



如何使用SciFinder获取科技信息

复旦大学

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)
 - SciPlanner使用简介
- 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



CAS——构建最高质量的化学数据库





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ACS
chemical
biology



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OF ORGANIC CHEMISTRY

 division of polymer chemistry, inc
American Chemical Society 

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

ACS Chemical
Neuroscience

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A CAS Solution

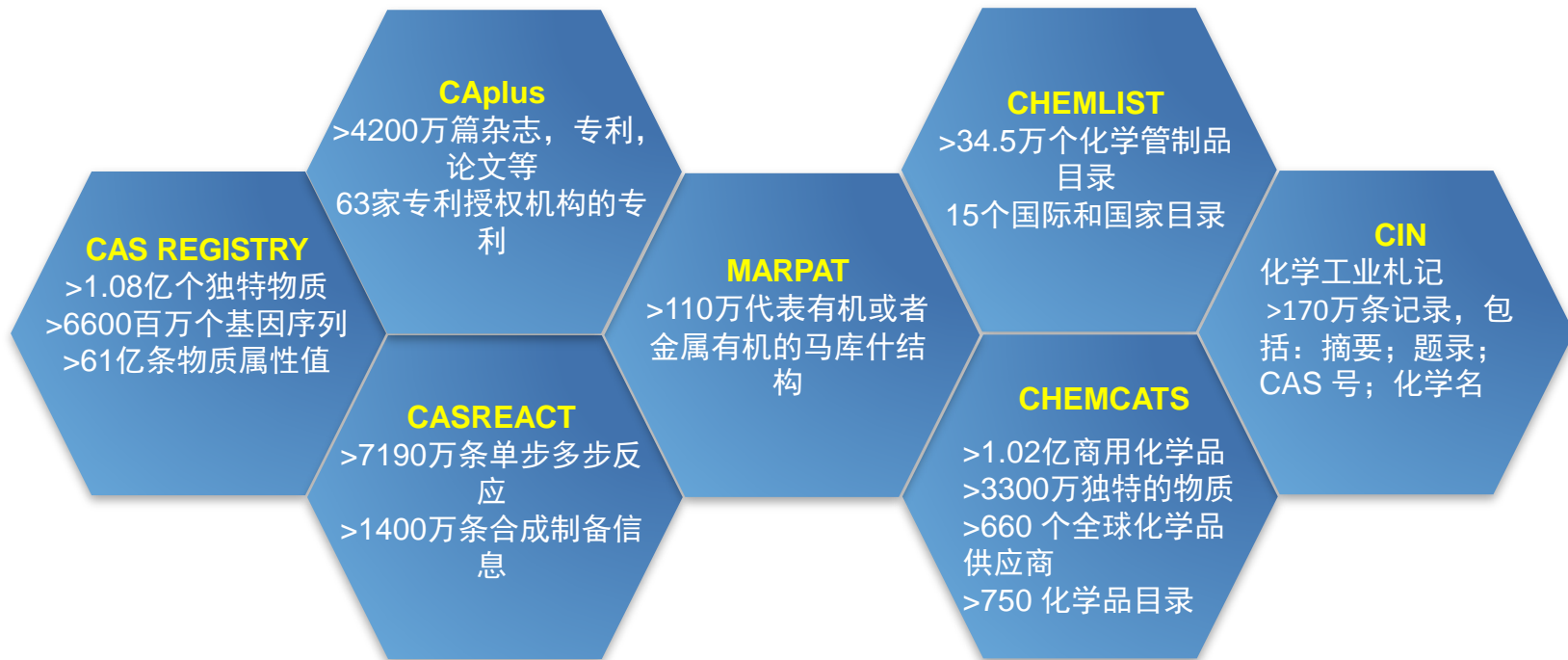
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THE JOURNAL OF
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Letters

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CAS——构建最高质量的化学数据库



CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料 ;合成橡胶 ;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

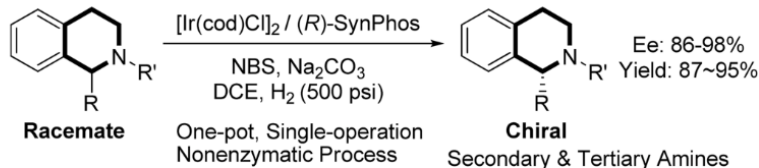
表面化学,催化剂,相平衡,核现象,电化学

CAS数据库最具价值的内容——人工索引

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

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
CAN163:331216
CAPLUS

PUBLISHER

American Chemical Society

Tips:

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

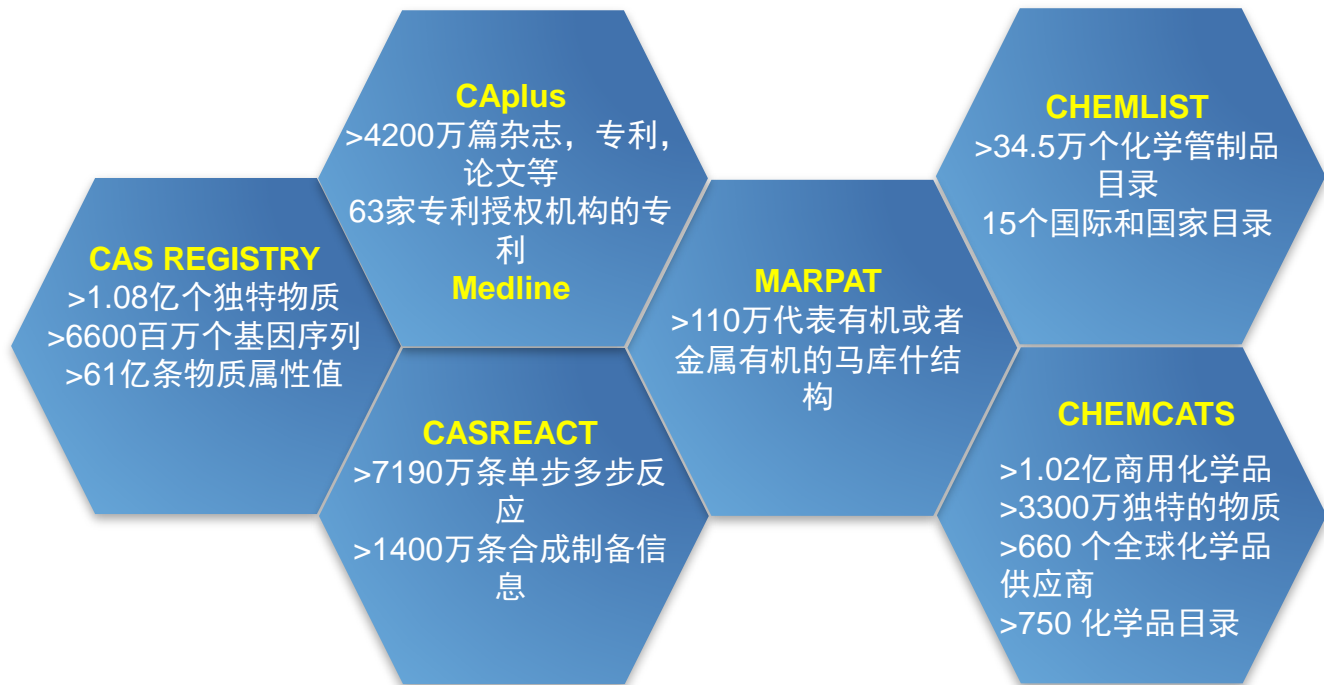
CAS人工标引解决的问题

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

提纲

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

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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.

SciFinder主界面

检索完，请点击退出

工具栏

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Preferences | SciFinder Help | Sign Out

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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

检索入口

已保存的结果集

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

定题追踪

KEEP ME POSTED

You have no profiles.
Learn how to:
Create Keep Me Posted

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: 杀虫剂的合成

- 检索式 : synthesis of pesticide

CAS Solutions

SciFINDER
A CAS SOLUTION

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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

synthesis of pesticide

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

Search

Advanced Search

关键词之间可用介词连接 : in, with, of...

主题检索的候选项

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Research Topic "synthesis of pesticide"

REFERENCES

Select All Deselect All

1 of 5 Research Topic Candidates Selected

		References
<input type="checkbox"/>	112 references were found containing "synthesis of pesticide" as entered.	112
<input checked="" type="checkbox"/>	44932 references were found containing the two concepts "synthesis" and "pesticide" closely associated with one another.	44932
<input type="checkbox"/>	82807 references were found where the two concepts "synthesis" and "pesticide" were present anywhere in the reference.	82807
<input type="checkbox"/>	11236033 references were found containing the concept "synthesis".	11236033
<input type="checkbox"/>	376179 references were found containing the concept "pesticide".	376179

Get References

“Concepts” 表示对主题词做了同义词的扩展；

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

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

文献检索结果

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Explore | Saved Searches | Save | Print | Export

Research Topic: synthesis of pesticides

REFERENCES | 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 44932 References Selected | Page: 1 of 2247

Sample Analysis: Author Name

Arimori Sadayuki ≥ 237

Hammann Ingeborg ≥ 190

Watanabe Yuki ≥ 139

Stendel Wilhelm ≥ 124

Homeyer Bernhard ≥ 121

Drabek Jozef ≥ 114

Erdelen Christoph ≥ 113

Behrenz Wolfgang ≥ 106

Wachendorff Neumann Ulrike ≥ 84

Maurer Fritz ≥ 77

Show More

1. Presence of pesticides in breast milk and...
Quick View | Other Sources
By Sharma, Neel...
From International Journal of Environmental Analy...
This study documents the levels of pesticide residues in milk samples of mothers from Himachal Pradesh, India, and time trend comparison of pesticides conducted around the world. The regional difference in xenobiotic levels of breast milk varied with demog. characteristics of mothers and altitudinal variations. The single or multiple pesticides contamination of p,p'-DDE, p,p'-DDT and chlorpyrifos was revealed in 27.45% mothers' milk samples. Among these p,p'-DDE was the major contaminant found in 26.79% samples followed by p,p'-DDT (1.31%) and chlorpyrifos (0.65...)

