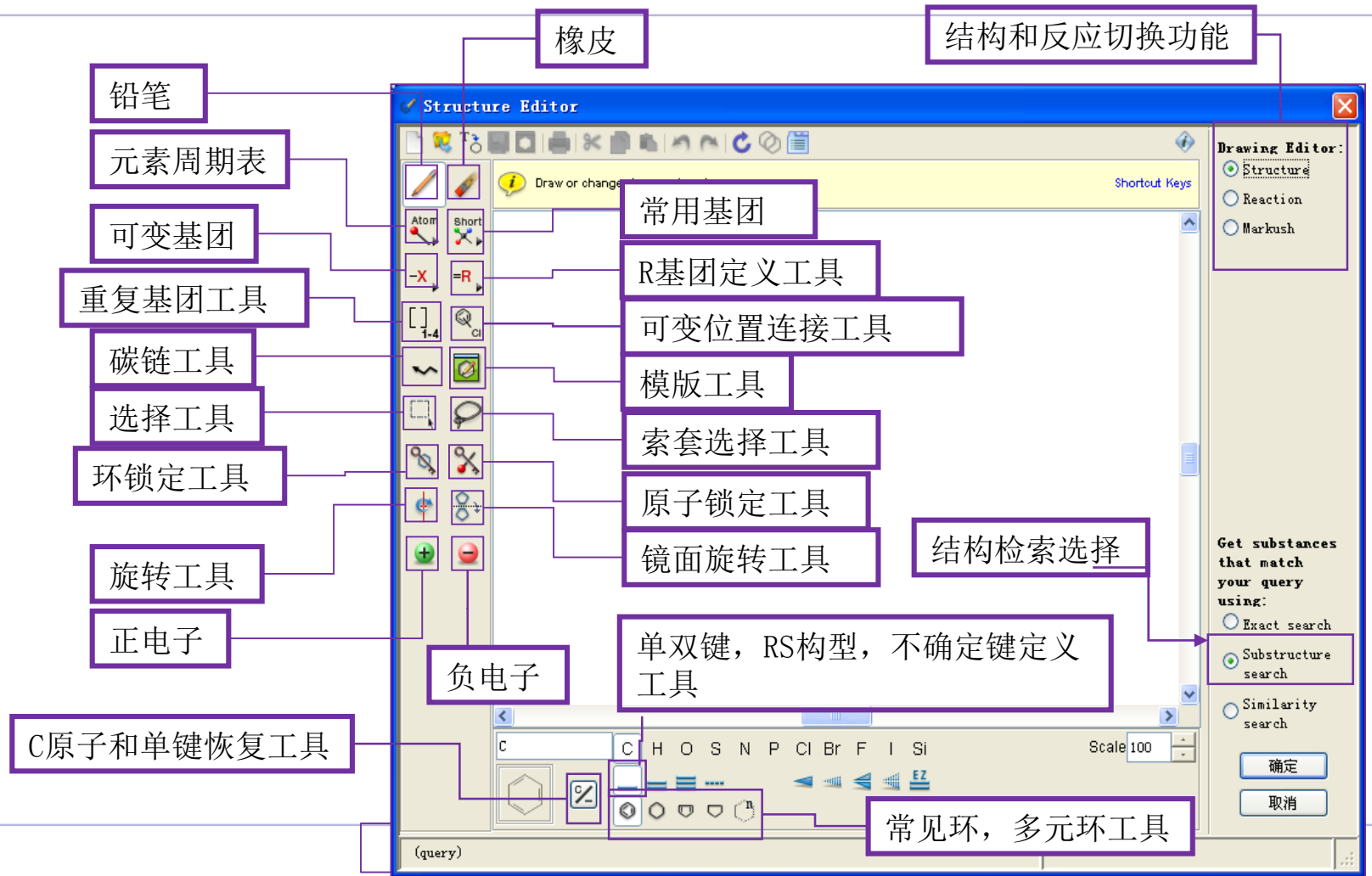
 **ChemDraw**
Launch a SciFinder substructure search
[More](#)

从PatentPak Viewer直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

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
 - 有机物化合物、天然产物：结构检索
 - 无机化合物、合金：分子式检索
 - 高分子化合物：分子式检索和结构检索





直接导入已保存的.cxf或者.mol文件

将绘制结构存为模板

Structure Editor

Select and draw structures with templates.

Shortcuts

CH	CH ₂	Me	OMe	Et	OEt	Pr-n	Pr-i	OPr-n
OPr-i	Bu-n	Bu-i	Bu-s	Bu-t	OBu-n	OBu-i		
OBu-s	OBu-t	Ph	OPh	o-C ₆ H ₄	m-C ₆ H ₄			
p-C ₆ H ₄	CF ₂	CF ₃	CCl ₂	CCl ₃	CBr ₂	CBr ₃	Cl ₂	
Cl ₃	CHO	CN	C(O)CH ₃	CO ₂ H	COOH	COSH		
CS ₂ H	CSSH	NH	NH ₂	NH ₃	NO ₂	OH		
OPO ₃ H ₂	OSO ₃ H	PO ₃ H ₂	SH	SO ₂	SO ₃ H			

Close

常用基团

环锁定工具

原子锁定工具

常用模板

Templates

Enter 3 or more characters...

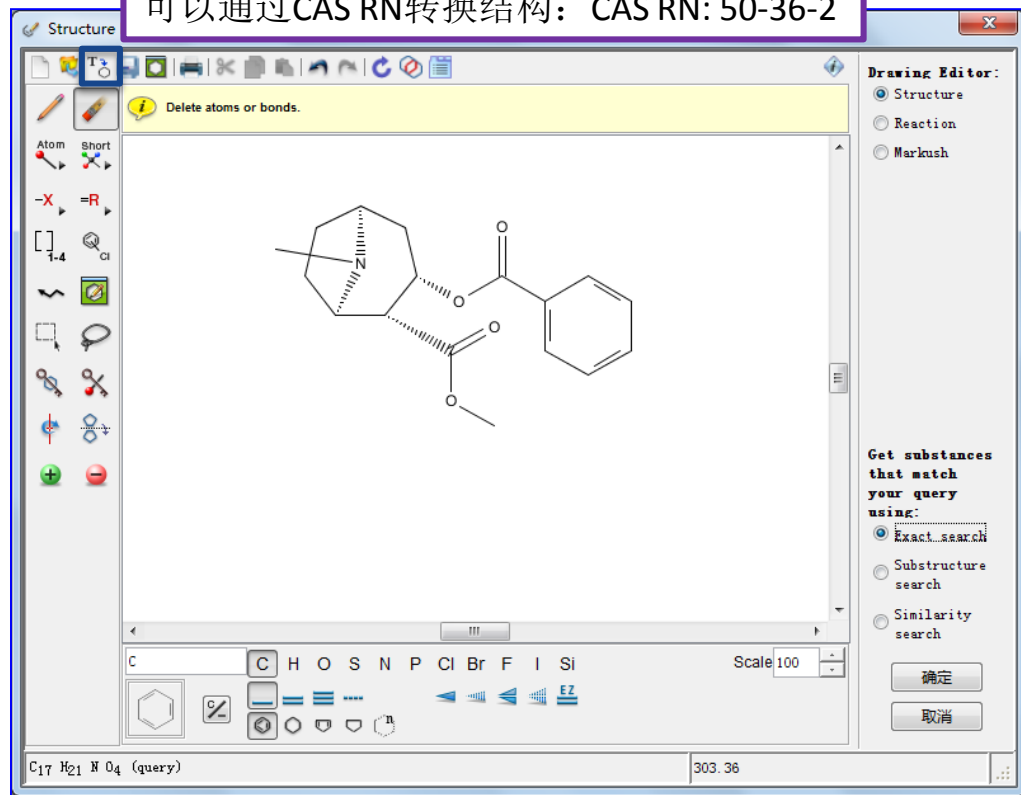
- Alkaloid (9)
- Amino Acid (25)
- Bicarboyclic (8)
- Carbohydrate (7)
- Coordination (14)
- Cycloalkane (13)
- Miscellaneous (6)
- Monocarbocyclic (19)
- N-containing (19)
- NOS-containing (10)
- Nucleic Acid (5)
- O-containing (11)
- Polycarbocyclic (13)
- Rings (4)
- S-containing (6)
- Steroid (7)
- User-Defined (0)

Close

C₇H₅NO 119.12

物质检索——精确结构检索

可以通过CAS RN转换结构: CAS RN: 50-36-2



精确结构检索

浏览精确结构检索结果

可以通过分析/限定筛选结果集

Analyze Refine

Analyze by: Substance Role

Preparation 30

Analytical Study 21

Properties 13

Biological Study 11

Reactant or Reagent 10

Uses 9

Formation, Nonpreparative 8

Sort by: Relevance

0 of 81 Substances Selected

1. 50-36-2
~21151 ~26
Absolute stereochemistry., Rotation (-).
C₁₇ H₂₁ N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1R,2R,3S,5S)-

2. 53-21-4
(Component: 50-36-2)
~1707 ~28
Absolute stereochemistry., Rotation (-).
HCl
C₁₇ H₂₁ N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl-*d*₅ ester, (1R,2R,3S,5S)-

3. 65266-73-1
~13 ~8
Absolute stereochemistry.
C₁₇ H₁₈ D₃ N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl-*d*₅ ester, (1R,2R,3S,5S)-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

88-89-1
C₆ H₃ N₃ O₇
2,4,6-Trinitrophenol

50-36-2
C₁₇ H₂₁ N O₄
Absolute stereochemistry., Rotation (-).

可卡因

盐酸可卡因

同位素取代可卡因

可卡因组合物

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

物质检索结果——Analyze

六种分析选项

Analyze Refine

Analyze by: ?

- Bioactivity Indicators
- Bioactivity Indicators
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Target Indicators

生物活性

Analyze Refine

Analyze by: ?

Bioactivity Indicators

Nervous system agents (all) 2

Show More

可以按照生物活性，商业可获得性，元素，反应可获得性，物质角色和靶点进行分析

物质角色

Analyze Refine

Analyze by: ?

Substance Role

Preparation 30

Analytical Study 21

Properties 13

Biological Study 11

Reactant or Reagent 10

Uses 9

Formation, Nonpreparative 8

Occurrence 3

Process 3

Miscellaneous 2

Show More

靶点

Analyze Refine

Target Indicators

DNA-binding proteins (all) 1

Enzymes (all) 1

Growth factors, animal (all) 1

Neuropeptides (all) 1

Opioid peptides (all) 1

Phosphoproteins (all) 1

Prolactin (all) 1

Pro-opiomelanocortin (all) 1

Proteins 1

Receptors (all) 1

Show More

物质检索结果——Refine

Analyze Refine

Refine by: ?

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

可以按照化学结构，
包含同位素化合物/金属化合物，
商业可获得性，
性质可获得性，
性质数值，文献可获得性
对结果进行限定

Only retrieve substances that:

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

Refine

Analyze Refine

Refine by: ?

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

Retrieve substances with:

- ☒ Any property
- ☐ Any predicted property
- ☐ Any experimental property
- ☐ Any selected experimental property

Refine



SCIFINDER[®]
A CAS SOLUTION

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1. **50-36-2** 🔍

~21151 ~26

Absolute stereochemistry., Rotation (-).

C₁₇H₂₁NO₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*,2*R*,3*S*,5*S*)-

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

2. **53-21-4** 🔍

CAS Registry Number: 50-36-2

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

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

SciFinder中的物质记录

SUBSTANCE DETAIL ?



Get
References



Get
Reactions



Get Commercial
Sources

获得文献，反应，供应商信息

[Return](#)

1. CAS Registry Number 50-36-2

~21,151  ~26 

C₁₇ H₂₁ N O₄

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

Molecular Weight

303.35

Melting Point (Experimental)

Value: 98 °C

Boiling Point (Experimental)

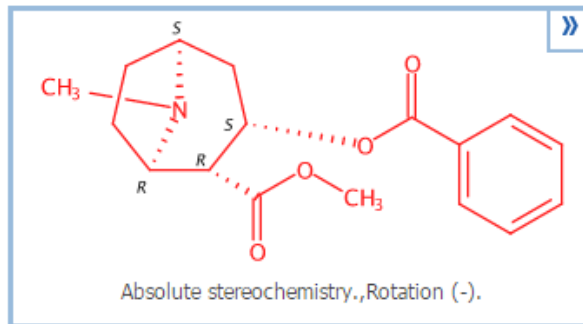
Value: 187 °C | Condition: Press: 0.1 Torr

Density (Predicted)

Value: 1.22±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

Value: 8.97±0.60 | Condition: Most Basic Temp: 25 °C



物质信息详情



SCIFINDER®
A CAS SOLUTION

EXPERIMENTAL PROPERTIES

EXPERIMENTAL SPECTRA

实验数据与实验谱图

¹H NMR IR Mass Raman UV and Visible

¹H NMR Properties

Value

Condition

Note

Proton NMR Spectrum

[See spectrum](#)

(13)BIORAD

Notes

(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.

