

CAS SciFinder Discovery Platform (Academic)

全面高效获取科技信息



杜德鑫

ddu@acs-i.org

美国化学文摘社 (CAS) 北京代表处

© 2023 American Chemical Society. All rights reserved.



大纲

- CAS 与 CAS SciFinder Discovery Platform (Academic) 简介
- 科研信息的高效查阅
 - 如何拓展文献调研?
 - 如何调研某类物质?
 - 如何调研反应信息?
 - 怎么查、怎么选具体的实验方案?
- 常见问题



CAS SciFinder Discovery Platform 查找路径

学校官网
(图书馆)



图书馆官网
(电子资源)
(外文数据库)



外文数据库
(SciFinder Academic 数据库)



CAS SciFinder Discovery Platform 简介与注册说明

注册和登录方式






您所在位置: 【电子资源】 外文数据库 正文 发布时间: 2023-01-16 点击次数: 3711

SciFinder Academic数据库

数据库名称	SciFinder Academic数据库
访问地址	https://scifinder.cas.org
资源类型	文摘型和数值型数据库
语种	英语
收录年限	1907年以来的5万多种科技期刊(包括目前仍在出版的数千种期刊)文献、63个专利授权机构的专利文献、会议论文、技术报告、图书、学位论文、评论、会议摘要、e-only期刊、网络预印本等。
学科范围	涵盖的学科包括应用化学、化学工程、普通化学、物理、生物学、生命科学、医学、聚合体学、材料学、地质学、食品科学和农学等诸多领域。
数据库简介	SciFinder由美国化学会(American Chemical Society, ACS)旗下的美国化学文摘社(Chemical Abstracts Service, CAS)出品,是一个研发应用平台,提供全球最大、最权威的化学及相关学科文献、物质和反应信息。SciFinder涵盖了化学及相关领域如化学、生物、医药、工程、农学、物理等多学科、跨学科的科技信息。SciFinder收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论和网络资源

4 © 2023 American Chemical Society. All rights reserved.

- 开通时间:** 2023年01月01日至2025年12月31日。
- 在校园网IP地址范围内用学校域名邮箱注册SciFinder帐号后在校园网IP地址范围内登陆网站: <https://scifinder.cas.org/>
 - SciFinder注册须知:
读者在使用SciFinder之前须使用学校的后缀名邮箱注册账号密码。注册后系统将自动发送一个链接到您所填写的email邮箱中,48小时内激活此链接即可完成注册。参考“SciFinder用户注册指南”。
- SciFinder注册地址:
<https://scifinder.cas.org/registration/index.html?corpKey=3A35186EX86F35055X1AA5171E17AE354E59>
- 3. 特别提示:**
- 如果进入系统后20分钟没有操作,系统将自动断开您与服务器的连接。
 - SciFinder经常更新,请大家留意图书馆或美国化学文摘社主页(www.cas.org)的相关消息。
 - 注意保护知识产权,合理使用数据库,只用于学术研究,实名使用,不与他人分享,禁止过量下载(以电子形式存储不超过5,000条记录),禁止在商业机构使用。
 - 在使用过程中出现问题,请参考“SciFinder常见问题解答”,如无法解决,请填写“SciFinder问题报告”,并发送至China@acs-i.org或联系图书馆。
- 4. 附件:**
-  [SciFinder用户注册指南.pdf](#): 提供了详细的注册流程介绍,便于用户顺利完成账号注册。
 -  [SciFinder常见问题解答.docx](#): 总结了用户在使用SciFinder数据库时常见的问题及解决办法,便于用户遇到问题时快速自查和应对。
 -  [SciFinder问题报告.doc](#): 用户在遇到账号问题时,



如何获取 CAS SciFinderⁿ 账号 (登录贵校图书馆网站, 查看注册相关的链接和说明)

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: Tips

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: Why?

请注意:

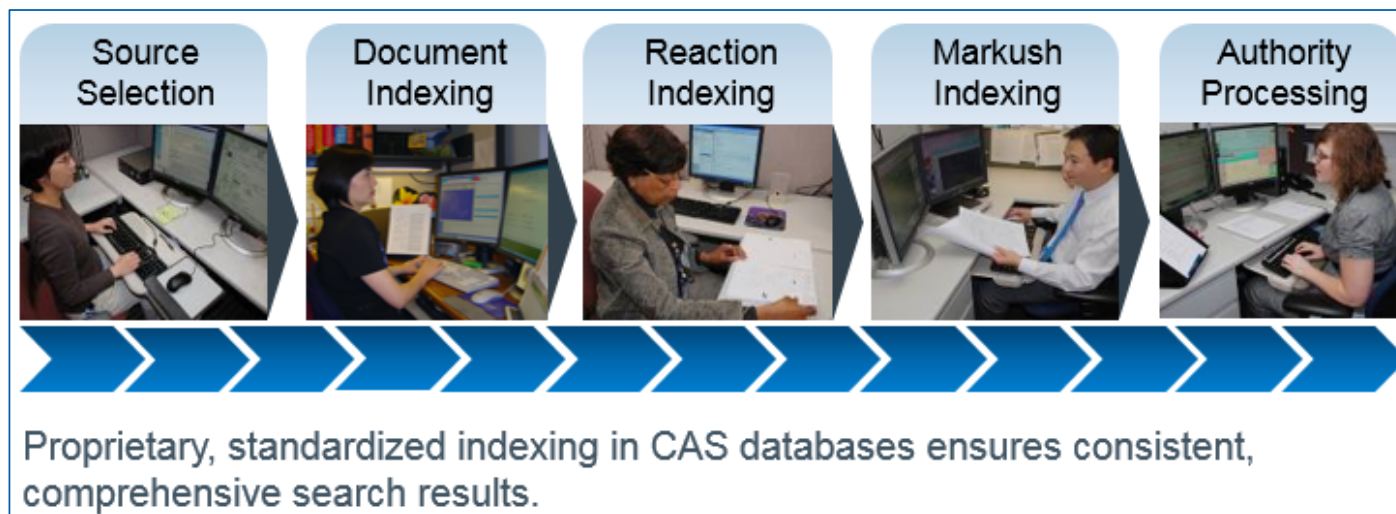
1. 必须输入真实姓名和**学校**邮箱
 2. 用户名必须是唯一的, 且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符:
 - - (破折号)
 - _ (下划线)
 - . (句点)
 - @ (表示“at”的符号)
 3. 密码必须包含 7-15 个字符, 并且至少包含**三种以下字符**:
 - 字母
 - 混合的大小写字母
 - 数字
 - 非字母数字的字符 (例如 @、#、%、&、*)
- 例: abc@123
4. 从下拉列表中选择一个密码提示问题并给出答案
单击 Register (注册)

Registration Already Complete

You have already completed your registration. For assistance with accessing SciFinder, consult the key contact for your organization.

点击激活链接后注册成功; 之后直接点击 <https://scifinder-n.cas.org> 访问

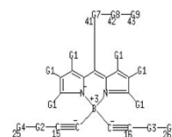
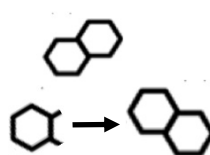
CAS 科学家智力标引



Data
pre-repository



1990
Smith, M.
anthracene



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17 β)-

CAS 科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS 具有最全面的学科连接内容合集



Over
50K
scientific journals
and documents

Over
279
million substances

Over
50
languages
translated

109
patent offices
worldwide

内容合集



CAS SciFinder Discovery Platform 涵盖的工作流程 解决方案



新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具




专业的配方数据库，助力配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息



独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立

CAS SciFinderⁿ 登录

<https://scifinder-n.cas.org>




Log In to SciFinderⁿ

Username or Email Address

Next

[Create an account.](#) | [Can't log in?](#)



Log In to SciFinderⁿ

Welcome, ddu@acs-i.org [Not You?](#)

Password

Log In

Keep me signed in

[Create an account.](#) | [Can't log in?](#)

CAS SciFinder[®] 主界面

The screenshot shows the CAS SciFinder main interface. On the left, a sidebar menu is highlighted with a blue box and labeled "CAS 应用". The main content area features a search bar with a "Draw" button highlighted in yellow. Below the search bar are three search options: Retrosynthetic Analysis, Search CAS Lexicon, and Search CAS Sequences. At the bottom, a "Recent Search History" section is highlighted with a blue box and labeled "历史记录". On the right, a user profile dropdown menu is highlighted with a blue box and labeled "账户信息".

CAS 应用

- SCIFINDER DISCOVERY PLATFORM
- CAS SciFinder[®]
- CAS Analytical Methods
- CAS Formulus
- STN IP PROTECTION SUITE
- STNext
- CAS Scientific Patent Explorer
- REGULATORY
- CAS Chemical Compliance Index
- ACCOUNT MANAGEMENT
- CAS Profile

账户信息

- What's New?
- Help and Support
- My CAS Profile
- Settings
- Log Out

历史记录

Recent Search History	历史记录	View All Search History
August 22, 2023		
References 2:29 PM	Toripalimab and "chemotherapy" and "non-small-cell lung cancer" (41 Results)	Rerun Search Edit Search

大纲

- CAS 与 CAS SciFinder Discovery Platform (Academic) 简介
- 科研信息的高效查阅
 - **如何拓展文献调研?**
 - 如何调研某类物质?
 - 如何调研反应信息?
 - 怎么查、怎么选具体的实验方案?
- 常见问题



如何拓展文献检索？

- 主题词怎么选择？如何构建？
- 研究某结构相关的文献？
- 如何筛选文献？追踪最新进展？
- 关注某篇文献的被引文献和引文——引文地图

检索目标课题研究文献

主题词、物质名称、CAS 登记号、专利号、PubMed ID、文献号、DOI 号

All Substances Reactions References Suppliers

Solid wast| 自动提示

- Solid waste
- Solid wastes
- Solid wastes, food
- Solid wastes, dross
- Solid waste slurries
- Solid waste treatment
- Solid wastes treatment
- Solid wastes, cuttings

Solid waiste| 辅助纠错

- Solid waste
- Solid wastes
- Solid wastes, food
- Biol. solid wastes
- Toxic solid wastes
- Animal solid wastes
- Solid wastes, dross
- Solid waste slurries

利用布尔逻辑运算符 & 通配符精准检索相关文献

- 支持布尔逻辑运算符 (or/and/not), 默认运算顺序 or > and > not
- “ ” 不允许词形变化, 但可出现单数或复数; () 优先运算, 括号中表达式还可以和其他术语交互
- 支持通配符 * 或 ?, * 代表 0 或多个字符, ? 代表 0 或 1 个字符

The screenshot displays the CAS search interface. At the top, there are navigation tabs: All, Substances, Reactions, References (highlighted), and Suppliers. The main search bar contains the query: "Solid wastes" and (treatment or disposal). To the right of the search bar are icons for clearing the search, drawing a structure, and a search icon. Below the search bar, there is an advanced search section with a dropdown menu set to "AND", a field for "Author Name" with the placeholder text "Enter last name, first name middle name.", and an example "Example: Schubert, J A". A button labeled "+ Add Advanced Search Field" is also present. At the bottom, there are three featured search options: "Retrosynthetic Analysis" (Make reaction plans with conditions, yields, catalysts, and experimental procedures.), "Search CAS Lexicon" (Build powerful searches using CAS concepts, chemical classes, and taxonomy.), and "Search CAS Sequences" (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.).

CAS Lexicon 词库检索近义词和相关技术术语

Search CAS Lexicon

Wastewater treatment

Your Query
You may include up to 1,000 terms in a search.

^ Preferred Term

Wastewater treatment
This will search synonyms: Sewage **treatment**; Spent liquor **treatment**;
Wastewater purification
[View fewer synonyms](#)

^ Broader Terms (1)

Waste management

^ Narrower Terms (94)

Acoustic wastewater treatment
 Advanced wastewater treatment
 Aeration wastewater treatment

Wastewater treatment
Wastewater treatment - Narrower Terms (4 Concepts)

Wastewater treatment, anion exchange
 Wastewater treatment, bromination
 Wastewater treatment, bromochlorination
 Wastewater treatment, carbonation
 Wastewater treatment, cation exchange
 Wastewater treatment, chloramination
 Wastewater treatment, chlorination

^ Related Terms (9)

Biochemical oxygen demand
 Chemical oxygen demand
 Purification
 Sewers

Select a boolean operator

Learn more about

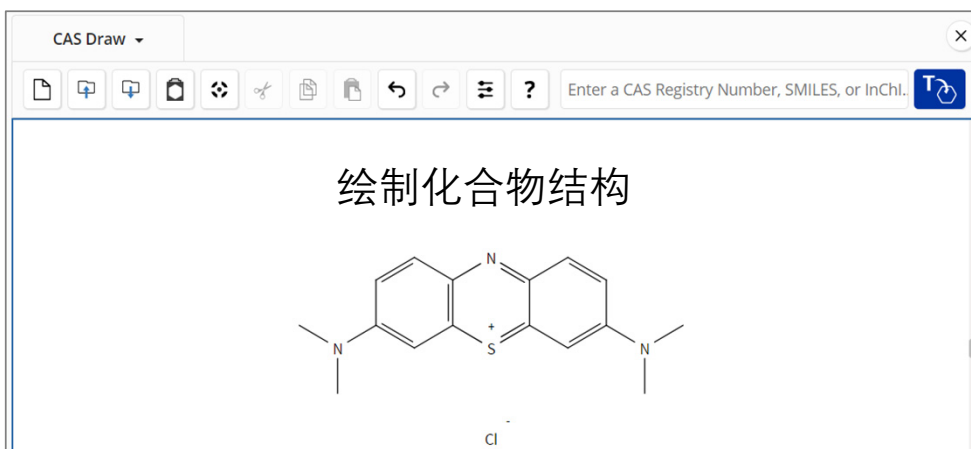
➤ Preferred Terms
➤ Broader Terms
➤ Narrower Terms
➤ Related Terms

根据作者/出版物/研究机构/物质结构检索相关文献

The screenshot displays the CAS search interface. At the top, navigation tabs include 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The search bar contains the query '"Solid wastes" and (treatment or disposal)'. Below the search bar, there are options for 'AND' and 'Abstract/Keywords'. A yellow box highlights the '+ Add Advanced Search Field' button, with an arrow pointing to a dropdown menu. The dropdown menu lists the following search fields: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked with a 'NEW' badge), Publication Year, Document Identifier, Patent Identifier, and Publisher. To the right of the search bar, there is a 'Draw' button and a search icon. Below the search bar, there are three main sections: 'Retrosynthetic Analysis' (Make reaction plans with conditions, yields, catalysts, and experimental procedures), 'Search CAS Sequences' (Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences), and a partially visible section 'es using'. The text '物质结构' (Material Structure) is written in yellow on the right side of the interface.

自定义高级检索项

物质结构与关键词联合检索文献



文本与物质结构检索是“and”关系

All Substances Reactions **References** Suppliers

wastewater and (treatment or disposal)

AND Author Name Enter last name, first name middle name. Example: Schubert, J A

+ Add Advanced Search Field

Edit Drawing Remove

检索结果分析与筛选

➤ As Drawn 精确结构

绘制结构中可出现 R 基团、可变基团；绘制结构中价态未达饱和的原子只能接氢；如有环系，不与其他环耦合或成桥环

➤ Substructure 亚结构

包括 As Drawn 检索结果，价态未达饱和的原子可以连接氢以外的其他原子；如果有环系，可形成其他环

References search for "wastewater and (treatment or disposal)" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

- AS Drawn (19K)
- Substructure (19K)

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Substance Role

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

19,328 Results

Sort: Times Cited View: Partial Abstract

1

Adsorption of methylene blue on low-cost adsorbents: A review

By: Rafatullah, Mohd.; Sulaiman, Othman; Hashim, Rokiah; Ahmad, Anees
Journal of Hazardous Materials (2010), 177(1-3), 70-80 | Language: English, Database: CPlus and MEDLINE

A review. In this article, the use of low-cost adsorbents for the removal of methylene blue (MB) from solution has been reviewed. Adsorption techniques are widely used to remove certain classes of pollutants from waters, especially those which are not easily biodegradable. The removal of MB, as a pollutant, from waste waters of textile, paper, printing and other industries has been addressed by the researchers. Currently, a combination of biol. treatment and adsorption on activated carbon is becoming more common for removal of dyes from wastewater. Although com. activated carbon is a preferred...