2. Sulfur(VI) fluoride exchange (SuFEx): Another good reaction for click chemistry
Quick View | Other Sources
By Zheng, Qinhe; Dong, Jiajia; Wu, Peng; Sharpless, Karl B.
From Abstracts of Papers, 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, 2016 (2016), CARB-102. | Language: English, Database: CAPLUS
It has been 14 years since the Cu(I)-catalyzed azide-alkyne cyclization (CuAAC) was introduced as a premier example of click chem., which conceptually describes a few good reactions making stable covalent connections between small units. Recently, another good reaction for click chem., sulfur(VI) fluoride exchange (SuFEx) was developed in our laboratory, which virtually consists of three near-perfect recipes. First, satd. aq. KFHF soln. was discovered as a general method for converting a sulfonyl chloride to the corresponding sulfonyl fluoride, which is stable on-standing while robust in presen...

3. Occurrence and removal of organic micropollutants: An overview of the watch list of EU Decision 2015/495
Quick View | Other Sources
By Barbosa, Marta O.; Moreira, Nuno F. F.; Ribeiro, Ana R.; Pereira, Manuel F. R.; Silva, Adrian M. T.
From Water Research (2016), 94, 257-279. | Language: English, Database: CAPLUS
Although there are no legal discharge limits for micropollutants into the environment, some regulations have been published in the last few years. Recently, a watch list of substances for European Union-wide monitoring was reported in the Decision 2015/495/EU of 20 March 2015. Besides the substances previously recommended to be included by the Directive 39/2013/EU, namely two pharmaceuticals (diclofenac and the synthetic hormone 17-alpha-ethinylestradiol (EE2)) and a natural hormone (17-beta-estradiol (E2)), the first watch list of 10 substances

文献检索结果

The screenshot shows the SciFinder interface with the search topic "synthesis of pesticide" and 14759 references. The left sidebar has "Publication Year" selected. The main area displays three search results:

- 1. Presence of pesticides in breast milk and infants' formulae in Himachal Pradesh, India**
By Sharma, Neeta Devi; Sharma, Ishwar D.; Chandel, Rajeshwar Singh; Wise, John C.
From International Journal of Environmental Analytical Chemistry (2016), 96(3), 225-236. | Language: English, Database: CAPLUS
This study documents the levels of pesticide residues in milk samples of mothers from Himachal Pradesh, India, and time trend comparison of pesticide load based on various studies conducted around the world. The regional difference in xenobiotic levels of breast milk varied with demog. characteristics of mothers and altitudinal variations. The single or multiple pesticides contamination of p,p'-DDE, p,p'-DDT and chlorpyrifos was revealed in 27.45% mothers' milk samples. Among these p,p'-DDE was the major contaminant found in 26.79% samples followed by p,p'-DDT (1.31%) and chlorpyrifos (0.65...
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Refine可以迅速
获得所需文献

文献检索结果

Research Topic "synthesis of pesticide" > references (44932) > refine "2010-" (14759)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Tools

Sort by: Accession Number | Accession Number | Author Name | Citing References | Publication Year

1. **Presence of pesticides in breast milk and infants' formulae in Himachal Pradesh, India**
By Sharma, Neeta Devi; Sharma, Ishwar D.; Chandel, Rajeshwar Singh; Wise, John C.
From International Journal of Environmental Analytical Chemistry (2016), 96(3), 225-236. | Language: English, Database: CAPLUS

This study documents the levels of **pesticide** residues in milk samples of mothers from Himachal Pradesh, India, and time trend comparison of **pesticide** load based on various studies conducted around the world. The regional difference in xenobiotic levels of breast milk varied with demog. characteristics of mothers and altitudinal variations. The single or multiple **pesticides** contamination of p,p'-DDE, p,p'-DDT and chlorpyrifos was revealed in 27.45% mothers' milk samples. Among these p,p'-DDE was the major contaminant found in 26.79% samples followed by p,p'-DDT (1.31%) and chlorpyrifos (0.65...

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By Barbosa, Marta O.; Moreira, Nuno F. F.; Ribeiro, Ana R.; Pereira, Manuel F. R.; Silva, Adrian M. T.
From Water Research (2016), 94, 257-279. | Language: English, Database: CAPLUS

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获得相关物质/反应

5种排序方式，可以按照进入数据库的时间、作者名、引文、公开年限、标题对文献检索结果进行重新排序

Citing Reference: 可以帮助找到最重要的文献

文献检索结果：Analyze

12种文献分析选项

Analyze Refine Categorize

Analyze by: ?

- Author Name
- 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

主要研究人员

Analyze Refine Categorize

Analyze by: ?

Author Name

Arimori Sadayuki	216
Schmutzler Dirk	123
Shioda Takayuki	118
Rosinger Christopher Hugh	107
Chen Foxiang	102
Dietrich Hansjoerg	97
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Zhang Zhiwei	89
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Wang Liwen	88

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主要研究机构， 合作伙伴，竞争对手

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Company-Organization

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主要发表期刊

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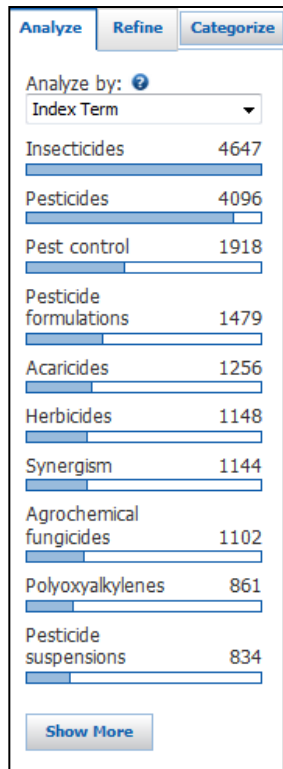
Analyze by: ?

Journal Name

Faming Zhuanli Shenqing	6720
PCT Int. Appl.	1868
Jpn. Kokai Tokkyo Koho	259
Journal of Agricultural and Food Chemistry	235
U.S. Pat. Appl. Publ.	148
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Repub. Korean Kongkae Taebo Kongbo	94
Indian Pat. Appl.	86
Youji Huaxue	67

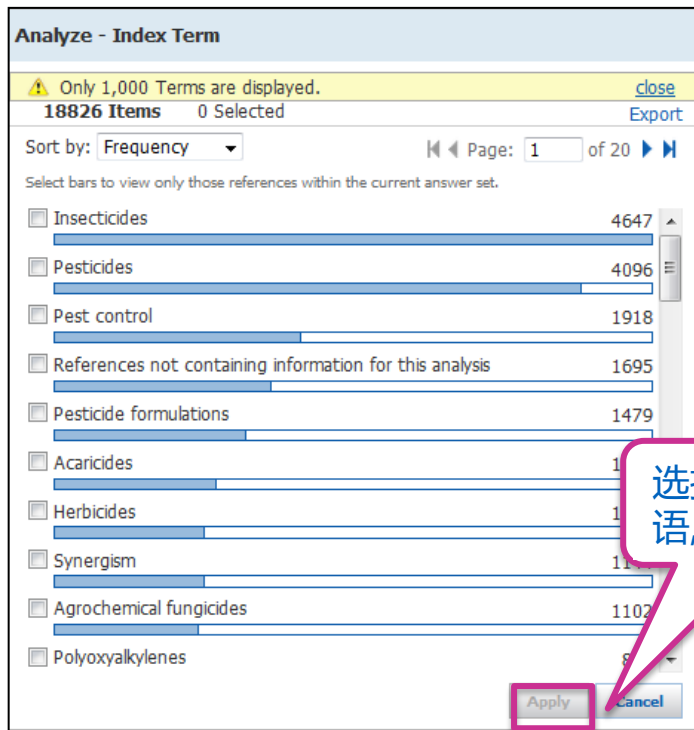
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文献检索结果：Analyze



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



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

选中的重要技术术语

1. Select a heading and category.

Category Heading	Category
All	Prepared substances (35973)
General chemistry	
Biotechnology	Reactants & reagents (12459)
Synthetic chemistry	Reactions (274)
Biology	Manufactured substances (1059)
Technology	Purified substances (1087)
Genetics & protein chemistry	Bio-prepared substances (397)
Physical chemistry	
Polymer chemistry	
Analytical chemistry	
Environmental chemistry	
Catalysis	

2. Select index terms of interest.

Index Terms	
Page: 1 of 360	
Select All Deselect All	
<input type="checkbox"/> Multinutrient fertilizers	62
<input checked="" type="checkbox"/> Organic fertilizers	53
<input type="checkbox"/> Fertilizers	50
<input checked="" type="checkbox"/> (3-Chloropyridin-2-yl) hydrazine	34
<input checked="" type="checkbox"/> 3-Pyrazolidinecarboxylic acid, 2-(3-chloro-2-pyridinyl)-5-oxo-, ethyl ester	33
<input type="checkbox"/> 3-Bromo-1-(3-chloro-2-pyridinyl)-1H-pyrazole-5-carboxylic acid	32
<input type="checkbox"/> Amides	31
<input type="checkbox"/> Complex fertilizers	31
<input type="checkbox"/> 1H-Pyrazole-5-carboxylic acid	30

Selected Terms

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

- Synthetic chemistry >
- Prepared substances (3 Terms)

文献信息详情

17. Plant biological source chive fertilizer maggot-eliminating pesticide

By: Li, Shi

Assignee: Qingdao Changlv Biology Research Institute, Peop. Rep. China

The title plant biol. source chive fertilizer maggot-eliminating pesticide contains effective ingredients of Nymphaea tetragona ext., chitin, plant ash, matrine, bios, and probiotics (prebiotic including Lactobacillus acidophilus, Bifidobacterium, Bacillus subtilis, and culture media raw material including soya-bean milk, wheat bran, fish bone powder, brown sugar), and is obtained through special process. The inventive plant biol. source chive fertilizer maggot-eliminating pesticide is mainly used as fertilizer in chive growth cycle to dispel chive maggot for sterilization of leek soil. There is synergistic effect of plant and biogenic cytokines, jointly being absorbed by chive, while providing nutritive substance, and avoiding chive maggot to infringe chive. The inventive plant biol. source chive fertilizer maggot-eliminating pesticide has efficient germicidal action, can purify soil, create good chive growing environment, can repair the chive injured by chem. pesticide, promote the absorption of nutritive substance, and resist chive maggot infringement, is nontoxic, easy to degrade, and pollution-free harmless, and has simple prepn., low pesticide amt., and low cost.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 104513104	PATENTPAK	A	Apr 15, 2015	CN 2013-10448242	Sep 27, 2013

