

CAS SciFinder Discovery Platform (Academic)

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杜德鑫

ddu@acs-i.org

美国化学文摘社 (CAS) 北京代表处

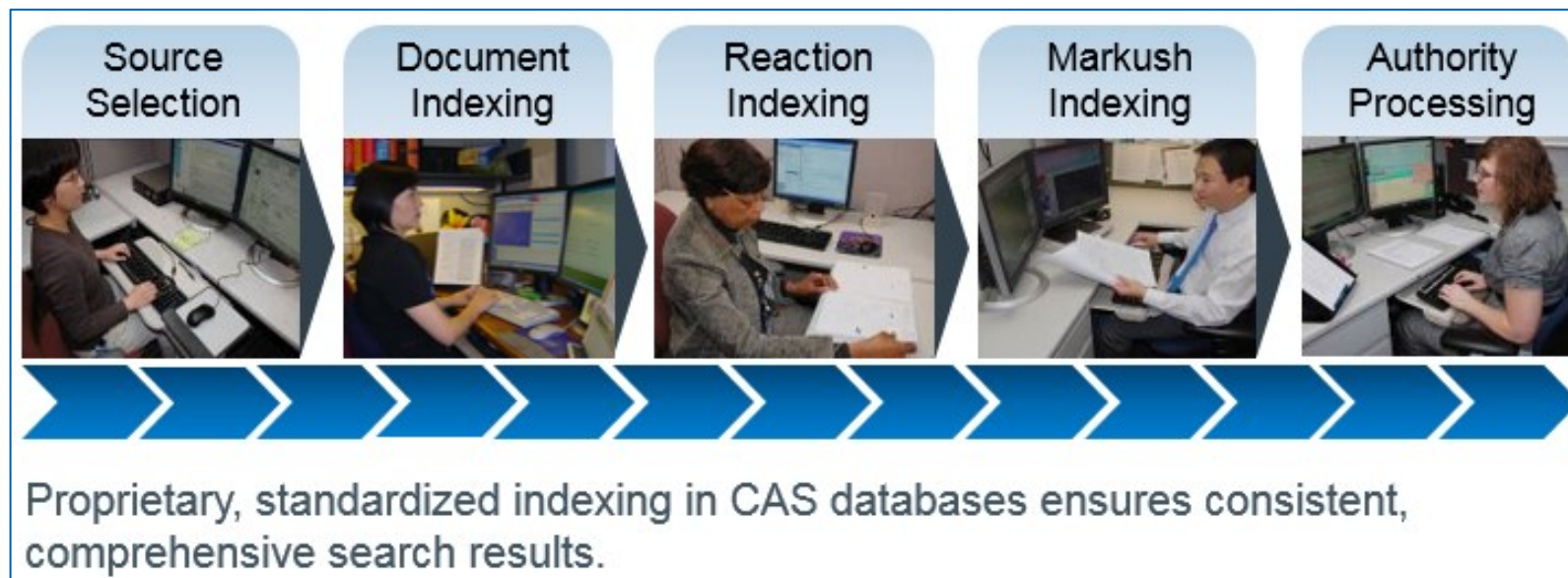
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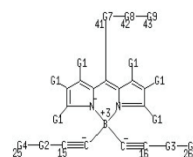
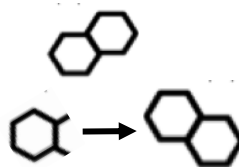
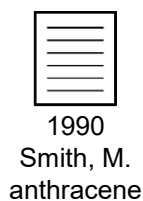
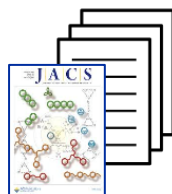
大纲

- 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 科学家智力标引



Data
pre-repository



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
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109
patent offices
worldwide

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



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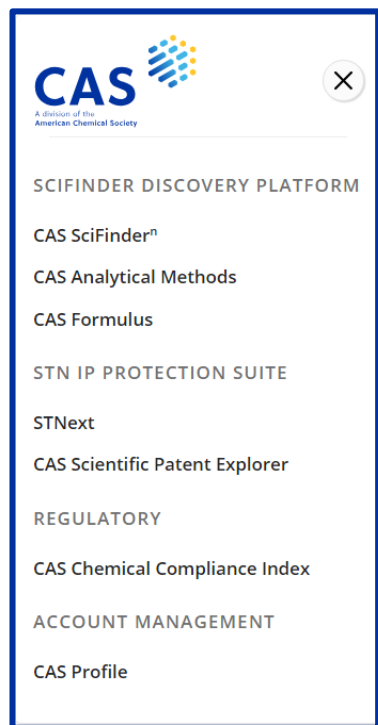
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CAS SciFinder[®] 主界面



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SCIFINDER DISCOVERY PLATFORM

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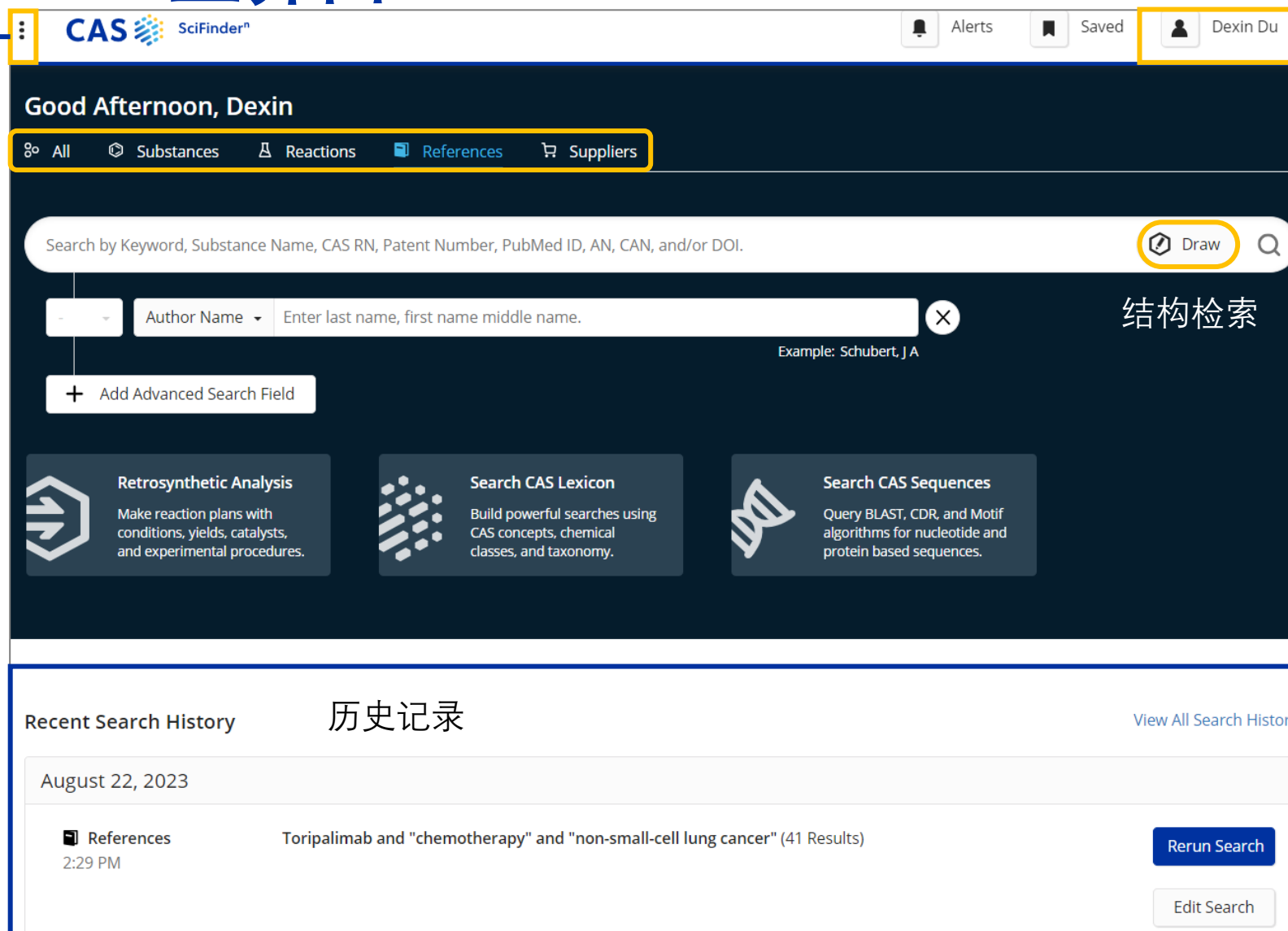
REGULATORY

- CAS Chemical Compliance Index

ACCOUNT MANAGEMENT

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CAS 应用



CAS SciFinder[®] Alerts Saved Dexin Du

Good Afternoon, Dexin

All Substances Reactions References Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Draw

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

+ Add Advanced Search Field

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.

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

Recent Search History 历史记录 View All Search History

August 22, 2023

References Toripalimab and "chemotherapy" and "non-small-cell lung cancer" (41 Results) Rerun Search

2:29 PM Edit Search

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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

lign

×

Draw

Q

Lignin
Lignan
Lignol
Lignox
Lignans
Lignite
Lignone
Lignase

自动提示

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. A search bar contains the query "Lignin and depolymerize or deconstruction and enzyme". 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 a dropdown menu set to "AND" and a field for "Author Name" with the placeholder text "Enter last name, first name middle name." and an example "Schubert, J A". A button labeled "+ Add Advanced Search Field" is also visible. At the bottom, there are three main service tiles: "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). The "Search CAS Lexicon" tile is highlighted with a yellow border.

CAS Lexicon 词库检索近义词和相关技术术语

Search CAS Lexicon

Biomass hydrotreatment

Your Query
You may include up to 1,000 terms in a search. [Clear All](#)

Preferred Term

Biomass hydrotreatment
This will search synonyms: Biomass hydrogenation; Biomass refining h...
[View fewer synonyms](#)

Broader Terms (1) [Select All](#)

Biomass refining

Narrower Terms (2) [Select All](#)

Biomass hydrocracking
 Biomass hydroisomerization

Related Terms (2) [Select All](#)

Biomass hydrotreatment catalysts
 Petroleum hydrotreating

Biomass hydrotreatment
Biomass hydrotreatment - Narrower Terms (2 Concepts)
Biomass hydrotreatment catalysts

Select a boolean operator [Learn more about CAS Lexicon searching.](#)

➤ 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 text 'Lignin and depolymerize or deconstruction and enzyme'. To the right of the search bar is a 'Draw' button and a search icon. Below the search bar, there are filters for 'AND', 'Abstract/Keywords', and the search term 'depolymerize'. A yellow box highlights the '+ Add Advanced Search Field' button, with a yellow arrow pointing to a dropdown menu. The dropdown menu lists various search criteria: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked with a 'NEW' badge), Publication Year, Document Identifier, Patent Identifier, and Publisher. On the right side of the interface, the text '物质结构' (Material Structure) is visible. Below the search bar, there are three promotional cards: 'Retrosynthetic Analysis', 'Search CAS Sequences', and another card partially visible on the right.

自定义高级检索项

检索结果分析与筛选

References search for "Lignin and depolymerize or deconstruction and enzyme" + 1 Advanced Field

Substances Reactions Citing Knowledge Graph

Sort: Relevance View: Partial Abstract

140 Results

1

Glycosylated linkers in multimodular lignocellulose-degrading enzymes dynamically bind to cellulose

By: Payne, Christina M.; Resch, Michael G.; Chen, Liqun; Crowley, Michael F.; Himmel, Michael E.; Taylor, Larry E. II; Sandgren, Mats; Stahlberg, Jerry; Stals, Ingeborg; Tan, Zhongping; et al

Proceedings of the National Academy of Sciences of the United States of America (2013), 110(36), 14646-14651, S14646/1-S14646/11 | Language: English, Database: CAlplus and MEDLINE

Plant cell-wall polysaccharides represent a vast source of food in nature. To depolymerize polysaccharides to soluble sugars, many organisms use multifunctional enzyme mixtures consisting of glycoside hydrolases, lytic polysaccharide mono-oxygenases, polysaccharide lyases, and carbohydrate esterases, as well as accessory, redox-active enzymes for lignin depolymerization. Many of these enzymes that degrade lignocellulose are multimodular with carbohydrate-binding modules (CBMs) and catalytic domains connected by flexible, glycosylated linkers. These linkers have long been thought to simply serve...