PREDICTED PROPERTIES

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties

Value

Condition

Note

Freely Rotatable Bonds

3

(21)

H Acceptors

3

(21)

H Donors

1

(21)

H Donor/Acceptor Sum

4

(21)

logP

5.471±1.252

Temp: 25 °C

(21)

Molecular Weight

278.33

(21)

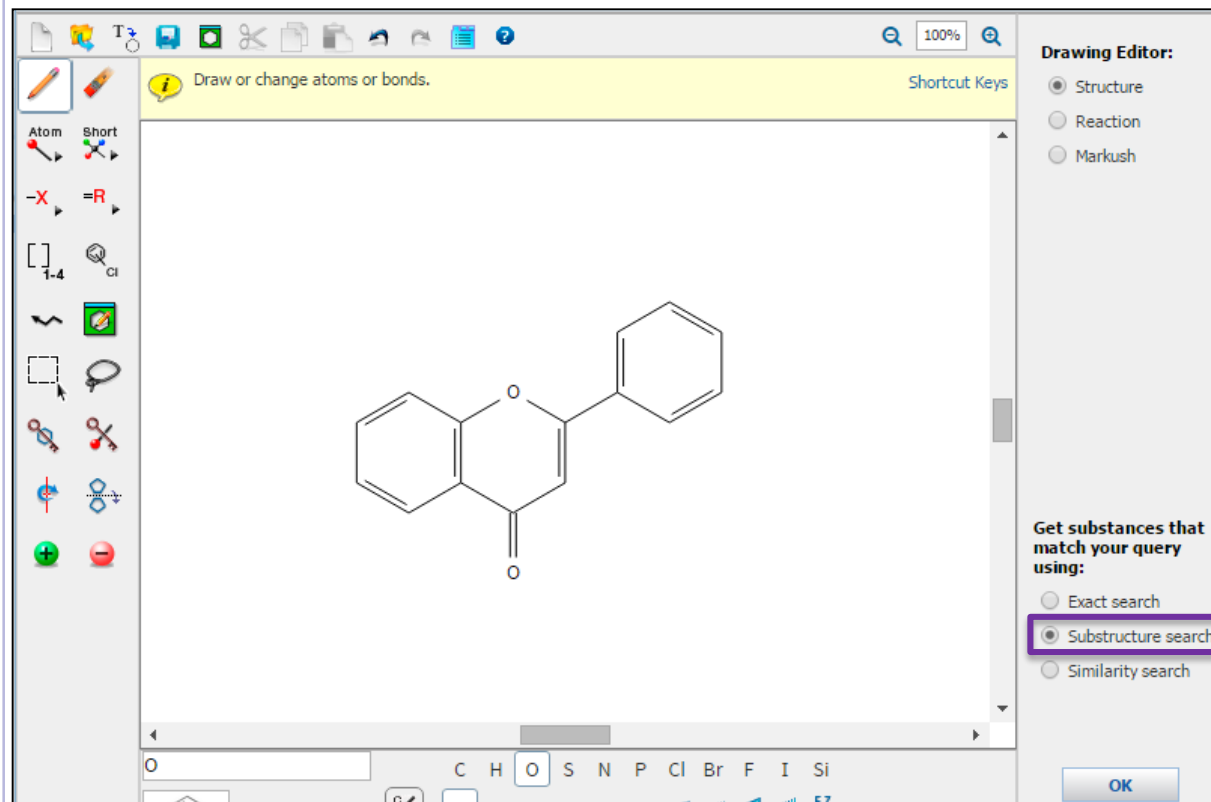
Notes

(21) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2015 ACD/Labs)

预测数据与预测谱图

PREDICTED SPECTRA

物质检索——亚结构检索



浏览亚结构检索结果

☐

0 of 63231 Substances Selected

☐ 1. 525-82-6 🔍

~3509

~78

»

🔍

C₁₅ H₁₀ O₂
4H-1-Benzopyran-4-one, 2-phenyl-

▶ **Key Physical Properties**

Regulatory Information

Spectra

Experimental Properties

☐ 2. 54849-75-1 🔍

~6

»

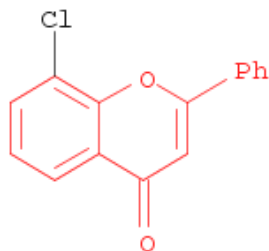
🔍

C₁₅ H₅ D₅ O₂
4H-1-Benzopyran-4-one, 2-(phenyl-d₅)-

Spectra

浏览亚结构检索结果

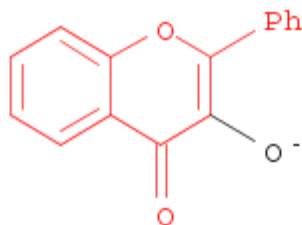
251. Substance Detail
1148-20-5



C₁₅ H₉ Cl O₂
4#1-Benzopyran-4-one, 8-chloro-2-phenyl-

取代物

261. Substance Detail
85481-91-0

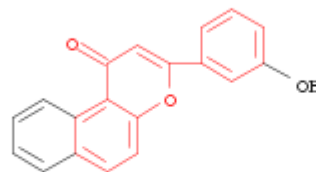


C₁₅ H₉ O₃
4#1-Benzopyran-4-one, 3-hydroxy-2-phenyl-, ion

Experimental Properties

离子

273. Substance Detail
136116-17-1



C₁₉ H₁₂ O₃
1#Naphtho[2,1-*b*]pyran-1-one, 3-(3-hydroxyphenyl)-

稠环物质



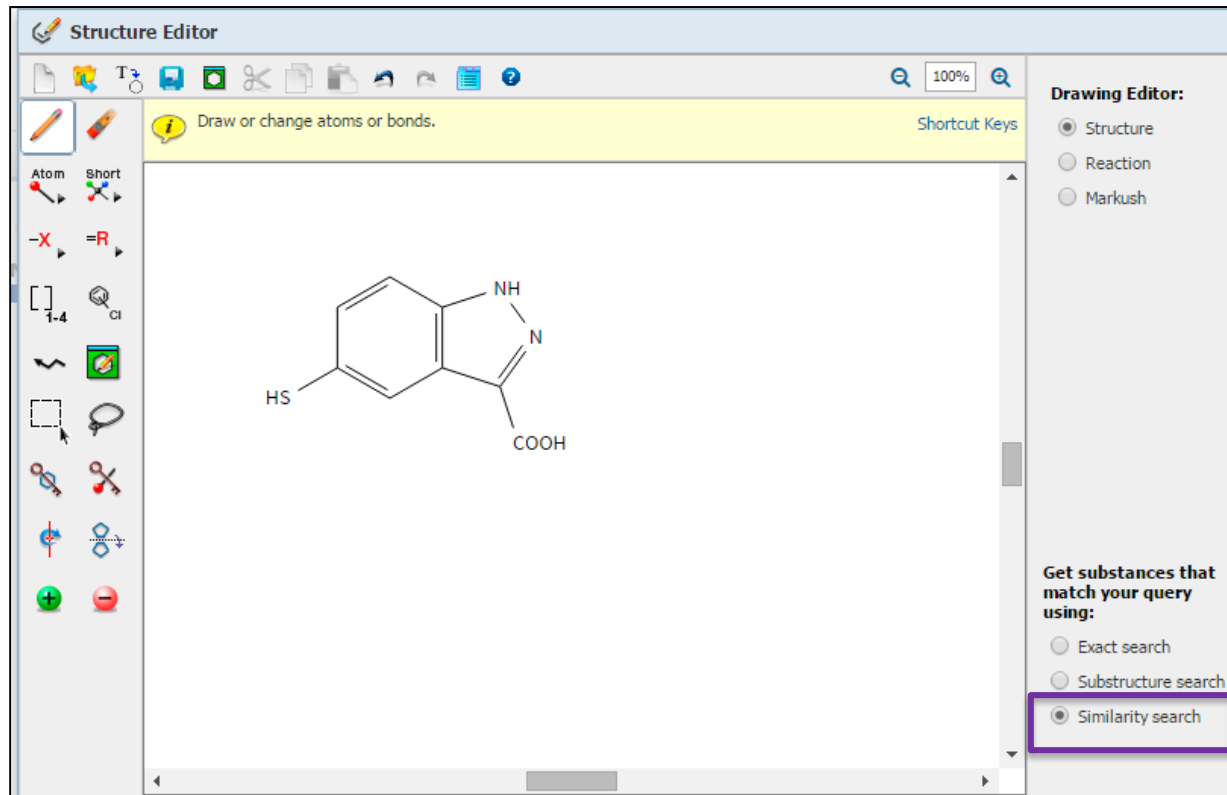
SciFINDER[®]
A CAS SOLUTION

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



Select All Deselect All

相似结构检索候选项

1 of 6 Similarity Candidates Selected

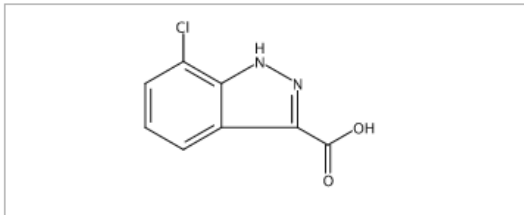
	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input checked="" type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	82
<input type="checkbox"/> 70-74	254
<input type="checkbox"/> 65-69	633
<input type="checkbox"/> 0-64 (least similar)	1636

相似度越高，结构越相似

相似结构检索结果

☐ 1. 129295-32-5

~3 ~96



$C_8 H_5 Cl N_2 O_2$
1H-Indazole-3-

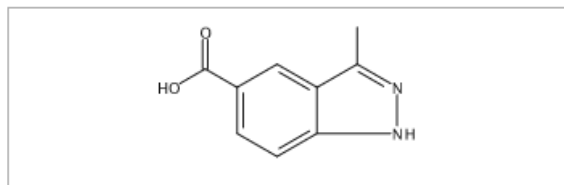
Key Physical

取代基变化

Score: 79

☐ 3. 885223-58-5

~11 ~34



$C_9 H_8 N_2 O_2$

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

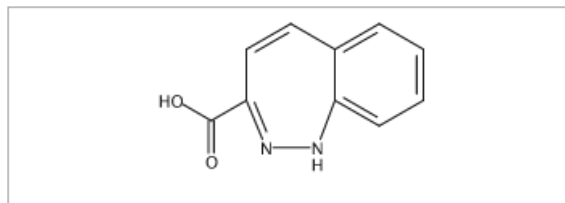
Key Physical Properties

取代基位置变化

Score: 71

☐ 117. 72119-92-7

~1



$C_{10} H_8 N_2 O_2$

1H-1,2-Benzodiazepine-3-carboxylic acid

Key Physical Properties
Experimental Properties

母体结构变化




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

物质检索——性质检索

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: 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

物质检索——性质检索

The screenshot displays the SciFinder web application interface. On the left, a sidebar contains navigation links for REFERENCES, SUBSTANCES, and REACTIONS. The main content area features a 'Select Property...' dropdown menu with a list of properties including 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 (highlighted), and pKa. Below the dropdown is a 'Search' button. To the right of the dropdown, there are input fields with examples: 'Examples: 44, 25-35, >125'.

寻找分子量在250-400之间的物质

物质检索——分子式检索

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction

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——标识符检索

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

sudan red

Enter one per line.