Priority Application

CN 2013-10448242	Sep 27, 2013
------------------	--------------

Indexing

Agrochemical
Section cross-reference(s): 19

重要技术术语

Concepts

Hormones, microbial
bios; plant biol. source chive fertilizer maggot-eliminating pesticide
Fish
bone meal of; plant biol. source chive fertilizer maggot-eliminating pesticide
Maggot
control of; plant biol. source chive fertilizer maggot-eliminating pesticide

Substances

519-02-8 Matrine
1398-61-4 Chitin
plant biol. source chive fertilizer maggot-eliminating pesticide
Agricultural use; Biological study; Uses
57-50-1 Sucrose, biological studies
plant biol. source chive fertilizer maggot-eliminating pesticide
Biological use, unclassified; Biological study; Uses

重要物质

QUICK LINKS

0 Tags, 0 Comments

PATENT INFORMATION

Apr 15, 2015
CN 104513104
A

APPLICATION

Sep 27, 2013

文献详情界面包括：

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

文献检索小结

- 主题检索时，使用介词作为连接
- 尽量选择包含**Concept**和**Closed Associated with**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

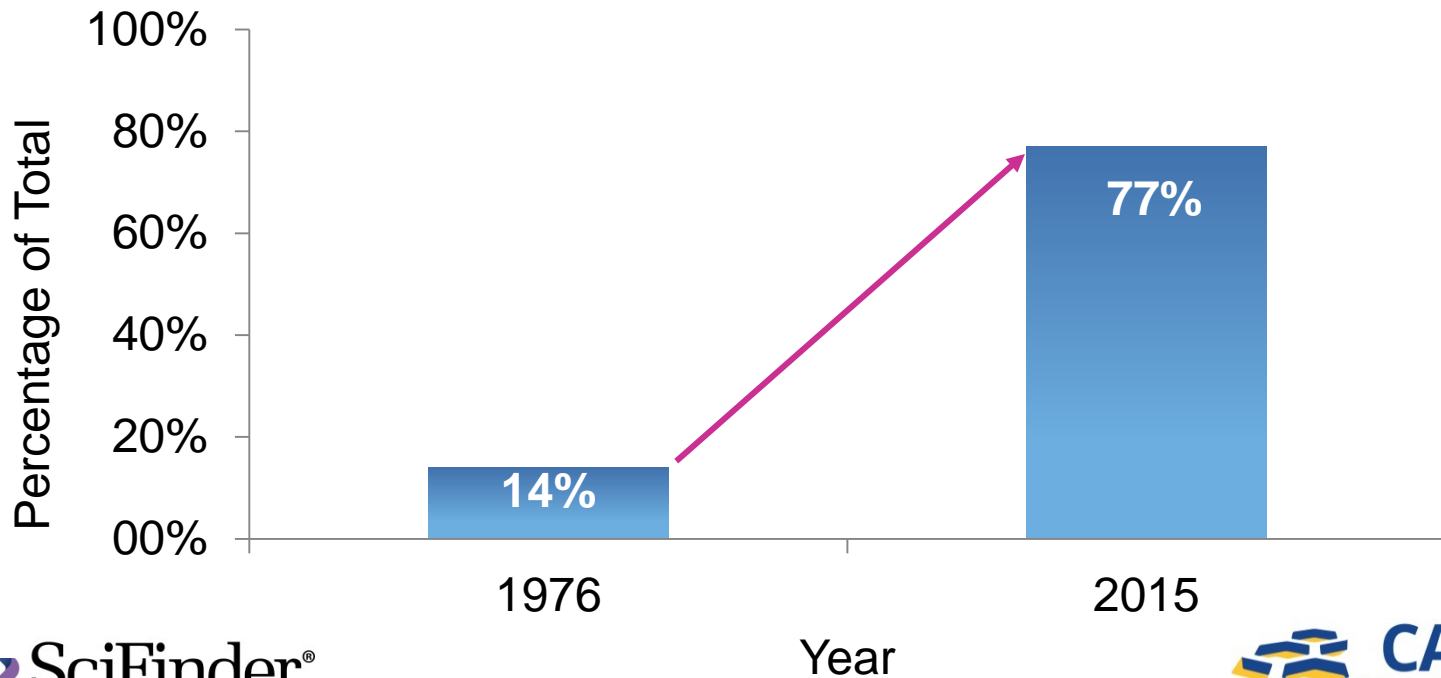
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- SciFinder常见问题及解决

PatentPak™

专利工作流程解决方案

越来越多的新化合物倾向于首先通过专利公布

Percentage of New Compounds from Patents



PatentPak——专利工作流程解决方案

在SciFinder检索结果中，看到PatentPak图标即可点击

The claimed herbicidal formulations contain active ingredients from the group of N-(1,3,4-oxadiazol-2-yl)-arylcarboxylic acid amides (I; where A = N or C-alkyl, C-halogenalkyl, etc., R = alkyls, halogenalkyls, etc., X = alkyls and substituted alkyls, and Z = H, halogens, and substituted alkyls). The claimed amides can be formulated in mixts. with other herbicides and optional herbicide safeners. The herbicide combinations were evaluated against 15 test weeds. The herbicidal formulations are suitable for weed control in agricultural crops (esp. genetically modified crops) and other useful pl...

8. Preparation of 6-fluor-9-methyl- β -carboline for the treatment of ear disease

Quick View **PatentPak**

By Rommelspacher, Hans; Enzensperger, Christoph
From Eur. Pat. Appl. (2015), WO 2015044434 A2 20150402. | Language: **German**, Database: CAPLUS

Patent No.	Kind	Language
EP 2853533	Interactive	German

Patent Family

WO 2015044434	A2	German
WO 2015044434	A3	German

Click PatentPak, get PatentPak Viewer

The invention relates to 6-fluor-9-methyl- β -carbolines (I) and pharmaceutical compns. thereof useful in the treatment of acute and chronic inner ear diseases. (6-1-methyl-1H-Indole-3-ethanamine hydrochloride with 2,2-dihydroxyacetic acid followed by decarboxylation and redn. and

9. Preparation of fluoro-substituted 9-methyl- β -carbolines for the treatment of ear diseases

Quick View **PatentPak**

By Rommelspacher, Hans; Enzensperger, Christoph
From PCT Int. Appl. (2015), WO 2015044434 A2 20150402. | Language: **German**, Database: CAPLUS

PatentPak——专利工作流程解决方案

PatentPak浏览器

下载带有物质信息汇总表格的专利PDF文件

PatentPak™

PAGE 38 / 75 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 1689575-79-8

CN1C(=O)N2CCc3cc(F)ccc3N2

Search in SciFinder | View Detail

Analyst Markup Location

page 38

page 60

CAS RN 24335-20-4

CN1C(=O)N2CCc3cc(F)ccc3N2

HCl

Beispiele

Beispiel 1a: Synthese von 6-Fluor-9-methyl- β -carbolin

5 Analog zur Vorschrift von Ho und Walker (Beng T. Ho und K. E. Walker; *Org. Synth.* **1971**, 51, 136 oder *Org. Synth.* **1988**, Coll. Vol. 6, 136) wird 3,5 mmol (800 mg) 5-Fluor-1-methyltryptamin (AKos GmbH, Steinen) gelöst und mit einer 10 Glyoxalsäurehydrat (**Figur 1a, Formel III**) in 810 μ L NMP (Sigma) wird dann eine Lösung aus 3,4 mmol (190,4 mg) NMP (Sigma) wobei der pH auf etwa 4 eingestellt wird. Die Mischung wird bei Raumtemperatur gerührt und zur Vervollständigung der Kristallisation noch eine weitere Stunde ins Eisbad gestellt. Der orange-beige Niederschlag des Betains (**Figur 1a, Formel IVa**) wird abfiltriert und mit wenig Eiswasser gewaschen. 15 Zur Decarboxylierung wird der noch feuchte Filterkuchen des Betains (**Figur 1a, Formel IVa**) in einen Kolben überführt und in verdünnter Salzsäure (6,48 mL Wasser und 918 μ L konzentrierte Salzsäure) gelöst. Die Reaktionsmischung wird unter

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

节省您最宝贵的资源——时间



- 即时获得来自世界上主要专利授权机构的专利PDF文件
- 专利族涵盖了多种语言
- 通过CAS登记号获得物质在专利文献中的相关信息
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器

文献检索练习

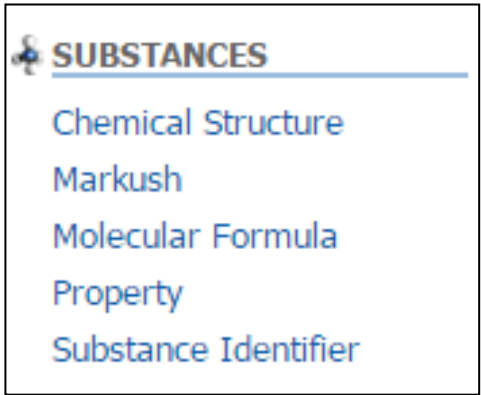
1. 检索有关合成除草剂 (herbicide) 的文献，该领域最大的研究机构是什么？有多少综述文献？最重要的那篇是什么？有多少篇专利？来自中国的专利有多少？主要的除草剂有哪些？
2. 检索你导师发表的文献，找出他的主要研究方向。

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
 - SciPlanner使用简介
- 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
 - Markush结构检索
 - 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



☞ **SUBSTANCES**

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

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 ?