View More

Full Text

Substance (1) Reactions (0) Citing (2,182) Citation Map

2

Photocatalytic degradation pathway of methylene blue in water

By: Houas, A.; Lachheb, H.; Ksibi, M.; Elaloui, E.; Guillard, C.; Herrmann, J.-M.
Applied Catalysis, B: Environmental (2001), 31(2), 145-157 | Language: English, Database: CPlus

The TiO₂/UV photocatalytic degradation of methylene blue (MB) was studied in aqueous heterogeneous suspensions. In addition to a prompt removal of the color, TiO₂/UV-based photocatalysis was simultaneously able to oxidize the dye, with an almost complete mineralization of C and of N and S heteroatoms into CO₂, NH₄⁺, NO₃⁻ and SO₄²⁻, resp. A detailed degradation pathway was determined by a careful identification of intermediate products, in particular aromatics, whose successive hydroxylations lead to the aromatic ring opening. These results suggest that TiO₂/UV photocatalysis may be envisaged a...

View More

Full Text

Substances (3) Reactions (0) Citing (2,137) Citation Map

Sort: Relevance

- Relevance
- Times Cited
- Accession Number: Ascending
- Accession Number: Descending
- Publication Date: Newest
- Publication Date: Oldest

结果集二次检索研究内容: Search Within Results

^ Search Within Results

Search for up to 3 text strings within the result set.

Adsorption

Search

References search for "wastewater and (treatment or disposal)" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (19K)

Substructure (19K)

Filter Behavior

Filter by Exclude

^ Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Searching for... Clear All

Adsorption X

Document Type

Substance Role

Language

Filtering: Search Within Results: Adsorption X Clear All Filters

10,167 Results Sort: Times Cited View: Partial Abstract

1

Adsorption of methylene blue on low-cost adsorbents: A review

By: Rafatullah, Mohd.; Sulaiman, Othman; Hashim, Rokiah; Ahmad, Anees
Journal of Hazardous Materials (2010), 177(1-3), 70-80 | Language: English, Database: CPlus and MEDLINE

A review. In this article, the use of low-cost adsorbents for the removal of methylene blue (MB) from solution has been reviewed. **Adsorption** techniques are widely used to remove certain classes of pollutants from waters, especially those which are not easily biodegradable. The removal of MB, as a pollutant, from **waste waters** of textile, paper, printing and other industries has been addressed by the researchers. Currently, a combination of biol. **treatment** and **adsorption** on activated carbon is becoming more common for removal of dyes from **wastewater**. Although com. activated carbon is a preferred...

View More

Full Text Substance (1) Reactions (0) Citing (2,182) Citation Map

2

Kinetics and mechanism of removal of methylene blue by adsorption on various carbons - a comparative study

By: Kannan, Nagarethinam; Sundaram, Mariappan Meenakshi
Dyes and Pigments (2001), 51(1), 25-40 | Language: English, Database: CPlus

The kinetics and mechanism of methylene blue **adsorption** on com. activated C (CAC) and indigenously prepared activated carbons from bamboo dust, coconut shell, groundnut shell, rice husk, and straw, were studied. The effects of various exptl. parameters were studied using a batch **adsorption** technique to obtain information on treating **effluents** from the dye industry. The extent of dye

物质角色筛选文献: Substance Role

- ^ Substance Role
- Process (9,604)
 - Occurrence (7,386)
 - Properties (645)
 - Uses (437)
 - Reactant or Reagent (266)
- [View All](#)

排序:

文献数量

字母顺序

Substance Role

By Count | Alphanumeric

3 Selected

- Process (9,604)
- Removal or Disposal (9,021)
- Pollutant (7,378)
- Occurrence (7,386)
- Physical, Engineering, or Chemical Process (5,569)
- Properties (645)
- Uses (437)
- Reactant or Reagent (266)
- Reactant (257)
- Technical or Engineered Material Use (227)
- Biological Study (162)
- Other Use, Unclassified (134)
- Biochemical P
- Occurrence, U
- Analytical Stu
- Analyte (54)
- Modifier or Ad
- Preparation (3
- Catalyst Use (
- Purification o
- Adverse Effic
- Biological Stu
- Analytical Rol
- Biological Use

Substance Role

By Count | Alphanumeric

3 Selected

- Adverse Effect (19)
- Analyte (54)
- Analytical Reagent Use (9)
- Analytical Role, Unclassified (12)
- Analytical Study (74)
- Biochemical Process (110)
- Biological Study (162)
- Biological Study, Unclassified (18)
- Biological Use, Unclassified (12)
- Catalyst Use (22)
- Formation, Non-preparative (4)
- Formation, Unclassified (3)
- Geological or Astronomical Formation (1)
- Miscellaneous (5)
- Modifier or Additive Use (35)
- Nanoscale (7)
- Occurrence (7,386)
- Occurrence, Unclassified (105)
- Other Use, Unclassified (134)
- Pharmacological Activity (1)
- Physical, Engineering, or Chemical Process (5,569)
- Pollutant (7,378)
- Polymer in Formulation (2)
- Preparation (32)
- Process (9,604)
- Properties (645)
- Purification or Recovery (21)
- Reactant (257)
- Reactant or Reagent (266)
- Reagent (9)
- Removal or Disposal (9,021)
- Synthetic Preparation (11)
- Technical or Engineered Material Use (227)
- Therapeutic Use (3)
- Uses (437)

OK Cancel

确定文献核心研究内容: Concept

Concept

Top Count Alphanumeric Search

7 Selected

- Adsorptive wastewater treatment (6,189)
- Adsorption (5,796)
- pH (3,185)
- Adsorbents (3,177)
- Surface area (2,804)
- Surface structure (2,453)
- Decolorization wastewater treatment (1,696)
- Wastewater treatment (1,666)
- Temperature (1,479)
- Dyes (1,376)
- Pore size distribution (1,298)
- Pore size (1,174)

OK Cancel

Concept 自定义检索

Top Count Alphanumeric Search

Concept Name

wastewater Search

8 Selected

<input checked="" type="checkbox"/> Absorptive wastewater treatment (78)	<input type="checkbox"/> Degassing wastewater treatment (1)	<input type="checkbox"/> Oxidative wastewater treatment (107)
<input type="checkbox"/> Acidic wastewater (2)	<input type="checkbox"/> Demineralization wastewater treatment (4)	<input type="checkbox"/> Oxidative wastewater treatment, wet air oxidation (2)
<input type="checkbox"/> Acidification wastewater treatment (2)	<input type="checkbox"/> Deodorization wastewater treatment (2)	<input type="checkbox"/> Oxygenation wastewater treatment (1)
<input type="checkbox"/> Acoustic wastewater treatment (27)	<input type="checkbox"/> Dephosphorization wastewater treatment (2)	<input type="checkbox"/> Petroleum refining wastewater (1)
<input type="checkbox"/> Activated-sludge process wastewater treatment (6)	<input type="checkbox"/> Detoxication wastewater treatment (2)	<input type="checkbox"/> Photocatalytic oxidation wastewater treatment (44)
<input checked="" type="checkbox"/> Adsorptive wastewater treatment (6,189)	<input type="checkbox"/> Dialysis wastewater treatment (1)	<input type="checkbox"/> Photocatalytic wastewater treatment (872)
<input type="checkbox"/> Advanced wastewater treatment (2)		

← Prev 1 2 Next →

OK Cancel

筛选不同研究领域文献：CA Section

- ^ CA Section
- Waste Treatment and Disposal (7,876)
 - Unit Operations and Processes (513)
 - Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (460)
 - Water (236)
 - Surface Chemistry and Colloids (222)
- [View All](#)

CA Section

By Count | Alphanumeric

3 Selected

<input checked="" type="checkbox"/> Waste Treatment and Disposal (7,876)	<input type="checkbox"/> Industrial Carbohydrates (24)	<input type="checkbox"/> Sewage and Wastes (4)
<input type="checkbox"/> Unit Operations and Processes (513)	<input checked="" type="checkbox"/> Plastics Manufacture and Processing (23)	<input type="checkbox"/> Biochemical Methods (3)
<input type="checkbox"/> Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (460)	<input type="checkbox"/> Pharmaceuticals (20)	<input type="checkbox"/> Industrial Organic Chemicals, Leather, Fats, and Waxes (3)
<input type="checkbox"/> Water (236)	<input type="checkbox"/> Textiles and Fibers (15)	<input type="checkbox"/> Organic Analytical Chemistry (3)
<input checked="" type="checkbox"/> Surface Chemistry and Colloids (222)	<input type="checkbox"/> Electrochemistry (14)	<input type="checkbox"/> Ferrous Metals and Alloys (2)
<input type="checkbox"/> Industrial Inorganic Chemicals (116)	<input type="checkbox"/> Electric Phenomena (13)	<input type="checkbox"/> Inorganic Analytical Chemistry (2)
<input type="checkbox"/> Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms (107)	<input type="checkbox"/> Fossil Fuels, Derivatives, and Related Products (10)	<input type="checkbox"/> Nuclear Technology (2)
<input type="checkbox"/> Plastics Fabrication and Uses	<input type="checkbox"/> Magnetic Phenomena (10)	<input type="checkbox"/> Thermodynamics, Thermochemistry, and Thermal Properties (2)
	<input type="checkbox"/> Air Pollution and Industrial Hygiene (8)	<input type="checkbox"/> Cement, concrete, and Related Building Materials (1)
	<input type="checkbox"/> Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers (8)	<input type="checkbox"/> Coatings, Inks, and Related





OK Cancel

文献结果集管理

合并、下载、分享和保存

References search for "wastewater and (treatment or disposal)" + drawn structure

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

    Save and Alert

Structure Match

As Drawn (19K)

Substructure (19K)

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Substance Role

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Filtering: Search Within Results: Adsorption X Substance Role: 5 Selected X Clear All Filters

Concept: 3 Selected X CA Section: 3 Selected X

7,458 Results Sort: Times Cited View: Partial Abstract





1

Adsorption of methylene blue on low-cost adsorbents: A review
By: Rafatullah, Mohd.; Sulaiman, Othman; Hashim, Rokiah; Ahmad, Anees
Journal of Hazardous Materials (2010), 177(1-3), 70-80 | Language: English, Database: CAPLUS and MEDLINE

A review. In this article, the use of low-cost adsorbents for the removal of methylene blue (MB) from solution has been reviewed. **Adsorption** techniques are widely used to remove certain classes of pollutants from waters, especially those which are not easily biodegradable. The removal of MB, as a pollutant, from **waste waters** of textile, paper, printing and other industries has been addressed by the researchers. Currently, a combination of biol. **treatment** and **adsorption** on activated carbon is becoming more common for removal of dyes from **wastewater**. Although com. activated carbon is a preferred...

[View More](#)

Full Text ▾

 Substance (1)  Reactions (0)  Citing (2,182)  Citation Map

2

Kinetics and mechanism of removal of methylene blue by adsorption on various carbons - a comparative study
By: Kannan, Nagarethinam; Sundaram, Mariappan Meenakshi

保存和提醒



Save Results and Create Alert

Name

"Solid wastes" and (treatment or disposal)

Save Options

Query Only

Selected Answers

All Answers (Up to 20,000)

Alert Frequency

No Alerts

As Available

Weekly

Monthly

Add Existing Tags (Optional)

Innocare

New Tag (Optional)

Tag Color

- 结果保存
- 自定义提醒频率
- 标签分类

下載和分享



Share Results

Use My Default Mail App

Send with CAS SciFinder[®]

Share Results

Email(s)

ddu@acs-i.org ×

Include Message (Optional)

Send Cancel 3000 Characters Remaining



Download Reference Results

File Type: PDF

Select Quantity: All Results, Selected Results, Range (ex. 2 to 20)

Display: Result Summary, Result Details

File Name: Reference_20230628_1301

Include: Task History, Abstract, Concepts, Substances, Formulations, Analytical Methods, Citations

Download Cancel Learn more about downloads.

File Type

PDF

Citation (.ris)

Excel (.xlsx)

PDF

Quoted (.txt)

Rich Text (.rtf)

Tagged (.txt)

合并



Combine Reference Results

Select a Combine Option:

Add
[Select](#)

Intersect
[Select](#)

Subtract
[Select](#)

[Learn More About Combine](#)

- 并集
- 交集
- 差集

Combine Reference Results: Subtract

Select 1 Saved Item: [← Return to Combine Option](#)

<input checked="" type="radio"/>	"Solid wastes" and (treatment or disposal)	Query	September 13, 2023
<input type="radio"/>	Test 0907	Query	September 7, 2023
<input type="radio"/>	Molecular sieves	Query	September 1, 2023
<input type="radio"/>	Orthosteric binding pocket	1,531 Saved Results	August 8, 2023
<input type="radio"/>	PD-Rotigotine	237 Saved Results	August 8, 2023
<input type="radio"/>	Parkinson disease	Query	August 8, 2023

Select 1 Saved Item to Subtract:

Subtract the **selected saved item** from the **current answer set**.

Subtract the **current answer set** from the **selected saved item**.

[View Results](#) [Cancel](#) [Learn More About Combine](#)

查看目标文献详情

Use of cellulose-based wastes for adsorption of dyes from aqueous solutions

Substances (7) Reactions (0) Citing (1,175) Citation Map

JOURNAL

Source
Journal of Hazardous Materials
Volume: 92
Issue: 3
Pages: 263-274
Journal: Article; Research Support, Non-U.S. Gov't
2002
DOI:
[10.1016/s0304-3894\(02\)00017-1](https://doi.org/10.1016/s0304-3894(02)00017-1)

CODEN: JHMAD9
ISSN: 0304-3894
ISSN-L: 0304-3894

Database Information
AN: 2002:372829
CAN: 137:205692
PubMed ID: 12031611
CAlplus and MEDLINE

Company/Organization
Department of Chemical Engineering
National Taiwan University
Taipei 106
Taiwan

By: Annadurai, Gurusamy; Juang, Ruey-Shin; Lee, Duu-Jong

Low-cost banana and orange peels were prepared as adsorbents for the adsorption of dyes from aqueous solutions. Dye concentration and pH were varied. The adsorption capacities for both peels decreased in the order methyl orange > methylene blue > Rhodamine B > Congo Red > methyl violet > Amido Black 10B. The isotherm data could be well described by the Freundlich and Langmuir equations at concentrations 10-120 mg/L. An alk. pH was favorable for the adsorption of dyes. Based on the adsorption capacity, it was shown that banana peel was more effective than orange peel. Kinetic parameters of adsorption such as the Lagergren rate constant and the intraparticle diffusion rate constant were determined. For the present adsorption process intraparticle diffusion of dyes within the particle was identified to be rate limiting. Both peel wastes were promising materials for adsorption of dyes from aqueous solutions

Keywords: cellulose waste adsorption dye wastewater

View Source Full Text

Similar References NEW Get Similar References

- Adsorption of dyes from aqueous solution by chromium-containing leather waste**
Zhongguo Pige (2004), 33(13), 10-13 | Language: Chinese, Database: CAlplus
- Adsorptive removal of Methylene blue dye from an aqueous solution using wter hyacinth root powder as a low cost adsorbent**
International Journal of Chemical Sciences and Applications (2012), 3(3), 338-345 | Language: English, Database: CAlplus
- Equilibrium modelling of adsorptive removal of methylene blue using BGA**
Oriental Journal of Chemistry (2012), 28(1), 519-524 | Language: English, Database: CAlplus