Examples:

50-00-0

999815

Acetaminophen

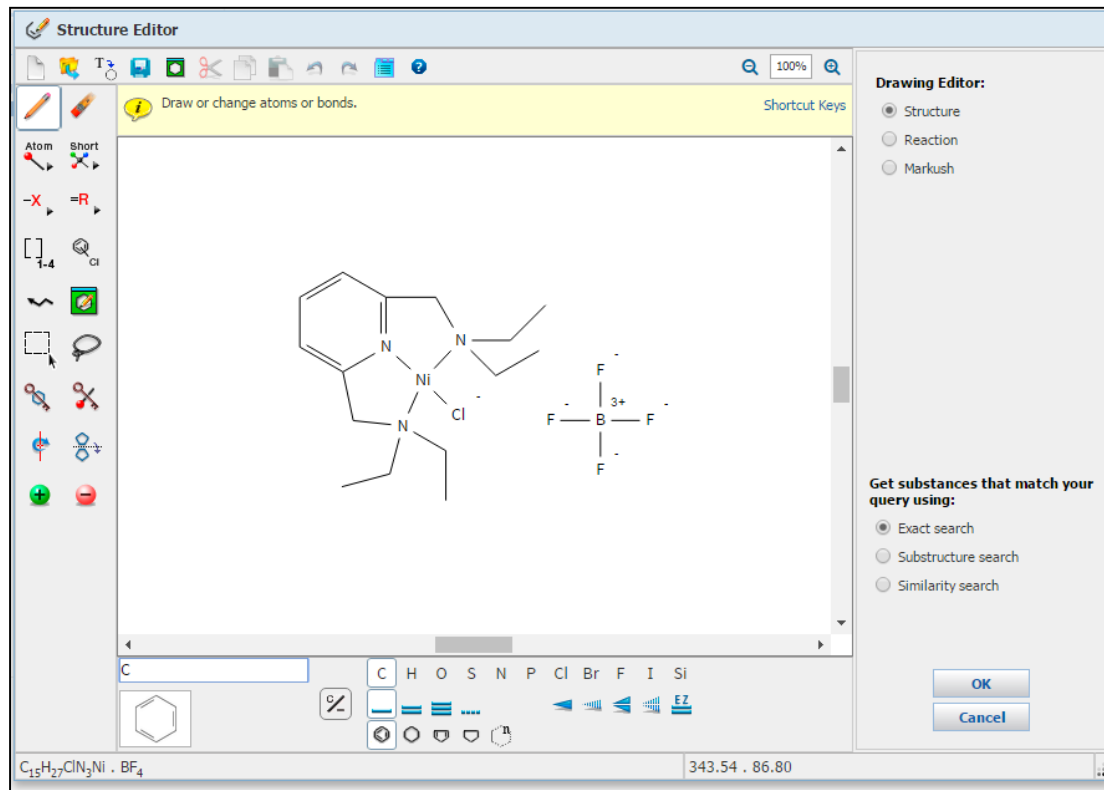
Search

提示:

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

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

精确结构检索配合物



获得精确结构检索结果

Characteristics

- ☒ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

- ☐ Alloys
- ☒ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☐ Polymers
- ☐ Organics, and others not listed

Studies

- ☐ Analytical
- ☐ Biological
- ☐ Preparation
- ☐ Reactant or reagent

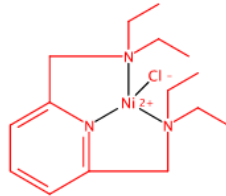
Sort by: CAS Registry Number

0 of 1 Substance Selected

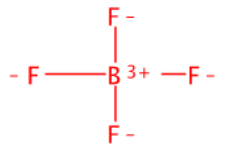
1. 1955541-98-6

~1

1955541-97-5
C₁₅ H₂₇ Cl N₃ Ni



14874-70-5
B F₄

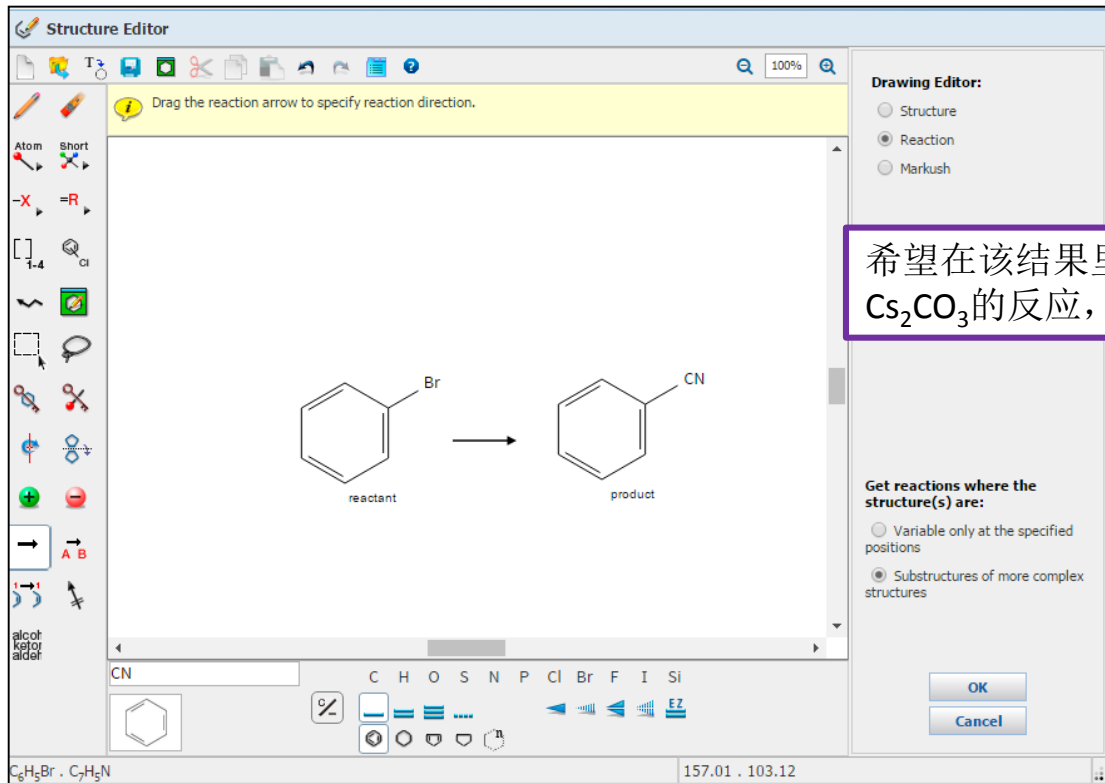


C₁₅ H₂₇ Cl N₃ Ni · B F₄
INDEX NAME NOT YET ASSIGNED

提纲

- 反应检索
 - 如何使用反应结构编辑器功能键提高反应检索精度
 - 如何使用Analyze/Refine处理反应结果集
 - 如何通过MethodsNow Synthesis快速获得权威可靠的合成方法

案例一：检索由溴苯转化为苯腈的反应



希望在该结果里进一步限定:溶剂为DMF, 试剂为 CS_2CO_3 的反应, 应如何操作?

获得34万多条反应，噪音较大

Reaction Structure substructure > reactions (343247)

REACTIONS

Get References Tools

Analyze Refine

Sample Analysis:
Reagent

HCl ≥ 8898

K_2CO_3 ≥ 5988

Et_3N ≥ 5774

H_2O ≥ 4430

$NaOH$ ≥ 4293

$EtH(Pr)_2$ ≥ 3928

$NaHCO_3$ ≥ 3884

Disodium carbonate ≥ 3711

CS_2CO_3 ≥ 3314

F_3CCO_2H ≥ 3183

Show More

Group by: No Grouping Sort by: Relevance

0 of 343247 reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

• 4 K^+
~24

~113

99%
~87

Overview

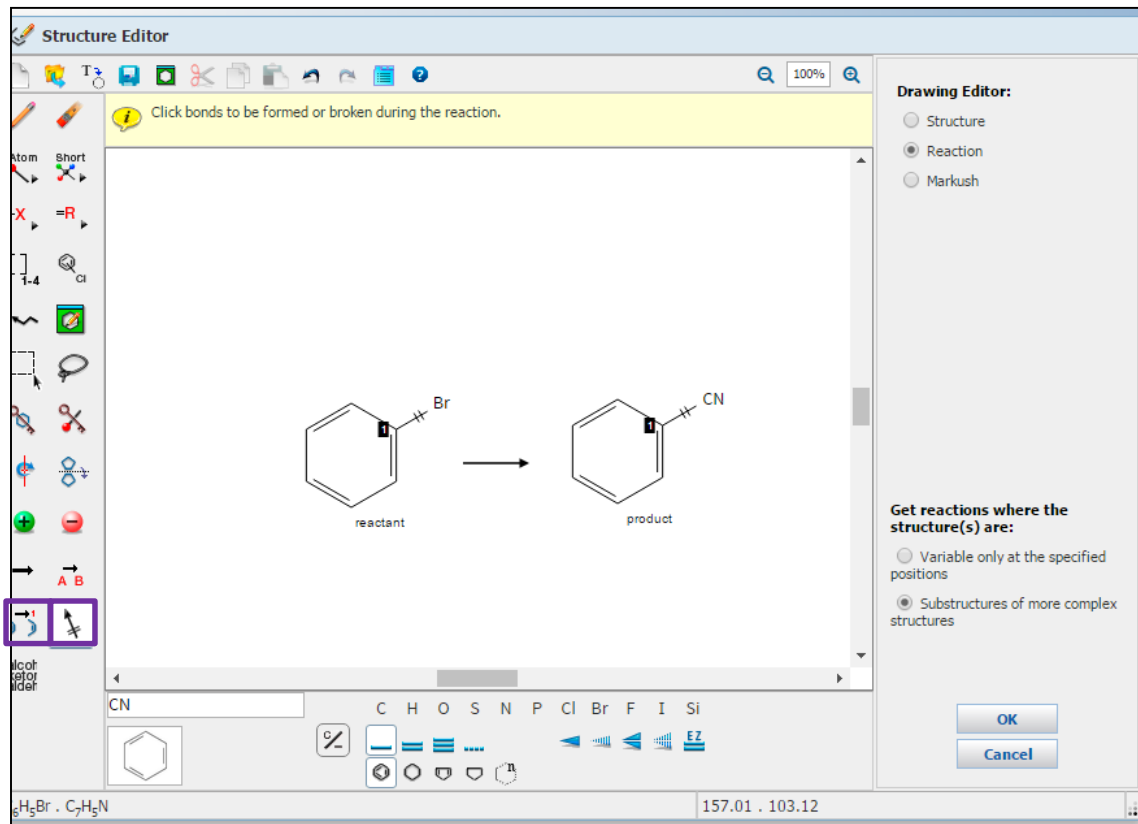
Steps/Stages

1.1 C:1863984-13-7 (inclusion complexes with palladium nanopar), S:DMF, 15 h, 140°C

Notes

alternative reaction conditions shown, nanoparticle cat.

可以通过反应原子标记工具和反应位置标记工具提高反应检索精度



获得反应97188条

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure substructure > reactions (97188)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Sample Analysis: ⓘ
Reagent ▾

HCl	≥ 9324
Et ₃ N	≥ 5595
H ₂ O	≥ 5573
NaHCO ₃	≥ 5064
NaOH	≥ 4585
K ₂ CO ₃	≥ 4516
EtN(Pr- <i>i</i>) ₂	≥ 3777
NH ₄ Cl	≥ 3625
F ₃ CCO ₂ H	≥ 3264

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

0 of 97188 reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

Single Step Hover over any structure for more options.

• 4 K⁺
~25 ⓘ

~116 ⓘ

99%
~93 ⓘ

使用反应结果集中的Analyze功能，需要将结果集压缩到20000以下

将反应限定为1步反应

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

0 of 9551 Reactions Selected

1. View Reaction Detail ⓘ Link ⓘ Similar Reactions

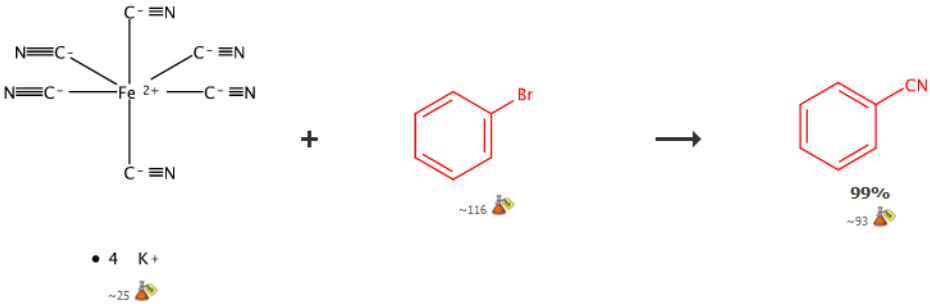
Single Step Hover over any structure for more options.