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

提示：

1. 一次最多可输入25个物质。
2. 每行一个物质标识符。

Search

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。

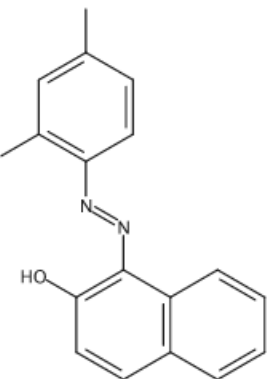
33
CAL SOCIETY

SciFinder中的物质记录

点击CAS RN 获得物质详细信息

1 3118-97-6

~894 ~58



C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

» 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

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

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



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SciFinder中的物质记录

SUBSTANCE DETAIL [?](#)

[Return](#)

[Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

CAS Registry Number 3118-97-6

~894 ~58

C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

Molecular Weight
276.33

Melting Point (Experimental)
Value: 166 °C

Boiling Point (Predicted)
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

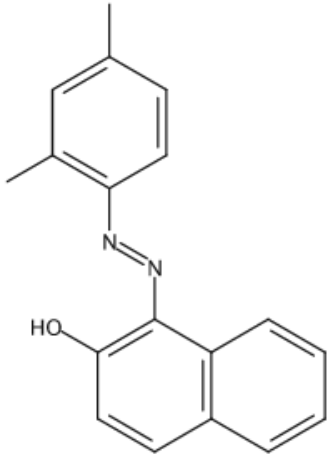
Density (Predicted)
Value: 1.14±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Rod No. 5

[View more...](#)

由物质获得文献，反应，供应商等信息



The chemical structure shows a naphthalene ring system with a hydroxyl group at the 2-position and an azo group at the 1-position. The azo group is connected to a 2,4-dimethylphenyl ring.

物质详情

EXPERIMENTAL PROPERTIES

实验数据与实验谱图

EXPERIMENTAL SPECTRA

¹H NMR IR Mass Raman UV and Visible

¹ H 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±1.282	Temp: 25 °C	(21)
Molecular Weight	276.33		(21)

预测数据与预测谱图

Notes

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

PREDICTED SPECTRA

物质检索——Property explore

The screenshot displays the 'Property explore' interface. At the top, there are navigation tabs: 'Explore' (selected), 'Saved Searches', and 'SciPlanner'. On the left side, there are three main sections: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property (highlighted), Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). The main content area is titled 'SUBSTANCES: PROPERTY' and features a radio button for 'Experimental'. Below this is a dropdown menu with the following options: 'Select Property...', 'Select Property...' (highlighted), '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', and 'Tensile Strength (MPa)'. To the right of the dropdown menu are two input fields, each with 'Examples: 44, 25-35, >125' below it.



物质检索——Property explore

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

寻找分子量在250-400之间的物质



物质结果集的筛选——Refine

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > **substances (35993816)**

SUBSTANCES Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: CAS Registry Number ▾

0 of 35993816 Substances Selected

Refine by:

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

Structure Editor:

Java Non-Java

Click to Edit

1. **1817853-33-0**

~1

C17H26NO5PS
INDEX NAME NOT YET ASSIGNED

▶ Key Physical Properties

2. **1817853-23-8**

~0

C20H20N2O3S
INDEX NAME NOT YET ASSIGNED

▶ Key Physical Properties

5. **1817853-08-9**

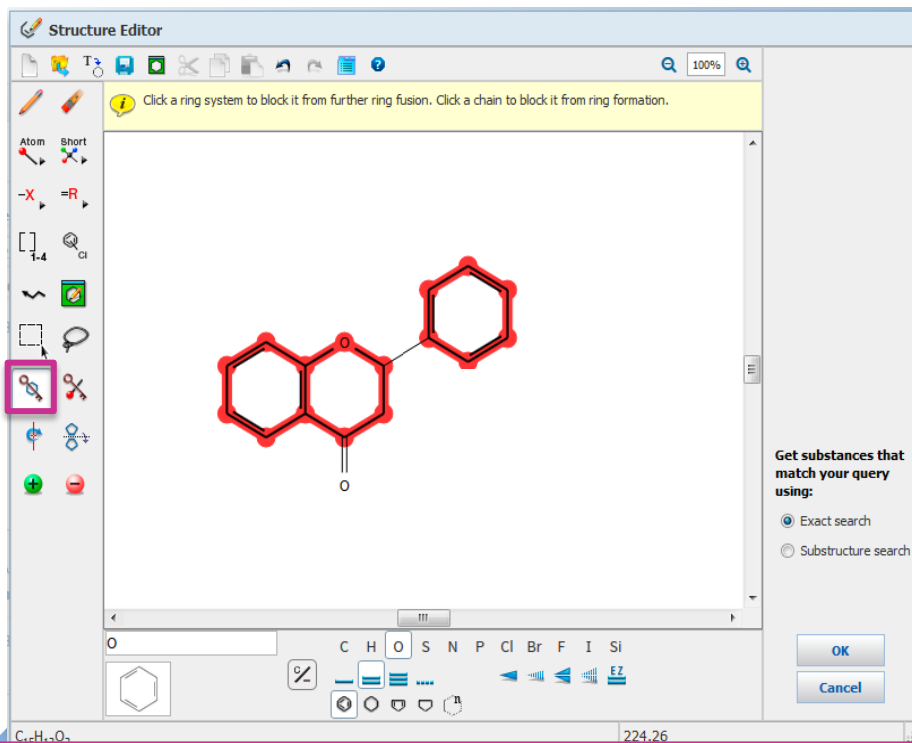
~1

6. **1817853-01-2**

~1

3500多万个结构，
如何筛选黄酮类物质？

物质结果集的筛选——Refine



锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES

Analyze Refine

Refine by:

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

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Exact Structure**

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

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物质结果集的筛选——Refine

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (35993816) > refine "substructure" (7896)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Sort by: Relevance ▾ ↓

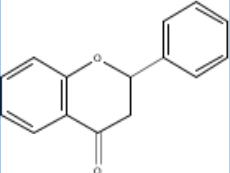
0 of 7896 Substances Selected

Refine by: ⓘ

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

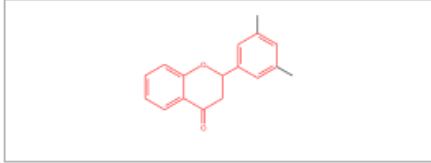
Structure Editor:

Java Non-Java



1. **1772897-96-7** 🔍

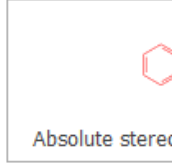
~0 ~1



C₁₇ H₁₆ O₂
4*H*-1-Benzopyran-4-one, 2-(3,5-dimethylphenyl)-2,3-dihydro-
▶ **Key Physical Properties**

2. **1438763-**


~2



C₁₇ H₁₆ O₂
4*H*-1-Benzopyran-4-one, 2,3-dihydro-, (2*R*)-
▶ **Key Physical Properties**

5. **21785-09-1** 🔍

~156 ~27



6. **72984-48**

~27

从3500多万个结构中
筛选出7800个黄酮类物质



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物质检索——分子式

REFERENCES

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

SUBSTANCES

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

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

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

C₁₂H₂₆O₄S · Na
Sulfuric acid monododecyl ester sodium salt (1:1)

Key Physical Properties

- Regulatory Information
- Spectra
- Experimental Properties

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

物质检索——结构

Explore ▾ Saved Searches ▾ SciPlanner

Author Name "yan, d" > references (1019)

REFERENCES

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

SUBSTANCES

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

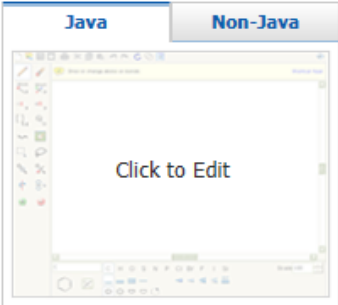
REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ⓘ

Structure Editor:

Java Non-Java



Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Import CXF

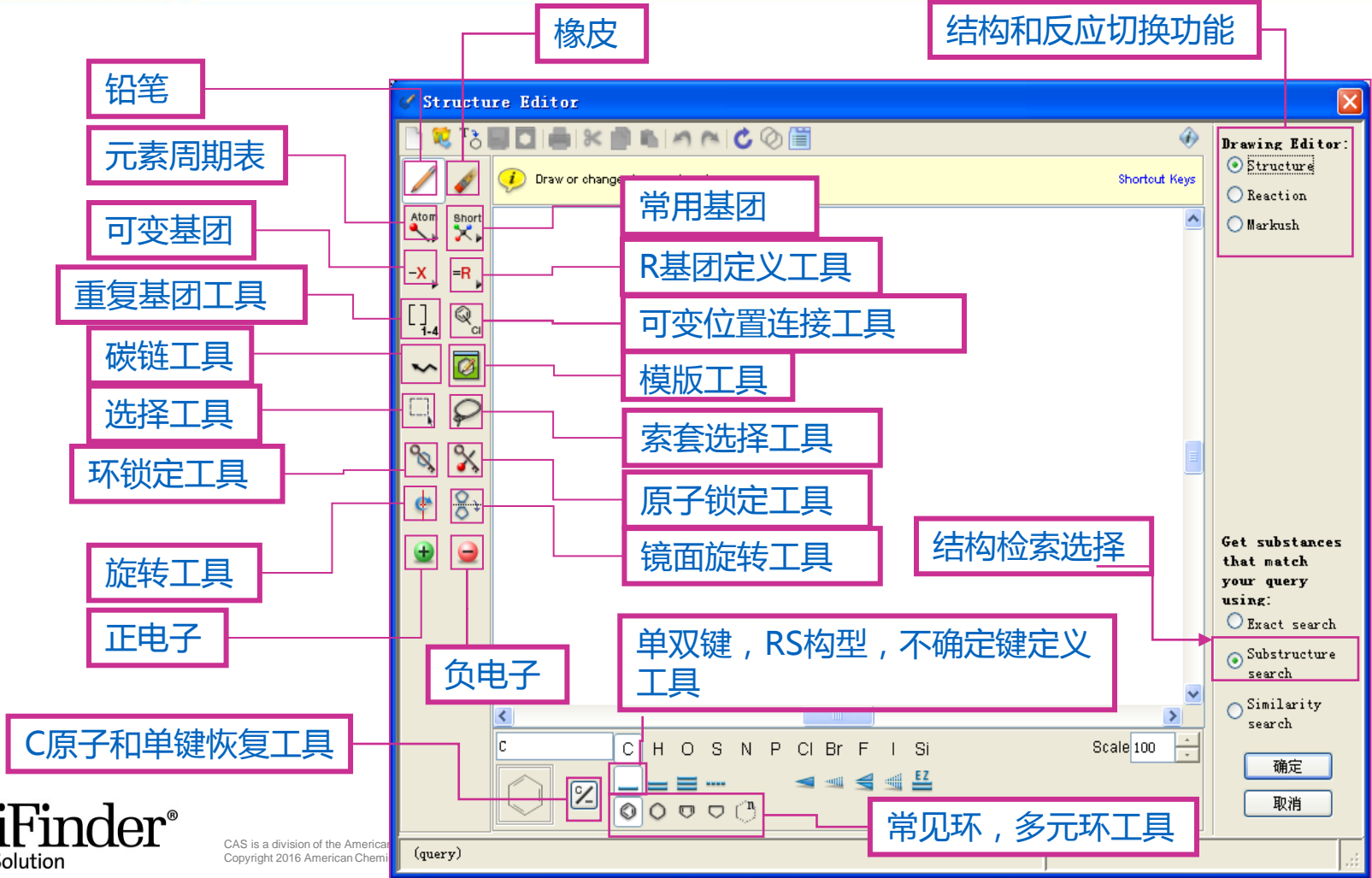
Search

Advanced Search



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物质检索——精确结构检索

The screenshot displays the Structure Editor window. The main canvas shows a chemical structure of a bicyclic compound with a benzoyl group and a methoxy group. A callout box points to the 'Structure' icon in the top toolbar, containing the text: 可以通过CAS RN转换结构：
CAS RN: 50-36-2

On the right side, the 'Drawing Editor' panel has 'Structure' selected. Below it, the 'Get substances that match your query using:' section has 'Exact search' selected. At the bottom, the status bar shows the molecular formula C₁₇H₂₁N O₄ (query) and the molecular weight 303.36.

