

化学及相关学科信息资源概述

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清华大学图书馆

主要内容

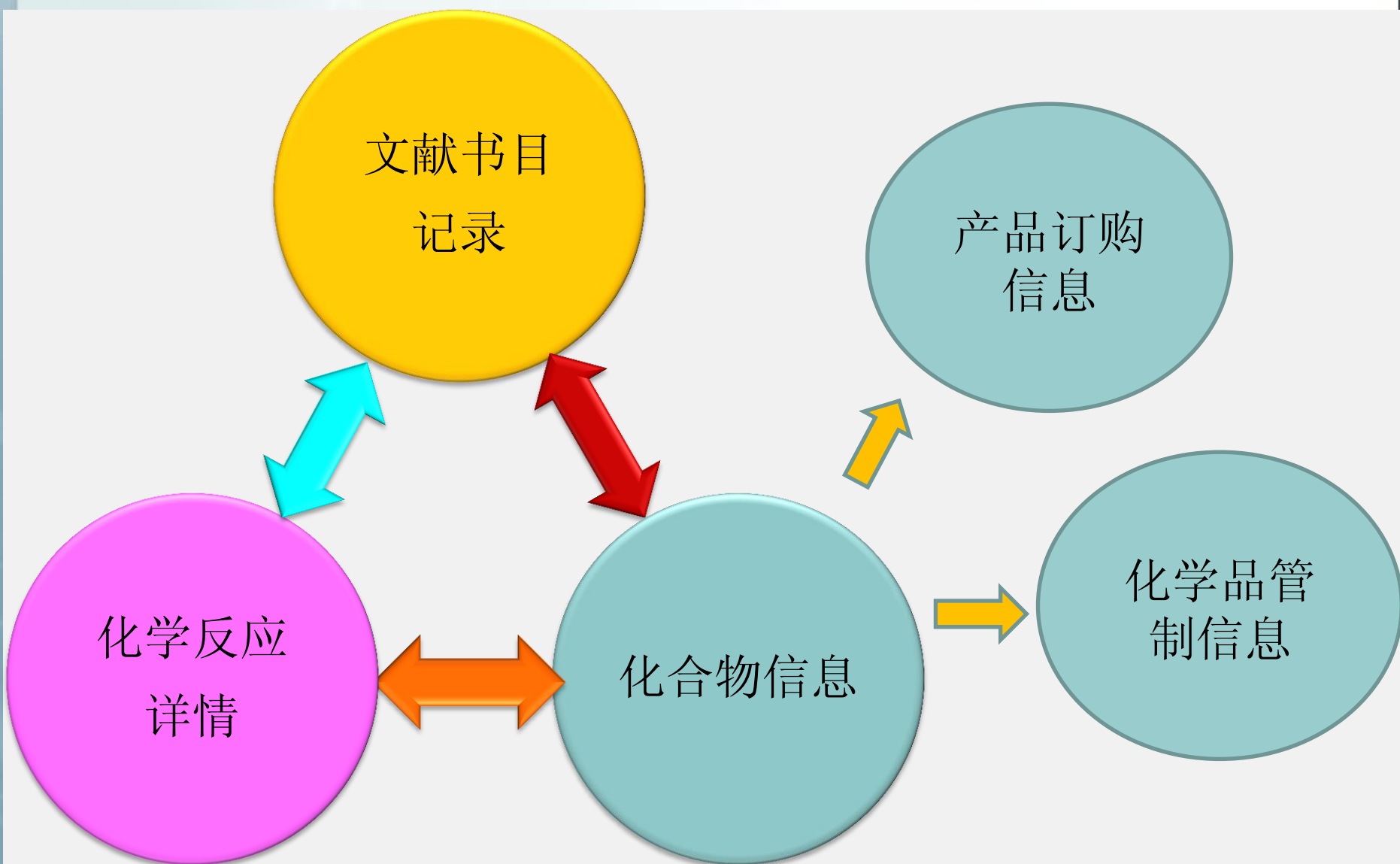
- 化学及相关学科文献信息源的特点
- 常用专业信息源概述
- 常用综合信息源概述
- 清华大学学术信息资源门户
- 清华大学电子期刊导航
- 清华大学水木搜索

1. 化学及相关学科文献信息源的特点

记录包含大量化学信息

- 书目信息（基本同其他学科信息资源）
 - 标题、责任者、来源、文摘……
- 反应信息
 - 反应式（步骤、条件、中间体、产率……）、反应条件……
- 化合物信息
 - 结构式、名称（系统命名、商品名、俗名、药品名……）、代码（CASRN……）、物理、化学、药理学、生物性质、商业信息及化学品管制信息₄

文献信息、化合物、反应之间无缝链接



文献信息、化合物、反应之间无缝链接

SciFinder®

Explore References Explore Substances Explore Reactions

Welcome Jia Lin | Sign Out

Add KMP Alert Research Topic "preparation of melamine" > references (224)

References **Get Substances** **Get Reactions** Get Related Tools Send to SciPlanner

224 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 12 Display:

1. **Preparation of melamine-formaldehyde microspheres and microcapsules based on poly(glutamic acid) by template method**
By Zhang, Ying; Yan, Shi-Feng; Rao, Shui-Qin; Zheng, Yan-Zhen; Yin, Jing-Bo; Chen, Xue-Si
From Gaodeng Xuexiao Huaxue Xuebao (2011), 32(10), 2447-2452. Language: Chinese, Database: CAPLUS
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)
2. **Preparation of melamine/formaldehyde resin-coated melamine phosphate flame retardant microcapsules**
By Wang, Zhengzhou; Xu, Shuo
From Faming Zhuanli Shenqing (2011), CN 102229712 A 20111102. Language: Chinese, Database: CAPLUS
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)
3. **Energy- and cost-saving melamine production system based on gas-phase quenching method**
By Tang, Yin; Yuan, Zhongwu; Gong, Yuande; Yin, Mingda; Yang, Xiuzhen; Chen, Duanyang; Yi, Jianglin; Lei, Lin; Liu, Chaohui; Li, Xuchu; et al
From Shiyong Xinxing Zhuanli Shuomingshu (2011), CN 201971766 U 20110914. Language: Chinese, Database: CAPLUS
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)
4. **Preparation of melamine cyanurate flame retardant with rod-like crystal**
By Niu, Minbu; Bao, Jinyuan; Xiao, Xuewen; Dai, Changlin
From Faming Zhuanli Shenqing (2011), CN 102174213 A 20110907. Language: Chinese, Database: CAPLUS
[Substances](#) [Reactions](#) [~0 Citings](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

SciFinder检索窗口示例

文献信息、化合物、反应之间无缝链接

SciFinder®

Welcome Jia Lin | Sign Out

Explore References | Explore Substances

SciFinder检索窗口示例

Add KMP Alert | Chemical Structure exact with limiters > substances (31)