Expand All | Collapse All

Concepts CAS 科学家提供的核心研究点

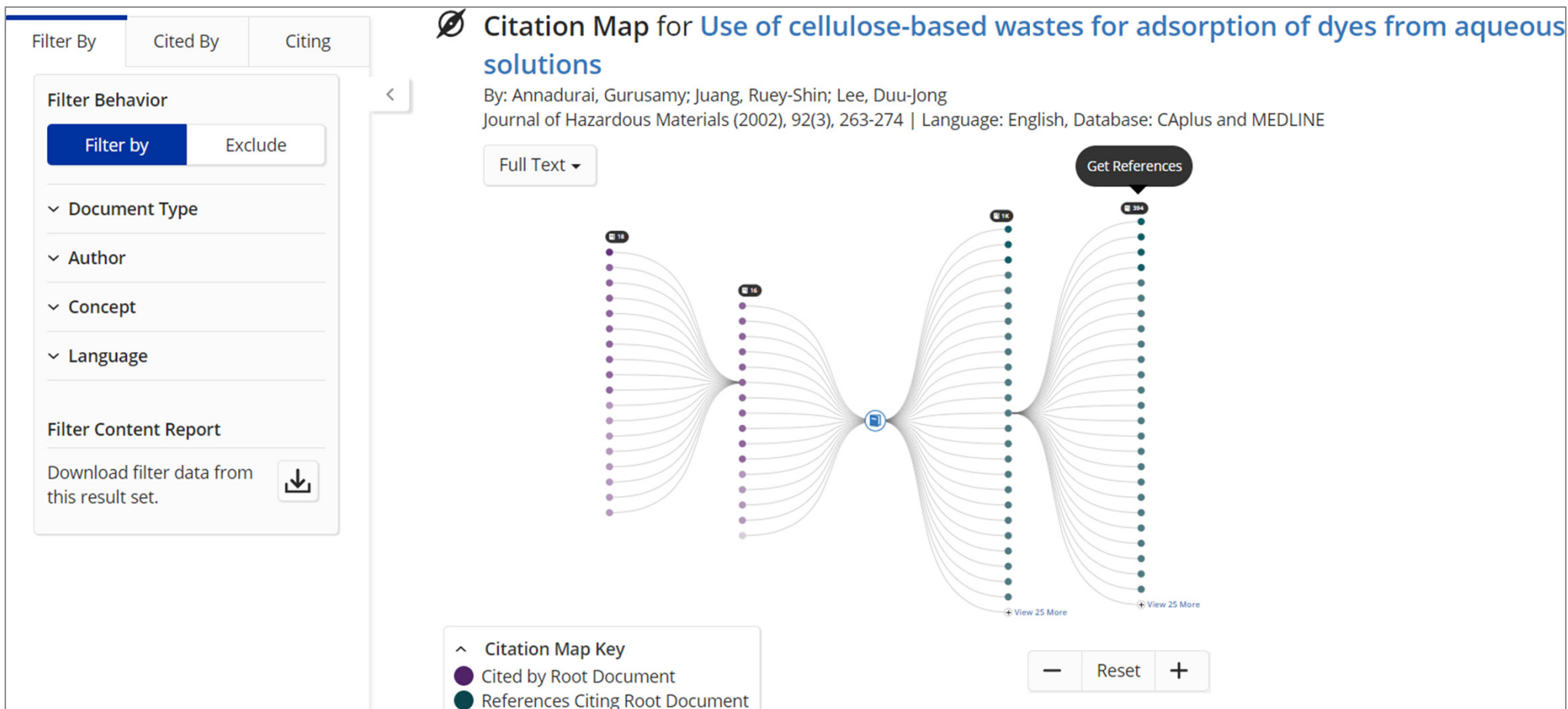
Adsorption	Dyes
Adsorptive wastewater treatment	Musa Modifier: peel of
Citrus sinensis Modifier: peel of	Orange Modifier: peel of
Decolorization wastewater treatment	

Substances 重点研究物质

Substances (7)

61-73-4 C ₁₆ H ₁₈ N ₅ S.Cl Phenothiazin-5-ium, 3,7-bis(dimethylamino)-, chloride (1:1) Role: Removal or Disposal, Process	9004-34-6 Image Not Available Unspecified Cellulose Role: Unspecified
1064-48-8 C ₂₂ H ₁₆ N ₆ O ₉ S ₂ .2Na 2,7-Naphthalenedisulfonic acid, 4-amino-5-hydroxy-3-[2-(4-nitrophenyl)diazenyl]-... Role: Removal or Disposal, Process	573-58-0 C ₃₂ H ₂₄ N ₆ O ₆ S ₂ .2Na 1-Naphthalenesulfonic acid, 3,3'-[[1,1'-biphenyl]-4,4'-diylbis(2,1-diazenediyl)]-... Role: Removal or Disposal, Process

绘制引文地图: Citation Map



查看专利详情

Method for treating organic dye in waste water

Substances (14) Reactions (0) Citing (1) Citation Map

By: Tong, Shanghai

A method for treating organic dye in waste water having effectively adsorbed organic dyes is provided. The method comprises the following steps: (1) soaking the sponge in the graphene oxide suspension emulsion to obtain a graphene oxide composite sponge, adding the graphene oxide composite sponge in a mixture of nanometer photocatalyst and reducing agent to obtain a photocatalyst-modified graphene composite sponge a hydrogel, washing and drying the photocatalyst-modified graphene composite sponge hydrogel to obtain a photocatalyst-modified graphene composite sponge; (2) adsorbing wastewater containing organic dyes through adsorption reactor equipped with photocatalyst-modified graphene composite sponge to adsorb organic dyes in the wastewater; and (3) taking out the adsorbed saturated photocatalyst-modified graphene composite sponge, and performing the catalytic decomposition of organic dyes under illumination to obtain regenerated photocatalyst-modified graphene composite sponge.

Keywords: organic dye wastewater adsorption reducing treatment

PatentPak Viewer Get Prior Art Analysis Full Text

Similar References

Recyclable preparation method of recyclable nano-carbon/titanium oxide-based photocatalytic materials for...
China CN116493003 A 2023-07-28 | Language: Chinese, Database: CAplus

Composite sponge containing modified graphene for adsorption of organic dye pollutants
World Intellectual Property Organization WO2020258930 A1 2020-12-30 | Language: Chinese, Database: CAplus

Preparation method of iron-based metal organogel/bacterial cellulose composite material, and its application in removing...
China CN113477229 A 2021-10-08 | Language: Chinese, Database: CAplus

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN110182887	Chinese	A	PDF PDF+ Viewer	2019-08-30	CN2019-10567857	2019-06-27
WO2020258931	Chinese	A1	PDF PDF+ Viewer	2020-12-30	WO2020-CN80333	2020-03-20

Priority Application

Priority Application Number	Application Date
CN2019-10567857	2019-06-27

IPC Data

Patent	Class	Patent Family Classification Codes
CN110182887	IPC1	C02F 0001/28; C02F 0001/30; C02F 0101/30
WO2020258931	IPC1	C02F 0001/28; C02F 0001/30; C02F 0101/30

Concepts

Substances

PatentPak Viewer 高效阅读专利

CAS PatentPak

PAGE 2 / 9 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

Analyst Markup Locations (1)
Page 2

CAS RN 61-73-4

• Cl⁻

Analyst Markup Locations (1)
Page 2

CAS RN 81-88-9

• Cl⁻

Analyst Markup Locations (1)
Page 2

废水中的有机染料；

(3) 将吸附饱和的光催化剂改性石墨烯复合海绵取出，在光照下催化分解有机染料，得到再生的光催化剂改性石墨烯复合海绵。

2. 根据权利要求1所述的处理方法，其特征在于，所述的氧化石墨烯悬乳液中氧化石墨烯的浓度为2~15mg/ml。

3. 根据权利要求1所述的处理方法，其特征在于，所述的纳米级光催化剂为纳米二氧化钛、纳米氧化锌或纳米氧化锡。

4. 根据权利要求1所述的处理方法，其特征在于，所述的还原剂为水合肼、抗坏血酸或氨水。

5. 根据权利要求1所述的处理方法，其特征在于，纳米级光催化剂与还原剂的质量比为1:5~30。

6. 根据权利要求1所述的处理方法，其特征在于，纳米级光催化剂和还原剂的混合液中，纳米级光催化剂的浓度为0.2~1mg/ml，且还原剂的浓度为2~10mg/ml。

7. 根据权利要求1所述的处理方法，其特征在于，所述的海绵选自聚氨酯海绵、三聚氰胺海绵、聚酯海绵、聚醚海绵或聚乙烯醇海绵中的一种。

8. 根据权利要求1所述的处理方法，其特征在于，步骤(2)中，含有机染料的废水经过3级以上吸附处理。

9. 根据权利要求1所述的处理方法，其特征在于，所述的有机染料选自甲基橙、亚甲基蓝、罗丹明B、甲基紫、中性红中的一种或多种。

10. 根据权利要求1~9任一项所述的处理方法，其特征在于，步骤(1)中，海绵在浸泡之前，经过超声清洗、洗涤和干燥。

精准定位

Mark	Page #	CAS RN	Name	Structure
2	p.2	1034343-98-0D	Graphene oxide	
4	p.2	1034343-98-0	Graphene	
5	p.2	13463-67-7	Titanium oxide (TiO ₂)	O=Ti=O
6	p.2	1314-13-2	Zinc oxide (ZnO)	Zn=O
7	p.2	1332-29-2	Tin oxide	
8	p.2	302-01-2	Hydrazine	H ₂ N—NH ₂
9	p.2	50-81-7	L-Ascorbic acid	
10	p.2	1336-21-6	Ammonium hydroxide ((NH ₄)(OH))	H ₄ N—OH
12	p.2	108-78-1	1,3,5-Triazine-2,4,6-triamine	
15	p.2	9002-89-5	Ethanol, homopolymer	
16	p.2	547-58-0	Benzenesulfonic acid, 4-[2-[4-(dimethylamino)phenyl]diazonyl]-, sodium salt (1:1)	
17	p.2	61-73-4	Phenothiazin-5-ium, 3,7-bis(dimethylamino)-, chloride (1:1)	

CAS 科学家增值标引的信息

小结

1. 检索词的构建：使用布尔逻辑算符及通配符连接主题词，CAS Lexicon 丰富选词
2. 利用高级检索选项以及文本与结构联合进行自定义组合检索
3. 通过聚类筛选工具快速获得目标文献
4. 利用引文地图拓展检索
5. 使用 PatentPak 高效阅读专利

如何调研某类物质？

- 快速检索聚合物或无机化合物？
- 利用谱图数值确认产物或杂质？从属性值出发，调研某类材料？
- 检索完整分子结构？通式结构？或含有某些片段的物质？
- 如何确认结构新颖性？

检索研究所需物质

Substances Reactions References Suppliers

物质/文献标识符

Search by Substance Name, CAS RN, Patent Number, P

AND Molecular Formula

+ Add Advanced Search Field

高级检索

- Molecular Formula
- CAS Registry Number >
- Chemical Identifier >
- Document Identifier
- Patent Identifier
- Experimental Spectra >
- Bioactivity Data **NEW** >
- Biological >
- Chemical Properties >**
 - Koc
 - logD
 - logP
 - Mass Intrinsic Solubility (g/L)
 - Mass Solubility (g/L)
 - Molar Intrinsic Solubility (mol/L)
 - Molar Solubility (mol/L)
 - Molecular Weight
 - pKa
 - Vapor Pressure (Torr)
- Density >
- Electrical >
- Lipinski >
- Magnetic >
- Mechanical >
- Optical and Scattering >
- Structure Related >
- Thermal >

结构检索

26CuN2O5.C2H3N

Search CAS Sequences

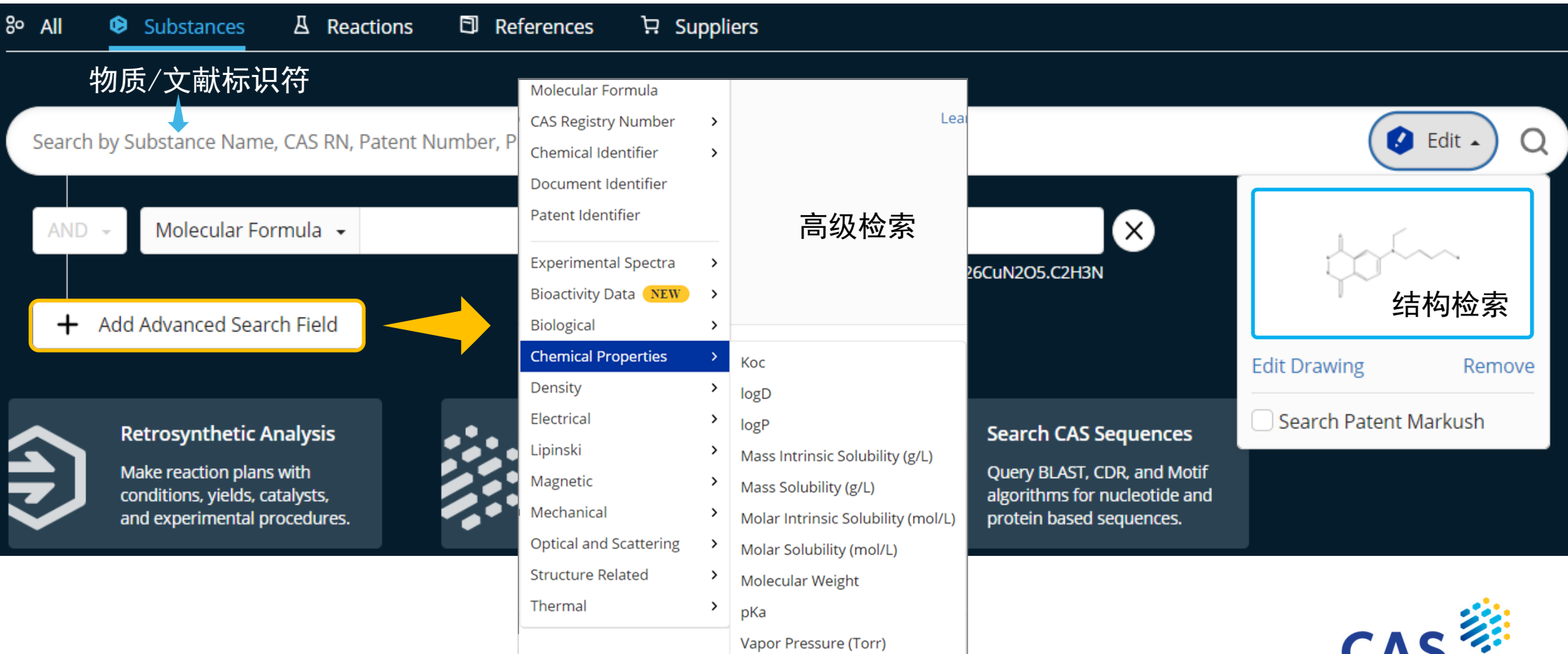
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

Retrosynthetic Analysis

Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Edit Drawing Remove

Search Patent Markush



物质/文献标识符检索与结果集排序

Substances search for "66612-29-1 Acridinium ester"

2 Results

Sort: Number of References: Descending

View: Partial

Filter Behavior: Filter by Exclude

Search Within Results

Reaction Role: Product (1), Reactant (1), Reagent (1)

Reference Role: Occurrence (2), Preparation (2), Process (2), Synthetic Preparation (2), Analyte (1)

Result 1: 66612-29-1
Chemical structure: C14H20N4O2
N-(4-Aminobutyl)-N-ethylisoluminol
426 References, 48 Reactions, 68 Suppliers

Result 2: 157321-55-6
Image Not Available
Notes: An acridinium ester (Hoechst Behring)
Unspecified
MA 70 (onium compound)
2 References, 0 Reactions, 0 Suppliers

Substances search for "10.1021/acs.analchem.6b00276"

11 Results

Sort: Relevance

View: Partial

Filter Behavior: Filter by Exclude

Search Within Results

Reaction Role: Product (10), Reactant (6), Reagent (8), Catalyst (7), Solvent (1)

Reference Role: Analytical Reagent Use (10), Analytical Study (10), Biological Study (10), Biological Use, Unclassified (10), Physical, Engineering, or Chemical Process (10)

Bioactivity Data

Commercial Availability

Result 1: 7440-57-5
Au
Gold
606K References, 20K Reactions, 1,306 Suppliers

Result 2: 7722-84-1
HO—OH
H₂O₂
Hydrogen peroxide
392K References, 268K Reactions, 128 Suppliers

Result 3: 1317-61-9
Image Not Available
Fe₃O₄
Iron oxide (Fe₃O₄)

Result 4: 58-85-5
Chemical structure: C10H16N2O3S
Absolute stereochemistry shown, Rotation (+)
C₁₀H₁₆N₂O₃S
Biotin

Result 5: 110-94-1
Chemical structure: C5H8O4
C₅H₈O₄
Glutaric acid

Sort: Relevance

- Relevance
- CAS RN: Ascending
- CAS RN: Descending
- Molecular Formula: Ascending
- Molecular Formula: Descending
- Molecular Weight: Ascending
- Molecular Weight: Descending
- Number of References: Ascending
- Number of References: Descending
- Number of Suppliers

- 可同时检索多个物质识别符（物质名称或 CAS 登记号）
- 双引号“ ”可精确识别物质识别符
- 不同物质用空格隔开，支持 **2000** 个字符

分子式检索物质

不含碳元素，按元素符号首字母顺序书写

含碳元素，碳排第一位，氢排第二位，
其他元素符号按首字母顺序书写

金属离子和阴离子间用点·隔开，
补充和阳离子等同个数的氢原子

Search by Substance Name, CAS RN, Patent Number, PubMed ID,
Molecular Formula Co_2O_3

Substances search for " Co_2O_3 " Molecular Formula

4 Results

1308-04-9
Image Not Available
 Co_2O_3
Cobalt oxide (Co_2O_3)

8,257 References 119 Reactions 12 Suppliers

Search by Substance Name, CAS RN, Patent Number, PubMed ID,
Molecular Formula CH_2O_3

Substances search for " CH_2O_3 " Molecular Formula

51 Results

463-79-6

 CH_2O_3
Carbonic acid

32K References 578 Reactions 8 Suppliers

Search by Substance Name, CAS RN, Patent Number, PubMed ID,
Molecular Formula $\text{H}_2\text{O}_4\text{S}\cdot 2\text{Na}$

Substances search for " $\text{H}_2\text{O}_4\text{S}\cdot 2\text{Na}$ " Molecular Formula

9 Results

7757-82-6

 $\text{H}_2\text{O}_4\text{S}\cdot 2\text{Na}$
Components: 2
Component RN: 7664-93-9
Sodium sulfate

116K References 57K Reactions 213 Suppliers

谱图和分子量联合检索物质

- H 谱化学位移：3.5, 6.5 至 7.5, 11.1
- 分子量：170 至 200

The screenshot shows the CAS search interface with the following elements:

- Navigation tabs: All, Substances, Reactions, References, Suppliers.
- Search bar: Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.
- Filter 1: Proton NMR, 3.5, 6.5 to 7.5, 11.1. Allowance of ± 0.2 ppm. Examples: 8.03, 7.2, 2.63 | 5.95, 7 to 8.5 | 6.3.
- Filter 2: AND, Molecular Weight, 170 to 200. Predicted values only. Examples: 46.07 | 125 to 350 | >300.
- Button: + Add Advanced Search Field.