View More

Full Text

Substances (4) Reactions (0) Citing (127) Citation Map

2

Glycosylated linkers in multimodular lignocellulose-degrading enzymes dynamically bind to cellulose

By: Payne, Christina M.; Resch, Michael G.; Chen, Liqun; Crowley, Michael F.; Himmel, Michael E.; Taylor, Larry E. II; Sandgren, Mats; Stahlberg, Jerry; Stals, Ingeborg; Tan, Zhongping; et al

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

References search for "Lignin and depolymerize or deconstruction and enzyme" + 1 Advanced Field

Substances Reactions Citing Knowledge Graph

Filter Behavior

Filter by Exclude

Search Within Results

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

ethanol

Search

Filtering: Search Within Results: ethanol X Clear All Filters

17 Results Sort: Relevance View: Partial Abstract

1

Lignocellulosic ethanol production without enzymes - Technoeconomic analysis of ionic liquid pretreatment followed by acidolysis

By: Oleskowicz-Popiel, Piotr; Klein-Marcuschamer, Daniel; Simmons, Blake A.; Blanch, Harvey W. Bioresource Technology (2014), 158, 294-299 | Language: English, Database: CAPlus and MEDLINE

Deconstruction of polysaccharides into fermentable sugars remains the key challenge in the production of inexpensive lignocellulosic biofuels. Typically, costly **enzymic** saccharification of the pretreated biomass is used to **depolymerize** its cellulosic content into fermentable monomers. In this work, we examined the production of lignocellulosic recovery, a process that does not require the use of **enzymes** to produce fermentable sugars. In the base case, the min. **ethano** selling price (MESP) was \$8.05/gal, but with improved performance of the hydrolysis, extraction, and sugar recovery, the MESP can be lowered to \$4.00/gal. Addnl., two scenarios involving **lignin** recovery were considered. Although the results based on current assumptions indicate that this process is expensive compared to more established technologies, improvements in the hydrolysis yield, the sugar extraction efficiency, and the sugar recovery were shown to result in more competitive processes.

View Less ^

Full Text

Substances (4) Reactions (0) Citing (28) Citation Map

Search Within Results

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

ethanol

Search

物质角色筛选文献: Substance Role

^ Substance Role

- Biological Study (32)
- Process (22)
- Reactant or Reagent (12)
- Preparation (6)
- Properties (6)

[View All](#)

排序:
文献数量
字母顺序

Substance Role ×

By Count Alphanumeric

0 Selected

- Biological Study (32)
- Biological Study, Unclassified (25)
- Process (22)
- Reactant (11)
- Reactant or Reagent (11)
- Physical, Engineering, or Chemical Process (10)

Substance Role

By Count **Alphanumeric**

0 Selected

| | | |
|--------------------------------------------------------------|--------------------------------------------------------------------------|-------------------------------------------------------|
| <input type="checkbox"/> Analyte (1) | <input type="checkbox"/> Industrial Manufacture (1) | <input type="checkbox"/> Properties (6) |
| <input type="checkbox"/> Analytical Study (1) | <input type="checkbox"/> Modifier or Additive Use (2) | <input type="checkbox"/> Purification or Recovery (1) |
| <input type="checkbox"/> Biochemical Process (6) | <input type="checkbox"/> Other Use, Unclassified (1) | <input type="checkbox"/> Reactant (11) |
| <input type="checkbox"/> Biological Study (32) | <input type="checkbox"/> Physical, Engineering, or Chemical Process (10) | <input type="checkbox"/> Reactant or Reagent (11) |
| <input type="checkbox"/> Biological Study, Unclassified (25) | <input type="checkbox"/> Preparation (6) | <input type="checkbox"/> Removal or Disposal (6) |
| <input type="checkbox"/> Biosynthetic Preparation (2) | <input type="checkbox"/> Process (22) | <input type="checkbox"/> Therapeutic Use (1) |
| | | <input type="checkbox"/> Uses (3) |

确定文献核心研究内容: Concept

^ Concept

- Lignin (37)
- Biomass (29)
- Depolymerization (27)
- Enzymic hydrolysis (14)
- Enzymes (13)

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Concept ×

Top Count Alphanumeric Search

0 Selected

- Lignin (37)
- Biomass (29)
- Depolymerization (27)
- Enzymic hydrolysis (14)
- Enzymes (13)
- Fermentation (13)
- Hydrolysis (12)
- Laccase (10)
- Trametes versicolor (10)
- Basidiomycota (9)
- Biofuels (9)
- Corn straw (9)
- Microbial gene (9)
- Cell wall (5)
- Crystallinity (5)
- Clitocybula dusenii (3)
- Decomposition (3)

Apply

Concept ×

Top Count Alphanumeric Search **自定义检索**

Concept Name

Select All on Page

- Depolymerization (27)
- Depolymerization catalysts (3)

筛选不同研究领域文献： CA Section

^ CA Section

- Cellulose, Lignin, Paper, and Other Wood Products (36)
- Fermentation and Bioindustrial Chemistry (30)
- Unavailable (21)
- Enzymes (14)
- Microbial, Algal, and Fungal Biochemistry (9)

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CA Section

By Count Alphanumeric

0 Selected

| | | |
|---------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|
| <input type="checkbox"/> Cellulose, Lignin, Paper, and Other Wood Products (36) | <input type="checkbox"/> Plant Biochemistry (4) | <input type="checkbox"/> General Biochemistry (1) |
| <input type="checkbox"/> Fermentation and Bioindustrial Chemistry (30) | <input type="checkbox"/> Electrochemical, Radiational, and Thermal Energy Technology (3) | <input type="checkbox"/> Mammalian Biochemistry (1) |
| <input type="checkbox"/> Unavailable (21) | <input type="checkbox"/> Textiles and Fibers (2) | <input type="checkbox"/> Optical, Electron, and Mass Spectroscopy and Other Related Properties (1) |
| <input type="checkbox"/> Enzymes (14) | <input type="checkbox"/> Waste Treatment and Disposal (2) | <input type="checkbox"/> Pharmaceuticals (1) |
| <input type="checkbox"/> Microbial, Algal, and Fungal Biochemistry (9) | <input type="checkbox"/> Biochemical Methods (1) | <input type="checkbox"/> Plastics Fabrication and Uses (1) |
| <input type="checkbox"/> Fossil Fuels, Derivatives, and Related Products (6) | <input type="checkbox"/> Fertilizers, Soils, and Plant Nutrition (1) | |
| <input type="checkbox"/> Biochemical Genetics (5) | <input type="checkbox"/> Food and Feed Chemistry (1) | |

文献结果集管理

References search for **"natural fibers" and high-density polyethylene** 合并、下载、分享和保存


Substances Reactions Citing Knowledge Graph Save and Alert

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: Search Within Results: wood flour × Concept: 5 Selected × [Clear All Filters](#)

45 Results 1

Sort: Relevance ▼ View: Partial Abstract ▼

Green high density polyethylene (HDPE) r...ber and agricultural fillers for technical applications
By: Mazur, Karolina; Jakubowska, Paulina; Romanska, Paulina; Kuciel, Stanislaw 
Composites, Part B: Engineering (2020), 202, 108399 | Language: English, Database: CAplus

In this study, the impact of natural fibers (NFs) on the mech., thermal and hydrodegrdn. behavior was assessed. Composites based on biobased high-d. polyethylene were manufactured with a 40 wt% of wood flour, basalt fibers, flax fibers, and walnut shell flour. The results confirmed the reinforcing effect of NFs on mech. properties, especially in relation to the stiffness of the composites. Significant improvement was visible in the case of composites with basalt fibers with about 600% and 156% improvements for Youngs modulus and tensile strength, resp. Moreover, to evaluate the viability of NF...

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Full Text ▼ Substances (2) Reactions (0) Citing (48) Citation Map

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

- Search Within Results
- Substance Role
- Concept
- CA Section

保存和提醒



Save Results and Create Alert

Name

天然纤维&HDPE

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

natural product drugs

SCU

New Tag (Optional)

Tag Color

Save Cancel

- 结果保存
- 自定义提醒频率
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Excel (.xlsx)

PDF

Quoted (.txt)

Rich Text (.rtf)

Tagged (.txt)

Download Reference Results

File Type: PDF

Select Quantity:

- All Results
- Selected Results
- Range (ex. 2 to 20)

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- Result Details

File Name: Reference_20230628_1301

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- Concepts
- Substances
- Formulations
- Analytical Methods
- Citations

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- 交集
- 差集

Combine Reference Results: Subtract

Select 1 Saved Item:

[← Return to Combine Option](#)

| | | | |
|----------------------------------|----------------------------------|-------|-------------------|
| <input checked="" type="radio"/> | 天然纤维&HDPE | Query | November 21, 2023 |
| <input type="radio"/> | 天然产物 & high-density polyethylene | Query | November 21, 2023 |
| <input type="radio"/> | eye pressure | Query | November 14, 2023 |
| <input type="radio"/> | melatonin | Query | November 14, 2023 |
| <input type="radio"/> | CLImaging | Query | November 3, 2023 |
| <input type="radio"/> | ECL-imaging | Query | November 3, 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.

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查看目标文献详情

Green high density polyethylene (HDPE) reinforced with basalt fiber and agricultural fillers for technical applications

Substances (2) Reactions (0) Citing (48) Citation Map

JOURNAL

Source

Composites, Part B: Engineering
Volume: 202
Pages: 108399
Journal
2020
DOI:
[10.1016/j.compositesb.2020.108399](https://doi.org/10.1016/j.compositesb.2020.108399)

CODEN: CPBEFF
ISSN: 1359-8368

Database Information

AN: 2021:621898
CAN: 174:734786
CAplus

Company/Organization

Institute of Materials Engineering,
Faculty of Materials Science and
Physics
Cracow University of Technology
Krakow 31-155
Poland

By: Mazur, Karolina; Jakubowska, Paulina; Romanska, Paulina; Kuciel, Stanislaw

In this study, the impact of natural fibers (NFs) on the mech., thermal and hydrodegrdn. behavior was assessed. Composites based on biobased high-d. polyethylene were manufactured with a 40 wt% of wood flour, basalt fibers, flax fibers, and walnut shell flour. The results confirmed the reinforcing effect of NFs on mech. properties, especially in relation to the stiffness of the composites. Significant improvement was visible in the case of composites with basalt fibers with about 600% and 156% improvements for Youngs modulus and tensile strength, resp. Moreover, to evaluate the viability of NFs as reinforcements, water absorption and its influence on mech. properties were investigated. Unmodified polymer and composites with basalt fibers showed similar relationships - low water absorption. Composites reinforced with lignocellulosic fibers exhibited high water uptake and progressive deterioration of properties over time.

Keywords: green HDPE basalt fiber agricultural filler composite stiffness application

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相似文献

Similar References NEW

Mechanical properties of bio-based epoxy composites reinforced with hybrid-interlayer ramie and recycled carbon fibres

Open Journal of Composite Materials (2020), 10(4), 118-133 | Language: English, Database: CAplus

A Sustainable Polymer Composite from Recycled Polypropylene Filled with Shrimp Shell Waste

Polymer-Plastics Technology and Engineering (2014), 53(2), 167-172 | Language: English, Database: CAplus

Mechanical properties and water absorption of fiber-reinforced polypropylene composites prepared by bagasse and beech...