Substances | Get References | Get Reactions | Tools | Send to SciPlanner

31 Substances | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [50]

View: [Grid] [List] [Table] [Full Screen]

1. Substance Detail
1260170-50-0

Nc1nc(N)c(N)n1

C₃ H₆ N₆

~1 References

Reactions

2. Substance Detail
1246816-14-7

Nc1nc(N)c(N)n1

15 NH₂

13 C

13 C

13 C

15 NH₂

文献信息、化合物、反应之间无缝链接

SciFinder®

Welcome Jia Lin | Sign Out

Explore References | Explore Substances | Explore Reactions

Research Topic "Photocyanation of aromatic com..." > references (15) > get reactions (27)

Reactions **Get References** Tools Send to SciPlanner

27 Reactions 0 Selected Save Print Export

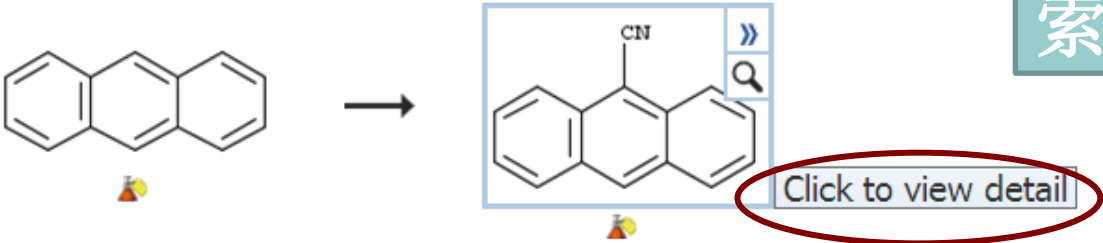
Group by: No Grouping Sort by: Accession Number

Answers per Page [15] 1 2

Select All Deselect All Display:

1. View Reaction Detail [Link](#)

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



Click to view detail

Overview

| Steps/Stages | Notes |
|--------------|---|
| 1.1 | Reactants: 1, Steps: 2, Stages: 2, Most stages in any one step: 1 |
| 2.1 | |

References

Photochemical reactions of aromatic compounds. Part 34. Direct photocyanation of arenes with sodium cyanide in the presence of electron acceptors [Full Text](#)

By Yasuda, Masahide et al

From Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1973-1999), (3), 746-50, 1981

SciFinder检索窗口示例

丰富实用的检索途径、检索字段和检索限定

- 书目信息（基本同其他学科信息资源）
 - 主题、人名、来源……
- 反应信息
 - 反应式（完整/部分）、反应条件、产率、反应步骤……
- 化合物信息
 - 结构式、名称、代码、数理化常数

可辅以多种限定条件

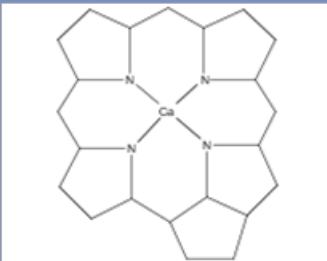
不同数据库有各自不同的检索字段

丰富实用的检索途径、检索字段和检索限定

Explore Substances

Chemical Structure Chemical Structure Search

Markush
Molecular Formula
Property **NEW**
Substance Identifier



Click image to change structure or view detail

Search type: Exact Structure Substructure Similarity

Show precision analysis

Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

Class(es)

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

Studies

- Analytical
- Biological
- Preparation
- Reactant or reagent

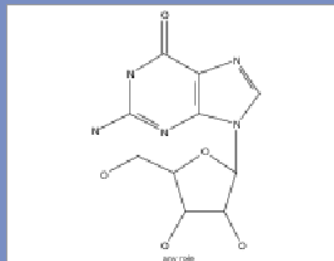
SciFinder检索窗口示例

Explore Reactions


Reaction Structure

Reaction Structure 

Search




Click image to change structure or view detail

Search type:  Allow variability only as specified
 Substructure


SciFinder检索窗口示例

Solvent(s) 


 Select Solvents

Non-participating
Functional Group(s) 

 Select Groups

Number of Steps 

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

Classification(s) 

- | | | |
|--|--|--|
| <input type="checkbox"/> Biotransformation | <input type="checkbox"/> Electrochemical | <input type="checkbox"/> Radiochemical |
| <input type="checkbox"/> Catalyzed | <input type="checkbox"/> Gas-phase | <input type="checkbox"/> Regioselective |
| <input type="checkbox"/> Chemoselective | <input type="checkbox"/> Non-catalyzed | <input type="checkbox"/> Stereoselective |
| <input type="checkbox"/> Combinatorial | <input type="checkbox"/> Photochemical | |

Source(s)

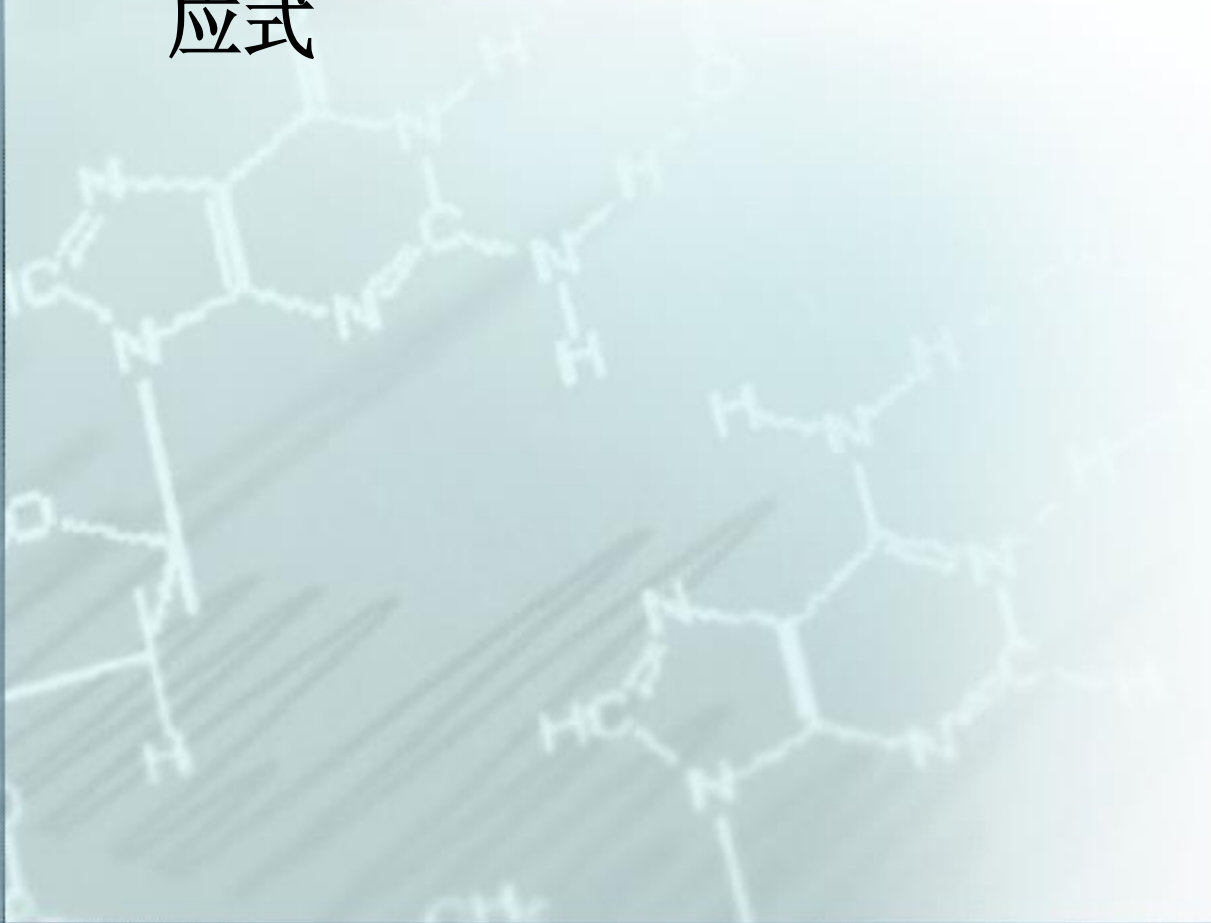
- Any source
 Patents only
 Sources other than patents