The screenshot shows the Experimental Spectra dropdown menu with the following options:

- Proton NMR
- Carbon-13 NMR
- Nitrogen-15 NMR
- Fluorine-19 NMR
- Phosphorus-31 NMR

The screenshot shows the Chemical Properties dropdown menu with the following options:

- Koc
- logD
- logP
- Mass Intrinsic Solubility (g/L)
- Mass Solubility (g/L)
- Molar Intrinsic Solubility (mol/L)
- Molar Solubility (mol/L)
- Molecular Weight
- pKa
- Vapor Pressure (Torr)

- 从小到大的顺序输入检索信息
- 英文模式下输入逗号和空格

谱图和分子量联合检索物质

Substances search for 2 Advanced Fields

References Reactions Suppliers Save and Alert

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

- Product (123)
- Reactant (103)
- Reagent (9)
- Catalyst (9)

Reference Role

- Preparation (123)
- Synthetic Preparation (122)
- Reactant (104)
- Reactant or Reagent (104)
- Properties (65)

Bioactivity Data

Commercial Availability

- Available (108)
- Not Available (15)

Number of Components

123 Results

Sort: Relevance View: Partial

1 5418-95-1

Nc1nc2c(c1)ccc2N=C

$C_8H_9N_5$
2-Guanidinobenzimidazole

277 References 397 Reactions 64 Suppliers

2 157086-07-2

O=C[C@H]1[C@@H](c2ccccc2)[C@H]3[C@@H](O)C=C[C@H]13

$C_{14}H_{14}O$
rel-(1*R*,2*R*,3*R*,4*S*)-3-Phenylbicyclo[2.2.1]hept-5-ene-2-carboxaldehyde

38 References 133 Reactions 2 Suppliers

3 74163-81-8

O=C(O)[C@@H]1c2ccccc2N1

$C_{10}H_{11}NO_2$
(-)-1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid

358 References 459 Reactions 116 Suppliers

4 712-53-8

COc1cc(O)c(C=O)cc1C(=O)O

$C_9H_8O_5$
3-Formyl-4-hydroxy-5-methoxybenzoic acid

5 1852487-06-9

CC(=O)N=Cc1ccn(C#CC)c1

$C_{10}H_{11}N_3O$
Acetic acid (2*Z*)-2-[[1-(2-propyn-1-yl)-1*H*-pyrrol-2-yl]methylene]hydrazide

6 1319734-00-3

COC1=CC=C2C3=CC=NC=C3N2=C1

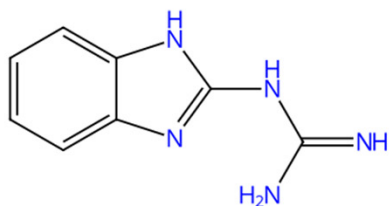
$C_{12}H_{10}N_2O$
7-Methoxy-5*H*-pyrido[3,2-*b*]indole

- 点击 CAS 登记号查看物质详情
- 查看物质相关的文献、反应和供应商信息

查看物质详情

CAS Registry Number: 5418-95-1

References (277) Reactions (397) Suppliers (64)



C₈H₉N₅

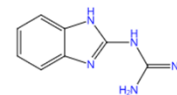
Guanidine, *N*-1*H*-benzimidazol-2-yl- (ACI)

Key Physical Properties	Value	Condition
Molecular Weight	175.19	-
Melting Point (Experimental)	245 °C (decomp)	-
Boiling Point (Predicted)	392.7±25.0 °C	Press: 760 Torr
Density (Predicted)	1.56±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.67±0.30	Most Basic Temp: 25 °C

Experimental Properties | Spectra

Proton NMR Spectrum for 5418-95-1

5418-95-1



C₈H₉N₅

CAS Name
2-Guanidinobenzimidazole

Conditions

Working Frequency

300 MHz

Solvent

DMSO-*d*₆ (2206-27-1)

Temperature

24 °C

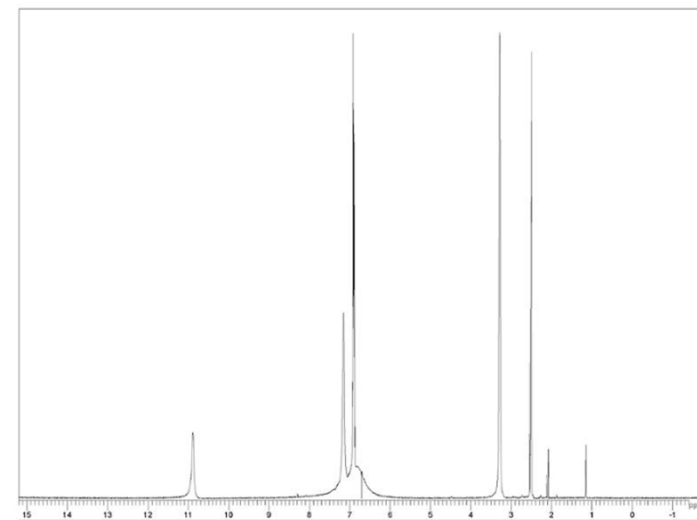
Spectrum Summary

Spectrum ID

ASL_6014117

Source

Spectral data were obtained from
John Wiley & Sons, Inc.



Experimental Spectra

¹H NMR

¹³C NMR

IR

Mass

Raman

Source

[View Proton NMR Spectrum](#)

(1) WSS

[View Proton NMR Spectrum](#)

(1) WSS

[View Proton NMR Spectrum](#)

(2) ENAMINE

利用结构信息检索物质

- X** 可变基团
- R** 自定义基团
- Fn** 片段结构
- []₁₋₄** 重复工具
- C_{cl}** 取代位点可变
- A B** 反应角色标记
- 🔑** 锁定工具

The screenshot displays the CAS Draw software interface. The central workspace shows a chemical structure of a benzothiazine derivative with two 'Ak' substituents. The interface includes a toolbar with various drawing tools, a search bar at the top, and a bottom panel with a zoom slider and OK/Cancel buttons.

41

检索结果集: Structure Match

CAS SciFinder[®] Substances Enter a query... Edit

Return to Home

Substances search for drawn structure

References Reactions Suppliers

Structure Match

- As Drawn (58)
- Substructure (3,742)
- Similarity (9,413)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. [Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

3,742 Results

1 1160823-78-8

C32H54O2S2Sn2
Stannane, 1,1'-[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl]dithiophene

553 References 946 Reactions 58 Suppliers

2 1160823-77-7

C26H38O2S2
Benzo[1,2-*b*:4,5-*b'*]dithiophene, 4,8-bis[(2-ethylhexyl)oxy]-

147 References 245 Reactions 58 Suppliers

3 1223479-75-1

(C40H53NO4S3)n
Poly[(5,6-dihydro-5-octyl-4,6-dioxo-4H-thieno[3,4-*c*]pyrrole-1,3-diyl)[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl]

127 References 94 Reactions 6 Suppliers

4 1044795-08-5

5 1098102-95-4

6 1320201-22-6

As Drawn: 绘制结构中可出现 R 基团和可变基团。绘制结构中价态未达饱和的原子只能接氢，环系（如有）不能与其他的环稠合或成桥环。

Substructure: 包括 As Drawn 的检索结果，另外价态未达饱和的原子可以连接氢以外的其他原子，环系（如有）可以与其他环稠合或成桥环。

Similarity: 获得片段或整体结构与被检索结构相似的物质，母体结构可以被取代和改变。

注意: Similarity 条件下不要绘制通式结构

检索结果集筛选目标物质: Filter Behavior

物质在反应中的角色

- Reaction Role
 - Product (54)
 - Reactant (3)
 - Reagent (1)
- Reference Role
 - Preparation (80)
 - Synthetic Preparation (75)
 - Biological Study (34)
 - Uses (34)
 - Reactant (24)

[View All](#)

物质在文献中的研究角色

Filter Behavior

-
-
-
- Commercial Availability
- Number of Components
- Molecular Weight
- LogP
- Stereochemistry
- Element
-
- Aromatic Rings
-
- Isotopes
- Metals
- Experimental Property
- Experimental Spectrum
- GHS Hazard Statements
- Bioactivity Indicator

<p>1044795-08-5</p>  <p>$C_{40}H_{70}O_2S_2Sn_2$ Stannane, 1,1'-[4,8-bis(dodecyloxy)benzo[1,2-b:4,5-b']]dithiophene-2,6-diylbis[1,1...</p> <p>93 References 171 Reactions 3 Suppliers</p>	<p>1098102-95-4</p>  <p>$C_{32}H_{54}O_2S_2Sn_2$ Stannane, 1,1'-[4,8-bis(octyloxy)benzo[1,2-b:4,5-b']]dithiophene-2,6-diylbis[1,1...</p> <p>87 References 161 Reactions 42 Suppliers</p>	<p>1320201-22-6</p>  <p>$C_{56}H_{102}O_2S_2Sn_2$ Stannane, 1,1'-[4,8-bis[(2-octyldodecyl)oxy]benzo[1,2-b:4,5-b']]dithiophene-2,6-d...</p> <p>67 References 110 Reactions 33 Suppliers</p>
<p>1098102-94-3</p>  <p>$C_{26}H_{38}O_2S_2$ Benzo[1,2-b:4,5-b']dithiophene, 4,8-bis(octyloxy)-</p> <p>7</p>	<p>1226782-13-3</p>  <p>$C_{26}H_{36}Br_2O_2S_2$ Benzo[1,2-b:4,5-b']dithiophene, 2,6-dibromo-4,8-bis[(2-ethylhexyl)oxy]-</p> <p>8</p>	<p>1237479-39-8</p>  <p>($C_{32}H_{54}O_2S_2Sn_2$, $C_{15}H_{17}Br_2F$... Components: 2 Thieno[3,4-b]thiophene-2-carboxylic acid, 4,6-dibromo-3-fluoro-, 2-ethylhexyl es...</p> <p>9</p>

特定官能团

Functional Group

- Amine (103)
- Tertiary amine (102)
- Amide (75)
- Ether (35)
- Alkene (30)

[View All](#)

Substance Class

- Polymer (2,613)
- Organic/Inorganic Small Molecule (1,066)
- Coordination Compound (87)
- Salt and Compound With (10)
- Incompletely Defined Substance (6)

物质类别



CAS Markush 检索，结构查新

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 登记号

预测性物质 (Prophetic Substance)

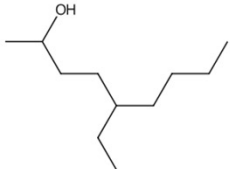
- 使用 Markush 结构陈述的预测物质，一个 Markush 可以陈述数千甚至更多的化学物质
- 被 Markush 结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，则不会被分配 CAS 登记号
- Markush 检索能够检索到仅通过 Substance 可能检索不到的结构

CAS PatentPak

PAGE 14 / 16 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

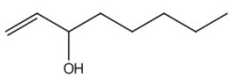
CAS RN 103-08-2



Analyst Markup Locations (2)

- Page 3
- Page 16

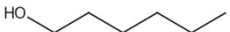
CAS RN 3391-86-4



Analyst Markup Locations (1)

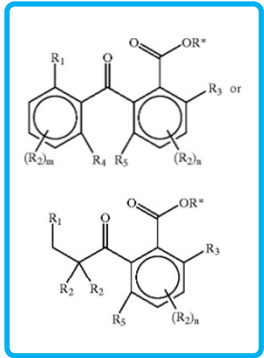
- Page 3

CAS RN 111-27-3



What is claimed is:


1. A perfuming composition containing a compound of formula




(I)

(II)

in which R represents a group of formula



in which X and Y can be identical or different and represent hydrogen, a linear or branched alkyl or alkoxy group from C₁ to C₁₂, a phenyl group, an olefinic group from C₂ to C₁₂, an alcohol group a CO₂M group, a —NR₆R₇ group or a group of formula



20
25
30
35
40
45
50
55

or a polyalcohol or polyether group;

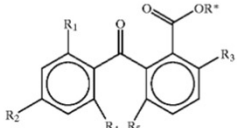
R₃ represents hydrogen, an alkyl or alkoxy group from C₁ to C₄, linear or branched, a OH group or a NH₂ group;

R₄ and R₅, taken separately, can be hydrogen or have the meaning given above for R₁ and can be identical to or different from R₁ or from each other; or R₄ and R₅, taken together, form a bridging group between the two aromatic rings, which bridging group can be a methylene or a keto group; m is an integer from 0 to 3 and n is an integer from 0 to 2; R₆ and R₇, taken separately, each represents hydrogen, an alkyl group from C₁ to C₄, an alcohol group having an alkyl chain from C₁ to C₁₂, or a phenyl group, or R₆ and R₇, taken together with the nitrogen atom form a 5-membered or 6-membered ring optionally containing another hetero atom; R₈ represents hydrogen, an alkyl group from C₁ to C₄, an alcohol group having an alkyl chain from C₁ to C₁₂ or a phenyl group;

M represents hydrogen or an alkali metal; and

R* is the organic part derived from a primary or secondary fragrant alcohol R*OH, wherein the fragrant alcohol is released upon exposure of the composition to light to provide a fragrance.