Journal of Applied Polymer Science (2009), 114(1), 653-657 | Language: English, Database: CAplus

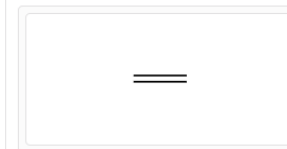
Concepts CAS 科学家提供的核心研究点

| | |
|-------------------------------------------------------|-------------------------------------------------------------------------------|
| Absorption Modifier: of water | Melting point |
| Bending strength | Microstructure Natural fibers |
| Charpy impact strength | Polymer fracture-surface morphology |
| Crystallinity | Stiffness |
| Crystallization temperature | Stress-strain relationship |
| Elongation at break | Surface roughness |
| Flax fibers | Synthetic fibers, basalt Role: Modifier or Additive Use |
| Flexibility | Synthetic polymeric fibers, lignocellulosic Role: Modifier or Additive Use |
| Flexural modulus | Tensile strength Walnut, flour and meal Modifier: Rehofix UNG 300 |
| Flours and Meals, walnut Modifier: Rehofix UNG 300 | Wood fibers |
| Fusion enthalpy | |
| Hydrolytic polymer biodegradation | |

Substances 重点研究物质

Substances (2)

9002-88-4



Role: Polymer in Formulation, Properties, Uses
Notes: SHC 7260

2072054-87-4

Image Not Available

Unspecified
Rehofix UNG 300

Role: Modifier or Additive Use, Uses
Notes: Rehofix UNG 300

查看专利详情

Continuous fiber composite reinforced synthetic wood elements

Substances (3) Reactions (0) Citing (5) Citation Map

By: Branca, Alfonso

The synthetic wood structural member comprises a synthetic wood body containing a synthetic polymer and having a longitudinal axis, such as wood fiber-filled recycled polyethylene; and ≥ 1 least one continuous fiber composite reinforcing rod element (such as glass fiber-reinforced recycled polyethylene) positioned within the synthetic wood body to increase the stiffness of the synthetic wood structural member, wherein the continuous fiber composite reinforcing rod element has a longitudinal axis of the synthetic wood structural member.

Keywords: synthetic wood element continuous fiber composite reinforced; recycled polyethylene glass fiber-reinforced recycled polyethylene

PatentPak Viewer Get Prior Art Analysis Full Text

Patent Family

| Patent | Language | Kind Code | PatentPak Options | Publication Date | Application |
|---------------|----------|-----------|---------------------|------------------|---------------|
| US20040048055 | English | A1 | PDF PDF+ Viewer | 2004-03-11 | US2002-242187 |
| US20070237940 | English | A1 | | 2007-10-11 | US2007-81 |

Priority Application

| Priority Application Number | Application Date |
|-----------------------------|------------------|
| US2002-242187 | 2002-09-11 |

PATENT

Patent Number: US20040048055

Publication Date: 2004-03-11

Application Number: US2002-242187

Application Date: 2002-09-11

Kind Code: A1

Assignee: Unknown

Source: United States
CODEN: USXXCO

Database Information: AN: 2004:203395
CAN: 140:236798
CAplus



IPC Data

| Patent | Class | Patent Family Classification Codes |
|---------------|-------|------------------------------------|
| US20040048055 | IPC | B32B 0027/04 A |
| US20070237940 | IPC | B32B 0027/04 |

Concepts

Substances

Substances (3)

9002-88-4



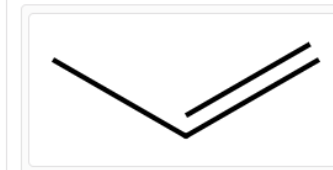
$(C_2H_4)_x$
Polyethylene

PatentPak

Role: Polymer in Formulation, Technical or Engineered Material Use, Uses

Notes: recycled

9003-07-0



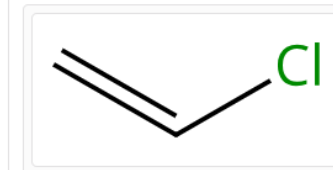
$(C_3H_6)_x$
1-Propene, homopolymer

PatentPak

Role: Polymer in Formulation, Technical or Engineered Material Use, Uses

Notes: (un)recycled

9002-86-2



$(C_2H_3Cl)_x$
Ethene, chloro-, homopolymer

PatentPak

Role: Polymer in Formulation, Technical or Engineered Material Use, Uses

PatentPak Viewer 高效阅读专利

CAS PatentPak

PAGE 14 / 15 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 10103-46-5

O=P(O)(O)O

• x Ca

Analyst Markup Locations (1)

Page 13

CAS RN 1302-42-7

O=[Al]=O

• Na⁺

EXAMPLE 4

Zeolite-pulp composite (100 g) obtained in Production Example 2 was impregnated with an aqueous solution of calcium chloride (0.30 mmol/1000 ml) and this zeolite was changed to 5A zeolite having larger pore size. To the 5A zeolite-pulp composite (10.0 g) were added collagen (5.0 g) and calcium phosphate (1.0 g) to give a molded product (5 cm×3 cm×1 cm).

EXPERIMENTAL EXAMPLE 4

The product (5 cm×3 cm×1 cm) obtained in Example 4 was immersed in an artificial body fluid (100 cm³) and preserved at 38° C. Thirty days later, the product was taken

PRODUCTION EXAMPLE 3

Pulp (300 g) was impregnated with an aqueous solution of sodium methasilicate 9 hydrate (190 g/5000 ml) and a mixed aqueous solution (5000 ml) of sodium aluminate (150 g) and sodium hydroxide (330 g) was added, which was followed by immersion at 90° C. for 2 hr to give a zeolite-pulp composite. The zeolite-pulp composite thus obtained had a zeolite-holding percentage of 30.1 wt %.

This zeolite-pulp composite was applied to an inclined wire-netting paper making machine (angle of inclination 50°, rate 10 m/min) to make a zeolite-holding paper (basic weight 100 g/m², paper width 50 cm).

US 6,372,333 B1

EXAMPLE 6

A rayon nonwoven fabric (basic weight 60 g/m², cloth width 50 cm) prepared by wet method was adhered to the

section of the rayon fiber when regenerating the rayon, and having polypropylene (core diameter 20 μm; fineness 50 μm; average fiber length 20 mm) was impregnated with an

精准定位

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？
- 如何查找相似的序列？

检索实验所需物质

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
 - Density > logD
 - Electrical > logP
 - Lipinski > Mass Intrinsic Solubility (g/L)
 - Magnetic > Mass Solubility (g/L)
 - Mechanical > Molar Intrinsic Solubility (mol/L)
 - Optical and Scattering > Molar Solubility (mol/L)
 - Structure Related > Molecular Weight
 - Thermal > pKa
 - Vapor Pressure (Torr)

结构检索 Edit

6CuN2O5.C2H3N

Edit Drawing Remove

Search Patent Markush

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.

筛选可用作催化剂的物质

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Filtering: Reaction Role: Catalyst X Reference Role: Catalyst Use X Clear All Filters

272 Results

Sort: Relevance View: Partial

Structure Match: As Drawn (4) Substructure (1,991) Similarity (19K) 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

Reaction Role: Catalyst (272) Reference Role: Catalyst Use (272)

Product (421) Reactant (109) Reagent (9) Solvent (1) Uses (272) Preparation (259) Synthetic Preparation (255) Properties (127) View All

1 161265-03-8 C39H32OP2 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-] 2,854 References 142K Reactions 134 Suppliers

2 2892148-77-3 C40H35OP2.I Components: 2 Component RN: 2139242-12-7 Phosphonium, [5-(diphenylphosphino)-9,9-dimethyl-9H-xanthen-4-yl]methyl-di phenyl-... 1 Reference 2 Reactions 0 Suppliers

3 2666309-71-1 C45H37OP2.Cl Components: 2 Component RN: 2242797-96-0 Phosphonium, [5-(diphenylphosphino)-9,9-dimethyl-9H-xanthen-4-yl]triphenyl-, chl... 1 Reference 3 Reactions 0 Suppliers

Sort: 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

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

Substances search for "Co2O3" Molecular Formula

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

4 Results

1308-04-9
Image Not Available
Co₂O₃
Cobalt oxide (Co₂O₃)

8,257 References 119 Reactions 12 Suppliers

Filter Behavior: Filter by, Exclude

Search Within Results

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

Reference Role: Properties (4), Reactant (3), Reactant or Reagent (3)

Substances search for "CH2O3" Molecular Formula

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

51 Results

463-79-6

CH₂O₃
Carbonic acid

32K References 578 Reactions 8 Suppliers

Filter Behavior: Filter by, Exclude

Search Within Results

Reaction Role: Product (11), Reactant (2), Reagent (2), Catalyst (2), Solvent (2)

Reference Role

Substances search for "H2O4S.2Na" Molecular Formula

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

9 Results

7757-82-6

• 2 Na
H₂O₄S.2Na
Components: 2
Component RN: 7664-93-9
Sodium sulfate

116K References 57K Reactions 213 Suppliers

Filter Behavior: Filter by, Exclude

Search Within Results

Reaction Role: Product (2), Reagent (2), Catalyst (1)

Reference Role: Process (6), Uses (6), Biological Study (5), Properties (5)

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 search criteria:

- Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.
- Criteria 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
- Criteria 2: AND, Molecular Weight, 170 to 200. Predicted values only. Examples: 46.07 | 125 to 350 | >300

Buttons: + Add Advanced Search Field

Experimental Spectra

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

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)

- 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

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

N#NC(=N)c1c[nH]c2ccccc12

$C_8H_9N_5$
2-Guanidinobenzimidazole

277 References 397 Reactions 64 Suppliers

2 157086-07-2

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

Relative stereochemistry shown

$C_{14}H_{14}O$
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]1CN2C=CC=CC=C2C1

Absolute stereochemistry shown, Rotation (-)

$C_{10}H_{11}NO_2$
(-)-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

C#CCN1C=CC=C1C(=O)N

Double bond geometry shown

$C_{10}H_{11}N_3O$
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=C3N2C=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)

Download Email Save

Nc1nc2ccccc2n1C(=N)N

$C_8H_9N_5$
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

$C_8H_9N_5$

CAS Name
2-Guanidinobenzimidazole

Conditions

- Working Frequency: 300 MHz
- Solvent: [DMSO-*d*₆ \(2206-27-1\)](#)
- Temperature: 24 °C

Spectrum Summary

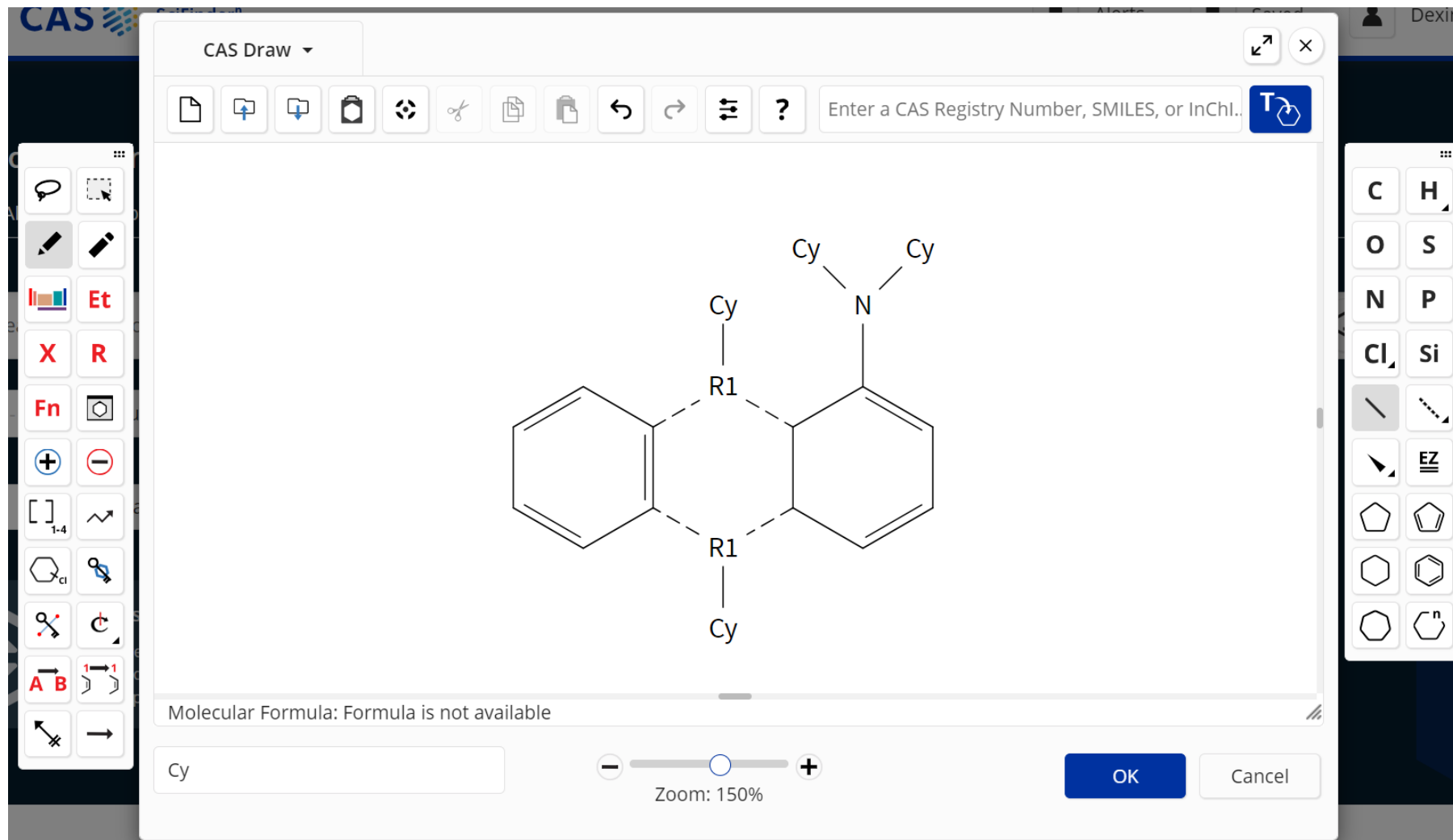
- Spectrum ID: ASI_6014117
- Source: Spectral data were obtained from John Wiley & Sons, Inc.