Publication Year(s) 

Examples: 1995, 1995-1999, 1995-, -1995

需要安装插件

- 通常需要安装插件，用于绘制/显示结构式和反应式



常用专业信息源概述

常用专业信息源

- **SciFinder**——主要用于检索研究文献及相关化学反应和化合物信息
- **Reaxys**——包含内容丰富的化学数值与事实
- **Web of Science**之**CCR**、**IC**
- **DII**之**Chemicals**
- **ACS Publications**
- **RSC Publishing**
- 其他? ——推荐使用“清华大学学术信息资源门户”
- 网络免费资源

SciFinder

- Chemical Abstracts Service出版发行的基于网络的检索系统
- 及时报道最新研究动态，丰富的化学反应、化合物信息，商业信息，药品管制信息.....，可以用书目信息、结构式、反应信息、化合物性质检索
- 需要注册个人账号（须用.....tsinghua.edu.cn邮箱，校园网内）
- 安装Java插件
- 访问入口：<https://scifinder.cas.org>
- 参见<http://www.lib.tsinghua.edu.cn/database/scifinder.htm>

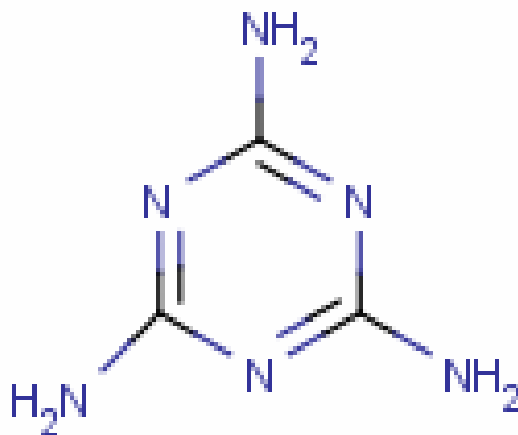
Reaxys

- Elsevier出版发行的网络数据库
- 丰富的化学反应和化合物信息，尤其是收集所有化合物之物理、化学、生物、药理学数据，所有数据经过试验验证.....，可用书目信息、结构式、反应信息、化合物性质检索
- 安装Java插件
- 访问入口：<https://www.reaxys.com>
- 参见：
<http://www.lib.tsinghua.edu.cn/database/reaxys.htm>

应用实例

检索三聚氰胺的制备方法、毒性等性质

Melamine (C₃H₆N₆)



SciFinder—利用书目信息检索

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions' are on the right. Below the navigation bar, a user greeting 'Welcome Jia Lin | Sign Out' is visible. The main search area features a search bar with the text 'preparaation of melamine' (note the typo) and a 'Search' button. A red circle highlights the 'Explore References' tab in the top navigation. Another red circle highlights the search bar. Below the search bar, a list of filters is shown on the left, including 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. The main content area displays search results with examples: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. Below the search results, there are several filter sections: 'Publication Year(s)' with a text input field and examples; 'Document Type(s)' with a grid of checkboxes for various document types; 'Language(s)' with a grid of checkboxes for various languages; 'Author Name' with three input fields for Last, First, and Middle names; and 'Company Name' with a text input field and examples.

SciFinder®

Welcome Jia Lin | Sign Out

Explore References | Explore Substances | Explore Reactions

Add KMP Alert | Research Topic "preparaation of melamine"

Explore References

Research Topic: preparation of melamine [Search]

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

Publication Year(s) []
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

| | | |
|---|---------------------------------------|-----------------------------------|
| <input type="checkbox"/> Biography | <input type="checkbox"/> Dissertation | <input type="checkbox"/> Patent |
| <input type="checkbox"/> Book | <input type="checkbox"/> Editorial | <input type="checkbox"/> Preprint |
| <input type="checkbox"/> Clinical Trial | <input type="checkbox"/> Historical | <input type="checkbox"/> Report |
| <input type="checkbox"/> Commentary | <input type="checkbox"/> Journal | <input type="checkbox"/> Review |
| <input type="checkbox"/> Conference | <input type="checkbox"/> Letter | |

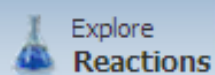
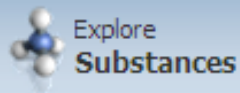
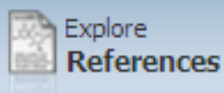
Language(s)

| | | |
|----------------------------------|-----------------------------------|----------------------------------|
| <input type="checkbox"/> Chinese | <input type="checkbox"/> German | <input type="checkbox"/> Polish |
| <input type="checkbox"/> English | <input type="checkbox"/> Italian | <input type="checkbox"/> Russian |
| <input type="checkbox"/> French | <input type="checkbox"/> Japanese | <input type="checkbox"/> Spanish |

Author Name [] [] []
Last * | First | Middle

Company Name []
Examples:
Minnesota Mining and Manufacturing
DuPont

SciFinder—利用书目信息检索



Welcome Jia Lin | Sign Out

Add KMP Alert Research Topic "preparation of melamine"

Research Topic Candidates

5 Topics 1 Selected

Select All Deselect All

| | Research Topic Candidates | References |
|-------------------------------------|---|------------|
| <input checked="" type="checkbox"/> | 232 references were found containing "preparation of melamine" as entered. | 232 |
| <input type="checkbox"/> | 13162 references were found containing the two concepts "preparation" and "melamine" closely associated with one another. | 13162 |
| <input type="checkbox"/> | 25647 references were found where the two concepts "preparation" and "melamine" were present anywhere in the reference. | 25647 |
| <input type="checkbox"/> | 9448561 references were found containing the concept "preparation". | 9448561 |
| <input type="checkbox"/> | 59007 references were found containing the concept "melamine". | 59007 |