Refine by: ⓘ

- ☐ Reaction Structure
- ☐ Product Yield
- ☒ Number of Steps
- ☐ Reaction Classification
- ☐ Excluding Reaction Classification
- ☐ Non-participating functional groups

Number of Steps:
Examples: 1, 1 - 3, 1 -, - 3

Refine


The reaction scheme shows an iron complex (Fe²⁺) with four cyanide (C≡N) ligands reacting with bromobenzene (a benzene ring with a bromine atom) to form a nitrile product (a benzene ring with a cyano group). The product is labeled with a 99% yield and a ~93 icon. The iron complex is labeled with a ~25 icon and 4 K⁺. The bromobenzene is labeled with a ~116 icon.

通过Analyze by Solvent选择在DMF溶剂中进行的反应

Explore ▾ Saved Searches ▾ SciPlanner

Save Print Export

⚠ 4,977 reactions with the Solvent **DMF** are displayed [Keep Analysis](#) [Clear Analysis](#)

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > refine "1 step" (9551)

REACTIONS ⓘ Get References Tools ▾ Send to SciPlanner

Analyze Refine

Group by: No Grouping ▾ Sort by: Relevance ▾ ↓

0 of 9551 Reactions Selected

1. View Reaction Detail 🔗 Link ⚙ Similar Reactions

Single Step Hover over any structure for more options.

Analyze by: ⓘ
Solvent ▾

DMF 4977

H ₂ O	2088
NMP	1510
THF	752
AcNMe ₂	586
CH ₂ Cl ₂	470
C ₆ H ₅ N	432
PhMe	284
MeCN	266

Chemical reaction scheme showing the reaction of a ferrocene complex (Fe²⁺ complexed with four nitrile ligands, C≡N) and a bromobenzene derivative (C₆H₅Br) to form a nitrile product (C₆H₅CN). The reaction is labeled "Single Step" and "99%".

• 4 K⁺ ~25

Waiting for scifinder.cas.org...

在反应结果集中继续通过Analyze by Reagent选择Cs₂CO₃作为试剂的反应

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > refine "1 step" (9551) > keep analysis "Solvent" (4977)

REACTIONS

Get References Tools

Analyze Refine

Analyze by:
Reagent

H ₂ O	345
HCl	300
K ₂ CO ₃	190
NH ₃	181
NH ₄ OH	164
FeCl ₃	155
Zn	134
Disodium carbonate	121
NaHCO ₃	115
NH ₄ Cl	100

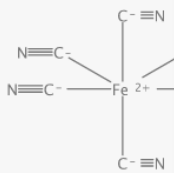
Show More

Group by: [No Grouping] Sort by: [No Grouping]

0 of 4977 Reactions Selected

1. View Reaction Detail

Single Step Hover over any structure



• 4 K⁺
~25

Overview
Steps/Stages

1.1 C:1863984-13-7 (incl...)

Analyze - Reagent

261 Items 1 Selected Export

Sort by: Frequency Page: 1 of 6

Select bars to view only those reactions within the current answer set.

<input type="checkbox"/> O ₂	60
<input type="checkbox"/> EtN=C=N(CH ₂) ₃ NMe ₂ • HCl	59
<input type="checkbox"/> LiOH	57
<input type="checkbox"/> CuCN	56
<input type="checkbox"/> H ₂ SO ₄	54
<input type="checkbox"/> TMEDA	52
<input type="checkbox"/> (NO)H(SO ₄)	51
<input type="checkbox"/> AcOH	49
<input checked="" type="checkbox"/> Cs ₂ CO ₃	48
<input type="checkbox"/> NaH	45

Apply Cancel

获得以 DMF为溶剂, Cs_2CO_3 为试剂的一步反应, 保存结果集

Analyze by: [?](#)

Reagent

Cs_2CO_3	48
KI	24
1427296-27-2	11
HCl	6
Et_3N	4
H_2O	4
CuCl_2	3
EtOH	3
$\text{F}_3\text{CCO}_2\text{H}$	3
Fe	3

[Show More](#)

0 of 48 Reactions Selected
1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

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

~116 ~111

Overview

Steps/Stages

1.1 R:

R: KI, R: Cs_2CO_3 , C: CuI, S: DMF, 8 h, 130°C

Notes

alternative preparation shown, pressure tube used, Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

A new oxazole ligand for the copper-catalyzed cyanation of aryl halides with $\text{K}_4[\text{Fe}(\text{CN})_6]$

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

By Sajadi, S. Mohammad and Maham, Mehdi

From Letters in Organic Chemistry, 11(2), 136-140; 2014

在初始反应结果集中限定2步反应，重复刚才的步骤

Explore ▼ Saved Searches ▼ SciPlanner

Reaction Structure substructure > reactions (97188)

REACTIONS ?

Get References Tools ▼

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 97188 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Number of Steps: 2

Examples: 1, 1 - 3, 1 -, - 3

Refine

The reaction scheme shows an iron complex reacting with bromobenzene to form a nitrile-substituted benzene. The iron complex is a central Fe²⁺ ion coordinated by six cyanide (C≡N) groups. The bromobenzene molecule is a benzene ring with a bromine atom. The product is a benzene ring with a nitrile group (CN). The reaction is labeled with a yield of 99% and a value of ~93.

获得以 DMF 为溶剂, Cs_2CO_3 为试剂的 2 步反应, 保存结果集

Reaction Structure substructure > reactions (97188) > refine "2 steps" (13339) > keep analysis "Solvent" (5734) > keep analysis "Reagent" (249)

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: Reagent

Cs_2CO_3	249
HCl	26
$\text{F}_3\text{CCO}_2\text{H}$	15
NH_4Cl	14
Zn	14
NaI	12
NMP	12
NaCl	11
H_2O	10

Group by: No Grouping Sort by: Relevance

0 of 249 Reactions Selected

1. View Reaction Detail Link

2 Steps Hover over any structure for more options.

Chemical reaction scheme showing the conversion of 1-bromo-4-iodobenzene (MW ~144) and hexamminecobalt(III) chloride (MW ~111) to 1,4-dicyanobenzene (MW ~106). The reaction involves 3 equivalents of K^+ ions.

在Saved Searches中的反应结果集中找到刚保存过的结果集

Explore ▾ **Saved Searches ▾** SciPlanner

Reaction Structure: [Saved Answer Sets](#)
[Keep Me Posted](#)
[History](#)

REACTIONS ? [Tools ▾](#)

Group by: No Grouping ▾ Sort by: Relevance ▾

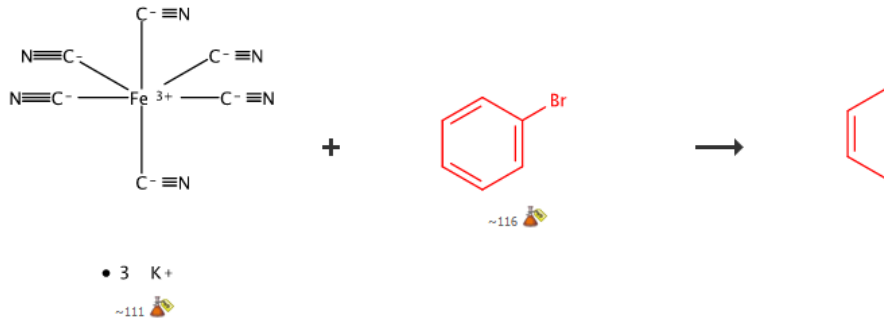
0 of 48 Reactions Selected

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

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

Analyze by: [?](#)
Reagent ▾

Cs ₂ CO ₃	48
KI	24
1427296-27-2	11
HCl	6
Et ₃ N	4
H ₂ O	4
CuCl ₂	3
EtOH	3
F ₃ CCO ₂ H	3



• 3 K⁺
~111



SciFinder®
A CAS SOLUTION

合并结果集

Explore ▾ Saved Searches ▾ SciPlanner

Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977) > keep analysis "Reagent" (48)

SAVED ANSWER SETS Combine selected saved answer sets and view combined set.

SAVED SEARCHES

- ☒ Saved Answer Sets
- ☐ Keep Me Posted
- ☐ History

2 of 49 Reaction Answer Sets Selected **References (38)** **Substances (8)** **Reactions (49)**

<input checked="" type="checkbox"/>	1010dmf1step (48) Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977) > keep analysis "Reagent" (48)	Edit	Link	Saved Oct 10, 2016
<input checked="" type="checkbox"/>	1010dmf2step (249) Reaction Structure substructure > reactions (97188) > refine "2 steps" (13339) > keep analysis "Reagent" (249)			
<input type="checkbox"/>	DMF-cyanation (4977) Reaction Structure substructure > reactions (97188) > refine "1 step" (9551) > keep analysis "Solvent" (4977)			
<input type="checkbox"/>	1010reaction2 (813) Chemical Structure substructure > substances (164) > get reactions (813)			
<input type="checkbox"/>	1010reaction1 (780) Chemical Structure substructure > substances (3920) > get reactions (780)			
<input type="checkbox"/>	a2 (3728) Chemical Structure exact with limiters > substances (11) > 1517-69-7 > get reactions (3728)			
<input type="checkbox"/>	a1 (697)			

Combine Answer Sets

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 1010dmf1step that are not in 1010dmf2step
- Exclude** Include only answers from 1010dmf2step that are not in 1010dmf1step

Combine Answer Sets **Cancel**

亚结构检索2：酮基的还原反应

Structure Editor

Drag the reaction arrow to specify reaction direction.

reactant

product

Drawing Editor:

- ☐ Structure
- ☒ Reaction
- ☐ Markush

Get reactions where the structure(s) are:

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

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

KEEP ME POSTED ?

C-N bond activation
Dec 12, 2015(1)
Dec 05, 2015(1)
Nov 28, 2015(1)

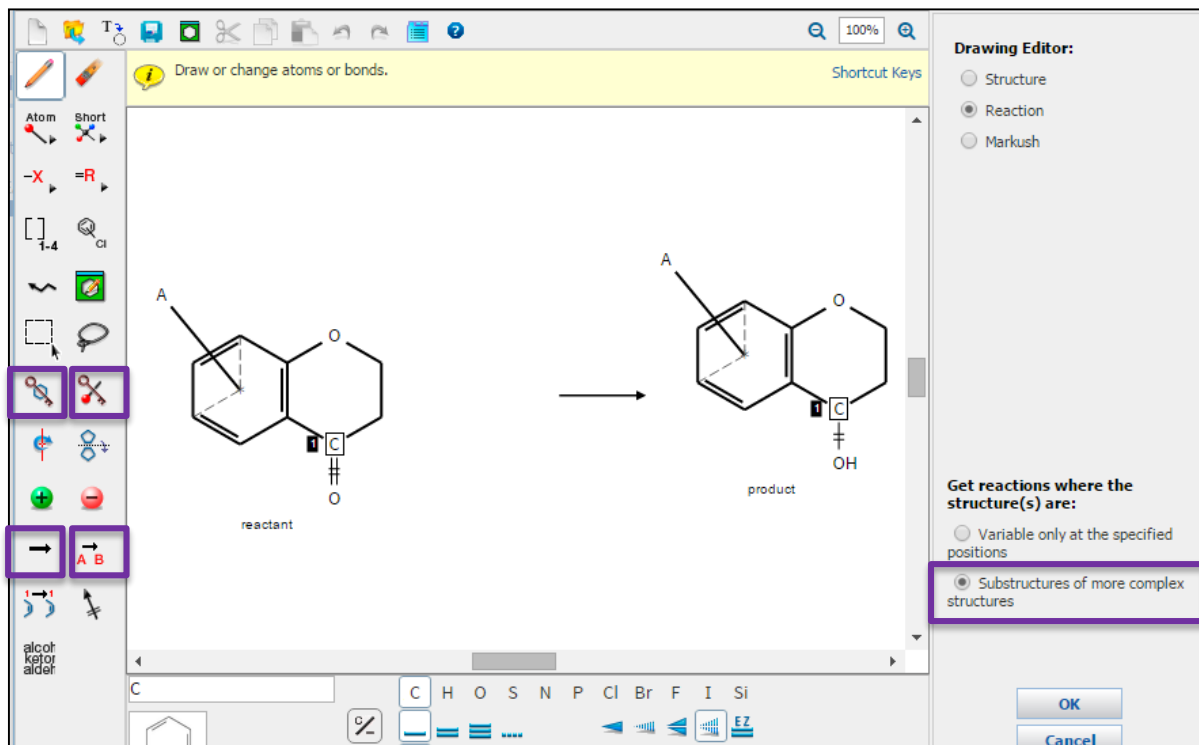
View All

alcohol
ketone
aldehyde



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亚结构检索2：酮基的还原反应



检索酮基的还原反应，
需将碳原子锁定

亚结构反应检索结果

通过Analyze或者Refine处理检索结果

Analyze Refine

Analyze by: Reagent

NaBH ₄	529
HCl	425
K ₂ CO ₃	387
Et ₃ N	367
H ₂	353
NaOH	299
NaHCO ₃	235
Et ₃ N • HCl	228
LiBH ₄	190
13289-97-9	149

Show More

Group by: No Grouping Sort by: Accession Number

0 of 1107 Reactions Selected

Display Options

Page: 1 of 23

1. View Reaction Detail Similar Reactions

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

~43

→

~5

Overview

Steps/Stages

1.1 R:NaBH₄, S:MeOH, overnight, rt

Notes

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

References

亚结构反应检索结果

AnalyzeRefine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups**

Non-participating Functional Group(s)
View: All 217 ▾

1 Selected Clear Selections

- ☐ Acetal
- ☐ Acetyl
- ☐ Acid Halide
- ☐ Alkene
- ☐ Alkyne
- ☐ Aldehyde
- ☐ Alcohols

Reactions must have

- ☒ all selections
- ☐ any selection

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

0 of 30 Reactions Selected

☐ 1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~5 ~3

Overview

Steps/Stages

1.1 R:NaBH₄, S:MeOH, rt

Notes

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

References

Identification of 3-hydroxy-4[3,4-dihydro-3-oxo-2H-1,4-benzoxazin-4-yl]-2,2-dimethyldihydro-2H-benzopyran derivatives as potassium channel activators and anti-inflammatory agents

Quick View Other Sources

限定某官能团参与

亚结构反应检索结果

AnalyzeRefine

Refine by: ?