Experimental Spectra

| ¹ H NMR | ¹³ C NMR | IR | Mass | Raman |
|------------------------------------------|---------------------|----|------|-------------------|
| View Proton NMR Spectrum | | | | Source (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
- Cl** 取代位点可变
- A B** 反应角色标记
- 🔒** 锁定工具



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 (0)

Substructure (21)

Similarity (46)

Analyze Structure Precision

Chemscaple Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscaple.

Create Chemscaple Analysis

21 Results

1 2873458-36-5 $C_{40}H_{28}BCIN_2$

2 2873458-38-7 $C_{44}H_{30}BCIN_2$
Benzo[c]phenazaborin-6-amine, 5-chloro-7,12-dihydro-*N*-2-naphthalenyl-*N*,7,12-trip...

3 2485009-17-2 $C_{57}H_{54}BN_3$
1,4-Phenazaborinediamine, 5,10-dihydro-*N*¹,*N*¹,*N*⁴,*N*⁴,5-pentaphenyl-10-[2,4,6-tris(...

1 Reference 1 Reaction 0 Suppliers

1 Reference 1 Reaction 0 Suppliers

1 Reference 0 Reactions 0 Suppliers

- **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。

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

Search Within Results

- Reaction Role
- Reference Role

Commercial Availability

Number of Components

Molecular Weight

LogP

Element

- Functional Group
- Aromatic Rings
- Substance Class

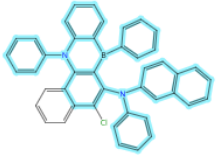
Isotopes

Metals

Reference Availability

4

2873458-38-7

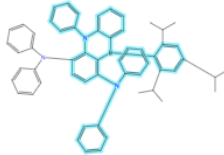


$C_{44}H_{30}BCIN_2$
Benzo[c]phenazaborin-6-amine, 5-chloro-7,12-dihydro-N-2-naphthalenyl-N,7,12-trip...

1 Reference 2 Reactions 0 Suppliers

5

2485009-17-2

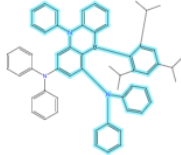


$C_{57}H_{54}BN_3$
1,4-Phenazaborinediamine, 5,10-dihydro-N¹,N¹,N⁴,N⁴,5-pentaphenyl-10-[2,4,6-tris(...]

1 Reference 0 Reactions 0 Suppliers

6

2485009-22-9

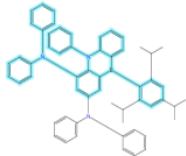


$C_{57}H_{54}BN_3$
1,3-Phenazaborinediamine, 5,10-dihydro-N¹,N¹,N³,N³,5-pentaphenyl-10-[2,4,6-tris(...]

1 Reference 0 Reactions 0 Suppliers

7

2485009-19-4

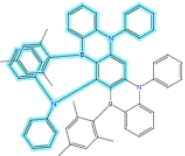


$C_{57}H_{54}BN_3$
2,4-Phenazaborinediamine, 5,10-dihydro-N²,N²,N⁴,N⁴,5-pentaphenyl-10-[2,4,6-tris(...]

1 Reference 0 Reactions 0 Suppliers

8

2410379-95-0

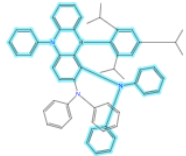


$C_{60}H_{51}B_2N_3$

1 Reference 0 Reactions 0 Suppliers

9

2485009-21-8



$C_{57}H_{54}BN_3$
1,2-Phenazaborinediamine, 5,10-dihydro-N¹,M¹,N²,N²,5-pentaphenyl-10-[2,4,6-tris(...]

1 Reference 0 Reactions 0 Suppliers

特定官能团

Functional Group

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

[View All](#)

Substance Class

- Organic/Inorganic Small Molecule (84)
- Salt and Compound With (11)
- Polymer (5)
- Protein/Peptide Sequence (3)

物质类别

CAS Markush 检索实现结构查新

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

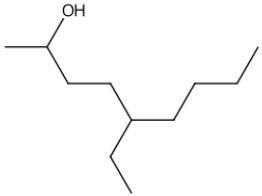
预测性物质 (Prophetic Substance)

- 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

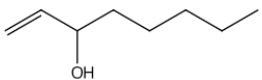
CAS RN 103-08-2



Analyst Markup Locations (2)

- Page 3
- Page 16

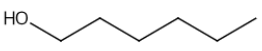
CAS RN 3391-86-4



Analyst Markup Locations (1)

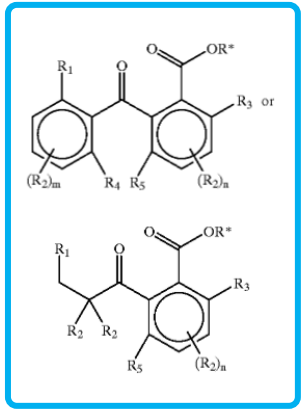
- Page 3

CAS RN 111-27-3



What is claimed is:

1. A perfuming composition containing a compound of formula



(I)

or a polyalcohol or polyether group;

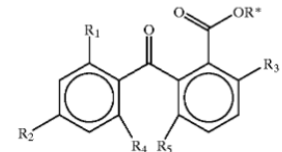
R_3 represents hydrogen, an alkyl or an alkoxy group from C_1 to C_4 , linear or branched, a OH group or a NH_2 group;

R_4 and R_5 , taken separately, can be hydrogen or have the meaning given above for R_1 and can be identical to or different from R_1 or from each other; or R_4 and R_5 , 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; R_6 and R_7 , taken separately, each represents hydrogen, an alkyl group from C_1 to C_4 , an alcohol group having an alkyl chain from C_1 to C_{12} , or a phenyl group, or, R_6 and R_7 , taken together with the nitrogen atom form a 5-membered or 6-membered ring optionally containing another hetero atom; R_8 represents hydrogen, an alkyl group from C_1 to C_4 , an alcohol group having an alkyl chain from C_1 to C_{12} or a phenyl group;

M represents hydrogen or an alkali metal; and

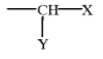
R^* is the organic part derived from a primary or secondary fragrant alcohol R^*OH , wherein the fragrant alcohol is released upon exposure of the composition to light to provide a fragrance.

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




(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 C_1 to C_{12} , a phenyl group, an olefinic group from C_2 to C_{12} , an alcohol group a CO_2M group, a $-NR_6R_7$ group or a group of formula



完整的结构检索流程

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

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

- As Drawn (13)
- Substructure (46)

Filter Behavior

Filter by Exclude

Patent Office

- China (6)
- World Intellectual Property Organization (4)
- United States (2)
- Japan (1)

CA Section

- Electric Phenomena (3)
- Heterocyclic Compounds (One Hetero Atom) (3)
- Chemistry of Synthetic High Polymers (2)
- Heterocyclic Compounds (More Than One Hetero Atom) (2)
- Benzene, Its Derivatives, and Condensed Benzenoid Compounds (1)

View All

13 Results

1

WO2018017478

Catalytic functional group removal from a polymer

By: Mattson, Kaila M.; Hawker, Craig J.; Pester, Christian W.; Gutekunst, Will R.; Schmidt, Bernhard V.K.J.
World Intellectual Property Organization, WO2018017478 A1 2018-01-25 | Language: English, Database: CPlus
Assignee: The Regents of University of California

Patent claim 1

PatentPak Full Text

258,259,261,262,264: opt. substd. by G6
302,303,305,306,308: opt. substd. by G6
358,359,361,362,364: opt. substd.

2

WO2011143563

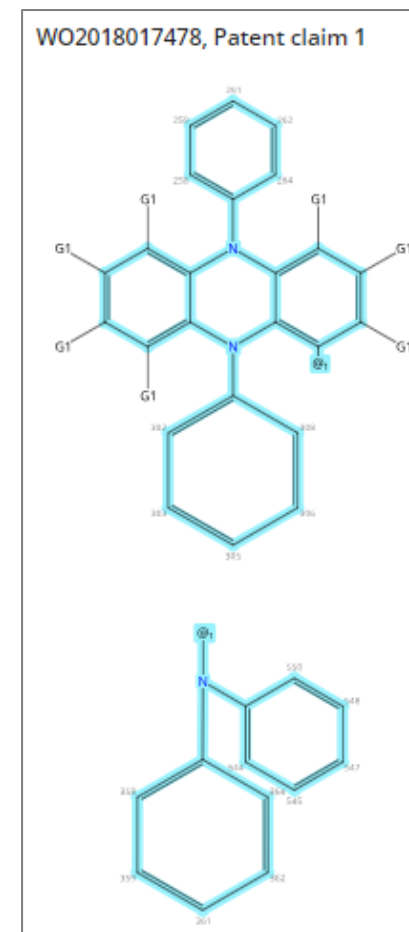
Azaborinine compounds as host materials and dopants for PHOLE DS

By: Kottas, Gregg; Kwong, Raymond C.
World Intellectual Property Organization, WO2011143563 A2 2011-11-17 | Language: English, Database: CPlus
Assignee: Universal Display Corporation

Patent claim 1

PatentPak Full Text

There are no notes to display for this structure.