Get References

SciFinder—利用书目信息检索

The screenshot displays the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this, a user is logged in as 'Jia Lin' with a 'Sign Out' option. A yellow alert banner reads 'Add KMP Alert'. The main search topic is 'preparation of melamine' with 232 references found. A toolbar contains buttons for 'References', 'Get Substances', 'Get Reactions' (circled in red), 'Get Related', 'Tools', and 'Send to SciPlanner'. The results table shows 232 references, 0 selected, and options to save, print, or export. The results are sorted by 'Accession Number' and displayed in a list format. The first six results are:

| Reference ID | Title | Author(s) | Source | Language | Database |
|--------------|---|---|--|----------|----------|
| 1. | Preparation of melamine polyol phosphate | Chen, Shuhua; Shen, Kemin; Ying, Lei | Faming Zhuanli Shenqing (2012), CN 102702262 A 20121003. | Chinese | CAPLUS |
| 2. | Method for preparation of melamine-formaldehyde resin for foams | Yang, Binfeng; Zhu, Guoqing; Yao, Yao; Shen, Tieqing; Ma, Lixin | Faming Zhuanli Shenqing (2012), CN 102675575 A 20120919. | Chinese | CAPLUS |
| 3. | Melamine production equipment | Wu, Zhongling; Sun, Youshen | Shiyong Xinxing Zhuanli Shuomingshu (2012), CN 202359048 U 20120801. | Chinese | CAPLUS |
| 4. | Preparation of melamine phosphonate flame retardant and flame retardant polyamide films | No Inventor data available | Faming Zhuanli Shenqing (2012), CN 102532600 A 20120704. | Chinese | CAPLUS |
| 5. | Method for preparation of melamine-modified halogen-free flameproof polyether | Liu, Ransheng; Zhao, Zengdian; Li, Jingtong | Faming Zhuanli Shenqing (2012), CN 102504244 A 20120620. | Chinese | CAPLUS |
| 6. | Study on preparation of melamine-formaldehyde foam | Xiang, Yixin; Feng, Shaohua; Wang, Wei | | | |

Reactions

Get References

Tools

Send to SciPlanner

58 Reactions

0 Selected

Save

Print

Export

NEW Group by: No Grouping

Sort by: Accession Number

Answers per Page [15]

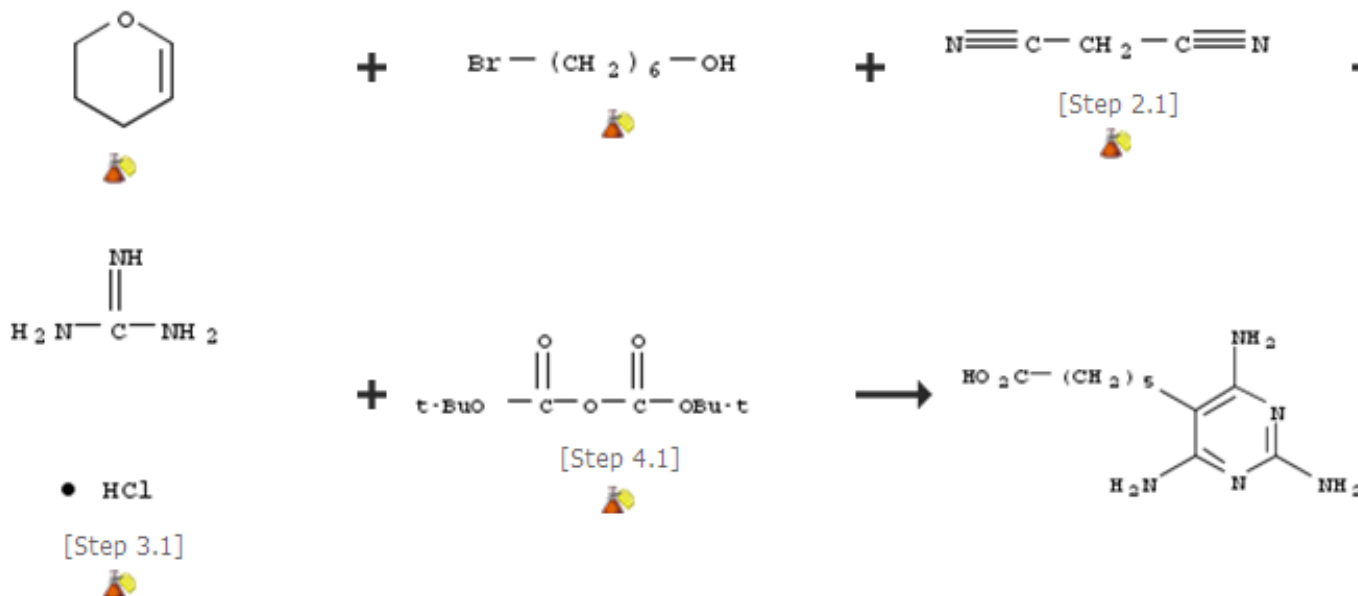
1 2 3 4

Select All Deselect All

Display:

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

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



Overview

Steps/Stages

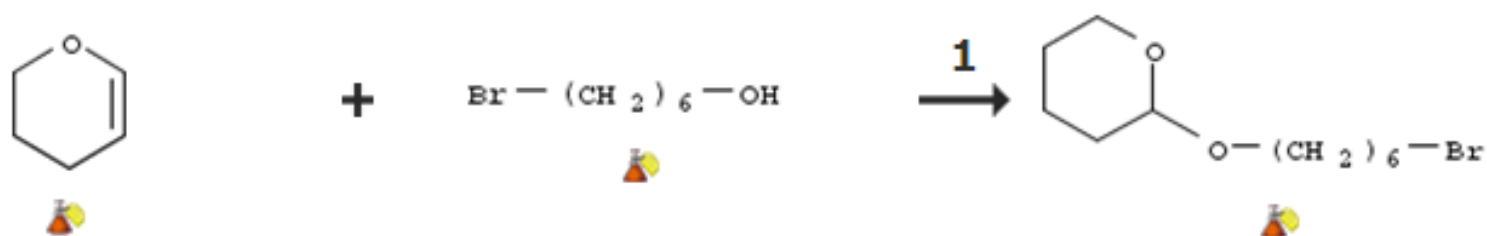
Notes

Reaction Detail

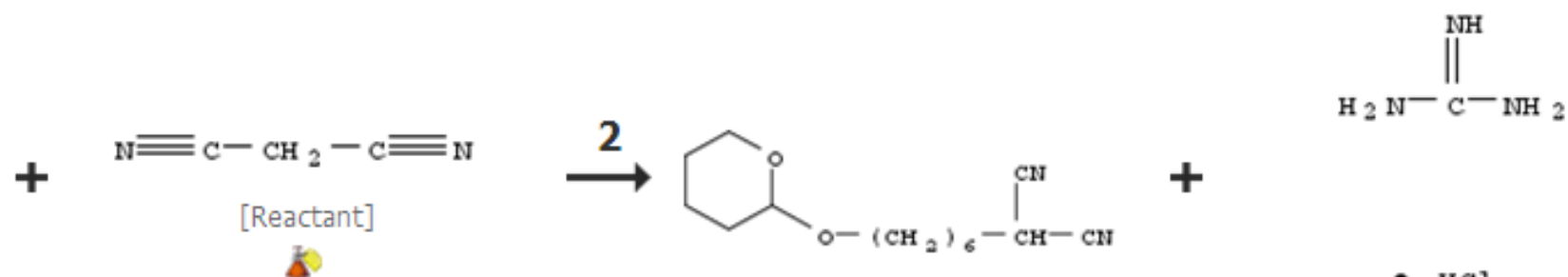
Get Reference Detail

Get Full Text

Send to SciPlanner

[Link](#) | [Save](#) | [Print](#) | [Export](#)
[Return](#)
[Previous](#) | [Next](#)
1. 8 Steps *Hover over any structure for more options.*


| Steps | Stages | Notes | Yield |
|----------|---|---|------------|
| 1 | 1.1 R:Py •p-MePhSO ₃ H, S:CH ₂ Cl ₂ , 23 h, rt | Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1 | 96% |



SciFinder—利用化合物信息检索

SciFinder®

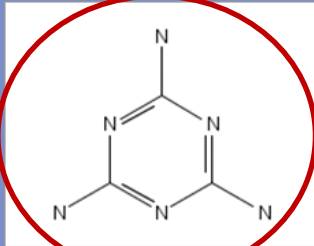
Welcome | [In Range](#) | [Sign Out](#)

[Explore References](#) [Explore Substances](#) [Explore Reactions](#)

Explore Substances

Chemical Structure [Chemical Structure](#) [Search](#)

Markush
Molecular Formula
Substance Identifier



Click image to change structure or view detail

Search type: [Exact Structure](#) [Substructure](#) [Similarity](#)

Show precision analysis

Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

Class(es) [Class\(es\)](#)

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

Studies [Studies](#)

- Analytical
- Biological
- Preparation
- Reactant or reagent

SciFinder—利用化合物信息检索

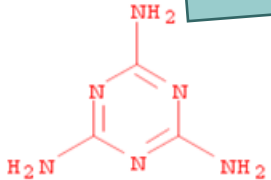
Add KMP Alert Chemical Structure exact with limiters > substances (9)

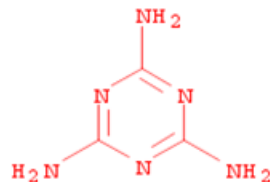
Substances Get References Get Reactions Send to SciPlanner

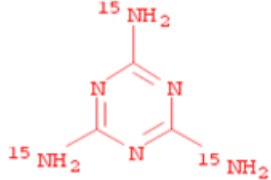
9 Substances 0 Selected Save Print Export

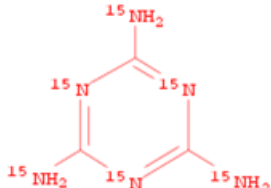
Sort by: Relevance Answers per Page [50]

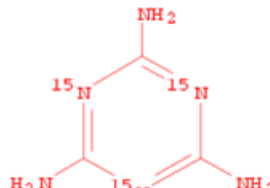
Select All Deselect All View: [Icons]

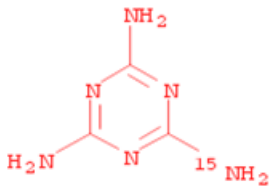
1. Substance Detail 108-78-1

C₃ H₆ N₆
1,3,5-Triazine-2,4,6-triamine
Spectra Experimental Properties

2. Substance Detail 25778-04-5
~16489
Reactions
108-78-1
C₃ H₆ N₆

(C₃ H₆ N₆)_x
1,3,5-Triazine-2,4,6-triamine, homopolymer

3. Substance Detail 287476-11-3
~78

C₃ H₆ N₆
1,3,5-Triazine-2,4,6-tri(amine-¹⁵N)

4. Substance Detail 603996-89-0
~2


5. Substance Detail 1182734-25-3
~1


6. Substance Detail 1182734-28-6
~1


SciFinder—利用化合物信息检索

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Jia Lin | Sign Out

Add KMP Alert Chemical Structure exact with limiters > substances (31) > 108-78-1

Substance Detail Get References **Get Reactions** Get Commercial Sources Get Regulatory Info NEW Send to SciPlanner

Link Save Print Export

CAS Registry Number: 108-78-1

C₃ H₆ N₆

1,3,5-Triazine-2,4,6-triamine

Melamine (8CI); s-Triazine, 4,6-diamino-1,2-dihydro-2-imino- (6CI); 1,3,5-Triazine-2,4,6(1H,3H,5H)-triimine; 2,4,6-Triamino-1,2,3-triazine; 2,4,6-Triamino-1,3,5-triazine; 2,4,6-Triamino-s-triazine; 2,4,6-Triaminotriazine; ADK Stab ZS 27; Cyanuramide; Cyanurotriamide; Cyanurotriamine; DG 002; DG 002 (amine); Flammex MEL; Isomelamine; Mark ZS 27; Melafine; Melamine 2020A; Mitsui 2020A; NSC 2130; PC 1; Pluragard; Pluragard C 133; Spinflam ML 94M; Teoharn; Theoharn; Triamino-s-triazine; Triaminotriazine; Virset 656-4; Yukamelamine; ZS 27; s-Triazinetriamine

Deleted CAS Registry Numbers: 504-18-7;65544-34-5;67757-43-1;68379-55-5;70371-19-6;94977-27-2;130392-03-9;169314-62-9

~15,110 References

Document Types: Book, Conference, Dissertation, Journal, Patent, Report

SciFinder—与化合物相关的记录内容（续）

对报道该化合物的文献，按研究内容、是否专利文献、是否含非取代衍生物，进行聚类分析

| CAS Role | Patents | Nonpatents | Nonspecific Derivatives from Patents | Nonspecific Derivatives from Nonpatents |
|---------------------------|----------------|-------------------|---|--|
| Analytical Study | ✓ | ✓ | ✓ | ✓ |
| Biological Study | ✓ | ✓ | ✓ | ✓ |
| Combinatorial Study | | | | ✓ |
| Formation, Nonpreparative | ✓ | ✓ | ✓ | ✓ |
| Miscellaneous | ✓ | ✓ | ✓ | |
| Occurrence | ✓ | ✓ | ✓ | ✓ |
| Preparation | ✓ | ✓ | ✓ | ✓ |
| Process | ✓ | ✓ | ✓ | ✓ |
| Properties | ✓ | ✓ | ✓ | ✓ |