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

Sort by: Relevance

0 of 80 Substances Selected

Page: 1 of 2

Refine by:

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

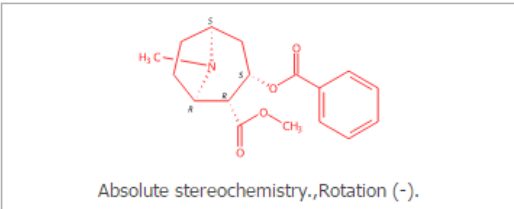
Select One:

- Include only metal-containing substances**
- Exclude metal-containing substances

Refine

1. 50-36-2

~20889



Absolute stereochemistry.,Rotation (-).

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

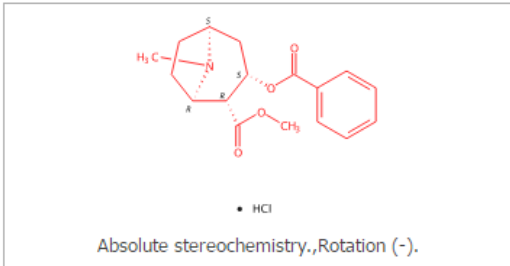
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

可卡因

2. 53-21-4

(Component: 50-36-2)

~1700



Absolute stereochemistry.,Rotation (-).

• HCl

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

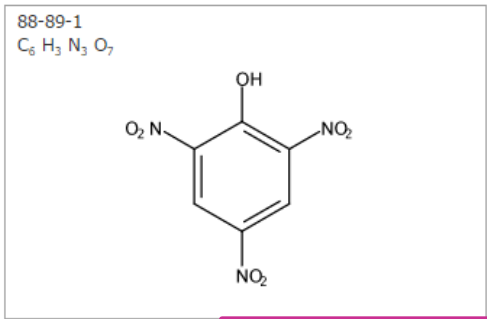
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

盐酸可卡因

3. 52748-70-6

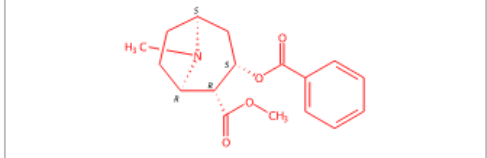
~11

88-89-1
C₆H₃N₃O₇



Absolute stereochemistry.,Rotation (-).

50-36-2
C₁₇H₂₁N O₄



Absolute stereochemistry.,Rotation (-).

可卡因组合物

物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索


The image shows a chemical drawing editor window. The central canvas displays a chemical structure of a benzopyrone derivative with a phenyl group attached to the 3-position of the pyrone ring. The interface includes a toolbar on the left with various drawing tools, a top status bar with a search icon and '100%' zoom, and a right-hand panel. The right panel has a 'Drawing Editor' section with radio buttons for 'Structure' (selected), 'Reaction', and 'Markush'. Below this is a section titled 'Get substances that match your query using:' with radio buttons for 'Exact search', 'Substructure search' (highlighted with a pink box), and 'Similarity search'. At the bottom of the right panel is an 'OK' button. The bottom of the window shows a chemical formula input field with 'O' and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si.






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物质检索——亚结构检索


0 of 63231 Substances Selected



1. 525-82-6 

~3509   ~78 

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

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

2. 54849-75-1 

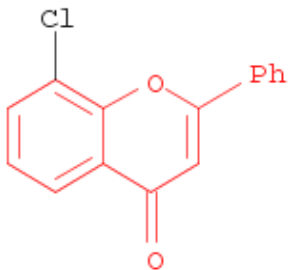
~6  

C₁₅ H₅ D₅ O₂
4*H*-1-Benzopyran-4-one, 2-(phenyl-*d*₅)-
Spectra

浏览亚结构检索结果

251. Substance Detail
1148-20-5

取代物

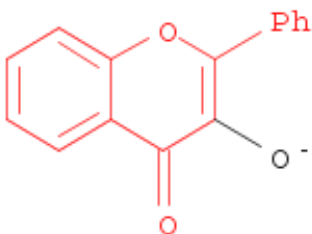


C₁₅ H₉ Cl O₂
4#1-Benzopyran-4-one, 8-chloro-2-phenyl-

[Experimental Properties](#)

261. Substance Detail
85481-91-0

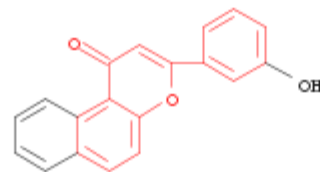
离子



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

273. Substance Detail
136116-17-1

稠环物质



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

亚结构检索结果的限定工具

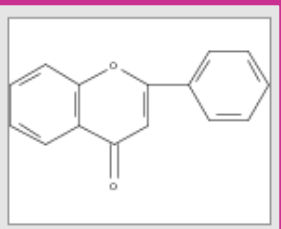
化学结构的再次限定

Analysis Refine

Refine by:

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

Chemical Structure:

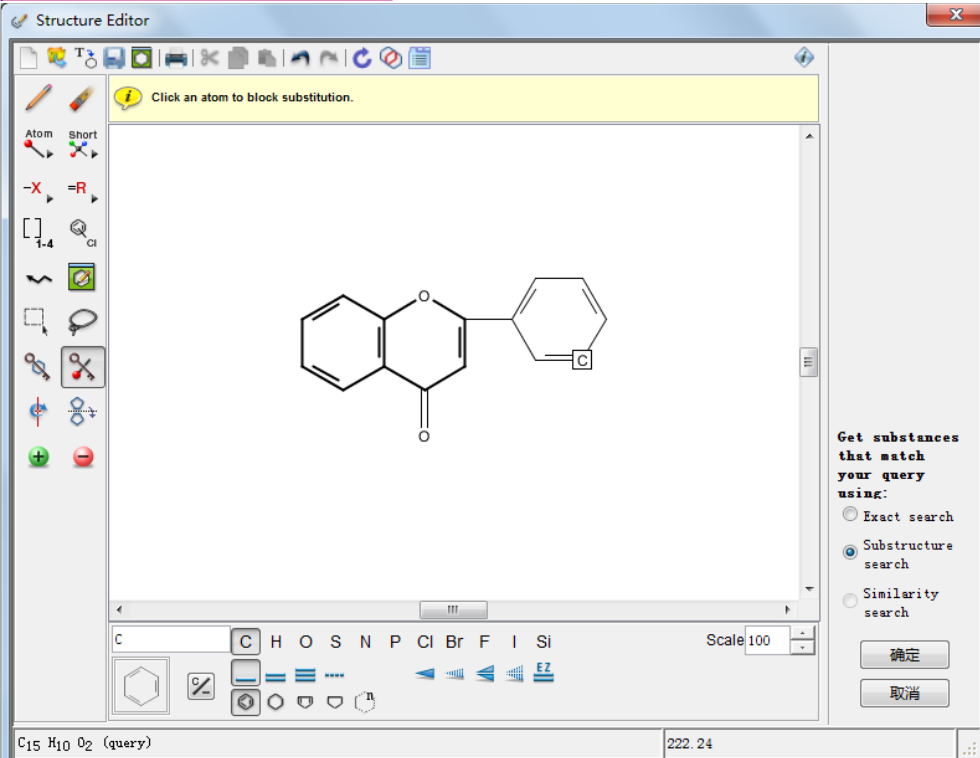


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C₁₅ H₁₀ O₂ (query) 222.24



环锁定



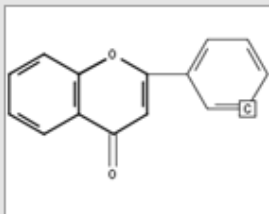
原子锁定



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化学结构的再次限定

Chemical Structure:



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

SciFinder®

Welcome Amy Qi | Sign Out

Add KMP Alert Chemical Structure substructure > substances (52072) > refine "substructure" (28699)

Substances Get References Get Reactions Tools Send to SciPlanner

28699 Substances 0 Selected

Select All Deselect All Sort by: Relevance (New) ↓

- 1. Substance Detail**
525-82-6
~2568

C₁₅ H₁₀ O₂
4#1-Benzopyran-4-one, 2-phenyl-
Spectra Experimental Properties
- 2. Substance Detail**
54849-75-1
~5

C₁₅ H₅ D₅ O₂
4#1-Benzopyran-4-one, 2-(phenyl-α₅)-
Spectra

同位素去除

Analysis **Refine**

Refine by:

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

Select One:

- Include only isotope-containing substances
- Exclude isotope-containing substances

Refine

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Amy Qi | Sign Out

Add KMP Alert Chemical Structure substructure > substances (52072) > refine "substructure" (28699) > refine "exclude isotope-containing" (28547)

Substances Get References Get Reactions Tools Send to SciPlanner

28547 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) ↓

Answers per Page [50] 1 2 3 4 5 6 ... 571

View:

1. Substance Detail
525-82-6 ~2568

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

Spectra
 Experimental Properties

2. Substance Detail
66585-04-4 ~1

C₁₅ H₁₀ O₂
4#-1-Benzopyran-4-one, 2-phenyl-, radical ion(1+) (9CI)

3. Substance Detail
64586-87-4
(Component: 525-82-6) ~5

• H⁺

C₁₅ H₁₀ O₂ · H
4#-1-Benzopyran-4-one, 2-phenyl-, conjugate acid (1:1)

物质检索——亚结构检索

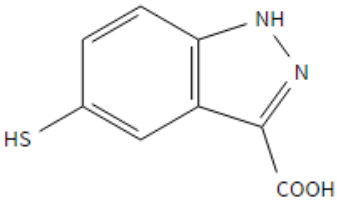
- 亚结构检索：

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

Structure Editor

Draw or change atoms or bonds. Shortcut Keys



The image shows a chemical structure editor interface. The central workspace displays a chemical structure of 5-mercapto-1H-benzotriazole-4-carboxylic acid, which consists of a benzene ring fused to a triazole ring, with a thiol group (-SH) at the 5-position and a carboxylic acid group (-COOH) at the 4-position. The left sidebar contains various drawing tools for atoms, bonds, and rings. The right sidebar, titled "Drawing Editor:", has three radio buttons: "Structure" (selected), "Reaction", and "Markush". Below this, under the heading "Get substances that match your query using:", there are three radio buttons: "Exact search", "Substructure search", and "Similarity search" (highlighted with a pink box).