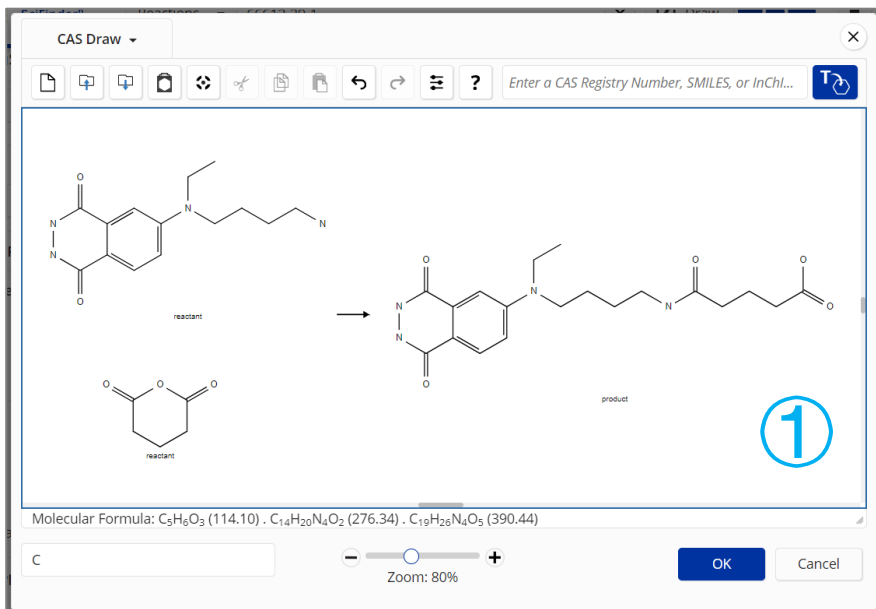
物质检索小结

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



Reactions search for drawn structure

References

3 Results

Group: By Document | Sort: Relevance | View: Collapsed

1

A new isoluminal 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: CAplus

Full Text

Suppliers (68)

Suppliers (92)

2

31-366-CAS-10683461

Steps: 1 Yield: 100%

Structure Match

- As Drawn (3)
- Substructure (5)
- Similarity (29K)

Filter Behavior

Filter by Exclude

Search Within Results

- Yield
 - 90-100% (3)
- Number of Steps
 - 1 (3)

检索具体物质能够发生的反应

Reactions search for "42196-31-6"

References

Filter Behavior

Filter by Exclude

Search Within Results

- Substance Role
 - Product (59)
 - Reactant (216)
 - Reagent (182)
 - Catalyst (23K)
 - Solvent (1)
- Non-Participating Functional Groups
- Experimental Protocols
 - Synthetic Methods (14K)
 - Experimental Procedure (2,773)
- Catalyst
 - Palladium trifluoroacetate (23K)
 - 2,2'-Bipyridine (1,270)

23,702 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (5 Reactions) Steps: 1 Yield: 99-100%

Suppliers (107) Suppliers (100) Suppliers (34)

31-239-CAS-1403436 Steps: 1 Yield: 100% Transition metal-catalyzed process for addition of amines to carbon-carbon double bonds

1.1 Reagents: [Trifluoroacetic acid](#)
Catalysts: [1,1-Bis\(diphenylphosphino\)ferrocene](#), [Palladium trifluoroacetate](#)
Solvents: [Toluene](#)

By: Hartwig, John; et al
World Intellectual Property Organization, WO2001064620 A1
2001-09-07

Experimental Protocols PatentPak Full Text

31-239-CAS-10342038 Steps: 1 Yield: 100% Palladium-Catalyzed Intermolecular Hydroamination of Vinylarenes Using Arylamines

1.1 Catalysts: [1,1-Bis\(diphenylphosphino\)ferrocene](#), [Palladium trifluoroacetate](#)
Solvents: [Toluene](#)
1.2 Reagents: [Trifluoromethanesulfonic acid](#)

Experimental Protocols Full Text

- Substance Role 限定反应角色
- Catalyst 筛选催化剂

如何检索某种催化剂能够催化的反应？

Reaction Role

- Product (2)
- Reactant (1)
- Reagent (1)
- Catalyst (2)
- Solvent (1)

Reference Role

- Catalyst Use (2)
- Preparation (2)
- Synthetic Preparation (2)
- Uses (2)
- Analyte (1)

[View All](#)

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

Return to Home

Substances search for drawn structure

References Reactions Suppliers

Structure Match

- As Drawn (64)
- Substructure (75)**
- Similarity (5,886)

Analyze Structure Precision

Chemscap Analysis

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

[Create Chemscap Analysis](#)

Filter Behavior

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

Search Within Results

Reaction Role

- Product (2)
- Reactant (1)
- Reagent (1)

Filtering: Reaction Role: Catalyst Reference Role: Catalyst

2 Results Sort: Number of References: Descending View: Partial

1

91742-21-1

• Na

$C_2HF_6NO_4S_2.Na$

Components: 2

Component RN: 82113-65-3

Methanesulfonamide, 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-, sodium salt ...

989 References **662 Reactions** 60 Suppliers

2

1449420-54-5

$C_{10}H_{20}NaO_5.C_2F_6NO_4S_2$

Components: 2

Sodium(1+), (1,4,7,10,13-pentaoxacyclopentadecane- $\kappa O^1, \kappa O^4, \kappa O^7, \kappa O^{10}, \kappa O^{13}$)-, salt ...

2 References 5 Reactions 0 Suppliers

查看某种催化剂能够催化的反应

🧪 Reactions for 91742-21-1

References ▾

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

- Product (354)
- Reactant (69)
- Reagent (153)
- Catalyst (84)
- Solvent (2)

Non-Participating Functional Groups

- Alkene (71)
- Halide (63)
- Alkyl halide (52)
- Acyclic alkene (46)
- Cyclic alkene (32)

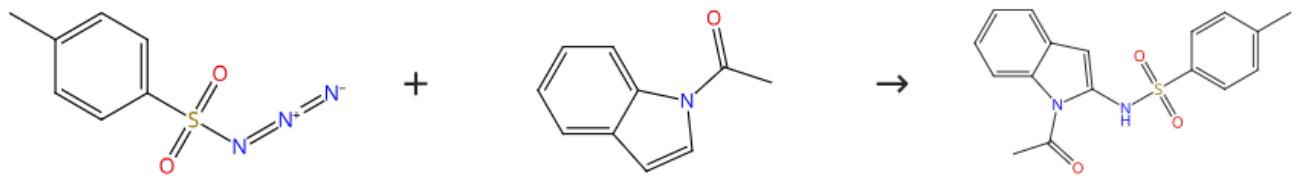
Filtering: Substance Role: Catalyst X

Clear All Filters

84 Results

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 93% ...



Suppliers (44) Suppliers (57)

31-080-CAS-19444697 Steps: 1 Yield: 93% ...

Delineating Physical Organic Parameters in Site-Selective H Functionalization of Indoles

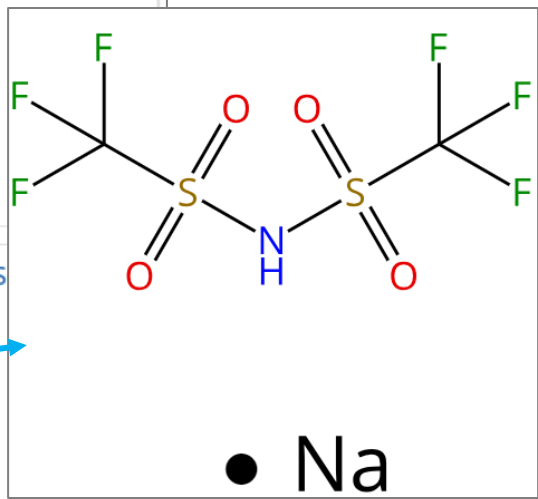
By: Kim, Youyoung; et al
ACS Central Science (2018), 4(6), 768-775

Full Text ▾

1.1 Catalysts:
[Iridium, \[\(1,2,3,4,5-η\)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl\]bis\(trifluoromethanesulfonyl\)imide](#)

Solvents: 1,2-Dichloroethane; 12 h, 40 °C

Collapse Scheme ^



● Na

查看文献中的重要反应

References for 50525-27-4

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

Sort: Times Cited ▾ View: No Abstract ▾

802 Results

1

Merging Photoredox Catalysis with Organocatalysis: The Direct Asymmetric Alkylation of Aldehydes
By: Nicewicz, David A.; MacMillan, David W. C.
Science (Washington, DC, United States) (2008), 322(5898), 77-80 | Language: English, Database: CAPLUS and MEDLINE
[View Abstract ▾](#)

Full Text ▾ Substances (33) Reactions (16) Citing (1,688) Citation Map

2

Efficient Visible Light Photocatalysis of [2+2] Enone Cycloadditions
By: Ischay, Michael A.; Anzovino, Mary E.; Du, Juana; Yoon, Tehshik P.
Journal of the American Chemical Society (2008), 130(39), 12886-12887 | Language: English, Database: CAPLUS and MEDLINE
[View Abstract ▾](#)

Full Text ▾ Substances (37) Reactions (21) Citing (808) Citation Map

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

- Journal (540)
- Patent (251)
- Review (2)
- Conference (8)
- Letter (2)
- Preprint (3)

Substance Role

- Uses (612)
- Analytical Study (255)
- Biological Study (175)

查看相似反应

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

- Product (354)
- Reactant (69)
- Reagent (153)
- Catalyst (84)
- Solvent (2)

Non-Participating Functional Groups

- Alkene (71)
- Halide (63)
- Alkyl halide (52)
- Acyclic alkene (46)
- Cyclic alkene (32)

Filtering: Substance Role: Catalyst X Clear All Filters

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 93%

Suppliers (44) Suppliers (57)

31-080-CAS-19444697 Steps: 1 Yield: 93% **Get Similar Reactions** Delineating Physical Organic P... H Functionalization of Indoles ACS Central Science (2018), 4(6), ... youyoung; et al

1.1 Catalysts:
[Iridium, \[\(1,2,3,4,5-η\)-1,2,3,4,5-pentamethylcyclopentadien-1-yl\]bis\(trifluoromethanesulfonyl\)imide](#), [Sodium bis\(trifluoromethanesulfonyl\)imide](#)
Solvents: [1,2-Dichloroethane](#); 12 h, 40 °C

Full Text

Collapse Scheme

检索相似反应

Get Similar Reactions

Set Reaction Similarity

Broad (3,535) Reaction centers only

Medium (110) Reaction centers plus adjacent atoms and bonds

Narrow (32) Reaction centers plus extended atoms and bonds

Get Reactions Cancel

催化剂可以催化的反应类型

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

- Product (354)
- Reactant (69)
- Reagent (153)
- Catalyst (84)
- Solvent (2)

Non-Participating Functional Groups

- Alkene (71)
- Halide (63)
- Alkyl halide (52)
- Acyclic alkene (46)
- Cyclic alkene (32)

[View All](#)

Experimental Protocols

- Synthetic Methods (56)

Catalyst

Number of Steps

Filtering: Substance Role: Catalyst X Clear All Filters

84 Results Group: By Transformation Sort: Reaction Count: Descending View: Expanded

1

Amination of Aromatic Compounds
[View 24 Related Reactions](#)

$$\text{Ar-H} \xrightarrow{\text{HN}_3} \text{Ar-NH}_2$$

2

Amination of Aromatic Nitrogen Heterocycles/ Chichibabin Reaction
[View 24 Related Reactions](#)

3

Reduction of Azides to Primary Amines/ Staudinger Reaction
[View 24 Related Reactions](#)

$$\text{R-N}_3 \longrightarrow \text{R-NH}_2$$

Sort: Reaction Count: Descending

- Reaction Count: Descending
- Reaction Count: Ascending
- Transformation Name: A to Z
- Transformation Name: Z to A

关注反应的机理研究或人名反应？

结构与关键词联用检索

Search interface showing "Friedel-crafts acylation" in the search bar. The "References" tab is selected in the top navigation bar. A drawn structure of indole is shown in a box with "Edit Drawing" and "Remove" buttons. Below the search bar, there are filters for "AND", "Author Name", and "Add Advanced Search Field".

References search for "Friedel-crafts acylation" + drawn structure

Search results for "Friedel-crafts acylation" + drawn structure. The "Reactions" filter is circled in blue. The first result is highlighted with a blue box and an arrow pointing to the "Reactions (21)" filter.

ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole
By: Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad
Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CAlus and MEDLINE

An efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides in the presence of ZrCl₄ has been discovered. It minimizes/eliminates common competing reactions that occur due to high and multiatom-nucleophilic character of indole. In this method, a wide range of aroyl, heteroaroyl, alkenoyl, and alkanoyl chlorides undergo smooth acylation with various indoles without NH protection and afford 3-acylindoles in good to high yields.

Full Text ▾ Substances (40) Reactions (21) Citing (99) Citation Map

Reactions search for "2011:601374". The "Reactions" filter is circled in blue. Two reaction schemes are shown with their respective reagents and suppliers.

21 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 82%

Reaction 1: A bicyclic ketone + Indole → A bicyclic ketone with an indole ring attached.

Suppliers (90) Suppliers (120) Suppliers (11)

Scheme 2 (1 Reaction) Steps: 1 Yield: 78%

Reaction 2: Indole + Benzoyl chloride → 3-benzoylindole.