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification**
- Excluding Reaction Classification
- Non-participating functional groups

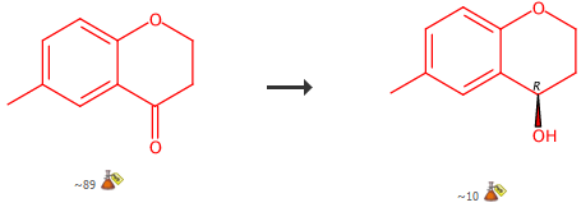
Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- ☒ Stereoselective

Refine

2. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



~89

~10

Overview

Steps/Stages

1.1 S: Me₂CO, 9 d, rt

Notes

biotransformation, enzymic, stereoselective, 100% ee, 100% conversion, Chaetomium sp.1 used, Reactants: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[selective reduction of 4-chromanone and its derivatives by selected filamentous fungi](#)
View Other Sources
ko, Tomasz et al
Journal of Molecular Catalysis B: Enzymatic, 97, 278-282; 2013

反应分类：生物转化反应，催化/非催化反应，光化学，电化学，顺反选择，手性立体选择等等）

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提纲

- 反应检索
 - 如何使用反应结构编辑器功能键提高反应检索精度
 - 如何使用Analyze/Refine处理反应结果集
 - 如何通过MethodsNow Synthesis快速获得权威可靠的合成方法

通过罗丹明物质获得反应

Substance Identifier "81-88-9" > substances (1) > get reactions (40)

SUBSTANCES ?

Get References Get Reactions Retrieve reactions for selected substances.

Analyze Refine

Analyze by: ?
Substance Role

Analytical Study 1
Biological Study 1
Formation, Nonpreparative 1
Miscellaneous 1
Occurrence 1
Preparation 1
Process 1
Properties 1

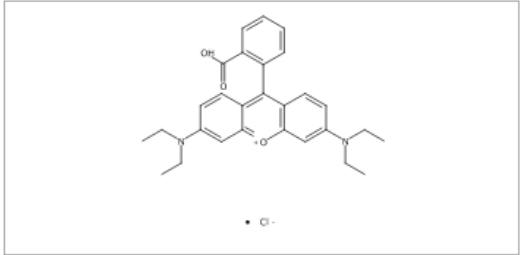
Sort by: CAS Registry Number

0 of 1 Substance Selected

1. **81-88-9**

(Component: 64381-98-2)

~20754 ~104



C₂₈ H₃₁ N₂ O₃ · Cl
Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, chloride (1:1)

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

由罗丹明的制备信息获得相关反应

Substance Identifier "81-88-9" > substances (1) > **get reactions (40)**

REACTIONS ?

Get References Tools

Analyze Refine

Analyze by: MethodsNow

MethodsNow Available 22

MethodsNow Not Available 18

Show More

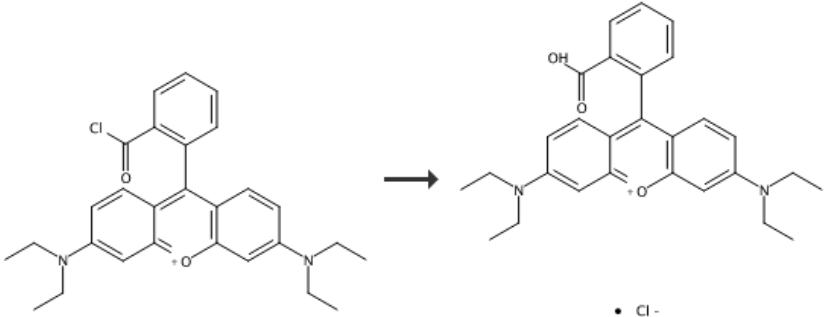
Group by: No Grouping Sort by: Accession Number

0 of 40 Reactions Selected

1. View Reaction Detail

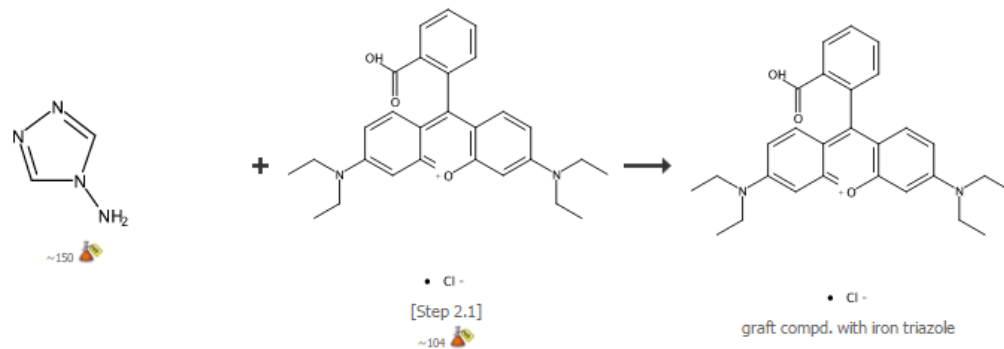
Single Step Hover over any structure

可以通过Analyze或者Sort by访问MethodsNow Synthesis



• Cl⁻

2 Steps Hover over any structure for more options.



► Overview

▼ METHODSNow™

Procedure

1. Add a 50 mL methanol solution containing 3 mmol 4-NH₂-1,2,4-triazole at room temperature into a 50 mL methanol solution containing 1 mmol Fe(ClO₄)₃·6H₂O and 5 mg ascorbic acid.
2. Stir the resulting limpid mixture for half an hour.

[View more...](#)

Available Experimental Data

Elemental Analysis, State

[View with MethodsNow](#)

Synergetic Spin Crossover and Fluorescence in One-Dimensional Hybrid Complexes

By Wang, Chun-Feng; Li, Ren-Fu; Chen, Xue-Yuan; Wei, Rong-Jia; Zheng, Lan-Sun; Tao, Jun
 From Angewandte Chemie, International Edition, 54(5), 1574-1577; 2015
 Published by Wiley-VCH Verlag GmbH & Co. KGaA

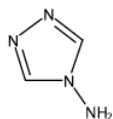
书目信息

Reaction Steps

1

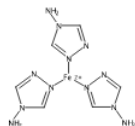
2

点击步数，获得相应步骤反应



~150

1



grafted by 1-pyrenecarboxaldehyde, by rhod

Products	Iron(2+), tris(4-1,2,4-triazol-4-amine- <i>M</i>), diperchlorate, hydrate, grafted by 1-pyrenecarboxaldehyde, by rhod, CAS RN: 151592-05-1
Reactants	4-1,2,4-Triazol-4-amine, CAS RN: 584-13-4
Reagents	Perchloric acid, iron(2+) salt (2:1), CAS RN: 13933-23-8 L-Ascorbic acid, CAS RN: 50-81-7
Solvents	Methanol, CAS RN: 67-56-1
Procedure	1. Add a 50 mL methanol solution containing 3 mmol 4-NH ₂ -1,2,4-triazole at room temperature into a 50 mL methanol solution containing 1 mmol Fe(ClO ₄) ₂ ·6H ₂ O and 5 mg ascorbic acid. 2. Stir the resulting limpid mixture for half an hour. 3. Evaporate the mixture to dryness by a rotary evaporator at about 333 K. 4. Precipitate the product as powder that turns purple on cooling.
Scale	milligram
Elemental Analysis	Calcd (%) for C ₆ H ₁₂ N ₁₂ O ₈ Cl ₂ Fe: C 14.21, H 2.38, N 33.15. Found: C 14.32, H 2.32, N 32.56.
State	purple powder.
CAS Method Number	3-562-CAS-1814872

Print/Export

Close

更清楚物质展示
更清楚实验过程展示

经过CAS科学家重写的实验步骤

物质表征信息

打印或者导出分析方法



FINDER
A CAS SOLUTION

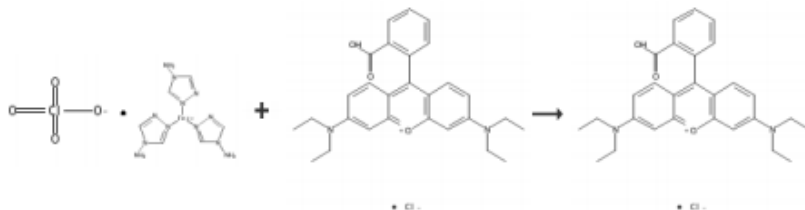
Synergetic Spin Crossover and Fluorescence in One-Dimensional Hybrid Complexes

By Wang, Chun-Feng; Li, Ren-Fu; Chen, Xue-Yuan; Wei, Rong-Jia; Zheng, Lan-Sun; Tao, Jun

From *Angewandte Chemie, International Edition*, 54(5), 1574-1577; 2015

Published by Wiley-VCH Verlag GmbH & Co. KGaA

Step 2



更好的阅读体验

Products	Rhodamine B, graft compd. with iron triazole, CAS RN: 81-88-9
Reactants	Iron(2+), tris(4 <i>H</i> -1,2,4-triazol-4-amine- <i>N</i> ¹)-, diperchlorate, hydrate, grafted by 1-pyrenecarboxaldehyde, by rhod, CAS RN: 151592-05-1 Rhodamine B, CAS RN: 81-88-9
Solvents	Toluene, CAS RN: 108-88-3
Procedure	<ol style="list-style-type: none"> 1. Disperse 100 mg FeL in 30 mL toluene. 2. Add 0.21 mmol rhodamine B. 3. Reflux the mixture under N₂ for 24 hours. 4. Collect the resulting materials by filtration. 5. Wash the resulting materials properly with ethanol to remove any unreacted reagent. 6. Dry the solids under vacuum.
Scale	milligram
Elemental Analysis	Calcd (%) for [Fe(C ₂ H ₄ N ₄) _{2.71} (C ₃₀ H ₃₃ N ₆ O ₂ Cl) _{0.29}](ClO ₄) ₂ : C 28.14, H 3.41, N 22.94. Found: C 28.13, H 2.97, N 26.92.
State	red solid.
CAS Method Number	3-614-CAS-1824301

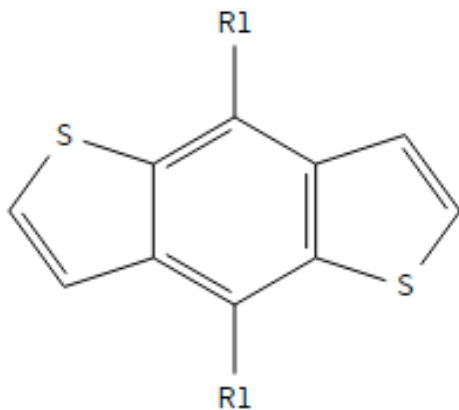

SciFinder®
 A CAS SOLUTION

提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
 - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
 - 尼龙1212（单体：十二胺、十二酸）的聚合方法

聚合物检索——结构式检索

- 案例：检索以下结构作为聚合单体的均聚物信息并对检索结果进行筛选



R1 = alkyl chains

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
- ☐ Preparation
- ☐ Reactant or reagent



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A CAS SOLUTION

通过化学结构限定检索结果

Analyze

Refine

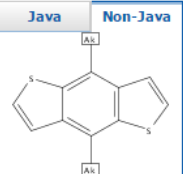
Refine by: ?