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search



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Select All Deselect All

相似结构检索候选项

1 of 6 Similarity Candidates Selected

Substances

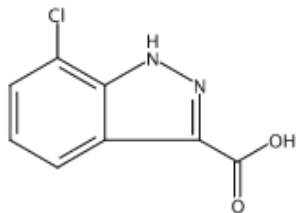
<input type="checkbox"/>	≥ 99 (most similar)	0
<input type="checkbox"/>	95-98	0
<input type="checkbox"/>	90-94	0
<input type="checkbox"/>	85-89	11
<input checked="" type="checkbox"/>	80-84	34
<input type="checkbox"/>	75-79	82
<input type="checkbox"/>	70-74	254
<input type="checkbox"/>	65-69	633
<input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



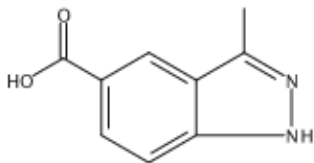
$C_8 H_5 Cl N_2 O_2$
 1H-Indazole-5-carboxylic acid, 7-chloro-
 ▶ Key Physical Properties

取代基变化

Score: 79

3. 885223-58-5

~11 ~34



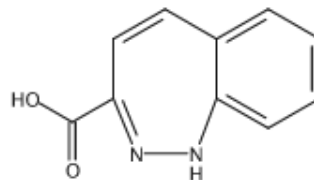
$C_9 H_8 N_2 O_2$
 1H-Indazole-5-carboxylic acid, 3-methyl-
 ▶ Key Physical Properties

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：

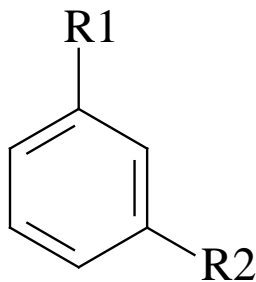
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

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

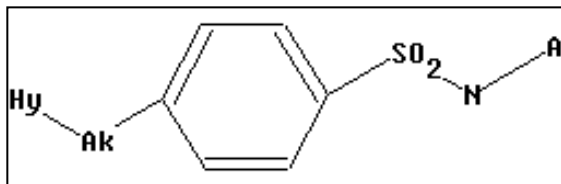
Markush检索

- 具体物质[Specific Substance] :
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance] :
 - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质，不会被分配CAS RN
 - Markush检索，能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH—halogen,
|
CH₃



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

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X =R

1-4 Cl

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

60

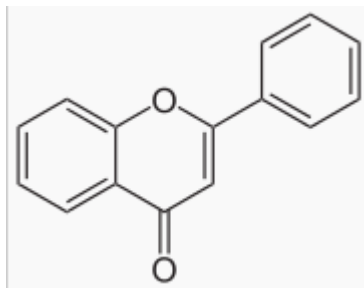


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物质检索练习

1. 检索 $(\text{NH}_4)_2\text{Sm}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
2. 检索青蒿素qinghaosu, 查看其HNMR谱图
3. 检索黄酮类物质



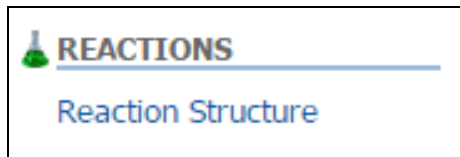
提纲

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

SciFinder检索选项——反应检索

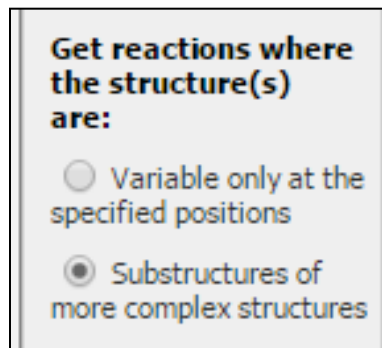
检索选项

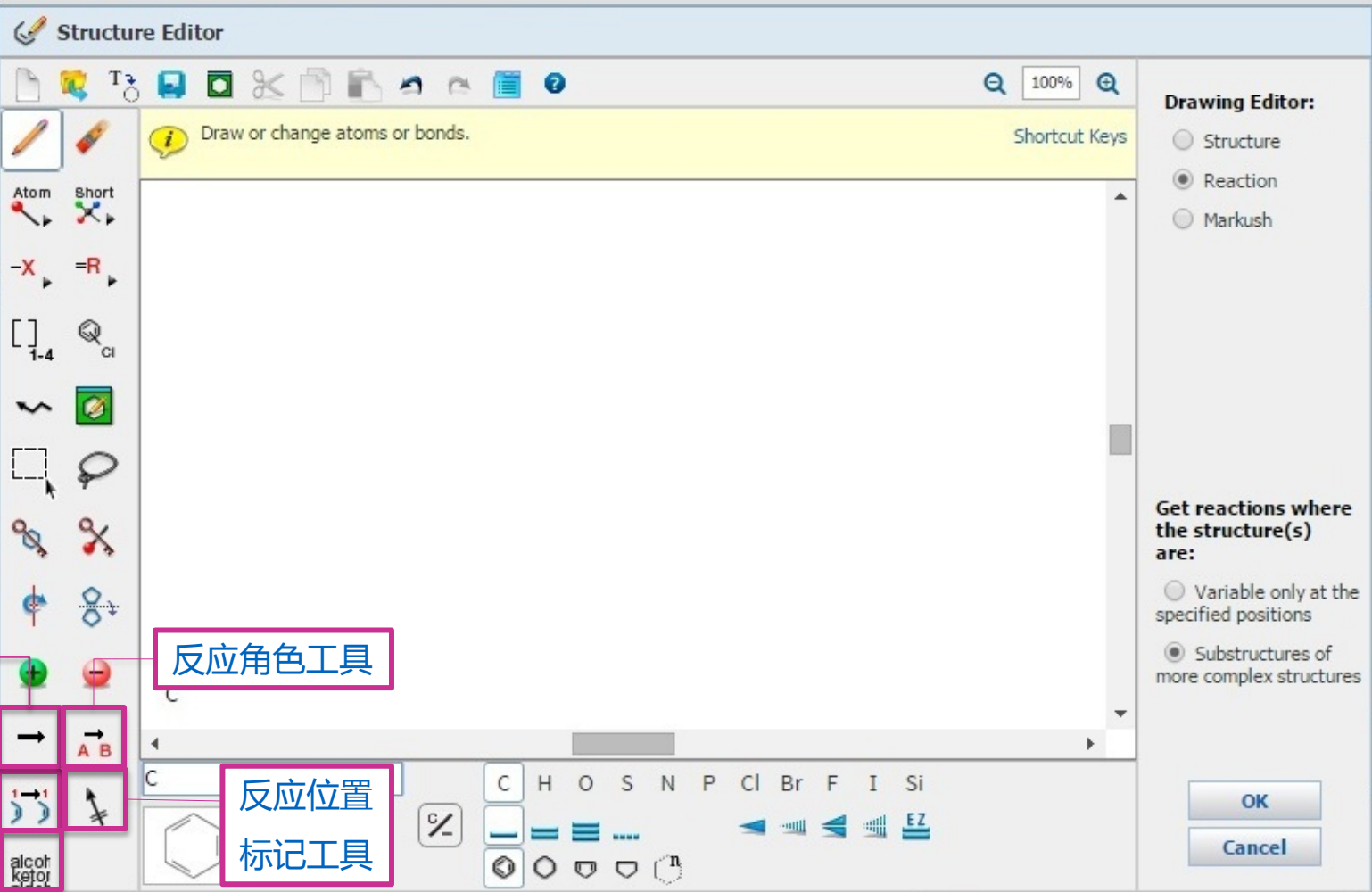
- 结构式



常用获取方法

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





反应箭头

反应原子
标记工具

官能团列表

反应角色工具

反应位置
标记工具

SciFinder反应检索——精确反应检索

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

The interface includes a toolbar on the left with various drawing tools, a search bar at the top right showing '100%', and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has three radio buttons: 'Structure', 'Reaction' (which is selected), and 'Markush'. Below these, there are two options for 'Get reactions where the structure(s) are:': 'Variable only at the specified positions' (which is highlighted with a pink box) and 'Substructures of more complex structures'. At the bottom of the panel are 'OK' and 'Cancel' buttons.

At the bottom of the window, the chemical formula $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_9\text{N}$ is displayed on the left, and the coordinates '137.14 . 107.16' are shown on the right.