Suppliers (109) Suppliers (73) Suppliers (10)

便捷查看详细反应操作

Structure Match

As Drawn (85)

Substructure (3,669)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Synthetic Methods (26)

Experimental Procedure (9)

Reaction Type

Stereochemistry

Reagent

Filtering: Experimental Protocols: Synthetic Methods X Clear All Filters

26 Results

Group: By Document Sort: Relevance View: Collapsed

1

Photoinduced Electron Transfer in Ruthenium Bipyridyl Complexes: Evidence for the Existence of a Cage with Molecular Oxygen

By: Yavin, Eylon; Weiner, Lev; Arad-Yellin, Rina; Shanzer, Abraham
Journal of Physical Chemistry A (2004), 108(42), 9274-9282 | Language: English, Database: CAPlus

Full Text View 4 Related Reactions

Absolute stereochemistry shown

Suppliers (75)

31-352-CAS-241330 Steps: 1 Yield: 100%

1.1 Solvents: [Ethanol](#); 4 h, rt

1.2 Reagents: [Trifluoroacetic acid](#)
Solvents: [Dichloromethane](#); 1 - 2 h, rt

Experimental Protocols

Reaction Overview

Steps: 1 Yield: 100%

JOURNAL

Photoinduced Electron Transfer in Ruthenium Bipyridyl Complexes: Evidence for the Existence of a Cage with Molecular Oxygen

By: Yavin, Eylon; et al
View All
Journal of Physical Chemistry A (2004), 108(42), 9274-9282

View Source Full Text

Company/Organization

Department of Organic Chemistry and Department of Chemical Research Support
Weizmann Institute of Science
Rehovot 76100
Israel

Step 1

| Stage | Reagents | Catalysts | Solvents | Conditions |
|-------|--------------------------------------|-----------|---------------------------------|-------------|
| 1 | - | - | Ethanol | 4 h, rt |
| 2 | Trifluoroacetic acid | - | Dichloromethane | 1 - 2 h, rt |

Alternative Steps (0)

Experimental Protocols

Synthetic Methods Experimental Procedure

Products [Ruthenium\(2+\), bis\(2,2'-bipyridine-κN¹,κN^{1'}\)\[\(N,N'-\(\(2,2'-bipyridine\)-4,4'-diyl-κN¹,κN^{1'}\)dicarbonyl\]bis\[alaninato\]\]\(2-\);-dihydrogen,\(OC-6-22\)-](#); Yield: 100%

Reactants [Tris\(2,2'-bipyridyl\)dichlororuthenium\(II\) hexahydrate](#)
[L-Alanine, N,N'-\(\(2,2'-bipyridine\)-4,4'-diyl\)dicarbonyl\]bis- bis\(1,1-dimethylethyl\) ester](#)

Reagents [Trifluoroacetic acid](#)

Solvents [Ethanol](#)
[Dichloromethane](#)

Procedure

1. Stir 2, 2'-bipyridyl derivative with equivalents amount of Ru-(bipy)₂Cl₂·6H₂O in 80% ethanolic solution for 4 hours under argon.
2. Remove the solvent.
3. Purify the product by column chromatography eluting with a CH₃CN/n-BuOH/0.4M KNO₃ (9/0.5/0.5) solution.
4. Remove the 'butyl ester group by stirring in trifluoroacetic acid/dichloromethane (1:4) solutions for 1-2 hours.
5. Evaporate the solvent.

Transformation Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters

Characterization Data

⁺ Ruthenium(2+), bis(2,2'-bipyridine-κN¹,κN^{1'})[(N,N'-((2,2'-bipyridine)-4,4'-diyl-κN¹,κN^{1'})dicarbonyl]bis[alaninato]](2-);-dihydrogen,(OC-6-22)-

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 Suppliers

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

Author Name Enter last name, first name middle name

+ Add Advanced Search Field

Retrosynthetic Analysis

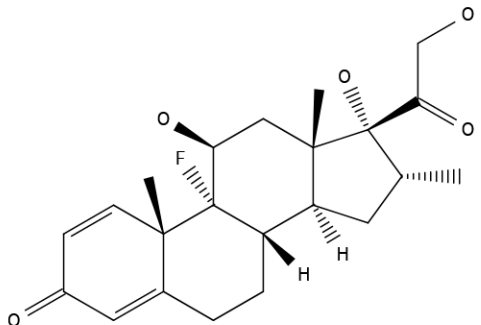
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search CAS L

Build reaction plans with CAS concepts, classes, and tax

Retrosynthetic Analysis
Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI..



Molecular Formula: C₂₂H₂₉FO₅ (392.47)

C

Zoom: 100%

Start Retrosynthetic Analysis Cancel

逆合成反应路线设计

Substances search for drawn structure

References ▾ Reactions ▾ Suppliers ▾

Structure Match

As Drawn (1)

Substructure (5)

Similarity (880K)

Analyze Structure Precision

Chemscape Analysis

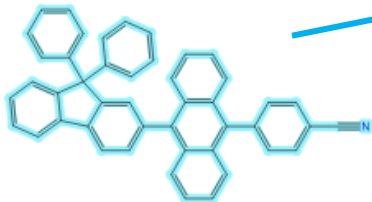
Visually explore structure similarity with a powerful new tool.
[Learn more about Chemscape.](#)

Create Chemscape Analysis

1 Result

1

2414255-10-8

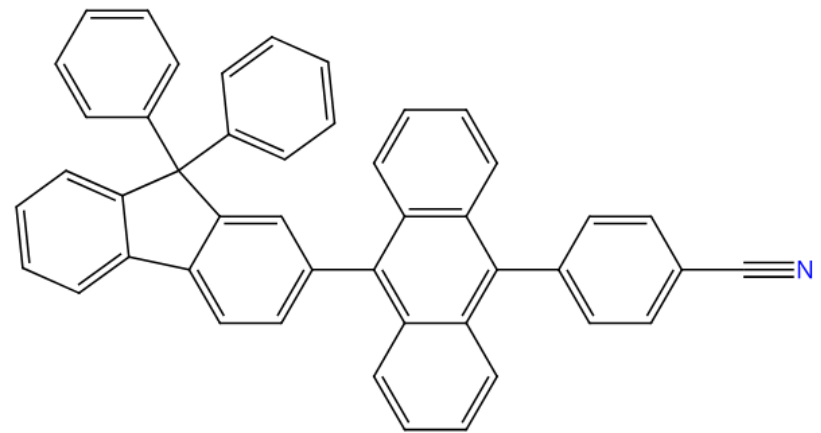


$C_{46}H_{29}N$
Benzonitrile, 4-[10-(9,9-diphenyl-9H-fluoren-2-yl)-9-anthracenyl]-

2 References 6 Reactions 0 Suppliers

CAS RN
2414255-10-8

CAS Name
Benzonitrile, 4-[10-(9,9-diphenyl-9H-fluoren-2-yl)-9-anthracenyl]-



Get Substance Details

Get Bioactivity Data

Get Reactions (6)

Synthesize (6)

Start Retrosynthetic Analysis

Get References (2)

Get Suppliers (0)

Edit Structure - Reset + Download

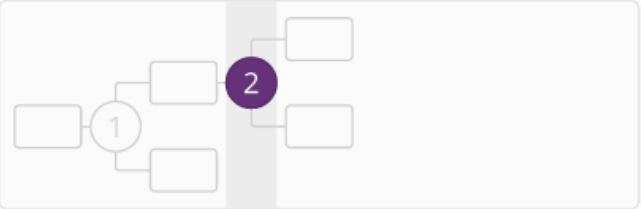
- 先进行物质检索
- 点击目标化合物，弹出物质菜单
- 点击 Start Retrosynthetic Analysis

预设路线参数

Retrosynthesis Plan Options for 2414255-10-8 Powered by ChemPlanner®

Select Synthetic Depth 合成深度 [Learn more.](#)

1
 2
 3
 4



Set Rules Supporting Predicted Reactions [Learn more.](#)

Common 反应规则是否常见
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

Set Starting Materials Cost Limit [Learn more.](#)

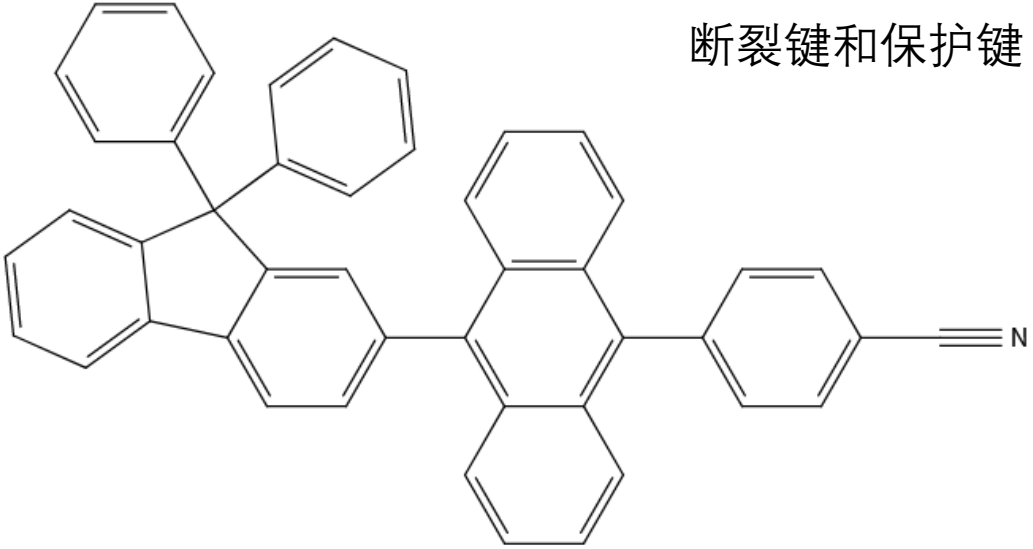
1000 起始原料费用 USD/mol

Email me when my plan is complete

[Create Retrosynthesis Plan](#)

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

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



断裂键和保护键

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

Plan Information

Estimated Yield: 74%
Overall Price: \$190.19
(USD per 100 grams)

Scoring Profiles

参数调节

Complexity Reduction

Convergence

High

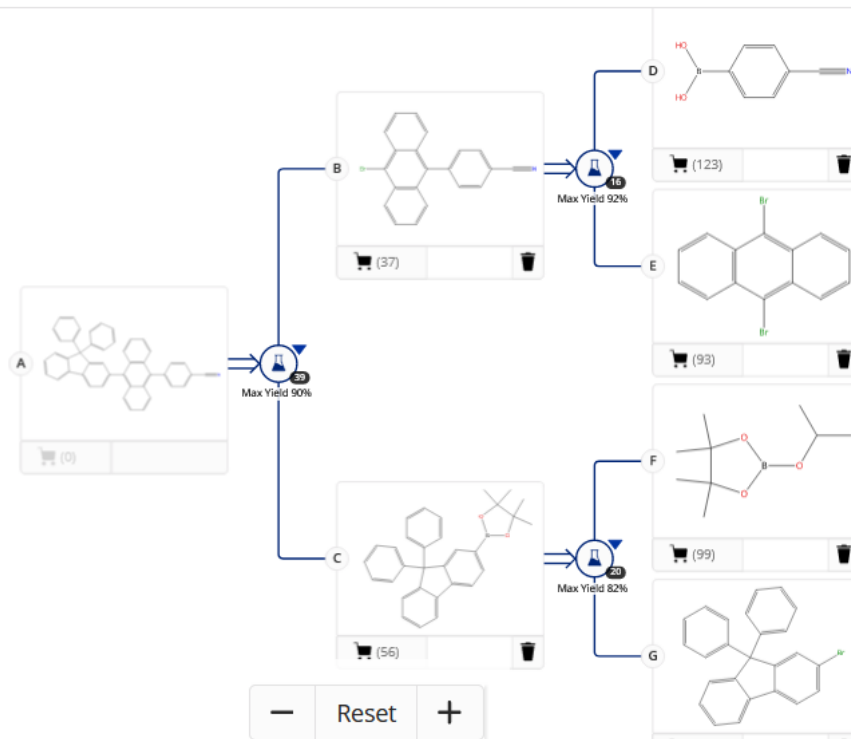
Evidence

Medium

Cost

Low

Yield



Step

Evidence

路线概览

A ⇒ B + C

Maximum Yield: 90%
Evidence (1)
Alternative Steps (39)