2. A perfuming composition according to claim 1, wherein the 2-benzoyl benzoate is of formula



完整的结构检索流程

Substances search for drawn structure

References - Reactions - Suppliers

Filtering: Number of Components: 1

Sort: Number of References: Descending View: Partial

485 Results

Structure Match

- As Drawn (0)
- Substructure (0)
- Similarity (501)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Create Chemscape Analysis

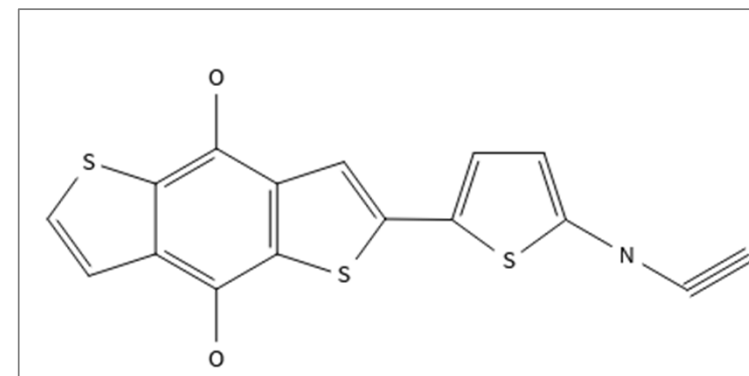
Filter Behavior

Filter by Exclude

Search Within Results

- Similarity
- 80-84 (1)
- 75-79 (5)
- 70-74 (8)
- 65-69 (68)
- 60-64 (403)

Item	Number of Components	Number of Results	References	Reactions	Suppliers
1352642-35-3	1	61	138	250	36
85903-02-2	2	61	32	49	5
1357156-35-4	3	62	31	44	4
1414596-18-1	4	65			
1431705-25-7	5	64			
1173479-25-8	6	61			



Step 1: 物质结构检索

- As Drawn, Substructure 结果为 0
- Similarity 结果中物质最大相似度仅 80-84%

完整的结构检索流程

The screenshot shows the CAS SciFinder interface for a Patent Markush search. At the top, there is a search bar with the text "Substances" and "Enter a query...". To the right of the search bar are buttons for "Edit", a search icon, a notification bell, a bookmark icon, and a user profile icon. Below the search bar, there is a "Return to Home" link and a "Patent Markush search for drawn structure" section. A "References" dropdown menu is visible. On the left side, there is a "Patent Markush Match" section with two buttons: "As Drawn (0)" and "Substructure (1)". Below this is a "Filter Behavior" section with "Filter by" and "Exclude" buttons. Further down are sections for "Patent Office" (Korea, Republic of (1)) and "CA Section" (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers (1)). The main search results area shows "1 Result" and "1" item. The first result is for patent KR2014061623, titled "Organic dyes for dye-sensitized solar cells with good photoelectric conversion efficiency". The chemical structure is shown with substituents G5, G1, and Ak. The authors are Lee, Yun Gu; Kim, Ha Yeong; Kim, Dae Hwan; Sim, Gyo Seung. The patent is from the Korea, Republic of, dated 2014-05-22. The assignee is Daegu Gyeongbuk Institute of Science and Technology. The patent claim 1 is shown with "PatentPak" and "Full Text" dropdown menus. A table of results is also visible:

Patent	Language	Kind Code	PatentPak Options
KR2014061623	Korean	A	PDF PDF+ Viewer
KR1465454	Korean	B1	PDF

Step 2: Markush 结构检索

- 直观呈现检索的结构与专利原文中 Markush 匹配的部分
- 标引结构在专利中的位置
- 详细的结构取代信息描述

物质检索小结

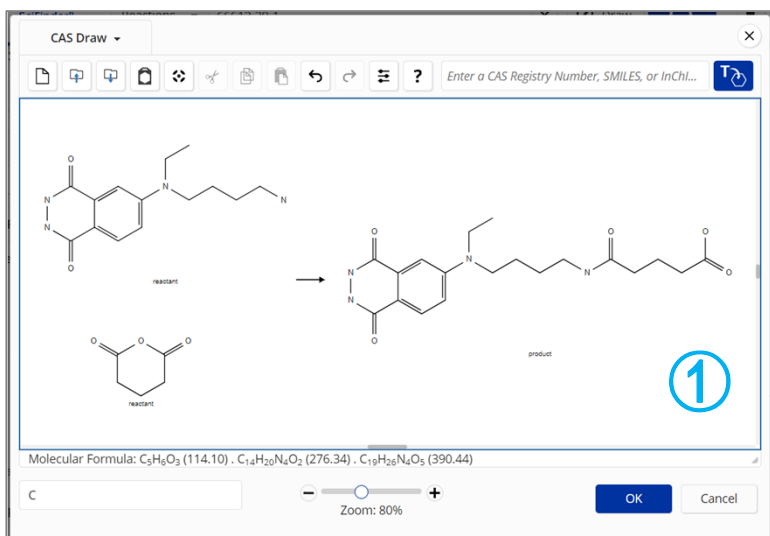
1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解 As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息

3. 如何进行反应调研?

- 如何从我感兴趣的底物、产物或催化剂出发，找到关联的反应？
- 如何查找相似反应？
- 如何关注特定转化类型的反应？
- 如何在大量反应结果中，快速找到最想要的反应？
- 如何查找涉及机理研究的反应？或人名反应？
- 如何设计新化合物的逆合成路线？

反应检索

直接反应检索



Reactions search for drawn structure

References

3 Results

Group: By Document Sort: Relevance View: Collapsed

1

A new isoluminol reagent for chemiluminescence labeling of proteins

By: Palmioli, Alessandro; Crisma, Marco; Peggion, Cristina; Brusasca, PierNatale; Zanin, Davide; et al
Tetrahedron Letters (2013), 54(33), 4446-4450 | Language: English, Database: CPlus

Full Text

Suppliers (68)

Suppliers (92)

2

31-366-CAS-10683461

Steps: 1 Yield: 100%

反应检索结果再编辑

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

- Product (52)
- Reactant (223)

Yield

- 90-100% (41)
- 80-89% (49)
- 70-79% (14)
- 50-69% (9)
- 30-49% (5)

View All

Number of Steps

- 1 (244)
- 2 (12)
- 3 (9)

275 Results

Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (8 Reactions) Steps: 1 Yield: 70-100%

Suppliers (67) Suppliers (129)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 100%

Suppliers (129) Suppliers (52) Suppliers (6)

Expand Scheme

Steps: 1 Yield: 100%

Send to Structure Editor

CAS Draw

Draw or change atoms or bonds.

Molecular Formula: C₈H₇N₃O₂ (207.15) · C₂H₃Cl₂ (98.96)

反应式再编辑

检索物质能够发生的反应

The screenshot shows the CAS SciFinder interface for a search of "1207-12-1". The search results are filtered by "Substance Role: Reactant", yielding 186 results. The interface includes a sidebar with filter options for Substance Role (Product, Reactant, Reagent, Catalyst), Yield (90-100%, 80-89%, 70-79%, 50-69%, 30-49%), and Number of Steps (1). The main content area displays two reaction schemes. Scheme 1 shows a reaction with 6 reactions, 1 step, and a yield of 37-100%. Scheme 2 shows a reaction with 68 reactions, 1 step, and a yield of 100%. Both schemes include chemical structures and supplier information.

物质标识符

The screenshot shows the CAS SciFinder interface for a search of a drawn structure. The search results are filtered by "Substance Role: Reactant", yielding 1,679 results. The interface includes a sidebar with filter options for Substance Role (Product, Reactant, Reagent) and Yield (90-100%, 80-89%, 70-79%, 50-69%, 30-49%). The main content area displays two reaction schemes. Scheme 1 shows a reaction with 1 reaction, 1 step, and a yield of 100%. Scheme 2 shows a reaction with 11 reactions, 1 step, and a yield of 100%. Both schemes include chemical structures and supplier information.

物质结构式

在物质结果集中查看能够发生的反应

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match: As Drawn (114), Substructure (370K), Similarity (8,561)

Filtering: Number of Components: 1

Sort: Number of References: Descending

363,361 Results

Item	Chemical Name	Formula	References	Reactions	Suppliers
1	Dibenzothiophene	C ₁₂ H ₈ S	13K	2,435	118
2	Dibenzothiophene, 4,6-dimethyl-	C ₁₄ H ₁₂ S	2,646	238	79
3	Boronic acid, B-4-dibenzothenyl-	C ₁₂ H ₉ BO ₂ S	1,390	2,596	112
4	Dibenzothiophene, 5,5-dioxide	C ₁₂ H ₈ O ₂ S	1,264	804	82
5	Dibenzothiophene, 4-methyl-	C ₁₃ H ₁₀ S	1,228	154	49
6	Dibenzothiophene, 2-bromo-	C ₁₂ H ₇ BrS	1,048	2,125	91

- 查找系列衍生物
- 数据关联查阅相关反应

关注反应的催化剂/机理研究或人名反应？

References search for "Petroleum hydrodesulfurization and catalyst"

Substances ▾ **Reactions ▾** Citing ▾ Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#)

[Load More Results](#)

Filter Behavior

[Filter by](#) [Exclude](#)

Search Within Results

Document Type

Language

Publication Year

Available at My Institution

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

13,703 Results Sort: Times Cited View: Partial Abstract

1

An overview of new approaches to deep desulfurization for ultra-clean gasoline, diesel fuel and jet fuel

By: Song, Chunshan
Catalysis Today (2003), 86(1-4), 211-263 | Language: English, Database: CPlus

This review with references discusses the problems of sulfur reduction in highway and non-road fuels and presents an overview of new approaches and emerging technologies for ultra-deep desulfurization of refinery streams for ultra-clean (ultra-low-sulfur) gasoline, diesel fuels and jet fuels. The issues of gasoline and diesel deep desulfurization are becoming more serious because the **crude oils** refined in the US are getting higher in sulfur contents and heavier in d., while the regulated sulfur limits are becoming lower and lower. Current gasoline desulfurization problem is dominated by the is...

[View More](#)

Full Text ▾ Substances (0) Reactions (0) Citing (1,755) Citation Map

2

Science and technology of novel processes for deep desulfurization of oil refinery streams: a review

By: Babich, I. V.; Moulijn, J. A.
Fuel (2003), 82(6), 607-631 | Language: English, Database: CPlus

A review. Oil refinery related catalysis, particularly **hydrodesulfurization** (HDS) processes, is viewed as a mature technol., but his view could also stifle potential new ideas. The applicability and perspectives of various desulfurization technologies are evaluated taking into account the requirements of the produced fuels. The progress achieved during recent years in catalysis-based HDS technologies (synthesis of improved **catalysts**, advanced reactor design, combination of distillation and HDS) and in non-HDS processes of sulfur removal (alkylation, extraction, precipitation, oxidation, and ad...

[View More](#)

Full Text ▾ Substances (4) Reactions (0) Citing (1,373) Citation Map

- 查找特定研究领域中的文献
- 数据关联查阅文献中的反应

反应检索结果集分组与排序

Reactions from References

References ▾

Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

1,720 Results

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (80)

80-89% (55)

70-79% (54)

50-69% (73)

30-49% (39)

View All


Number of Steps

1 (943)

2 (407)

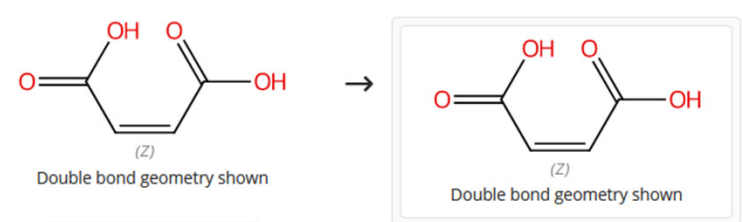
3 (153)

Scheme 1 (1 Reaction) Steps: 1 Yield: 100% ⋮



Expand Scheme ▾

Scheme 2 (1 Reaction) Steps: 1 Yield: 100% ⋮



Double bond geometry shown (Z)

Double bond geometry shown (Z)

- Relevance
- Publication Date: Newest
- Publication Date: Oldest
- Yield
- Number of Steps: Ascending
- Number of Steps: Descending

根据不参与反应的官能团筛选反应

Reactions from References

出现在反应前后，但未发生变化的官能团

References ▾

1,720 Results

Group: By Scheme ▾ Sort: Relevance ▾ View: Collapsed ▾

Filter Behavior

Filter by Exclude

Search Within Results


Yield

Number of Steps

Non-Participating Functional Groups

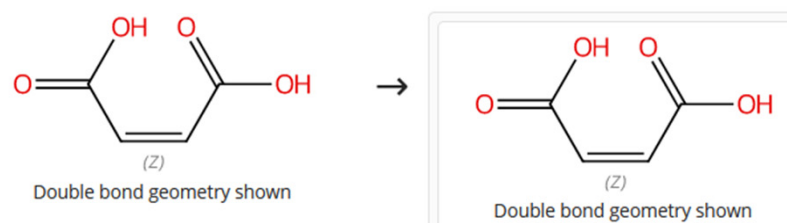
- Alkene (190)
- Cyclic alkene (151)
- Sulfide (126)
- Organometal (120)
- Diene (118)
- Alkene (190)
- Secondary amine (28)
- Ether (22)
- Alcohol (14)
- Cyclic alcohol (14)
- Alkyl halide (11)
- Cyclic ketone (10)
- Ketone (10)
- Acyclic alkene (9)
- Alkyne (7)
- Imine (7)

Scheme 1 (1 Reaction)



Expand Scheme ▾

Scheme 2 (1 Reaction)



Double bond geometry shown (Z)

Double bond geometry shown (Z)

便捷查看详细反应操作

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Synthetic Methods (633)

Experimental Procedure (369)

Reaction Type

Stereochemistry


Reagent

Catalyst

Filtering: Experimental Protocols: Experimental Procedure X Clear All Filters

369 Results Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%



31-138-CAS-6276270 Steps: 1 Yield: 100% Carbon-Sulfur Bond Cleavage and Hydrodesulfurization of Thiophenes by Tungsten


1.1 Reagents: Hydrogen Solvents: Benzene-d₆; 30 min, 1 atm, rt

By: Sattler, Aaron; et al Journal of the American Chemical Society (2011), 133(11), 3748-3751

Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 100%



Reaction Overview

Steps: 1 Yield: 100%

JOURNAL

Carbon-Sulfur Bond Cleavage and Hydrodesulfurization of Thiophenes by Tungsten

By: Sattler, Aaron; et al View All Journal of the American Chemical Society (2011), 133(11), 3748-3751

View Source Full Text

Company/Organization

Department of Chemistry Columbia University new York, New York 10027 United States

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrogen	-	Benzene-d ₆	30 min, 1 atm, rt

Alternative Steps (0)

Experimental Protocols

Synthetic Methods Experimental Procedure

Products (2-Ethylbenzenethiolato)trihydrotetraakis(trimethylphosphine)tungsten, Yield: 100%

Reactants ((Dimethylphosphino-κP)methyl-κC)[2-(η²-ethenyl)benzenethiolato-κ5]tris(trimethylphosphine)tungsten

Reagents Hydrogen

Solvents Benzene-d₆

Procedure

1. Treat a solution of (κ¹, η²-CH₂CHC₆H₄S)W(PMe₃)₃(η²-CH₂PM₂) (5 mg, 0.01 mmol) in d₆-benzene (ca. 0.7 mL) in an NMR tube equipped with a J. Young valve with H₂ (ca. 1 atmosphere).
2. Monitor the sample by ¹H NMR spectroscopy, there by demonstrating that (κ¹, η²-CH₂CHC₆H₄S)W(PMe₃)₃(η²-CH₂PM₂) converts to W(PMe₃)₄(SC₆H₄Et)H₃ over a period of ca. 30 minutes at room temperature.

Transformation Replacement of Metals by Hydrogen/ Demetallation Reduction of Double or Triple Bonds/ Hydrogenation

Scale milligram

- Experimental Protocols
- 查看详细合成方法或实验过程

无需浏览原文即可获取详细的实验信息

逆合成反应路线设计

Good Evening, Dexin

All Substances Reactions **References**

Search by Keyword, Substance Name, CAS RN, Patent Number, PubM

Author Name Enter last name, first name middle

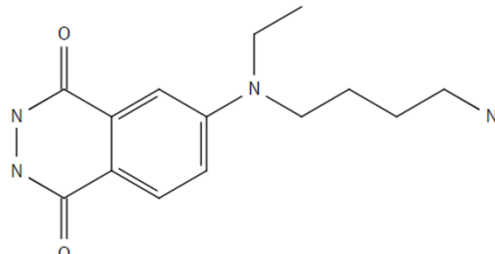
+ Add Advanced Search Field

Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search C...
CAS conce...
classes, and

Retrosynthetic Analysis
Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI.



Molecular Formula: C₁₄H₂₀N₄O₂ (276.34)

Zoom: 100%

Start Retrosynthetic Analysis Cancel

逆合成反应路线设计

The screenshot displays the CAS search interface. On the left, the 'Substances search for drawn structure' panel shows search filters: 'References' (81), 'Reactions' (37), and 'Suppliers' (28). The 'Structure Match' section includes 'As Drawn (1)', 'Substructure (29)', and 'Similarity (12K)'. The search results show one result for CAS RN 194357-64-7, with its chemical structure and name: Acridinium, 9-[[4-[[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-2,6-dimethylphenoxy]...]. A blue arrow points from the structure to the 'Start Retrosynthetic Analysis' button in the substance details panel. The details panel also includes options for 'Get Substance Details', 'Get Bioactivity Data', 'Get Reactions (37)', 'Synthesize (30)', 'Get References (81)', and 'Get Suppliers (28)'. A large chemical structure of the target molecule is shown on the right.