SciFinder—与化合物相关的记录内容（续）

预测得到的该化合物的性质（生物、化学、密度、利宾斯基及其相关、光谱、结构相关、热），“**Note**”为数据来源引文序号

Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

| Biological Properties | Value | Condition | Note | Te |
|-------------------------|-------|------------------|------|----|
| Bioconcentration Factor | 1.0 | pH 1 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 2 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 3 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 4 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 5 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 6 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 7 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 8 Temp: 25 °C | (39) | |
| Bioconcentration Factor | 1.0 | pH 9 Temp: 25 °C | (39) | |
| | 1.0 | | (39) | |

SciFinder—与化合物相关的记录内容（续）

实验得到的该化合物的性质（生物、化学、密度、光学和散射、光谱、结构相关、热），“**Note**”为数据来源引文序号

Experimental Properties: Biological Chemical Density Optical and Scattering Spectra Structure-related Thermal

| Biological Properties | Value | Condition | Note |
|--|---------------|-----------------------------------|---------|
| ADME (Absorption, Distribution, Metabolism, Excretion) | See full text | | (2)CAS |
| Half-Life (Biological) | See full text | | (2)CAS |
| LD50 | See full text | | (19)CAS |
| Median Lethal Dose(LD50) | 6000 mg/kg | Organism: rat Route: intragastric | (20)CAS |
| Median Lethal Dose(LD50) | 4300 mg/kg | Organism: rat Route: intragastric | (20)CAS |

SciFinder—与化合物相关的记录内容（续）

报道前述预测和实验性质的文献信息

- (1) Li, Yuan-Yuan; *Chromatographia* 2011, V74(7-8), P523-530CAPLUS
- (2) Chu, C. Y.; *Toxicology Letters* 2010, V199(3), P398-402CAPLUS
- (3) WSS: Spectral data were obtained from Wiley Subscription Services, Inc. (US)
- (4) AIST: Integrated Spectral Database System of Organic Compounds. (Data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan))
- (5) Lagoja, Irene M.; *Chemistry & Biodiversity* 2007, V4(4), P818-822CAPLUS
- (6) Pravica, Michael; *Diamond and Related Materials* 2011, V20(7), P1090-1092CAPLUS
- (7) Cousson, A.; *Acta Crystallographica, Section E: Structure Reports Online* 2005, VE61(2), Po222-o224CAPLUS
- (8) "International Chemical Safety Cards" data were obtained from the National Institute for Occupational Safety and Health (US)
- (9) Klema, Friedrich; *Mitteilungen des Chemischen Forschungsinstitutes der Wirtschaft Oesterreichs* 1954, V8, P152-6CAPLUS
- (10) Rochow, T. G.; *Journal of Industrial and Engineering Chemistry (Washington, D. C.)* 1940, V32, P1187-8CAPLUS
- (11) "Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)
- (12) Knaggs, I. Ellie; *Proceedings of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences* 1940, V177, P140-7CAPLUS
- (13) Singh, Man; *Pakistan Journal of Scientific and Industrial Research* 2006, V49(3), P160-169CAPLUS
- (14) Zhao, Xiaodan; *Journal of Hazardous Materials* 2011, V189(3), P732-740CAPLUS
- (15) Mathieu, Didier; *Thermochimica Acta* 2002, V384(1-2), P369-375CAPLUS
- (16) Liu, Peng; *Wuli Huaxue Xuebao* 2009, V25(12), P2417-2421CAPLUS
- (17) BIORAD: Infrared spectral data from the Bio-Rad/Sadtler IR Data Collection was obtained from Bio-Rad Laboratories, Philadelphia, PA (US). Copyright © Bio-Rad Laboratories. All Rights Reserved.
- (18) Marchewka, M. K.; *Journal of Physics and Chemistry of Solids* 2003, V64(11), P2169-2181CAPLUS
- (19) Ph... .. *Kidney International* 2009, V75(8), P774-779CAPLUS

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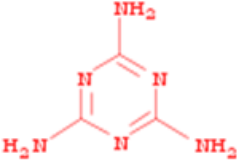
Substances Get References **Get Reactions** Tools NEW Send to SciPlanner

31 Substances 0 Selected Save Print Export

Select All Deselect All Sort by: Answers per Page [50]

View: ■■■■

1. **Substance Detail**
1260170-50-0



C₃ H₆ N₆

- ~1 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

Get Reactions

Retrieve reactions for:

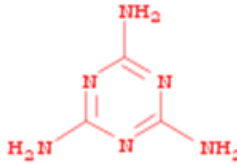
- All substances
- Selected substances

Limit results by reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get Cancel

4. **Substance Detail**
1220748-50-4
(Component: 108-78-1)



• 5 H₂O

C₃ H₆ N₆ · 5 H₂O

1,3,5-Triazine-2,4,6-triamine, hydrate (1:5)

C₃ H₆ N₆ · 6 H₂O

1,3,5-Triazine-2,4,6-triamine, hydrate (1:6)

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Explore Reactions

Reaction Structure

Reaction Structure

Search

C1=NC=NC=N1
product

Click image to change structure or view detail

Search type: Allow variability only as specified Substructure

Solvent(s) [Select Solvents](#)

Non-participating Functional Group(s) [Select Groups](#)

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

Classification(s)

| | | |
|--|--|--|
| <input type="checkbox"/> Biotransformation | <input type="checkbox"/> Electrochemical | <input type="checkbox"/> Radiochemical |
| <input type="checkbox"/> Catalyzed | <input type="checkbox"/> Gas-phase | <input type="checkbox"/> Regioselective |
| <input type="checkbox"/> Chemoselective | <input type="checkbox"/> Non-catalyzed | <input type="checkbox"/> Stereoselective |
| <input type="checkbox"/> Combinatorial | <input type="checkbox"/> Photochemical | |

Source(s)





Any source
 Patents only
 Sources other than patents


Publication Year(s)
Examples: 1995, 1995-1999, 1995-, -1995

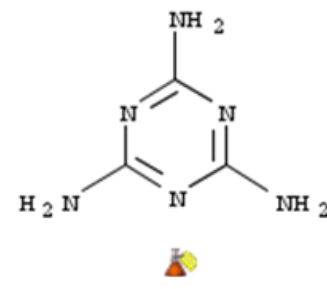
SciFinder—命中的反应式

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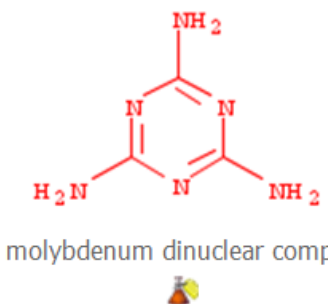
Display:    