1.1 Reagents: Potassium carbonate
Catalysts: Tetrakis(triphenylphosphine) palladium
Solvents: TolueneWater; 12 h, 90 °C

B ⇒ D + E

Maximum Yield: 92%
Evidence (8)
Alternative Steps (16)

1.1 Reagents: Potassium carbonate
Catalysts: Tetrakis(triphenylphosphine) palladium
Solvents: EthanolTolueneWater; 12 h, 110 °C

C ⇒ F + G

Maximum Yield: 82%
Evidence (9)
Alternative Steps (20)

1.1 Reagents: Butyllithium
Solvents: Tetrahydrofuran; -78 °C; 1 h, -78 °C
View All
Experimental Protocols



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

Step **Evidence**

| | |
|----------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| A ⇒ B + C Maximum Yield: 90% Evidence (1) Alternative Steps (39) | 1.1 Reagents: Potassium carbonate Catalysts: Tetrakis(triphenylphosphine) palladium Solvents: TolueneWater; 12 h, 90 °C |
| B ⇒ D + E Maximum Yield: 92% Evidence (8) Alternative Steps (16) | 1.1 Reagents: Potassium carbonate Catalysts: Tetrakis(triphenylphosphine) palladium Solvents: EthanolTolueneWater; 12 h, 110 °C |
| C ⇒ F + G Maximum Yield: 82% Evidence (9) Alternative Steps (20) | 1.1 Reagents: Butyllithium Solvents: Tetrahydrofuran; -78 °C; 1 h, -78 °C View All Experimental Protocols |

Max Yield 90%

Reset

Feedback

[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 ▾ 🔗 📄 ✉ 🔖 Save

8 Results Group: By Scheme ▾ Sort: Relevance ▾ View: Expanded ▾

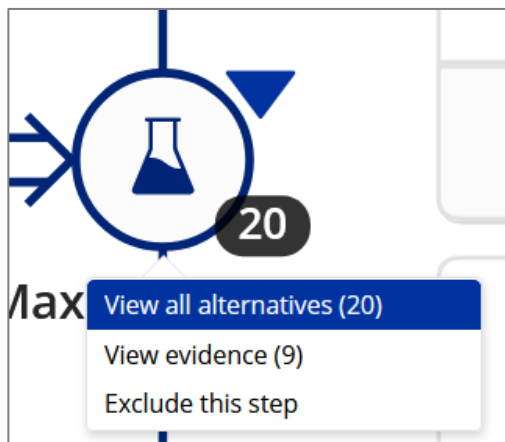
Scheme 1 (8 Reactions) Steps: 1 Yield: 55-92% ⋮

The reaction scheme shows the synthesis of a brominated anthracene derivative. The starting materials are 4-cyano-phenylboronic acid and 1,4-dibromoanthracene. The product is 1,4-dibromoanthracene-9-yl 4-cyanophenyl ether.

[Suppliers \(123\)](#) [Suppliers \(93\)](#) [Suppliers \(37\)](#)

| | | |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <input type="checkbox"/> | 31-179-CAS-22392291 Steps: 1 Yield: 92% ⋮ | Anthracene-based dark blue light organic electrolu minescent material and application in organic light-emitting device thereof By: Wang, Lei; et al China, CN111303009 A 2020-06-19 |
| | 1.1 Reagents: Potassium carbonate Catalysts: Tetrakis(triphenylphosphine)palladium Solvents: EthanolTolueneWater ; 12 h, 110 °C | PatentPak ▾ Full Text ▾ |
| <input type="checkbox"/> | 31-614-CAS-25144957 Steps: 1 Yield: 55% ⋮ | Anthracene-based fluorescent emitters toward superior-efficiency nondoped TTA-OLEDs with deep blue emission and low efficiency roll-off |
| | 1.1 Reagents: Potassium carbonate | |

选择替代路线



20

Max

- View all alternatives (20)
- View evidence (9)
- Exclude this step

C ⇒ F + G

Maximum Yield: 82%

Evidence (9)

Alternative Steps (20)

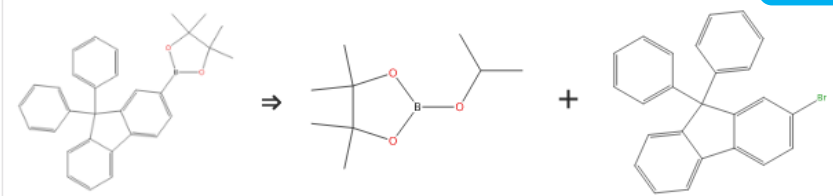


C ⇒ F + G Alternative Steps (20)

Filter by

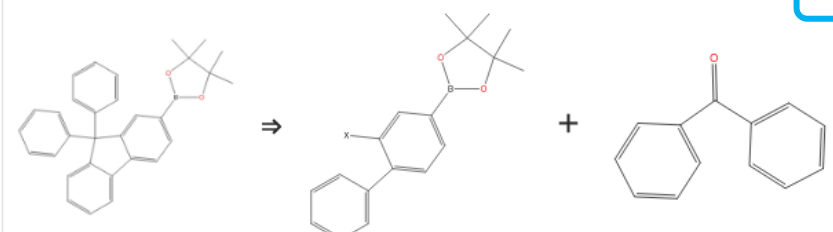
- Alternative Step Type
 - Experimental (3)
 - Predicted (17)
- Stereochemistry
 - Non-Selective (20)

1 of 8 Experimental Step



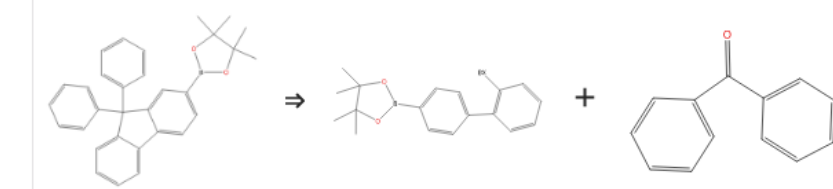
Selected View 6 similar Alternatives View Evidence (9) Maximum Yield: 82%

2 of 8 Predicted Step

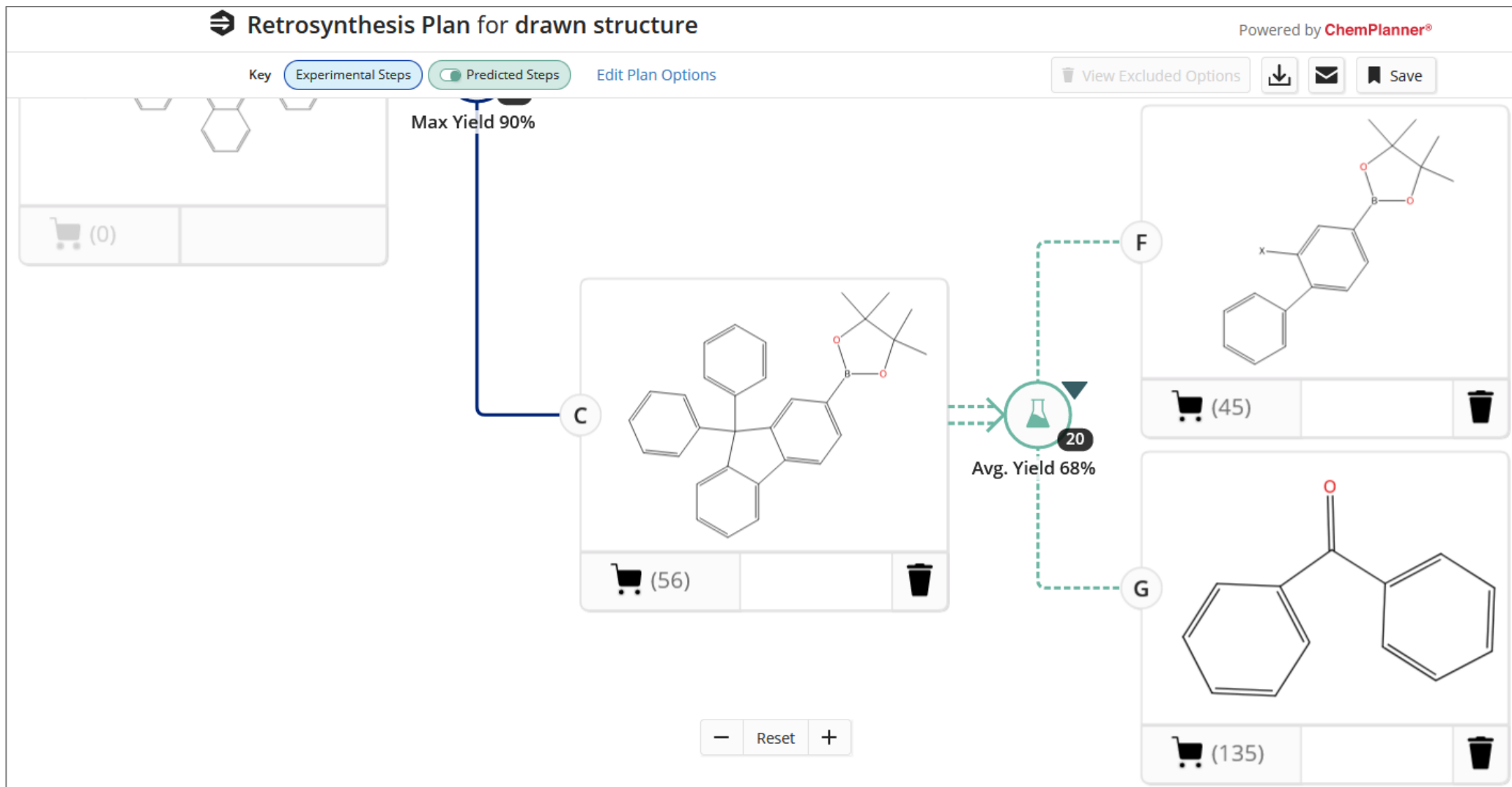


Select Hide 1 similar Alternative View Evidence (455) Average Yield: 68%

2.1 Predicted Step



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、结构式进行反应检索
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 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. 反应路线参数的预先设定与调节
6. 查看反应路线详情和文献支持，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)

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, Teija; 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

[Full Text](#)

[View in CAS SciFinder](#)

[Abstract](#)

文献来源

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

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

分析仪器

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.

Validation

Linearity Range 0-400 μg/L

Concentration < 1 μg

操作步骤

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

The screenshot shows a search interface for "steel and impurity". The main results list includes a highlighted entry: "Validation of an HPLC method for analysis of nifedipine residues on stainless-steel the manufacture of pharmaceuticals". A callout box highlights the "Analytical Methods" link in the article's metadata. Another callout box shows a table of related analytical methods with their CAS Method Numbers.

References search for "steel and impurity"

Substances Reactions Citing Knowledge Graph Save and Alert

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

Filtering: CAS Solutions: Analytical Methods Clear All Filters

23 Results Sort: Relevance View: Partial Abstract

1

Validation of an HPLC method for analysis of nifedipine residues on stainless-steel the manufacture of pharmaceuticals

By: Milenovic, D. M.; Lazic, M. L.; Veljkovic, V. B.; Todorovic, Z. B.
Acta Chromatographica (2008), 20(2), 183-194 | Language: English, Database: CPlus
[Analytical Methods](#)

A simple, sensitive, and convenient HPLC method has been developed, validated, and applied to anal. of nifedipine residues on stainless-steel surfaces of equipment used in drug manufacture Cotton swabs moistened with methanol were used to collect residues of the drug from the surfaces; recoveries were 82.26, 86.88, and 88.95% for 25, 125, and 250 µg per swab the results, as relative standard deviation (RSD), was <5%. The method was validated over the concentration range of 25-250 µg per swab Small quantities of residues of the drug and its main impurities were determined by HPLC

View More

Substances (2) Reactions (0) Citing (10)

electrolyte and arsenic in 10% acetylacetonone electrolyte were in good agreement with industrial data. Titanium and aluminum were measured from the dissolved steel matrix but titanium was also detected in the inclusions. It was concluded that the anal. results for titanium and aluminum measured using an optical emission spectrometer is affected by the inclusions within the stainless steel.