- 先进行物质检索
- 点击目标化合物，弹出物质菜单
- 点击 Start Retrosynthetic Analysis

预设路线参数

Retrosynthesis Plan Options for 194357-64-7 Powered by ChemPlanner®

Select Synthetic Depth **反应深度** [Learn more.](#)

1 2 3 4



Set Rules Supporting Predicted Reactions **反应规则常见性** [Learn more.](#)

Common Uncommon (includes Common Rules) Rare (includes Common and Uncommon Rules)

Set Starting Materials Cost Limit **起始原料费用** [Learn more.](#)

1000 USD/mol

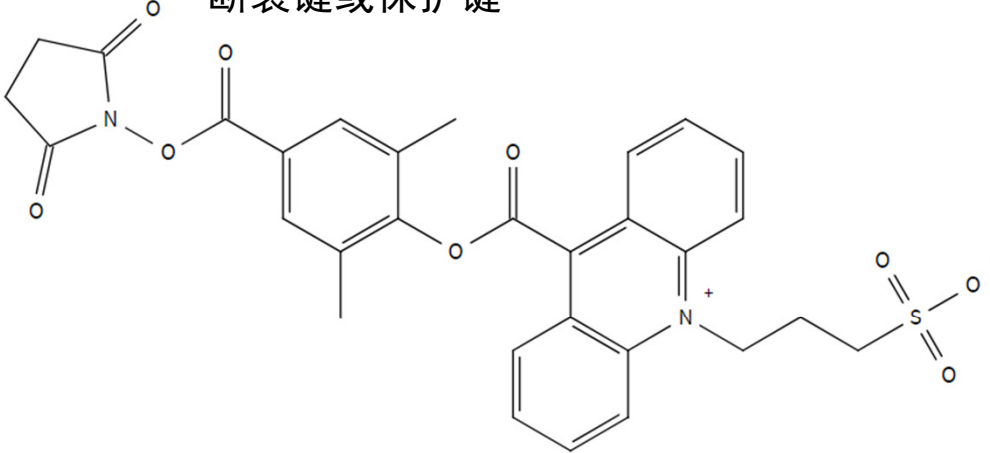
Email me when my plan is complete

[Create Retrosynthesis Plan](#)

Break and Protect Bonds [Learn more.](#)

Break Bond Protect Bond [Clear All Bond Selections](#)

断裂键或保护键



路线概览和参数调节

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options Save

路线概览

Estimated Yield: 14%
Overall Price: \$31,964.74
(USD per 100 grams)

Scoring Profiles 参数调节

Complexity Reduction

Convergence High

Evidence

Cost

Yield Low

Atom Efficiency Medium

Apply Reset Scoring

Retrosynthesis Plan Diagram:

Step 1: A (33) → B (13) + C (96) (Max Yield 56%)

Step 2: B (13) + C (96) → D (27) + E (33) (Max Yield 28%)

Step 3: D (27) + E (33) → F (146) + G (97) (Max Yield 87%)

Step	Evidence
A ⇒ B + C	1.1 Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate; 16 h, rt → 155 °C; 155 °C → 40 °C View All Experimental Protocols
B ⇒ D + E	1.1 Reagents: Tosyl chloride Solvents: Pyridine; rt → 100 °C
D ⇒ F + G	1.1 Reagents: Dicyclohexylcarbodiimide Solvents: Dimethylformamide; rt → 0 °C; 0 °C; < 5 °C; 5 °C → rt

Feedback

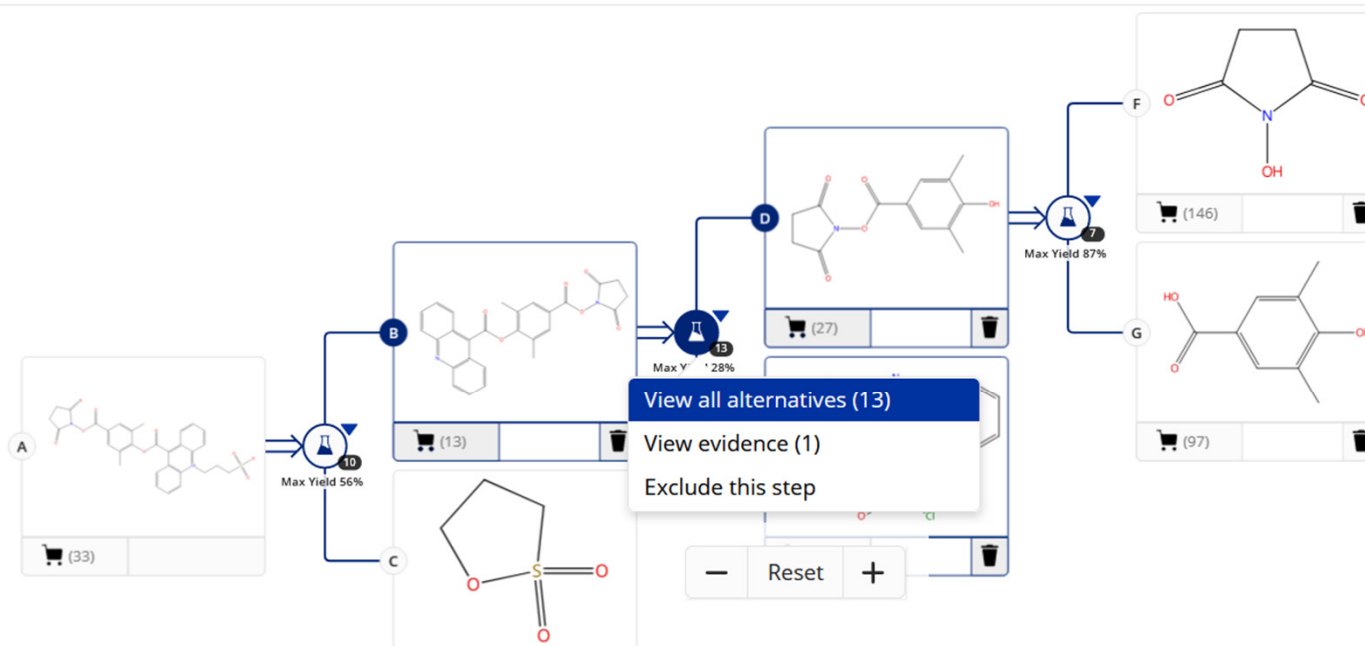
路线详情

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options Download Email Save







- View All Alternatives
查看所有替代路线
- View Evidence
查看某步路线的支持报道
- Exclude This Step
删除不感兴趣的步骤



查看逆合成反应路线中的实验报道

Reactions from Retrosynthesis Plan Evidence

References    

18,384 Results Group: By Scheme Sort: Relevance View: Collapsed

Filter Behavior

Search Within Results

Yield

- 90-100% (2,592)
- 80-89% (2,430)
- 70-79% (1,790)
- 50-69% (1,965)
- 30-49% (740)

[View All](#)

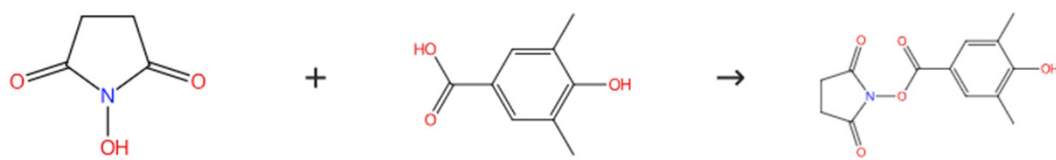
Number of Steps




- 1 (18K)

Non-Participating Functional Groups

- Amide (17K)
- Ether (4,066)

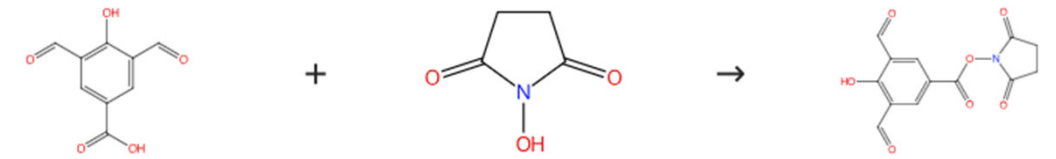
Scheme 1 (2 Reactions) Steps: 1 Yield: 37-87% ...





 Suppliers (145)  Suppliers (98)  Suppliers (27)

[Expand Scheme](#)

Scheme 2 (1 Reaction) Steps: 1 Yield: 39% ...



 Suppliers (7)  Suppliers (145)

选择替代路线

Step	Evidence
A ⇒ B + C Maximum Yield: 56% Evidence (1) Alternative Steps (10)	1.1 Solvents: 1-Butyl-3-methylimidazolium hexafluorophosphate ; 16 h, rt → 155 °C; 155 °C → 40 °C View All ▾ Experimental Protocols
B ⇒ D + E Maximum Yield: 28% Evidence (1) Alternative Steps (13)	1.1 Reagents: Tosyl chloride Solvents: Pyridine ; rt → 100 °C

A ⇒ B + C Alternative Steps (10)

Filter by

- Alternative Step Type
 - Experimental (1)
 - Predicted (9)
- Stereochemistry
 - Non-Selective (10)

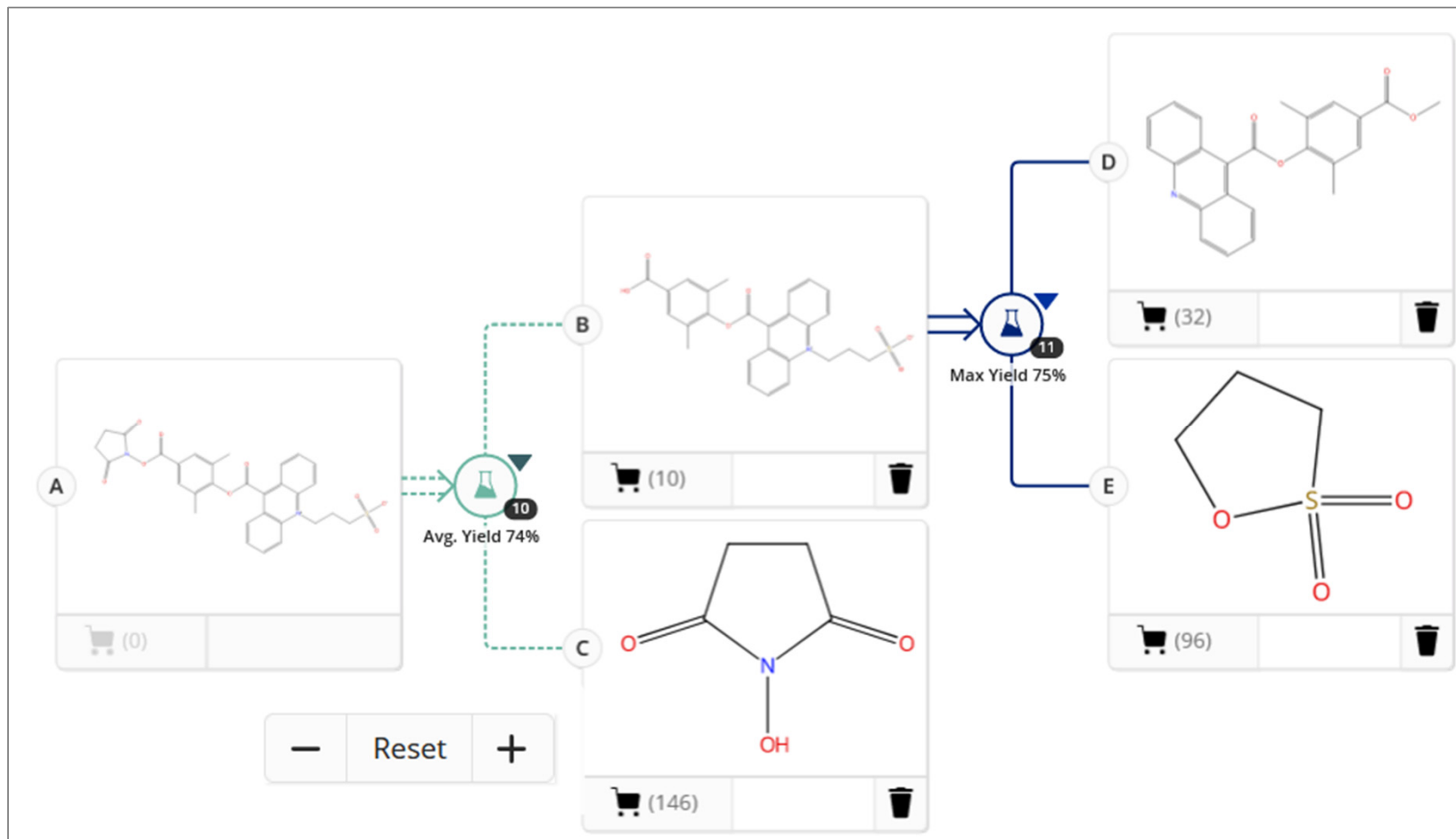
1 of 8 Experimental Step

Selected [View Evidence \(1\)](#) Maximum Yield: 56%

2 of 8 Predicted Step

[Select](#) [View Evidence \(18,500\)](#) Average Yield: 74%

新的逆合成反应路线



反应检索小结

1. 反应检索方法：通过物质标识符、文献标识符、结构式以及文本信息等进行检索
2. 反应结果集筛选精炼：
 - Non-Participating Functional Groups 确定不参与反应的官能团
 - Search Within Results 可在结果集中进行二次筛选
3. 反应详情：Experimental Protocols 获取 CAS 科学家增值标引的反应详情
4. Retrosynthesis 支持化合物的反应路线预测（未知和已知化合物）
5. 支持查看反应路线详情和文献支持，也可以自定义选择替代路线或删除不感兴趣的路线

具体的实验方案怎么查、怎么选？

- 如何获取获得具体的实验操作和表征数据等信息？
- 能一键获取从原文中提取的分析操作和数据详情吗？
- 如何对多种分析方法进行充分评估？
- 我研究的物质有什么具体的配方应用？
- 专利配方的组成和制备工艺是什么？如何进行实验评估？

直观的合成实验详情 Synthetic Methods™

- CAS科学家标引的合成详情
- 节省阅读全文的时间，高效获得所需的合成实验信息

CAS Reaction Number: 31-614-CAS-24450288

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Reaction Overview

Yield: 98%

Suppliers (15)

Suppliers (89)

98%

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl₃)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products [Methyl 2-\(4-bromophenyl\)-7-fluoro-1,2,3,4-tetrahydro-3-\(1-methyl-1H-1,2,4-triazol-5-yl\)-4-oxo-5-quinolinecarboxylate](#), Yield: 98%

Reactants [4-Bromobenzaldehyde](#)
[Benzoic acid, 5-fluoro-2-\(2-\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\)-3-nitro-, methyl ester](#)

Reagents [Hydrochloric acid](#)
[Titanium chloride \(TiCl₃\)](#)
[Water](#)

Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

View PDF Full Text

Company/Organization
Werner Siemens Imaging Center,
Department of Preclinical Imaging
and Radiopharmacy
Eberhard Karls University
Tuebingen 72076
Germany

Procedure

1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature.
3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
4. Quench the mixture by the slow addition of water (260 mL).
5. Pour the reaction mixture into a separating funnel.
6. Extract the mixture with ethyl acetate (4 x 140 mL).
7. Pool the organic fractions.
8. Wash the organic fractions with NaHCO₃ (3 x 60 mL) and NaHSO₃ (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na₂SO₄).
10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
12. Dry the resulting yellow syrup under high vacuum to obtain product.