精确反应检索

Get reactions where the structure(s) are:

Variable only at the specified positions

Substructures of more complex structures

OK

Cancel

反应检索结果

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

获取相似反应

The screenshot displays a web interface for chemical reaction search. At the top, there are navigation options like 'Get References' and 'Tools'. A dropdown menu for 'Group by:' is open, showing 'No Grouping', 'Document', and 'Transformation', with 'Document' selected. Below this, a list of results is shown, with the first one highlighted: '1. View Reaction Detail'. A callout box points to the 'Group by:' menu with the text '浏览记录，发现很多反应来自同一篇文章，通过Group by Document合并。'. Another callout box points to the 'Similar Reactions' link with the text '获取相似反应'. The main reaction shown is the reduction of nitrobenzene to aniline, with a yield of 100%. Below the reaction, there is a detailed overview section with the following content:

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

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

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

获取相似反应

选择相似反应的相似限制：

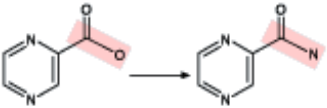
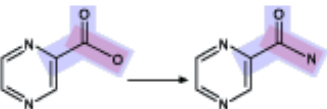
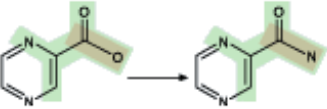
- Broad：仅反应中心相似
- Medium：反应中心及附属原子和键
- Narrow：反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (117007)

- Medium - Reaction centers plus adjacent atoms and bonds (111636)

- Narrow - Reaction centers plus extended atoms and bonds (106767)


按照反应类型排序

Get References | Tools

Group by: Transformation | Sort by: Frequency

0 of 512 Reactions Selected

1. Reduction of Nitro Compounds to Amines
491 Reactions
$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds
10 Reactions
$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{Ar} \quad \text{Ar} \\ \quad \quad \backslash \quad / \\ \quad \quad \text{N}=\text{N} \end{array}$$

3. Reduction of Nitro to Azoxy Compounds
10 Reactions
$$\text{Ar-NO}_2 \longrightarrow \begin{array}{c} \text{O}^- \\ | \\ \text{Ar} \quad \text{N}^+ = \text{N} \quad \text{Ar} \end{array}$$

4. Formation of C=C from Alcohols via Dehydration
2 Reactions
$$\begin{array}{c} \text{R}^1 \quad \text{R}^3 \\ | \quad | \\ \text{C} - \text{C} \\ | \quad | \\ \text{H} \quad \text{OH} \end{array} \longrightarrow \begin{array}{c} \text{R}^1 \quad \text{R}^3 \\ \backslash \quad / \\ \text{C} = \text{C} \\ / \quad \backslash \\ \text{R}^2 \quad \text{R}^4 \end{array}$$

更精确的查找需要的反应

反应检索结果的筛选

REACTIONS ?

Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 512 Reactions Selected

Page: 1 of 11

Analyze by: Reagent

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

1. View Reaction Detail Link Similar Reactions

获得特定物质做还原剂的反应

~102

100%

~122

Overview

Steps/Stages

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

Notes

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

References

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

Quick View Other Sources

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



Overview

Steps/Stages

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

Notes

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

References

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

Quick View Other Sources

By Sabater, Sara et al
From ACS Catalysis, 4(6), 2038-2047; 2014

不用阅读全文，直接获得包含
实验过程的反应记录

Experimental Procedure

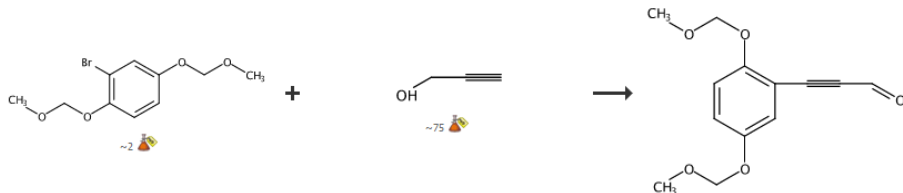


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene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

SciFinder囊括最大的反应实验过程合集

6. [View Reaction Detail](#) [🔗 Link](#)

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



Experimental Procedure: 我们可以做得更好

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

Experimental Procedure

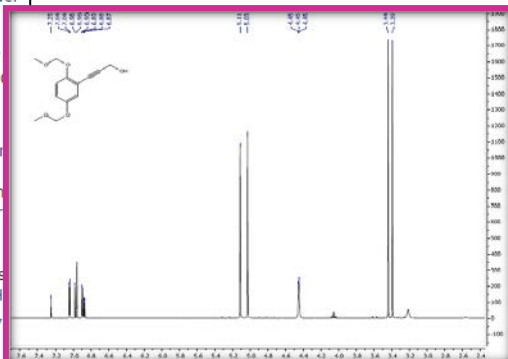
NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in *n*-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in *n*-butylamine (10 mL) and Pd(Ph₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). **3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol** (**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 room temperature and quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. **3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal** (**9**). Yield 91%; colorless oil. IR (KBr) ν_{\max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



MethodsNow

Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
Published by Royal Society of Chemistry

Reaction Steps

1

2

3

4

5

6

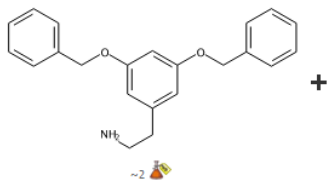
7

8

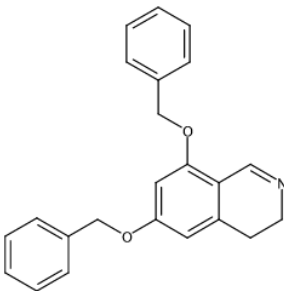
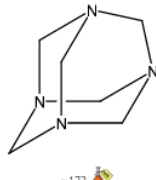
9

10

11



+



Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	<ol style="list-style-type: none">1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon2. Stir the mixture for 3 hours at 90°C.3. Dilute the reaction mixture with H₂O.4. Basify with potassium carbonate and extract with CH₂Cl₂.5. Wash the combined organic layers with brine.6. Dry over MgSO₄ and concentrate in vacuo.7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
¹H NMR	(CDCl ₃ , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, J = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
¹³C NMR	(CDCl ₃ , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹

HRMS	(FAB+) calcd for C ₂₃ H ₂₂ NO ₂ (M+H ⁺) 344.1651; found 344.1658
Mass Spec	(FAB+) m/z 344 (M+H ⁺)
State	yellow solid
CAS Method Number	3-614-CAS-200055

多步反应中，原文没有描述
的实验过程以灰色展示

物质信息

实验过程

图谱信息

保存/导出方法

Print/Export

Close

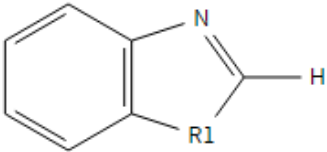
亚结构反应检索——通过C-H活化对苯并噻唑或者恶唑进行烷基化

Structure Editor

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

Atom Short

-X =R



R-group Definitions

ceramic 2 of 4

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

R1 = O, S

▼ Atoms

H																			He
Li	Be										B	C	N	O	F				Ne
Na	Mg										Al	Si	P	S	Cl				Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br			Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I			Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At			Rn
Fr	Ra																		

► Variables / Shortcuts

Close

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

Structure Editor ceramic 2 of 4

Draw or change atoms or bonds. Shortcut Keys

Atom Short

-X **=R**

1-4 Cl

R1 H

product

Drawing Editor:

- Structure
- Reaction
- Markush

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

Close

Create Saved Answ
View All | Import

KEEP ME POSTED

C-N bond activation
Dec 05, 2015(1)
Nov 28, 2015(1)
Nov 21, 2015(1)

View All

Get reactions where the structure(s) are:

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

74 SOCIETY

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Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Get reactions where the structure(s) are:

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

reactant → product

Formula is not available

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通过后处理选项筛选反应

Analyze Refine

Analyze by:
 Catalyst

CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
658062-48-7	9
1365572-73-1	8
166330-10-5	8

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通过催化剂筛选反应

Get References

Tools

Group by

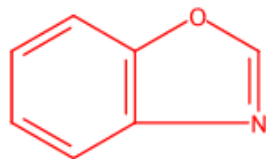
No Grouping
No Grouping
Document
Transformation

Sort by: Accession Number

Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



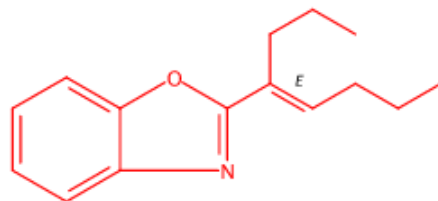
~99

+



~44

→



99%

Overview

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Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 99 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~99 ~93 85% ~6

2 Selected Clear Selections

- Acetal
- Acetyl
- Acid Halide
- Acyclic Alkene
- Acyclic Ketone
- Acylmetal
- ALCOHOLS

Reactions must have

- all selections
- any selection

Overview

Steps/Stages

1.1 C: Pd(PPh₃)₄, C: Ph₂P(CH₂)₃PPh₂, S: 98-08-8, 10 min, rt
1.2 R: Cs₂CO₃, 44 h, 110°C

Notes

alternative preparation shown, in-situ generated
1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1

References

A General Palladium-Catalyzed Method for the Synthesis of Tertiary Alkyl Halides
Quick View Other Sources
By Wu, Xiaojin et al
From Angewandte Chemie, International Edition, 5

通过后处理工具筛选反应


Analyze Refine

Group by: No Grouping Sort by: Relevance

0 of 99 Reactions Selected

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.



~99 ~93

Overview

Steps/Stages

1.1 C: Pd(PPh₃)₄, C: Ph₂P(CH₂)₃PPH₂, S: 98-08-8, 10 min, rt
1.2 R: Cs₂CO₃, 44 h, 110°C



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反应检索练习

1. 检索苯甲醛氧化成苯甲酸的反应，有哪些常用的氧化剂？
用高锰酸钾做氧化剂的反应条件？

2. 底物上有伯羟基和仲羟基，寻找伯羟基氧化成醛而仲羟基不变的反应条件？

提纲

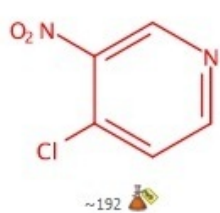
- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- SciFinder常见问题及解决

关于SciPlanner使用简介

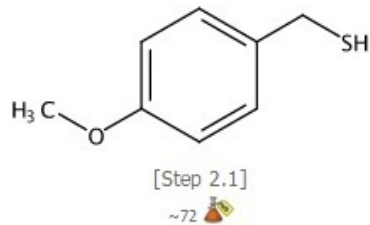
3. View Reaction Detail Link

勾选想要的反应

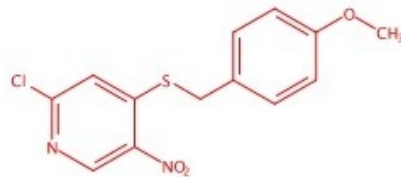
3 Steps Hover over any structure for more options.