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

Structure Editor:

Java

Non-Java



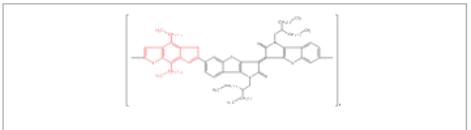
Click image to change structure or view detail.
Search type: **Substructure**

Sort by: CAS Registry Number

0 of 118 Substances Selected

1. 1809608-17-0

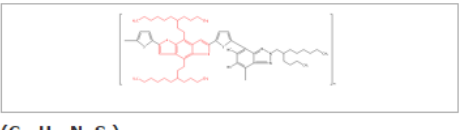
~1



$(C_{94}H_{140}N_2O_2S_4)_n$
INDEX NAME NOT YET ASSIGNED

2. 1807885-40-0

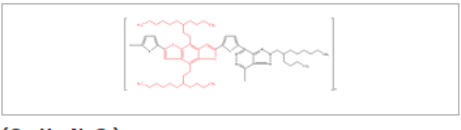
~1



$(C_{64}H_{85}N_5S_4)_n$
INDEX NAME NOT YET ASSIGNED

3. 1807885-37-5

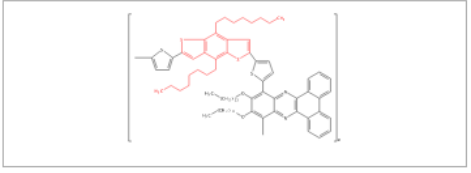
~1



$(C_{60}H_{85}N_5S_4)_n$
INDEX NAME NOT YET ASSIGNED

4. 1778703-42-6

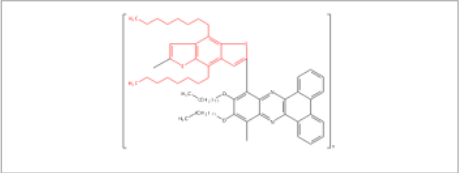
~1



INDEX NAME NOT YET ASSIGNED

5. 1778703-40-4

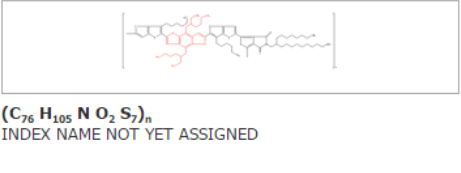
~1



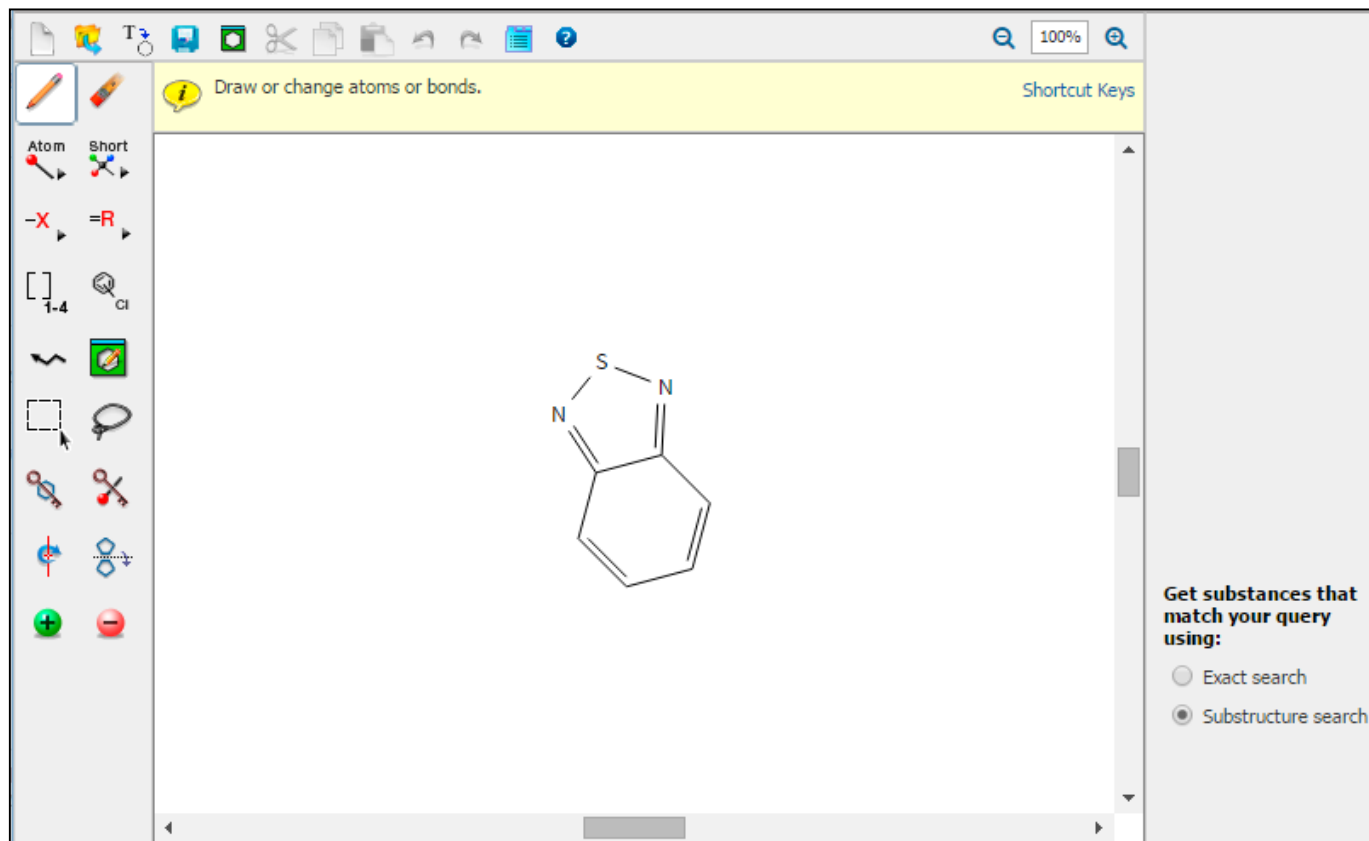
INDEX NAME NOT YET ASSIGNED

6. 1702435-34-4

~1



$(C_{76}H_{105}N_5O_2S_7)_n$
INDEX NAME NOT YET ASSIGNED



SUBSTANCES ?

Get References

Get Reactions

Get Commercial Sources

Tools ▾

Create Keep Me Posted Alert

Send to SciPlanne

Analyze Refine

Analyze by: ?

Substance Role ▾

Preparation 20

Uses 20

Properties 14

Process 7

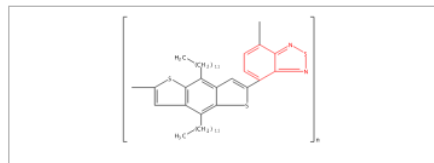
Prophetic in Patents 1

Show More

Sort by: Relevance ▾

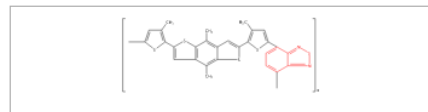
- Relevance
- CAS Registry Number
- Number of References
- Number of Commercial Sources
- Molecular Weight
- Molecular Formula

~1

**(C₄₀ H₅₄ N₂ S₃)_n**Poly[2,1,3-benzothiadiazole-4,7-diyl(4,8-didodecylbenzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl)]

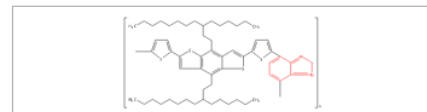
2. 1616403-92-9 🔍

~2

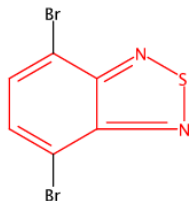
**(C₂₈ H₁₈ N₂ S₃)_n**Poly[2,1,3-benzothiadiazole-4,7-diyl(4-methyl-2,5-thiophenediyl)-(4,8-dimethylbenzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl)(3-methyl-2,5-thiophenediyl)]

3. 1227363-53-2 🔍

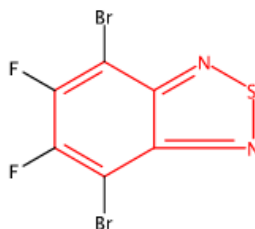
~3

**(C₅₈ H₇₈ N₂ S₃)_n**Poly[2,1,3-benzothiadiazole-4,7-diyl-2,5-thiophenediyl[4,8-bis(3-hexylundecyl)benzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl]-2,5-thiophenediyl]

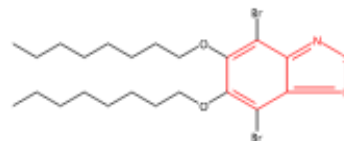
15155-41-6

C₈ H₂ Br₂ N₂ S

1295502-53-2

C₆ Br₂ F₂ N₂ S

1192352-08-1

C₂₂ H₃₄ Br₂ N₂ O₂ S
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提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
 - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
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聚合物检索——分子式检索

- 聚合物的分子式表现形式

分子式中带有括号

括号外为 n ，嵌段聚合物（有首尾端或无首尾段都可）

有端基嵌段聚合物分子式： $(C_6H_{10}O_2)_n C_3H_4O_2$

无端基嵌段聚合物分子式： $(C_{12}H_{12}O_4)_n$

括号外为 x ，对于均聚物和共聚物，将以单体进行标引，聚合度不影响标引

共聚物： $(C_2H_4 . C_2F_4)_x$

均聚物： $(C_2H_4)_x$

(C₂ H₄ . C₂ F₄)_x——SciFinder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

0 of 5 Substances Selected

Analyze by: Substance Role

Uses 5

Preparation 4

Properties 4

Process 3

Reactant or Reagent 3

Analytical Study 2

Biological Study 2

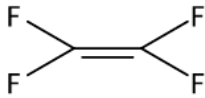
Formation, Nonpreparative 2

Miscellaneous 1

Occurrence 1

1. 1056460-80-0

116-14-3
C₂ F₄



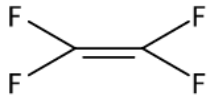
74-85-1
C₂ H₄

CH₂ = CH₂

(C₂ H₄ . C₂ F₄)_x
Ethene, 1,1,2,2-tetrafluoro-, polymer with ethene, triblock

2. 136846-15-6

116-14-3
C₂ F₄



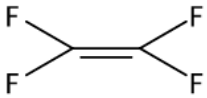
74-85-1
C₂ H₄

CH₂ = CH₂

(C₂ H₄ . C₂ F₄)_x
Ethene, 1,1,2,2-tetrafluoro-, polymer with ethene, graft

3. 132201-85-5


116-14-3
C₂ F₄



74-85-1
C₂ H₄

CH₂ = CH₂

(C₂ H₄ . C₂ F₄)_x
Ethene, tetrafluoro-, polymer with ethene, block (9CI)

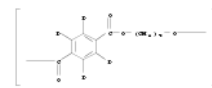
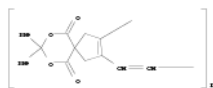