Transformation

Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/
Knoevenagel Reaction
Reduction of Nitro Compounds to Amines

Scale gram

Characterization Data

5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-, methyl ester

State yellow amorphous solid

Transformations

1. Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
2. Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/ Knoevenagel Reaction
3. Reduction of Nitro Compounds to Amines

CAS Method Number 3-315-CAS-33168860

CAS 分析实验方法详情

- CAS科学家标引的分析实验详情
- 无需下载全文，高效获得所需的分析实验信息

Analysis of Vanadium in Stainless steel by Electrochemical extraction

CAS MN: 1-119-CAS-286328

Method Category: Element Detection

Technique: Electrothermal atomic absorption spectroscopy; Decomposition; Electrochemical extraction

Materials	Role	Image	CAS RN	
Vanadium	analyte	View Structure	7440-62-2	
Stainless steel	matrix		12597-68-1	
Al ₂ O ₃ cutting wheel	material	实验原料		
SiC grinding paper	material			
0.05 μm pore size polycarbonate filter	material			
Standard calomel reference electrode	material			
Platinum ring counter electrode	material			
Hollow cathode lamps	material			
Electrodeless discharge lamp	material			
THGA graphite tubes	material			
Nitric acid	reagent		View Structure	7697-37-2
Hydrofluoric acid	reagent		View Structure	7664-39-3
Acetylacetone	reagent		View Structure	123-54-6
Chromium	reagent		View Structure	7440-47-3
Methanol	reagent		View Structure	67-56-1
Tetramethylammonium chloride	reagent		View Structure	75-57-0

Source

Determination of alloying and impurity elements from matrix and inclusions from a process sample of a double stabilized stainless steel

Sipola, Teijja; Alatarvas, Tuomas; Fabritius, Timo; Peramaki, Paavo

ISIJ International (2016), 56 (8), 1445 - 1451. Iron and Steel Institute of Japan

CODEN: IINTEY | ISSN: 09151559 | DOI: 10.2355/isijinternational.isijint-2016-071

文献来源

[Full Text](#) [View in CAS SciFinder](#)

[Abstract](#) ^

Equipment Used

Cutting machine, Secotom-10, Struers

Ultrasonic cleaning unit, P 30 H, Elmasonic

Grinding machine, Labopol-6, Struers

Potentiostat, SP-150, BioLogic

Vacuum pump, BUSCHI

Graphite furnace atomic absorption spectrometer, AAnalyst 600, PerkinElmer

Autosampler, AS-800, PerkinElmer

分析仪器

Conditions

Instrument

internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm; injection volume: 10 μL

分析条件

Instructions

Preparation of stainless steel process samples

1. Cut stainless steel pieces from a corner piece of different slabs using a Struers Secotom-10 cutting machine with an Al₂O₃ cutting wheel.
2. Grind and polish the steel samples using a Struers Labopol-6 grinding machine with SiC grinding paper to a size of approximately 15 x 10 x 5 mm.
3. Clean the sample from grinding paper traces using an Elmasonic P 30 H ultrasonic cleaning unit (frequency 37 kHz, room temperature).
4. Clean all glassware in an acid bath, rinse with ultrapure water and methanol sequentially.

Electrolytic extraction of stainless steel using 10% acetylacetone

1. Perform electrolytic extraction on a BioLogic SP-150 potentiostat.
2. Use 10% acetylacetone (10 v/v% acetylacetone, 1 w/v% tetramethylammonium chloride and methanol) as the electrolyte.
3. Use the sample as the working electrode and set the potential to 0.150 V vs. the standard calomel electrode (SCE).
4. Suspend the sample in the electrolyte in a platinum basket and use a platinum ring as a counter electrode.
5. Filter the electrolyte through a 0.05 μm pore size polycarbonate filter with the help of a BUSCHI vacuum pump.
6. Expose the sample to ultrasound in methanol and filter the methanol with the electrolyte.

Decomposition of inclusions

1. Dry the polycarbonate filter containing the extracted inclusions overnight in a desiccator.
2. Place the dry filter in a PTFE container with 5 mL concentrated nitric acid and 2 mL HF and close gently.
3. Perform decomposition for 30 minutes at 120 °C (393.15 K).
4. Cool the containers to room temperature, remove the filter and dilute to the volume with water.
5. Prepare a blank sample similarly by filtering a fresh electrolyte through a polycarbonate filter.

Quantification of inclusions using graphite furnace atomic absorption spectrometry (GFAAS) with Cr as a matrix modifier

1. Perform GFAAS on a PerkinElmer AAnalyst 600 graphite furnace atomic absorption spectrometer equipped with an AS-800 autosampler and PerkinElmer THGA graphite tubes (standard platform B0504033).
2. Use a hollow cathode lamp (HCL) as the radiation source.
3. Use the following furnace program: ramp for 10 s to 110 °C, hold for 30 s; ramp for 10 s to 140 °C, hold for 30 s; ramp for 10 s to 1300 °C, hold for 20 s; perform atomization at 2400 °C for 6 s; ramp for 1 s to 2500 °C and hold for 5 s.
4. Set the instrument parameters as follows: internal gas flow rate: 250 mL/min (non-atomization), 0 mL/min (atomization); current: 15 mA; wavelength: 318.4 nm; slit width: 0.7 nm.
5. Add 0.05 μg Cr as a matrix modifier.
6. Inject 10 μL of the sample and perform measurements.

操作步骤

Validation

Linearity Range 0-400 μg/L

Concentration < 1 μg

数据有效性

关注文献关联的分析实验方法？

方法一：文献结果集页面点击 CAS Solutions中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法

References search for "Water pollutants Analysis"

Substances Reactions Citing Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? Learn about result relevance. [Load More Results](#)

Filtering: CAS Solutions: Analytical Methods [Clear All Filters](#)

90,278 Results Sort: Times Cited View: Partial Abstract

1

Determination of organic compounds in water using dispersive liquid-liquid microextraction
By: Rezaee, Mohammad; Assadi, Yaghoub; Milani Hosseini, Mohammad-Reza; Aghaee, Elham; Ahmadi, Fardin; Berijani, Sana
Journal of Chromatography A (2006), 1116(1-2), 1-9 | Language: English, Database: CAplus and MEDLINE
[Analytical Methods](#)

A new microextraction technique termed dispersive liquid-liquid microextraction (DLLME) was developed. DLLME is a very simple and rapid method for extraction and preconcentration of organic compounds from H₂O samples. In this method, the appropriate mixture of extraction solvent (8.0 μL C₂Cl₄) and disperser solvent (1.00 mL acetone) are injected into the aqueous sample (5.00 mL) by syringe, rapidly. Therefore, cloudy solution is formed. In fact, it is consisted of fine particles of extraction solvent which is dispersed entirely into aqueous phase. After centrifuging, the fine particles of extr...
[View More](#)

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Substance Role

Language

Publication Year

Available at My Institution

CAS Solutions

Analytical Methods (23)

Formulus (9)

Reactions (0) Citing (2,797) Citation Map

Concepts	
MEDLINE® Medical Subject Headings	
Substances	
Analytical Methods	
Title	CAS Method Number
Analysis of Naphthalene in Water by Liquid-liquid microextraction	1-143-CAS-36077
Analysis of Naphthalene in Water by Liquid-liquid microextraction	1-143-CAS-43362
Analysis of Naphthalene in Surface waters by Liquid-liquid microextraction	1-143-CAS-91087
Analysis of Naphthalene in Water by Liquid-liquid microextraction	1-143-CAS-119593
Analysis of Naphthalene in Water by Liquid-liquid microextraction	1-143-CAS-187909

直接检索感兴趣的分析实验方法

方法二：登录 <https://methods.cas.org> 进行主题检索或分类浏览

CAS Solutions Analytical Methods

★ Saved Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

Agricultural Applications / Analysis	Fuels / Geology / Biofuels	Pharmacology / Toxicology
Bioassays	Historical Analysis / Dating	Polymer Analysis
Biomolecule Isolation	Miscellaneous	Water Analysis
Environmental Analysis	Organic Compound Analysis	
Food Analysis	Organometallics / Inorganics	

方法分类: 13大类, 45小类

农业应用、生物鉴定、
生物分子分离、环境、
食品、考古、有机物、
药学、毒理学等

Browse Method Categories > Environmental Analysis

Air Analysis	Pesticide Residue Analysis	Water / Wastewater / Sludge Analysis
Environmental Analysis	Soil Analysis	

如何选择合适的分析方法?

The screenshot displays a search interface with a left-hand filter panel and a main results area. The filter panel includes sections for Analyte, Matrix, Method Category, Technique, and Year. The main area shows two search results, each with a title, CAS number, and a list of keywords. The first result is for the analysis of Phenanthrene in Wastewater, and the second is for the analysis of Bisphenol M in Wastewater. Both results include buttons for 'View Details & Instructions' and 'Add to Compare' or 'Remove from Compare'.

Filter By

- Analyte**
 - Copper (2719)
 - Lead (2536)
 - Cadmium (2393)
 - Mercury(2+) (1769)
 - Zinc (1644)
 - [View All](#)
- Matrix**
 - Drinking waters (19706)
 - River waters (15404)
 - Wastewater (9690)
 - Water (9196)
 - Lake waters (6581)
 - [View All](#)
- Method Category**
 - Water / Wastewater / Sludge Analysis (57447)
 - Element Detection (8153)
 - Anion Cation Analysis (8060)
 - Environmental Analysis (4942)
 - Suboptimal Analysis (4846)
 - [View All](#)
- Technique**
 - Solid phase extraction (12386)
 - HPLC (5310)
 - Fluorescence spectroscopy (4756)
 - UV-visible spectroscopy (3586)
 - Spectrophotometry (3406)
 - [View All](#)
- Year**

57447 Results Sort Relevance

1

Analysis of Phenanthrene in Wastewater by Magnetic solid phase extraction
CAS MN: 1-143-CAS-553068

[View Details & Instructions](#) [Add to Compare](#)

Analyte: Pyrene; Acenaphthene; Anthracene; Acenaphthylene; Phenanthrene; Benzo[a]pyrene
Matrix: Wastewater
Other Materials: Reagent: Ethanol; 1,2-Dibromoethane; Sodium chloride; Ferrous sulfate heptahydrate; Ferric chloride hexahydrate; Ammonia; Acetonitrile; Sulfuric acid; Octadecylamine
[View All](#)

Method Category: **Water / Wastewater / Sludge Analysis**

Technique: Liquid-liquid microextraction; Magnetic solid phase extraction; Gas chromatography; Flame ionization detectors

Equipment Used: Gas chromatograph; Injector; Flame ionization detector

Source: Facile and rapid preparation of magnetic octadecylamine nanocomposite and its application as a capable adsorbent in magnetic dispersive solid phase extraction of some polycyclic aromatic hydrocarbons from wastewater samples
Farajzadeh, Mir Ali; Fazli, Nasim; Pezhhanfar, Sakha; Mogaddam, Mohammad Reza Afshar
Chemical Papers (2023), 77 (2), 781-794. Springer International Publishing AG
[Full Text](#) [View in CAS SciFinder](#)
[Abstract](#)

2

Analysis of Bisphenol M in Wastewater by Solid phase dispersive extraction
CAS MN: 1-143-CAS-552528

[View Details & Instructions](#) [Remove from Compare](#)

Analyte: Bisphenol M; Bisphenol G; Bis(4-hydroxyphenyl)diphenylmethane; 1,1-Bis(4-hydroxyphenyl)cyclohexane; 2,2-Bis(4-hydroxyphenyl)propane

- 根据待分析物、基质、方法类别、分析技术和发表年份筛选
- 查看分析原料、所用仪器和方法来源
- 支持多种分析实验方法对比

如何选择合适的分析实验方法？

	1	2	3	Preparation
Title	Analysis of Phenanthrene in Wastewater by Magnetic solid phase extraction	Analysis of Bisphenol M in Wastewater by Solid phase dispersive extraction	Analysis of Anthracene in Drinking waters by Solid phase extraction	<p>Preparation of stock and working standard solutions of polycyclic aromatic hydrocarbons (PAHs)</p> <ol style="list-style-type: none"> 1. Prepare a mixture stock solution of the selected PAHs at a concentration of 100 mg/L in acetonitrile (ACN). 2. Dilute this solution with deionized water to obtain working standard solutions. <p>Preparation of magnetic octadecylamine nanocomposite (octadecylamine@Fe₃O₄) by chemical co-precipitation method</p> <ol style="list-style-type: none"> 1. Add 100 mg of octadecylamine to 50 mL sulfuric acid solution (2 mol/L). 2. Adjust the temperature of the mixture to 80 °C, stir at a rate of 300 rpm for 20 min to dissolve octadecylamine and obtain a clear solution. 3. Add 0.53 g of ferric chloride hexahydrate (FeCl₃·6H₂O) and 0.36 g of ferrous sulfate heptahydrate (FeSO₄·7H₂O) to the solution. 4. Add 20 mL concentrated ammonia solution dropwise to obtain stable brownish color, indicating the generation of Fe₃O₄ nanoparticles. 5. Maintain the solution temperature at 80 °C and stir at 300 rpm. 6. Separate the produced magnetic <p>Collection of water samples</p> <ol style="list-style-type: none"> 1. Collect waste water treatment plant (WWTP) effluent sample, a river water sample and a bottled water sample for analysis. 2. Allow the sample to stand overnight in the dark so that the sedimentation of particulate matter would occur. 3. Spike the decanted supernatants at three concentration levels (25, 75, 125 mg/L) in triplicate and then analyze. <p>Preparation of bisphenol standard solutions</p> <ol style="list-style-type: none"> 1. Prepare individual stock solutions of 500 ppm in methanol and store at 4 °C in the dark until use. 2. Prepare the working solutions of 1 ppb daily by appropriate dilution with 1:10 diluted NH₄Cl-NH₄OH buffer, pH 8.0. <p>Synthesis of solid phase Fe(TTA)₃ complex</p> <ol style="list-style-type: none"> 1. Weigh 4 mmol of HTTA into a 20 mL glass vial and dissolve in 10 mL ethanol. 2. Add 3 mL of 1 mol/L NaOH to dissociate thenoyltrifluoroacetone (HTTA) to its enolate, TTA. 3. Place a magnetic stirrer in the vial and stir the mixture for 5 <p>Preparation of standard solution of polycyclic aromatic hydrocarbons (PAHs)</p> <ol style="list-style-type: none"> 1. Prepare a stock solution of PAHs (10 mg/mL) in methanol and keep in the dark at 4 °C. <p>Preparation of polypyrrole (PPy) coated stainless steel mesh</p> <ol style="list-style-type: none"> 1. Dip bare stainless steel mesh in hydrofluoric acid for 30 min, rinse with deionized water to produce a rough surface. 2. Cut a circle with an inner diameter equal to the syringe's inner diameter from the etched stainless steel mesh. 3. Deposit PPy coating on the pretreated meshes by electrochemical deposition by a Metrohm electroanalyzer Model 797 VA computrace. 4. Perform deposition by cyclic voltammetry based on the three-electrode system including stainless steel mesh as the working electrode, an Ag/AgCl electrode as the reference electrode and a platinum wire electrode as the auxiliary electrode. 5. Perform electropolymerization of PPy film on the meshes in a nitrogen-saturated solution containing 0.1 mol/L pyrrole monomer and 0.5 mol/L sulfuric
CAS Method Number	1-143-CAS-553068	1-143-CAS-552528	1-143-CAS-552414	
Method Category	Water / Wastewater / Sludge Analysis	Water / Wastewater / Sludge Analysis	Water / Wastewater / Sludge Analysis	
Technique	Liquid-liquid microextraction; Magnetic solid phase extraction; Gas chromatography; Flame ionization View All	Solid phase dispersive extraction	Gas chromatography; Solid phase extraction	
Analyte	Pyrene; Acenaphthene; Anthracene; Acenaphthylene; Phenanthrene; Benzo[a]pyrene	Bisphenol M; Bisphenol G; Bis(4-hydroxyphenyl)diphenylmethane; 1,1-Bis(4-hydroxyphenyl)cyclohexane; 2,2-	Pyrene; Anthracene; Acenaphthylene; Benzantracene; Acenaphthene; Naphthalene; Fluorene	
Matrix	Wastewater	Wastewater; River waters; Bottled drinking water	Wastewater; River waters; Well waters; Drinking waters	
Other Materials	Ethanol; 1,2-Dibromoethane; Sodium chloride; Ferrous sulfate heptahydrate; Ferric chloride View All	Sodium chloride; Sodium hydroxide; Thenoyltrifluoroacetone; Methanol; Iron chloride (FeCl ₃); Ethanol; View All	Sodium chloride; 1H-Pyrrole; Methanol; Hydrofluoric acid; Sulfuric acid; Toluene; CRP-5 column (25 m x View All	

详细的分析实验方法对比

研究课题在产品中的应用？配方/制剂的检索与设计

方法一：登<https://formulus.cas.org> 输入检索式

Searching for...