+



→

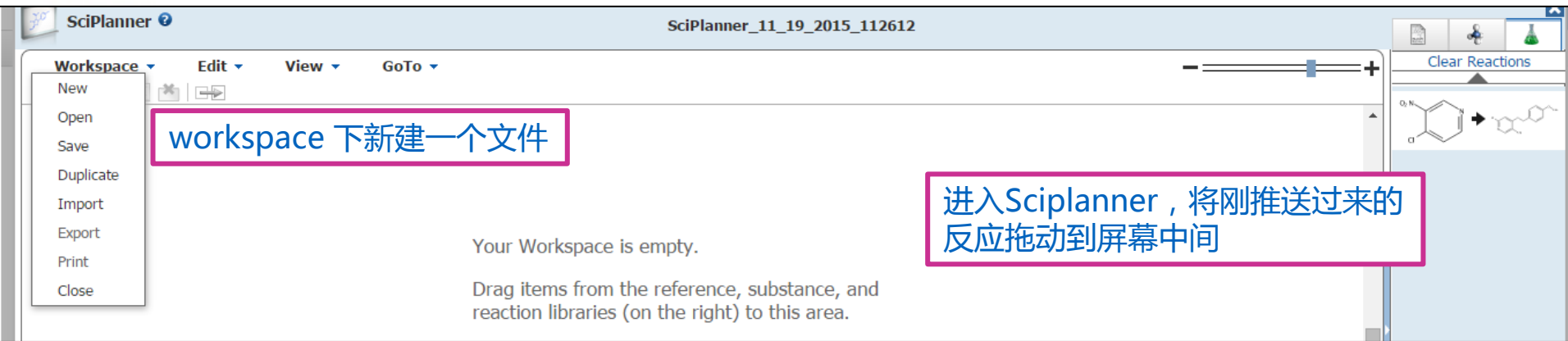



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SciPlanner

Display Options



SciPlanner  SciPlanner_11_19_2015_112612

Workspace    Edit View GoTo

workspace 下新建一个文件

Your Workspace is empty.

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

Clear Reactions

进入SciPlanner，将刚推送过来的反应拖动到屏幕中间

SciPlanner
SciPlanner_11_19_2015_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

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

1

2

3

点击反应中的一个中间产物，
单击上面的双向箭头，
选择Synthesis this

Send selected records to SciPlanner.

Send to
SciPlanner

Get
References

Tools

Group by: No Grouping Sort by: Accession Number

Display Options

1 of 34 Reactions Selected

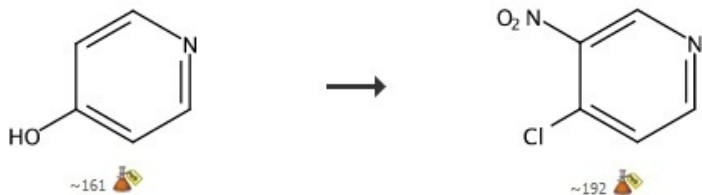
Page: 1 of 3

1. View Reaction Detail Link

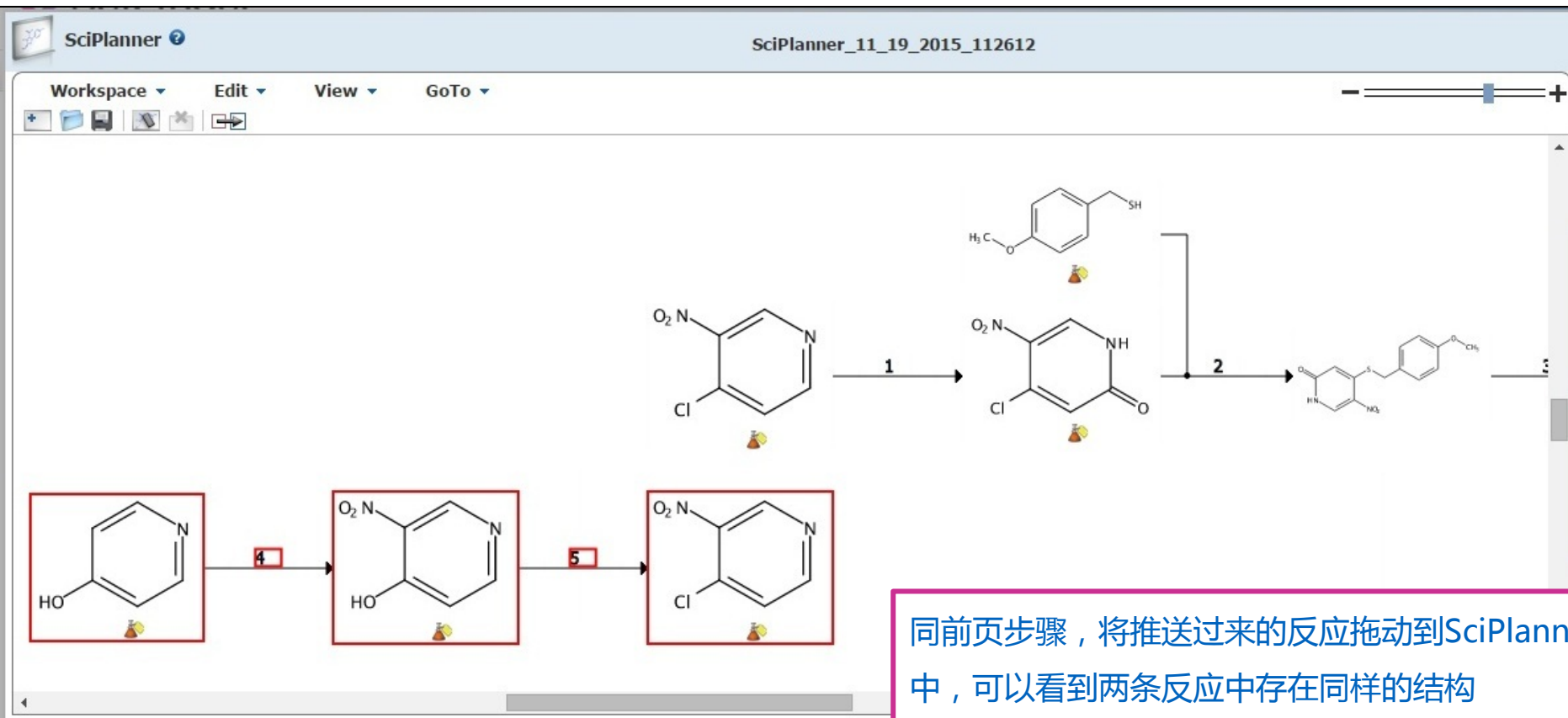
在检索到的反应中，选择感兴趣的一条反应

将该条反应继续推送到SciPlanner中

2 Steps Hover over any structure for more options.



关于SciPlanner使用简介

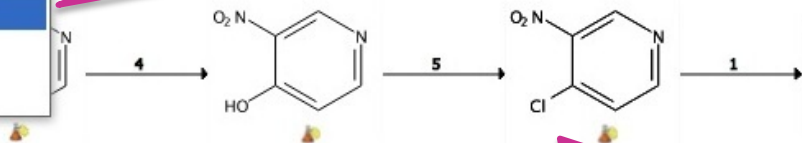




Workspace Edit View GoTo

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Open
Save
Duplicate
Import
Export
Print
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点击 Workspace, 选择其中的
Export 输出结果



用鼠标将两个同样的结构拖动至
重叠状态, 两条反应合并

选择适当的输出格式, 输出结果

Export ?

* Required

For:

Offline Review

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- Citations (*.ris)
- Image (*.png)

Saving Locally

- SciPlanner eXchange (*.pkx)

Details:

File Name: *

SciPlanner_11_19_2015_112612

Title

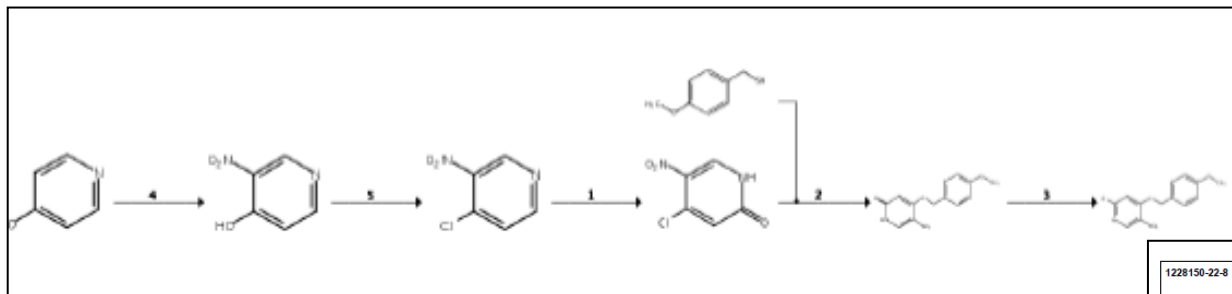
Include:

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

Export

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SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%
<p>References</p> <p>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</p> <p>By Poloek, Anurach et al</p> <p>From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p> <p>C₁₃H₁₂N₂O₄S 2-(1H-Pyridinone, 4-[[4-methoxyphenyl(methyl)thio]-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p> <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[4-methoxyphenyl(methyl)thio]-5-nitro- Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p> <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro- Related Info: ~ 361 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p> <p>C₅H₄N₂O₃ 4-Pyridinol, 3-nitro- Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p> <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy- Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p> <p>C₅H₅N O 4-Pyridinol Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p> <p>C₉H₅ClN₂O₃ 2-(1H-Pyridinone, 4-chloro-5-nitro- Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索
 - SciPlanner使用简介
- 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

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

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- USERNAME AND PASSWORD--**: Includes fields for Username (with a *Tips* link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a Security Question (dropdown menu) and an Answer field (with a *Why?* link).

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

请注意：

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

- - (破折号)
- _ (下划线)
- . (句点)

• @ (表示“at”的符号)

3. 密码必须包含 7-15 个字符，并且至少包含三种以下字符：

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

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

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