1. **View Reaction Detail**  [Link](#)
2 Steps *Hover over any structure for more options.*



NC1=NC(=N)C(=N1)N

→



molybdenum dinuclear complex

▼ Overview

| Steps/Stages | Notes |
|--|--|
| 1.1 R:MoO ₃ , R:HBr, S:H ₂ O, heated | 2) molybdenum dinuclear complex containing 2,4,6-triamine-[1,3,5]-triazine formed, Reactants: 1, Reagents: 3, Solvents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1 |
| 2.1 R:NH ₃ , R:HBr, S:H ₂ O, pH 8 | |

References

[Oxotetrabromomolybdenum\(V\) complex compounds with s-triazine derivatives](#)
By Chivu, Haritina et al
From Revista de Chimie (Bucharest, Romania), 62(3), 283-286; 2011

[Full Text](#)

Reaxys—利用化合物结构及其理化性质检索

The screenshot displays the Reaxys web interface. At the top left is the Reaxys logo. A navigation bar contains tabs for Query, Results, Synthesis Plans, History, My Alerts, My Settings, and Help. Below this, there are tabs for Reactions, Substances and Properties (which is selected), and Text, Authors and more. A text input field labeled "Generate structure from name" is present. The main area features a large frame with the instruction "Double click this frame and draw structure query". To the right of this frame are search options: "As drawn" (selected), "Substructure:" (with sub-options "on heteroatoms" and "on all atoms"), and a list of checkboxes: "Ignore stereo", "No salts", "No mixtures", "No isotopes", "No additional rings", and "Further options". A "Search" button is highlighted with a red box. Below the main area are tabs for "Properties (Form-based)" and "Properties (Advanced)". On the left, a sidebar lists search categories: Substance Data (with "Search text in all facts" and a search input field containing "is"), Identification Data, Physical Data, Spectroscopic Data, Bioactivity Data, Ecotoxicological Data, and Bibliographic Data. On the right, a detailed view of the "Spectroscopic Data" filter is shown, including checkboxes for "Spectroscopy data available", "NMR available or specify Nuclei", "IR available or specify Solvent", "UV available or specify Absorption Maxima", "ESR available or specify Nuclei", and "MS available". Each of these categories has associated dropdown menus and input fields, some with "in solvent" options.

Reaxys—利用化合物标识检索

Properties (Form-based)

Properties (Advanced)

Search

Substance Data

Search text in all facts

Search for

e.g. nitrobenzene; e.g. decrease AND 'enzyme activity'

Identification Data

Reaxys-RN

=

CAS Registry Number

is 108-78-1

Chemical Name / Synonyms

is

Molecular Formula

is

Molweight (g/mol)

=

No of Elements

=

No of Fragments

=

Physical Data

Spectroscopic Data

Bioactivity Data

Ecotoxicological Data

Natural Products

Bibliographic Data

Reaxys—利用化合物结构及其理化性质检索

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Reactions **Substances and Properties** Literature

Generate structure from name

Double click this frame and draw structure query **STRUCTURE EDITOR**

As drawn
 Substructure:
 on heteroatom
 on all atoms
 Similarity

Nc1nc(N)c(N)n1

Include tautomers
 Ignore stereo
 No salts
 No mixtures
 No isotopes
 No additional rings

Further options

Include related Markush
 Keep Fragments ...
 separate together
 No charges
 No radicals

Type values in fields e.g. 3-5)

of Atoms
 # of Fragments
 # of Ring Closures

Properties (Form-based) Properties (Advanced)

+ Substance Data

Reaxys—命中化合物及其相关反应和各项理化性质



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Query

Results

Synthesis Plans

History

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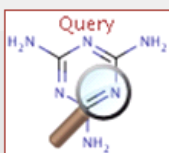
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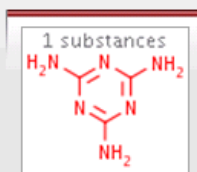
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Create Alert



1 substances out of 717 citations

Filter by:

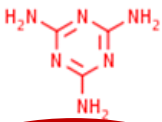


- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Availability
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Substances (Grid)

Substances (Table)

Citations

go to Page Page 1 of 1

| Structure | Chemical Name | N° of preparations All Preps All Reactions | Available Data | N° of ref. | Boiling Point |
|---|--|---|--|------------|---------------|
|  <input type="checkbox"/> 1   | 2,4,6-triamino-1,3,5-triazine 2,4,6-triamino-5-triazine melamine powder acetoguanamine cyanuramide Melamine melamina | 121 prep out of 403 reactions. | Identification Physical Data (292) Spectra (94) Bioactivity/Ecotox (42) Use/Application (49) Natural Product (3) Quantum Chemical Data (2) | 681 | |

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Reaxys—命中反应式及反应条件和反应详情

121 reactions out of 243 citations

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Reactions
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| | Yield | Conditions | References |
|-------------------------------|---|--|---|
| <input type="checkbox"/> 1 | <chem>N#C + CN(C)=[N+]#N >> Nc1nc(N)c(N)n1</chem> | Synthesize | Synthesize |
| | 93% | <p>With potassium hydroxide in water; dimethyl sulfoxide</p> <p style="text-align: center;">Show Experimental Procedure</p> | <p>Suddeutsche Kalkstickstoff-Werke Aktiengesellschaft</p> <p>Patent: US4069383 A1, 1978 ;</p> <p style="text-align: center;"> Title/Abstract Full Text Show Details </p> |
| <input type="checkbox"/> 2 | <chem>NC#N >> Nc1nc(N)c(N)n1</chem> | Synthesize | Synthesize |
| | | <p>With Catalyst M-Chromium oxide; ammonia T=450 - 750°C; oder anderen Katalysatoren;</p> | <p>Monsanto Chem. Co.</p> <p>Patent: US1855396 , 1958 ;</p> <p style="text-align: center;"> Full Text Show Details </p> |
| | | <p>With Catalyst M-Chromium oxide; ammonia T=350 - 400°C; P=35 Torr; oder anderen Katalysatoren;</p> | <p>Am. Cyanamid Co.</p> <p>Patent: US2577201 , 1950 ;</p> <p style="text-align: center;"> Full Text Show Details </p> |