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86

(C₁₂ H₁₂ O₄)_n——SciFinder检索结果

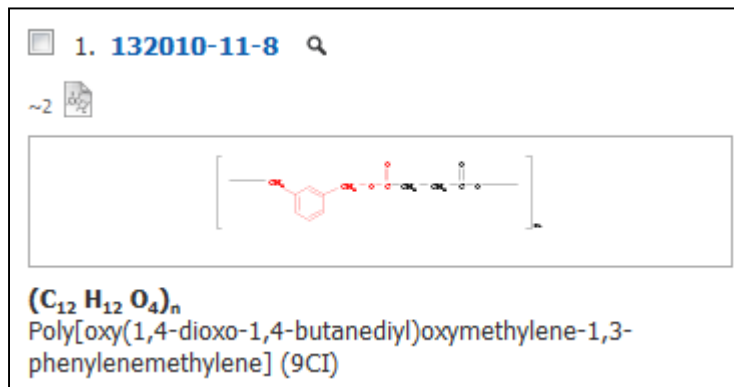
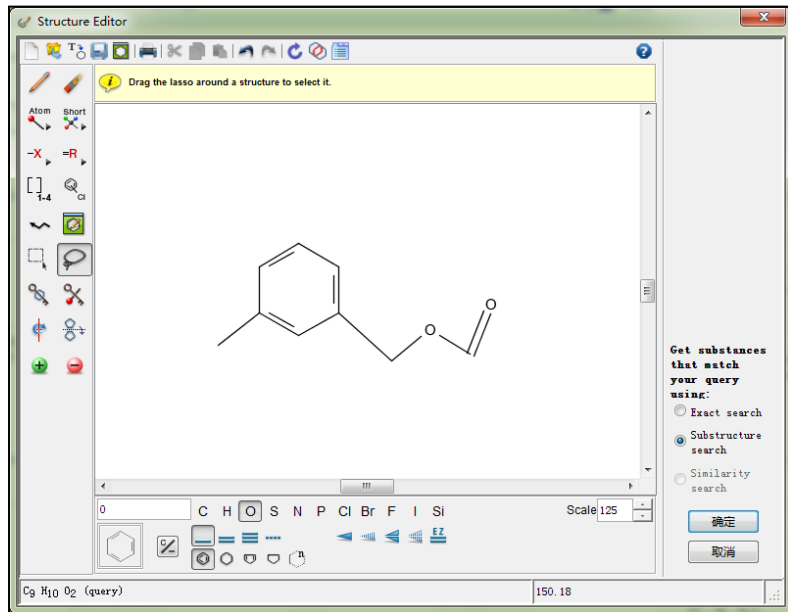
0 of 44 Substances Selected

<p>1. 1637772-98-5 🔍</p> <p>~1 </p>  <p>(C₁₂ H₈ D₄ O₄)_n INDEX NAME NOT YET ASSIGNED</p>	<p>2. 1421756-46-8 🔍</p> <p>~1 </p> <p>Substance Image Cannot Be Displayed 1421756-46-8</p> <p>(C₁₂ H₁₂ O₄)_n Poly[oxy[(R)-phenyl-1,2-ethanediyl]oxy(1,4-dioxo-1,4-butanediyl)]</p>	<p>3. 1392419-56-5 🔍</p> <p>~1 </p>  <p>(C₁₂ H₁₂ O₄)_n Poly[(8,8-dimethyl-6,10-dioxo-7,9-dioxaspiro[4.5]dec-2-ene-2,3-diyl)-1,2-ethenediyl]</p>
<p>4. 1353713-96-8 🔍</p> <p>~1 </p> <p>Substance Image Cannot Be Displayed 1353713-96-8</p> <p>(C₁₂ H₁₂ O₄)_n Poly[oxyphenyleneoxy(1,6-dioxo-1,6-hexanediyl)]</p>	<p>5. 1341223-97-9 🔍</p> <p>~1 </p> <p>Substance Image Cannot Be Displayed 1341223-97-9</p> <p>(C₁₂ H₁₂ O₄)_n Poly[[[(1-carboxyethoxy)methoxy-1,4-phenylene]-1,2-ethenediyl]</p>	<p>6. 1287722-74-0 🔍</p> <p>~1 </p>  <p>(C₁₂ H₁₂ O₄)_n Poly[oxy(2-methyl-1,3-propanediyl)oxycarbonyl-1,2-phenylenecarbonyl]</p>



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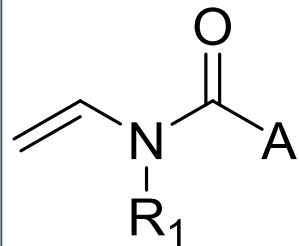
用结构限定



提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
 - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
 - 尼龙1212（单体：十二胺、十二酸）的聚合方法

检索案例：检索所有包含下列结构特征的乙烯作为单体的均聚物的反应 (文献)



R1 = H or alkyl group
A = any atom except H

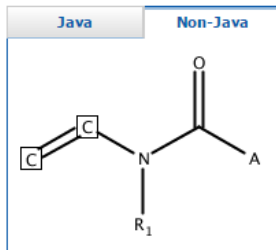
检索思路：

从结构检索出发，经过限定后，得到聚合物物质结果集

方案一：由物质获得反应，再获得相关合成制备文献；

方案二：由物质获得文献，再通过文献检索结果处理工具精选文献

Structure Editor:



Import CXF

Search

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

Search Type:

- ☐ Exact Structure
 - ☒ Substructure
 - ☐ Similarity
- ☐ Show precision analysis



Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

在Advanced Search中，选中Single component和Polymers



获得98个均聚物物质结果

Chemical Structure substructure with limiters > **substances (98)** > get reactions (70) > reaction 6 (of 70)

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools

Create Keep Me Posted Alert Send to SciFinder

Analyze Refine

Sort by: Number of References

0 of 98 Substances Selected

Analyze by: Substance Role

Preparation 61

Uses 43

Reactant or Reagent 24

Properties 18

Biological Study 16

Process 8

Analytical Study 3

Formation, Nonpreparative 2

Miscellaneous 1

1. **28408-65-3**

5202-78-8
 $C_4 H_7 N O$

单体CAS RN

$(C_4 H_7 N O)_x$
Acetamide, *N*-ethenyl-, homopolymer

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. **26616-03-5**

3195-78-6
 $C_5 H_9 N O$

聚合物CAS RN

$(C_5 H_9 N O)_x$
Acetamide, *N*-ethenyl-*N*-methyl-, homopolymer

Regulatory Information

3. **187035-78-5**

149993-19-1
 $C_6 H_{11} N O$

$(C_6 H_{11} N O)_x$
Propanamide, *N*-ethenyl-2-methyl-, homopolymer

方案一：
由物质获得反应，再获得相关合成制备文献

方案一：通过物质（限定为产物）获得反应

Chemical Structure substructure with limiters > **substances (98)** > get reactions (70) > reaction 6 (of 70)

SUBSTANCES ? Get References Get Reactions Retrieve reactions for selected substances.

Analyze Refine

Analyze by: ?
Substance Role

Preparation 61
Uses 43
Reactant or Reagent 24
Properties 18
Biological Study 16
Process 8
Analytical Study 3
Formation, Nonpreparative 2
Miscellaneous 1

Sort by: Number of References

0 of 98 Substances Selected

1. 28408-65-3
~583 ~3

5202-78-8
 C_4H_7NO

$(C_4H_7NO)_x$
Acetamide, *N*-ethenyl-, homopolymer

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 26616-03-
~173

3195-78-6
 C_5H_9NO

$(C_5H_9NO)_x$
Acetamide, *N*-ethenyl-, homopolymer

Regulatory Information

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



获得70条满足检索需要的反应

Chemical Structure substructure with limiters > substances (98) > get reactions (70)

REACTIONS ?

Get References Tools

Send to SciPlanner

Analyze Refine

Group by: No Grouping Sort by: Accession Number

0 of 70 Reactions Selected

Page: 1 of 2


Analyze by: Reagent

1321-74-0	21
HCl	15
AIBN	8
CaCO ₃	8
NaOH	6
(-)-Menthol	4
142648-73-5	4
AcOH	4
Cs ₂ CO ₃	4
H ₂ SO ₄	3

Show More

1. View Reaction Detail Link

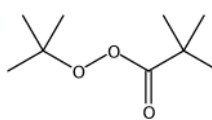
Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:



S: Me₂CO, 5 min, rt; 10 min, rt; 9 h, reflux; 1 h, reflux

Notes

incremental addition (reactant, reagent, solvent), optimization study, optimized on reagent, solvent, time, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Methods for making polymers from N-vinylacetamide monomer

Quick View PATENTPAK

By Chandran, Rama S. and Leblanc, Jean-pierre

From Eur. Pat. Appl., 870782, 14 Oct 1998

通过反应获得文献

CAS Solutions **SciFINDER**
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Welcome Cyrene Qian

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

Chemical Structure substructure with limiters > substances (98) > **get reactions (70)** > get references (30)

REACTIONS [Get References](#) Retrieve references for selected reactions. [Send to SciPlanner](#)

Analyze **Refine**

Analyze by: [?](#)
Reagent

1321-74-0	21
HCl	15
AIBN	8
CaCO ₃	8
NaOH	6
(-)-Menthol	4
142648-73-5	4
AcOH	4
Cs ₂ CO ₃	4
H ₂ SO ₄	3

Group by: No Grouping Sort by: Accession Number

0 of 70 Reactions Selected

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

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

Overview

Steps/Stages

1.1 R:

Notes

incremental addition (reactant, reagent, solvent), optimization study, optimized on reagent, solvent, time, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

获得30篇和聚合物制备相关的文献

Explore ▼
Saved Searches ▼
SciPlanner
Save
Print
Export

Chemical Structure substructure with limiters > substances (98) > get reactions (70) > get references (30)

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

Analyze
Refine
Categorize

Sort by: Accession Number ↑
Display Options

☐ 0 of 30 References Selected

Analyze by: ?
Author Name ▼

Ajiro Hiroharu	5
Akashi Mitsuru	5
Burke Steven K	4
Holmes Farley	
Stephen Randall	4
Momose Fumino	4
Nodono Mitsufumi	4
Shimonaka Ayako	4
Fujikawa Daisuke	3
Ishii Akihiro	3

☐ 1. Oral administration of iron-binding crosslinked amine polymers
Quick View
Other Sources

By Mandeville, W. Harry, III; Holmes-Farley, Stephen Randall
From U.S. (1997), US 5702696 A 19971230. | Language: English, Database: CAPLUS

Iron binding polymers are provided for decreasing the absorption of iron from the gastrointestinal tract. The polymers are orally administered, and are useful for treatment of iron overload disorders. In an example, N-vinylacetamide is copolymd. with divinylbenzene and the product is hydrolyzed to give a crosslinked vinylamine polymer.

☐ 2. Methods for making polymers from N-vinylacetamide monomer
Quick View
PATENTPAK ▼

By Chandran, Rama S.; Leblanc, Jean-pierre
From Eur. Pat. Appl. (1998), EP 870782 A2 19981014. | Language: English, Database: CAPLUS

Essentially non-crosslinked polymers prepd. from N-vinylacetamide (I) monomer exhibit reduced levels of residual non-polymerizable contaminants, particularly residual acetamide. The process includes contacting I with a polymn. medium contg. a diluent selected from Et acetate and acetone and a free-radical initiator, under conditions effective to polymerize I monomer, thereby forming a ppt. of the polymer in the polymn. medium; and isolating the pptd. polymer from the polymn. medium.

☐ 3. Hair-care preparations containing N-vinylcarboxamide copolymers
Quick View
PATENTPAK ▼

By Miyagawa, Satsuki; Hinata, Takehiko; Yamaguchi, Tetsuhiko
From Eur. Pat. Appl. (1998), EP 878185 A2 19981118. | Language: English, Database: CAPLUS

Disclosed is a hair-care prepn. contg. a homopolymer or copolymer comprising a repeating unit which is derived from an N-vinylcarboxamide monomer (I) wherein R¹ and R²

方案二：
由物质获得文献，再通过文献检索结果处理工具
精选文献

方案二：通过物质获得文献（限定为合成/制备/工艺）

CAS Solutions

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A CAS SOLUTION

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Chemical Structure substructure with limiters > substances (98) > get reactions (70) > get references (30)

SUBSTANCES ? **Get References** Retrieve references for selected substances. Tools ▾

Analyze Refine

Analyze by: ?
Substance Role ▾

Preparation 61
Uses 43
Reactant or Reagent 24
Properties 18
Biological Study 16
Process 8
Analytical Study 3
Formation, Nonpreparative 2
Miscellaneous 1

Sort by: Number of References ▾

0 of 98 Substances Selected

1. 28408-65-3
~583 ~3

5202-78-8
C₄ H₇ N O

(C₄ H₇ N O)_x
Acetamide, *N*-ethyl-, homopolymer
► **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

2. 26616-03-5
~173

3195-78-6
C₅ H₉ N O

(C₅ H₉ N O)_x
Acetamide, *N*-ethyl-
Regulatory Information

Get References

Retrieve references for:

☒ All substances
☐ Selected substances

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input checked="" type="checkbox"/> Preparation
<input type="checkbox"/> Analytical Study	<input checked="" 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 checked="" type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

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

Get Cancel

获得301篇文献

Explore ▼
Saved Searches ▼
SciPlanner

Save
Print
Export

Chemical Structure substructure with limiters > substances (98) > get references (301)

REFERENCES ⓘ

Get Substances
Get Reactions
Get Related Citations
Tools ▼

Create Keep Me Posted Alert
Send to SciPlanner

Analyze
Refine
Categorize

Sort by: Accession Number ▼

Display Options

☐
0 of 301 References Selected

Analyze by: ⓘ

Author Name ▼

Akashi Mitsuru	25
Holmes Farley	
Stephen Randall	12
Mandeville W Harry III	9
Ajiro Hiroharu	8
Kishida Akio	8
Lai Ta Wang	7
Bunes Leonard A	6
Burke Steven K	6
Momose Fumino	6

☐
1. Environment-friendly transparent film comprising water-soluble polymer and metal oxide nano particle

Quick View
PATENTPAK ▼

By Sawaguchi, Takashi; Suzuki, Shota; Tadano, Takeshi; Zhu, Rui; Hoshi, Toru; Sasaki, Daisuke; Hagiwara, Toshinori
From Jpn. Kokai Tokkyo Koho (2016), JP 2016053160 A 20160414. | Language: Japanese, Database: CAPLUS

Title film is prepd. by solvent casting a dispersion contg. a water-sol. polymer, a hydroxy group surface-modified metal oxide nanoparticle, and water. Thus, silica (PL-1-SL) particles were dispersed in poly(N-vinylacetamide) and blended with different ratios to obtain a dispersion soln. which was put into a petri dish after the evapn. of water to form the title film.