Formulations 原料、用途、物理形态、功能或文献识别符

Search for Formulations by Ingredient, Purpose, Form, Function, etc.

orthopedic and implant

Try Advanced Search for a more precise search experience

高级检索

Formulation Designer

Design custom formulations templates based on selections and ingredients.

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方/制剂结果集

- 利用聚类项精简结果：
行业、配方/制剂用途、物理形式、物质状态、递送方式、涵盖信息、文献类型、发表机构、发表年份
- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情

Formulations search for "Petroleum and Additive"

Get Additional References Compare (0/3) Save

749,219 Results Sort: Relevance

一次最多可以比较三种不同制剂或配方的信息详情

1

Asphalt Mastic Composition: Asphalt Mastic Utilizing Petroleum Refinery Operations

Location: Claim 9, 10
Purpose: asphalt mastic utilizing petroleum refinery Operations
Physical Form: Fuel emulsions, Liquids, Solids

[Add to Compare](#)

Component	Function	Amount Reported
Petroleum	-	-
recycled tire rubber	additive	-
liquid asphalt composition	-	-
hydrocarbon diluent	diluent	-

Additional components reported
[View Formulation Detail](#)

31 Similar Formulations - [View All](#) (opens in a new window)

2

Pharmaceutical Composition: Antiviral Agents or Antimalarials, Etc.--Controlled-Release Drug Delivery Systems

Location: Claim 1, 3, 5, 10, 11, 12, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 27, 28, 29, 30, 31, 32, 33, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 55, 64, 67

Purpose: Analgesics, Anti-inflammatory agents, Antiangiogenic agents, Antiarthritics, Antibiotics, Anticonvulsants, Antimalarials, Antipsychotics, Antitumor agents, Antiviral agents, Fungicides, Immunomodulators, Nervous system agents, Ophthalmic agents, inte...

View More

Target: Angiogenesis, Bipolar disorder, Bladder neoplasm, Colon neoplasm, Colorectal neoplasm, Digestive tract neoplasm, Endocrine system neoplasm, Epilepsy, Esophagus neoplasm, Glioblastoma, Gliosarcoma, Hepatocellular carcinoma, Homo sapiens, Immune diseas...

View More

Delivery Route: Mucosal drug delivery systems, Nasal drug delivery systems, Ophthalmic drug delivery systems, Oral drug delivery systems, Parenteral drug delivery systems, Pharmaceutical intravenous injections, Rectal drug delivery systems, Sublingual drug delivery ...

View More

Physical Form: Capsules, Liquids, Particles, Pharmaceutical liposomes, Pharmaceutical microspheres, Powders, Tablets

[Add to Compare](#)

配方/制剂的制备? 实验评估?

- 制剂或配方原料
- 相似的制剂或配方
- 专利来源

Additive Formulation: Production or Processing of Refining of Petroleum

Download Save

Purpose	Target	Delivery Route	Physical Form	Source
processing of refining of petroleum. production	-	-	-	View

Predicted value

Formulation Ingredients [Expand All Groups](#) | [Collapse All Groups](#)

Component	Function	Amount Reported	Optionality
Group: petroleum additive	additive. active agent	15-90 % wt	Mandatory
Demulsifying agents	demulsification agent	15-85 % wt	Mutually exclusive alternatives
desalting agent	desalting agent	15-85 % wt	Mutually exclusive alternatives
Corrosion inhibitors	corrosion inhibitor	70-90 % wt	Mutually exclusive alternatives
Group: Carriers	carrier, active agent	-	Mandatory
Nonionic surfactants	surfactants	-	Mandatory
Solvents	solvents	-	Mandatory

More Formulations like this... NEW

Petroleum Fuel Additive Formulation
Purpose: petroleum fuel additive
Target: -
Delivery Route: -
Physical Form: -

Petroleum Fuel Additive Formulation
Purpose: petroleum fuel additive
Target: -
Delivery Route: -
Physical Form: -

Petroleum Fuel Additive Formulation
Purpose: petroleum fuel additive
Target: -
Delivery Route: -
Physical Form: -

Petroleum Fuel Additive Formulation
Purpose: petroleum fuel additive
Target: -
Delivery Route: -
Physical Form: -

Source Patent

Oil production additive formulations

Assignee: Imperial Chemical Industries PLC
WO2001040410
Language: English
Location: Claim 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 26

Patent PDF

View in CAS SciFinder®

高级检索

[← Return to Home](#)

Advanced Formulations Search ?

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.

At least two search terms are required.

Search For Operator Enter one term

Function Optional Anticorrosion

Ex: binder, surfactant, carrier

Search For Operator Enter one term

All Fields Optional coating

General search of all fields

- All Fields
- All Fields
- Form
- Function
- Ingredient
- Purpose
- Route
- Target

Optional

- Required
- Optional
- Excluded

检索原料

Searching for...

Formulations

Ingredients

Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

propylene glycol

- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性

- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至设计工具

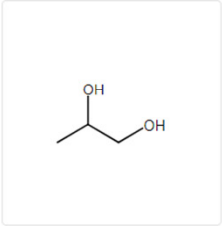
Formulation Designer

Ingredients search for "propylene glycol"

2 Selected 3 Results

1

CAS RN: 57-55-6
[View Details](#)



C₃H₈O₂

(±)-Propylene glycol
[Propylene glycol](#)

Key Physical Properties	Value	Condition
Molecular Weight	76.09	-
Melting Point (Experimental)	-59 °C	-
Boiling Point (Experimental)	188.2 °C	-
Density (Experimental)	1.036 g/cm ³	Temp: 25 °C

Commonly Used As: Solvents; Carriers; Plasticizers; Humectants; Antifreeze...

Similar Ingredients with Regulatory Information

- 27194-74-7 [Propylene glycol monolaurate](#)
- 29387-86-8 [Propylene glycol butyl ether](#)
- 30136-13-1 [Propylene glycol monopropyl ether](#)

[View 14 More](#)

[Commonly Formulated With](#) | [Regulatory Information](#) | [Experimental Properties](#)

Formulations Suppliers Add to Designer

设计配方/制剂

 Formulation Designer

Formulation Designer

[Clear All Selections](#)

Industry

Pharmaceutical
Cosmetics & Personal Care
Agrochemical
Cleaning & Surfactant Products
Food & Related
Inks, Paints, & Coatings

Purpose


Detergents
Cleaning compositions
Antibacterial agents
Disinfectants
Oral hygiene products
Fabric softeners
Antimicrobial agents
Toothpastes
Hand sanitizers
Bleaching detergents
[- View More Purposes -](#)

Physical Form

Liquids
Powders
Solutions
Tablets
Liquid detergents
Gels
Granular laundry detergents
Solids
Grains (particles)
Granular materials
[- View More Physical Forms -](#)

Add up to 5 Ingredients

Sodium polyacrylate

 [Add Another Ingredient](#)

Create Template

设计配方/制剂

Formulation Designer Clear All Selections

Industry	Purpose	Physical Form	Active or Featured Ingredient
Cleaning & Surfactant Products	Detergents	Liquid detergents	Sodium polyacrylate

[Edit Selections](#) ↓

Your Template

Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Sodium polyacrylate	Cosing; Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA Inactive Ingredients Database	-	
Function: Buffers	Boric acid (H ₃ BO ₃)	ANMAT; Cosing; Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients;	Triethanolamine; Sodium hydroxide; Ethanolamine; Sodium carbonate; Sulfuric acid	Approximately 1%

Alternative Ingredients (Showing all 11) ×

Select the ingredient you would like to use:

Triethanolamine	Sulfuric acid	Timnodonic acid
Sodium hydroxide	Hydrochloric acid	<i>p</i> -Toluenesulfonic acid
Ethanolamine	Glycolic acid	(±)-1-Amino-2-propanol
Sodium carbonate	Citric acid	

[View More Alternatives](#)

- 原料详情
- 原料管制信息
- 可替代的原料选项

文献关联的配方/制剂

方法二：在文献结果集页面，点击 CAS Solutions 中的 Formulus 获得有具体配方或制剂信息的文献，从文献详情页中链接获取

References search for "oil and dispersants"

Substances Reactions Citing Knowledge Graph

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

Filtering: CAS Solutions: Formulus [Clear All Filters](#)

2,972 Results Sort: Times Cited View: Partial Abstract

1

Physical and Chemical Stability of Curcumin in Aqueous Solutions and Emulsions: Impact of pH, Temperature, and Molecular Environment
By: Kharat, Mahesh; Du, Zheyuan; Zhang, Guodong; McClements, David Julian
Journal of Agricultural and Food Chemistry (2017), 65(8), 1525-1532 | Language: English, Database: CAplus and MEDLINE

The utilization of curcumin as a nutraceutical in food and supplement products is often limited because of its low water solubility, poor chem. stability, and low oral bioavailability. This study examined the impact of pH, storage temperature, and mol. environment on the phys. and chem. stability of pure curcumin in aqueous solutions and in oil-in-water emulsions. Unlike naturally occurring curcuminoid mixtures (that contain curcumin, demethoxy-curcumin, and bisdemethoxy-curcumin), pure curcumin was highly unstable to chem. degradation in alk. aqueous solutions (pH >7.0) and tended to crystall...

[View More](#)

Full Text Substance (1) Reactions (0) Citing (333) Citation Map

2

CAS Solutions

- Formulus (2,972)
- Analytical Methods (28)

Formulation Purpose

Top Count Alphanumeric Search

2 Selected

<input type="checkbox"/> Pesticides (378)	<input checked="" type="checkbox"/> Dispersing agents (14)
<input type="checkbox"/> Herbicides (338)	<input type="checkbox"/> Lubricating oil additives (13)
<input type="checkbox"/> Insecticides (172)	<input type="checkbox"/> Anticorrosive coating materials (12)
<input type="checkbox"/> Coating materials (151)	<input type="checkbox"/> Dietary supplements (12)
<input type="checkbox"/> Lubricants (107)	<input type="checkbox"/> Disinfectants (12)
<input type="checkbox"/> Cleaning compositions (105)	<input type="checkbox"/> Fabric softeners (12)
<input type="checkbox"/> Fungicides (90)	<input type="checkbox"/> Foundation cosmetics (12)
<input type="checkbox"/> Cosmetics and Personal care products (89)	<input type="checkbox"/> Fuel additives (12)
<input type="checkbox"/> Sunscreens (65)	<input type="checkbox"/> Lubricating oils (12)
<input type="checkbox"/> Agrochemical fungicides (58)	<input type="checkbox"/> Thermally insulating coating materials (12)
<input checked="" type="checkbox"/> Detergents (58)	<input type="checkbox"/> Analgesics (11)
<input type="checkbox"/> Drug delivery systems (56)	<input type="checkbox"/> Antibacterial coating materials (11)
<input type="checkbox"/> Antibacterial agents (46)	<input type="checkbox"/> Dermatological agents (11)
<input type="checkbox"/> Fertilizers (46)	

OK Cancel

文献关联的配方/制剂

Formulations

Dispersant Composition: Dispersing Agents

[View CAS Formulus® Detail](#)

Location: Claim 1, 12, 14

Purpose: Dispersing agents

Component	Function	Amount Reported
Group: hydrocarbon fluid	active agent	-
polyamine-polyester reaction products	-	-

成分

功能

用量

Dispersant Composition: Dispersing Agents

[View CAS Formulus® Detail](#)

Location: Claim 1, 12, 14, 15

Purpose: Dispersing agents

Component	Function	Amount Reported
Group: hydrocarbon fluid	active agent	-
polyamine-polyester reaction products	-	-
metal dialkyldithiophosphate	-	<0.6 w %

Dispersant Composition: Dispersing Agents

[View CAS Formulus® Detail](#)

Location: Table 1

Purpose: Dispersing agents

Component	Function	Amount Reported
Maleic anhydride	-	-
pilot 900 oil	-	40 %
Polyaziridine	-	-

Dispersant Composition: Dispersing Agents

[View CAS Formulus® Detail](#)

Location: Table 1

Purpose: Dispersing agents

Component	Function	Amount Reported
Maleic anhydride	-	-
pilot 900 oil	-	40 %
Polyaziridine	-	-

实验方案检索小结

1. 利用 Synthetic Methods™ 查看文献中合成方法详情
2. 利用 CAS Analytical Methods 进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
3. 利用 CAS Formulus 检索原料、配方/制剂，或通过文献结果集获得关联的配方/制剂信息；利用配方设计工具启发产品配方的开发

学习资源



ACS
Chemistry for Life®

运用化学的力量改善人们的生活



订阅号



服务号



美国化学会 ACS
ACS美国化学会来啦! 是官方! 是官方! 是官方!!!


关注 发消息

2023 CAS SciFinder Discovery Platform 论坛录课

日期	主题
3月1日	解锁CAS SciFinder Discovery Platform新功能
3月8日	巧用CAS SciFinder Discovery Platform文献检索快速进阶
3月15日	万物互联 CAS SciFinder Discovery Platform物质检索更高效
3月22日	CAS SciFinder Discovery Platform反应检索, 不止A to B
4月4日	不止化学: CAS SciFinder Discovery Platform序列检索技巧
4月12日	新手入门开题和文献综述? 巧用CAS SciFinder Discovery Platform事半功倍
4月19日	实验进展太慢? 巧用CAS SciFinder Discovery Platform寻找启发
5月10日	毕业季 CAS SciFinder Discovery Platform助力论文写作及答辩准备
5月24日	毕业季 巧用CAS SciFinder Discovery Platform 做足升学与择业准备



CAS SciFinder® 学习中心



ACS美国化学会
ACS作为权威科学信息的主要来源, 是全球化学企业、化学家、化学工程师和相关人员的职业家园。>
4096篇原创文章
视频号: ACS美国化学会
49个朋友关注

ACS美国化学会
ACS Cent. Sci. | 通过¹⁹F NMR从原子分辨水平实时检测活细胞内谷胱甘肽...
Nano Lett. | 基于合金工程的连续能级调控: 按需定制二维半导体SERS基底

SFn学习中心-首页
CAS SciFinder® 学习中心
注册 短视频 专题论坛 使用技巧
CAS SCIFINDER® 材料学专题
专题论坛推荐
CAS SCIFINDER-n: 聚合物相关信息获取策略

CAS SciFinder Discovery Platform 专题论坛时间表

2023 年 9 月 — 12 月

CAS SCIFINDER DISCOVERY PLATFORM 专题论坛涵盖多个科学研究领域, 为您带来全面的检索思路和丰富的检索技巧。

直播时间为 **周五 14:00 - 15:00**。点击论坛主题即可注册、观看直播。

9月15日 | [专利专题论坛](#)

9月22日 | [生物制药专题论坛](#)

10月13日 | [高分子材料专题论坛](#)

10月27日 | [金属有机与无机化学专题论坛](#)

11月10日 | [食品与个人护理品专题论坛](#)

11月24日 | [药物设计与合成专题论坛](#)

12月8日 | [电子信息与能源材料专题论坛](#)

常见问题

Unauthorized IP Address

User registration is available only from IP addresses specified by the key contact at your organization. Please try to register again from an authorized location.

- 检查注册链接是否正确
- 确认连入校园网，且不是通过 VPN 连接
- 如果链接正确，且在校园内，请联系图书馆或 china@acs-i.org



There was a problem verifying your account.

Try Again

Contact Us

Or [Log Out](#) and try again.

Reference Id: GU75LMF9IZnhTq6mymUog

- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告之后联系图书馆或 china@acs-i.org

CAS SciFinderⁿ 检索浏览器推荐

浏览器推荐:

- Windows (7, 8.1, 10): Chrome 60 及更高版本, Firefox 55 及更高版本, Firefox 52 (ESR)、Edge 15 及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3 及更高版本, Chrome 60 及更高版本, Firefox 55 及更高版本, Firefox 52 (ESR)

不建议使用 360 浏览器，相关功能或插件会被自动拦截

使用注意事项

- ▶ 一人注册一个账号
- ▶ 实名注册， 请提供真实姓名信息（中文名用汉语拼音全拼）
- ▶ 不得过量下载 (<https://www.cas.org/legal/infopolicy>)
- ▶ 不得账号分享
- ▶ 不得将账号用于非学术研究

THANK YOU!



美国化学文摘社北京代表处

ACS International, Ltd. – Representing CAS
Unit 1010, Tower B, Raycom InfoTech Park
2 Kexueyuan Nanlu, Haidian District, Beijing, China
+86-10-6250 8026/7

cas.org





扫描上方二维码答题