Reaxys—生物活性/生态毒性之药理学数据

⚡ Bioactivity/ Ecotox

⚡ Pharmacological Data (22)

| | | |
|---------|------------------------|--|
| 1 of 22 | Effect | pharmacokinetics |
| | Species or Test-System | Sprague-Dawley rat |
| | Sex | male |
| | Route of Application | intravenous |
| | Concentration | 10 mg/kg |
| | Kind of Dosing | title comp. dissolved in normal saline |
| | Further Details | mass of species: 200 g; maximum concentration (Cmax) |
| | Type | Cmax |
| | Value of Type | 2.29 µg/ml |
| | Reference | <p>Wu, Yu-Tse; Huang, Chih-Min; Lin, Chia-Chun; Ho, Wei-A. N.; Lin, Lie-Chwen; Tsai, Tung -H. U.; Chiu, Ting-Fang; Tarng, Der-Cherng; Lin, Chi-Hung Journal of Agricultural and Food Chemistry, 2010, vol. 58, # 1 p. 108 - 111</p> <p>Title/Abstract Full Text View citing articles Show Details</p> |
| 2 of 22 | Effect | pharmacokinetics |
| | Species or Test-System | Sprague-Dawley rat |
| | Sex | male |
| | Route of Application | intravenous |
| | Concentration | 10 mg/kg |
| | Kind of Dosing | title comp. dissolved in normal saline |
| | Further Details | mass of species: 200 g; half-life (t1/2) |
| | Type | t1/2 |

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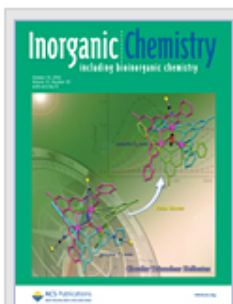
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Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, BCKV Campus PO, Mohanpur, Nadia, WB 741252, India

Inorg. Chem., 2012, 51 (19), pp 10129-10135

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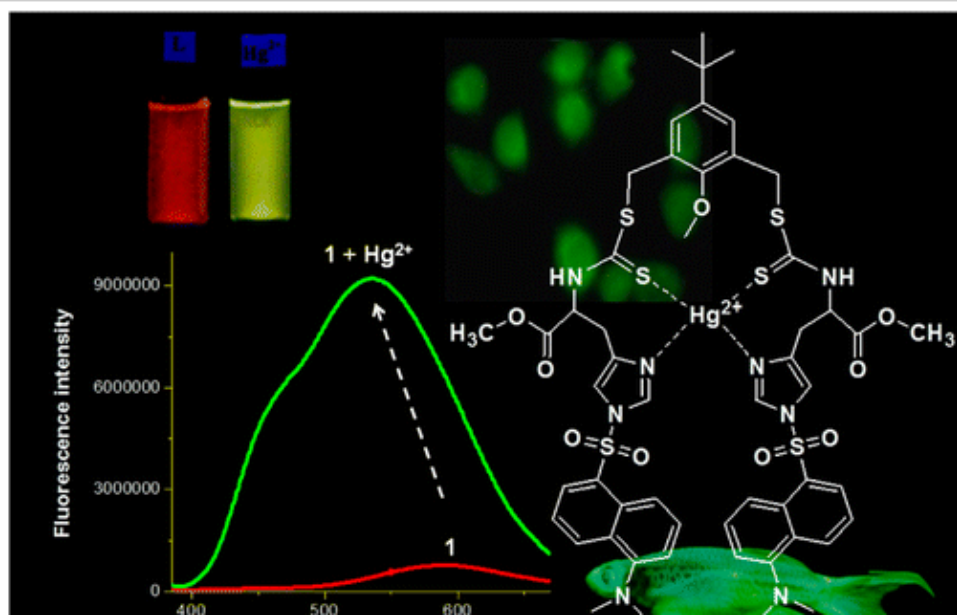
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CCS Section: Toxicology

Abstract



New Trick for an Old Ligand! The Sensing of Zn(II) Using a Lanthanide Based Ternary Yb(III)-cyclen-8-hydroxyquinoline System As a Dual Emissive Probe for Displacement Assay

Steve Comby, Sarah A. Tuck, Laura K. Truman, Oxana Kotova, and Thorfinnur Gunnlaugsson

Inorganic Chemistry 2012 51 (19), pp 10158-10168

Abstract: A novel near-infrared (NIR) emissive lanthanide-based zinc sensor was designed, based on the self-assembly in aqueous solution between the nonemissive coordinatively unsaturated Yb(III) cyclen complex 2·Yb and the sulfonated 8-hydroxyquinoline (8-HQS) ...

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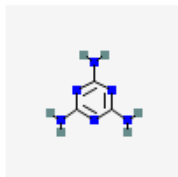
All: 101 Rule of 5: 35

Items 1 - 20 of 101

Page 1 of 6 Next

1: CID: 7955

Related Structures, BioAssays, BioSystems, Literature, Other Links



MELAMINE; Cyanurotriamide; Cyanurotriamine ...

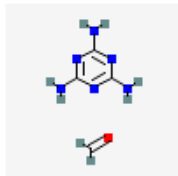
IUPAC: 1,3,5-triazine-2,4,6-triamine

MW: 126.119940 g/mol | MF: C₃H₆N₆

Tested in BioAssays: All: 19, Active: 2; BioActivity Analysis

2: CID: 93374

Related Structures



Cymel 481 resin; Methylated melamine, formaldehyde polymer;

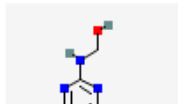
Formaldehyde, melamine polymer, methylated ...

IUPAC: formaldehyde; 1,3,5-triazine-2,4,6-triamine

MW: 156.145920 g/mol | MF: C₄H₈N₆O

3: CID: 70549

Related Structures, BioAssays



Cilag; Glazamine M; Resloom HP ...

IUPAC: [[4,6-bis(hydroxymethylamino)-1,3,5-triazin-2-yl]amino]methanol

MW: 216.197880 g/mol | MF: C₆H₁₂N₆O₃

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Pharmacological Actions 5

BioSystems 2

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melamine AND (([Element]... (0)

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10, Pages: 2143-2173, Journal; General
Review, 2006, CODEN: TETRAB, ISSN:
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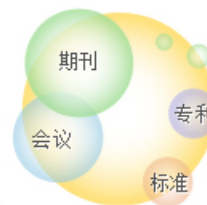
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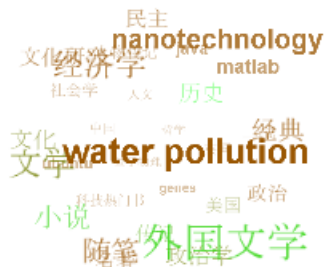
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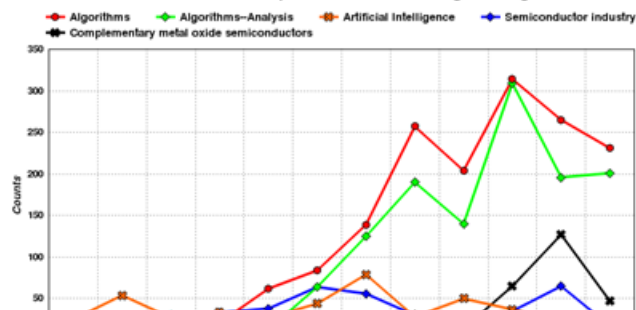
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