☐
2. Compositions and kits for treating pruritus and methods of using the same

Quick View
PATENTPAK ▼

By Salamone, Joseph Charles; Salamone, Ann Beal; Leung, Kelly Xiaoyu-Chen; Reilly, Katelyn Elizabeth
From PCT Int. Appl. (2016), WO 2016057789 A1 20160414. | Language: English, Database: CAPLUS

A treatment for pruritus is described that is based upon amylase. The amylases (α -, β -, γ -amylase) are noted for the cleavage of the α -glycosidic bonds of polysaccharides, yielding lower mol. wt. carbohydrate/sugar fragments. It has now been found that α -amylase is effective in the redn. of pruritus (itching) of affected tissue.

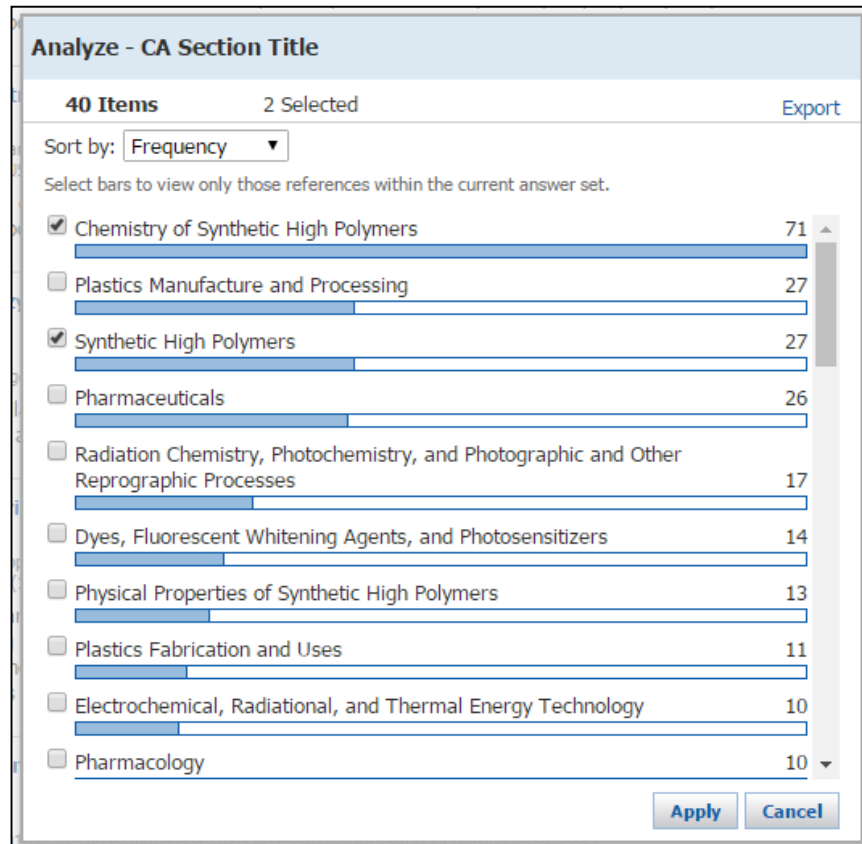
☐
3. Compositions and kits for treating pruritus and methods of using the same

Quick View
PATENTPAK ▼

By Salamone, Joseph Charles; Salamone, Ann Beal; Leung, Kelly Xiaoyu-Chen; Reilly, Katelyn Elizabeth
From U.S. Pat. Appl. Publ. (2016), US 20160101166 A1 20160414. | Language: English, Database: CAPLUS

A treatment for pruritus is described that is based upon amylase. The amylases (α -, β -, γ -amylase) are noted for the cleavage of the α -glycosidic bonds of polysaccharides, yielding lower mol. wt. carbohydrate/sugar fragments. It has now been found that α -amylase is effective in the redn. of pruritus (itching) of affected tissue.

可以通过CA Section Title等选项进行分析，甄选文献



通过分类工具，可以对反应类型/关键词等进行限定，筛选文献

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Prepared substances (1180)
Polymer chemistry	Reactants & reagents (567)
General chemistry	Manufactured substances (515)
Synthetic chemistry	Reactions (56)
Technology	Purified substances (9)
Biotechnology	
Physical chemistry	
Genetics & protein chemistry	
Catalysis	
Biology	
Analytical chemistry	
Environmental chemistry	

2. Select index terms of interest.

Index Terms	
Select All	Deselect All
<input type="checkbox"/> Polymerization	37 ▲
<input type="checkbox"/> Hydrolysis	13
<input checked="" type="checkbox"/> Crosslinking	10
<input type="checkbox"/> Radical polymerization	8
<input type="checkbox"/> Solvent effect	6
<input type="checkbox"/> Diels-Alder reaction	3
<input type="checkbox"/> Inverse emulsion polymerization	3
<input type="checkbox"/> Polymerization kinetics	3
<input type="checkbox"/> Radical solution polymerization	3
<input type="checkbox"/> Acetylation	2
<input type="checkbox"/> Acid hydrolysis	2
<input type="checkbox"/> Alkylation	2
<input type="checkbox"/> Graft polymerization	2
<input type="checkbox"/> Hydrogenation	2 ▼

Selected Terms

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

✱ Synthetic chemistry > Reactions (1 Terms)

Synthetic chemistry > Reactions > 1 Index Term(s) Selected

OK

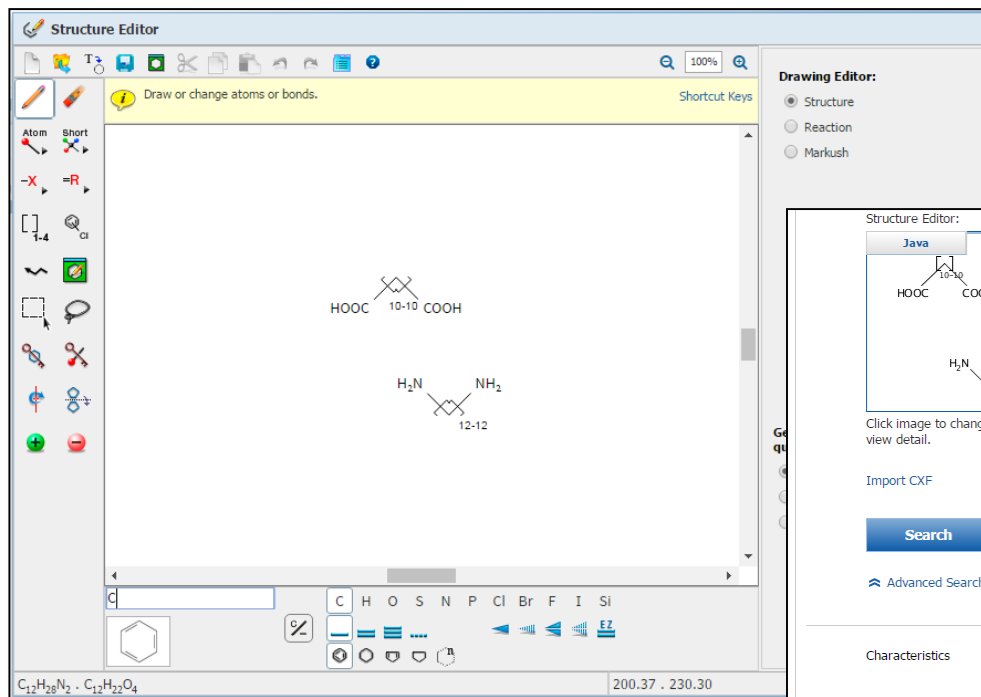
Cancel

均聚物合成/制备检索技巧总结

- 如果需要用结构式检索均聚物合成、制备信息，则可用以下操作步骤：
 1. 直接绘制单体的结构式，并在执行检索之前，将条件设置为单组分、聚合物
 2. 获取到物质结果集后：
 - A) 如果希望获取到精准的化学反应，则可通过物质获取化学反应，并限定物质在反应过程中的角色（产物）
 - B) 如果希望获取最完整、全面的文献信息，则可通过物质获取文献信息，并将结果限定为工艺，制备等

提纲

- 聚合物结构检索
- 聚合物分子式检索
- 聚合物反应检索
 - 检索所有包含下列结构特征的乙烯作为单体的均聚物的反应（文献）
 - 尼龙1212（单体：十二胺、十二酸）的聚合方法



Drawing Editor:

- ☒ Structure
- ☐ Reaction
- ☐ Markush

Structure Editor:

Java **Non-Java**

HOOC 10-10 COOH

H_2N 12-12 NH_2

Click image to change structure or view detail.

Import CXF

Search

[Advanced Search](#) ☐ Always Show

Search Type:

- ☒ Exact Structure
- ☐ Substructure
- ☐ Similarity

☐ Show precision analysis

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

Characteristics

- ☒ Single component
- ☐ Commercially available
- ☐ Included in references

Classes

- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☒ Polymers
- ☐ Organics, and others not listed

Analyze Refine

Sort by: CAS Registry Number

1 of 2 Substances Selected

1. 132512-65-3

~6

60180-78-1
 $C_{12}H_{28}N_2 \cdot C_{12}H_{22}O_4$

2783-17-7
 $C_{12}H_{28}N_2$

693-23-2
 $C_{12}H_{22}O_4$

$(C_{12}H_{28}N_2 \cdot C_{12}H_{22}O_4)_x$
 Dodecanedioic acid, compd. with 1,12-dodecanediamine (1:1), homopolymer

2. 36497-34-4

~566

2783-17-7
 $C_{12}H_{28}N_2$

693-23-2
 $C_{12}H_{22}O_4$

$(C_{12}H_{28}N_2 \cdot C_{12}H_{22}O_4)_x$
 Dodecanedioic acid, polymer with 1,12-dodecanediamine
[Regulatory Information](#)

Analyze by: Substance Role

Preparation 2

Properties 2

Uses 2

Biological Study 1

Process 1

Reactant or Reagent 1

Show More

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



SCIFINDER®
 A CAS SOLUTION

尼龙1212（单体：十二胺、十二酸）的聚合方法

Get References
Tools
Send to SciFinder

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

0 of 1 Reaction Selected

1. View Reaction Detail Link

Single Step Hover over any structure for more options.

Overview
Steps/Stages

1:1 C:O=PH₂OH, S:H₂O, rt → 220°C; 2 h, 20 bar; 220°C → 270°C; 1.5 h, 270°C; 6 h, heated

Notes
thermal, high pressure, reaction in an autoclave, pressure decreased to atmospheric levels while heating for 6 hours, Reactants: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References
Polymer powder with adapted melting behavior
Quick View PATENTPAK
By Diekmann, Wolfgang et al

注意事项

- 一人注册一个帐号
- 严禁过量下载
- 严禁将帐号用于非学术研究
- 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
- Mac电脑，如使用Safari浏览器请注意及时升级版本，不要拦截SciFinder插件，或者安装火狐或者谷歌浏览器使用SciFinder

谢谢关注！



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英文网站：www.cas.org (提供英文培训资料)