Keywords: double stabilized stainless steel alloying impurity element inclusion

Open Access Full Text

Expand All | Collapse All

Concepts

Substances

Analytical Methods

| Title | CAS Method Number |
|-----------------------------------------------------------------------|-------------------|
| Analysis of Aluminum in Stainless steel by Electrochemical extraction | 1-119-CAS-285768 |
| Analysis of Aluminum in Stainless steel by Electrochemical extraction | 1-119-CAS-286264 |
| Analysis of Vanadium in Stainless steel by Electrochemical extraction | 1-119-CAS-286328 |

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 ▾

CAS Analytical Methods

★ Saved Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

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

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 > Agricultural Applications / Analysis

除草剂、农药残留、土壤分析

Herbicide Analysis

Pesticide Residue Analysis

Soil Analysis

如何选择合适的分析方法?

CAS Solutions Analytical Methods

steel and sulfur

Results (13) Sort Relevance

Compare (2/3)

Remove from Compare

Analysis of Carbon in **Steel** by Laser induced breakdown spectroscopy
CAS MN: 1-119-CAS-267238

View Details & Instructions

| | |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Analyte | Sulfur; Carbon |
| Matrix | Steel |
| Other Materials | Material: Continuum Surelite laser |
| Method Category | Element Detection |
| Technique | Laser induced breakdown spectroscopy |
| Equipment Used | Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer; CCD camera; Gas environment controls |
| Source | Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel Jiang, X.; Hayden, P.; Costello, J. T.; Kennedy, E. T. Spectrochimica Acta, Part B: Atomic Spectroscopy (2014), 101, 106-113. Elsevier B.V. |

Full Text View in CAS SciFinder

Abstract

Analysis of Carbon in **Steel** by Laser induced breakdown spectroscopy

- 分析目标物
- 介质
- 方法类别
- 分析技术
- 发表年份

如何选择合适的分析实验方法?

Compare Methods

| | 1 | 2 |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Title | Analysis of Carbon in Steel by Laser induced breakdown spectroscopy | Analysis of Silver in Steel by Glow discharge mass spectrometry |
| CAS Method Number | 1-119-CAS-267238 | 1-119-CAS-101987 |
| Method Category | Element Detection | Element Detection |
| Technique | Laser induced breakdown spectroscopy | Time-of-flight mass spectrometry; Glow discharge mass spectrometry |
| Analyte | Sulfur ; Carbon | Titanium; Chromium; Antimony; Magnesium; Lead; Silicon; Cobalt; Sulfur ; Niobium; Tin; Nickel; Manganese; Vanadium; Boron; Molybdenum; Phosphorus; Silver; Tungsten; Copper; View All |
| Matrix | Steel | Steel |
| Other Materials | Continuum Surelite laser | Grimm-type chamber (with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube) |
| Equipment Used | Laser-induced breakdown spectrometer; Laser pulse generation system (two synchronized lasers); optical system; Ablation chamber; Spectrometer, VM-521, Acton View All | Orthogonal time-of-flight mass spectrometer, Tofwerk, Thun, Switzerland; Dry pump, Triscroll 300, Varian Inc., Palo Alto, USA; Radio frequency glow discharge orthogonal time View All |

| | | |
|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Source | Double-pulse laser induced breakdown spectroscopy with ambient gas in the vacuum ultraviolet: Optimization of parameters for detection of carbon and sulfur in steel View All | A comparison of non-pulsed radiofrequency and pulsed radiofrequency glow discharge orthogonal time-of-flight mass spectrometry for analytical purposes View All |
| Method | Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode View All | Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode View All |
| Limit of Detection | 2.9 ppm Carbon, 1.5 ppm, Sulfur | 0.3 µg/g, Boron, 0.2 µg/g, Magnesium, 0.3 µg/g, Aluminum, 1.9 µg/g, Silicon, 1.6 µg/g, Phosphorus, 1.0 µg/g, Sulfur , 2.3 µg/g, Titanium, 1.1 µg/g, Vanadium, 1.0 µg/g, Chromium, 5.5 View All |
| Precision | | 12% (RSD, reproducibility), Boron, 28% (RSD, reproducibility), Magnesium, 2% (RSD, reproducibility), Aluminum, 6% (RSD, reproducibility), Silicon, 5% (RSD, View All) |
| Sensitivity | | 6 - 165 cps/(µg/g) |

| | | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Method | <p>Laser-induced breakdown spectroscopic analysis using nitrogen as ambient gas in double pulse mode</p> <ol style="list-style-type: none"> 1. Perform the analysis using LIBS setup containing the laser pulse generation system (two synchronized lasers), the optical system (lenses, mirrors, polarizer and half-wave plate), an ablation chamber, spectrometer, detection system (CCD camera and computer) and finally the gas environment controls (needle valve, gauge, pressure meters). 2. Use the Q-switched Nd:YAG lasers to create the plasmas in double-pulse mode by Continuum Surelite (model III-10), operating at the fundamental wavelength of 1.06 µm with a pulse width of 6 ± 1 ns and maximum output energy of 800 mJ. 3. Operate the laser at a repetition rate of 10 Hz.. 4. Insert the optical combination of a half-wave plate and a polarizer into the Surelite laser beam to vary the pulse energy incident on the sample. 5. Focus the approximately 10-mm-diameter beams produced by Surelite laser onto the steel samples by plano-convex lenses of 125 mm and 150 mm focal | <p>Glow discharge orthogonal time-of-flight mass spectrometry in pulsed mode</p> <ol style="list-style-type: none"> 1. Collect the NIST 1262b certified reference steel. 2. Determine the performance of the pulsed RFGD-TOFMS. 3. The radiofrequency glow discharge orthogonal time-of-flight mass spectrometer (RFGD-TOFMS) includes a RFGD bay unit (RF generator, matching box, RF connector, refrigerator disc and sample mounting system with a pneumatic piston to press the sample against the source) (GD Profiler HR instrument (Horiba Jobin Yvon, Longjumeau, France)). 4. Use the GD source of a copper-based modified Grimm-type chamber with a 4 mm diameter anode and a 2.5 mm inner diameter flow tube (EMPA, Switzerland). 5. Extract the ions originating from the source at pressure of 800 Pa through a sampler of 500 µm diameter and a 1 mm diameter skimmer. 6. The following interface region includes electrostatic focusing and deflecting components and couples the |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

详细的分析实验方法对比

研究课题在产品中的应用？配方的检索与设计

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

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 "orthopedic and implant"

Get Additional References Compare (0/3)

1,064 Results Sort: Relevance

Filter by

- Industry
 - Cosmetics & Personal Care
 - Pharmaceutical
 - Unclassified
- Purpose
 - Drug delivery systems (296)
 - Antitumor agents (107)
 - Pharmaceutical formulations (81)
 - Ophthalmic agents (73)
 - Antipsychotics (65)
- Physical Form
 - Pharmaceutical implants (1,064)
 - Tablets (315)
 - Capsules (226)
 - Powders (207)
 - Suspensions (154)
- State of Matter
- Delivery Route
 - Ophthalmic drug delivery systems (177)
 - Subcutaneous drug delivery systems (138)
 - Intramuscular injections (81)
 - Pharmaceutical injections (74)
 - Pharmaceutical implants (61)
- Information Included
 - Component Amount (1,393)
 - Process (1,064)
 - Experimental Activity (721)

View All

1

Implants: Antitumor Agents

Location: Article page 3, 6, 7, 8, 9
Purpose: Antitumor agents
Physical Form: **implant**

Add to Compare

| Component | Function | Amount Reported |
|--------------------------------------|----------------|-----------------|
| Group: Ti-TNTs wire implants | implant | - |
| Ti wires | additives | - |
| Acetone | Solvents | - |
| Ethanol | Solvents | - |
| Perchloric acid | additives | 1 |
| Additional group components reported | | |
| Trail aqueous solution | - | 2 mg/mL |

[View Formulation Detail](#)

2

Composition for Promoting Bone Formation

Location: Claim 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41
Purpose: promoting bone formation
Target: Amphibia, Ape, Aves, Bos taurus, Canis familiaris, Capra, Cavia porcellus, Equus caballus, Felis catus, Fish, Gerbil, Hamster, Homo sapiens, Monkey, Mus musculus, Oryctolagus cuniculus, Ovis aries, Rattus, Reptilia, Swine
Delivery Route: Intraosseous prosthetic implants, intramedullary application
Physical Form: **pharmaceutical implants**

Add to Compare

| Component | Function | Amount Reported |
|--------------------------------|----------|-----------------|
| Group: surgical implant | - | - |
| Dental implants | - | - |

JOURNAL

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials
Language: English

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

PATENT

Use of pro-inflammatory compounds for promoting bone formation

Assignee : Imperial Innovations Limited

- 一次最多可以比较三种不同制剂或配方的信息详情

配方的制备? 实验评估?

Implants: Antitumor Agents

Download Save

| Purpose | Target | Delivery Route | Physical Form | Source |
|------------------|--------|----------------|---------------|--------|
| Antitumor agents | - | - | implant | View |

Formulation Ingredients Expand All Groups | Collapse All Groups

| Component | Function | Amount Reported | Optionality |
|------------------------------|------------------------|-----------------|-------------|
| Group: Ti-TNTs wire implants | implant | - | Mandatory |
| Ti wires | additives | - | Mandatory |
| Acetone | Solvents | - | Mandatory |
| Ethanol | Solvents | - | Mandatory |
| Perchloric acid | additives | 1 | Mandatory |
| butanol | Solvents | 6 | Mandatory |
| ethylene glycol electrolyte | solid support material | 9 | Mandatory |
| Water | Solvents | - | Mandatory |
| Trail aqueous solution | - | 2 mg/mL | Mandatory |

More Formulations like this... NEW

Ha-NP with HASE: Antitumor Agents
Purpose: Antitumor agents
Target: -
Delivery Route: -
Physical Form: Particles

CIPRODEX: Antibacterial
Purpose: Antibacterial agents
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (otic)
Physical Form: Liquids, Suspensions

CIPRODEX Ciprofloxacin and Dexamethasone Suspension/Drops: Antibacterial Agents or...
Purpose: Antibacterial agents, corticos...
Target: Haemophilus influenzae, Hom...
Delivery Route: AURICULAR (optic).
Physical Form: Liquids, Suspensions

Ha-NP-Loaded Microneedle Patch: Antitumor Agents
Purpose: Antitumor agents
Target: Neoplasm
Delivery Route: skin absorption
Physical Form: Pharmaceutical patches

Process

stage 1: Ti-TNTs wire implants were loaded overnight with 2 mg/mL Trail aqueous solution for in-vitro, ex-vivo and in-vivo studies. prior to loading, implants were cleaned with ethanol, dried under sterile conditions and placed in a 30 mL drops of Trail solutions placed on a parafilm strip. after overnight drug loading, implants were dabbed with a soft tissue and dried and placed in PBS solution to monitor drug release profile at 37 °C, over a range of selected time points.

- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

Experimental Activity

| Descriptor | Notes | Details |
|-----------------------|-------|-------------------------------------------------------------|
| Ex-vivo study | - | no caspase-3 activity was observed for PBS-TNTs samples |
| cell death | - | highest cell death was observed in Trail-TNTs |
| drug release | - | 45 % |
| in-vitro cytotoxicity | - | luciferase activity confirmed 100% cell death in Trail-TNTs |
| loading amount | - | 12.63 µg |

Source Journal

Titanium wire implants with nanotube arrays: A study model for localized cancer treatment

Biomaterials
Language: English
Location: Article page 3, 6, 7, 8, 9

Full Text 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

Add Another Term

 Search

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

- Optional
- Required
- Optional
- Excluded

Clear All

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"



Filter by

Industry

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

[View All](#)

Regulatory Information

- REACH (5)
- Cosing: Cosmetic Ingredient Inventory (3)
- EPA Pesticide Inactive Ingredients (3)
- FDA Inactive Ingredients Database (3)
- ANMAT (1)

[View All](#)

Experimental Properties

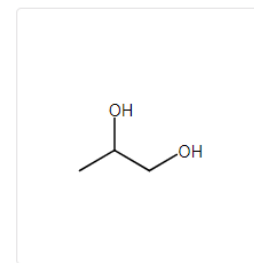
- Boiling Point (3)

2 Selected 3 Results

1

CAS RN: 57-55-6

[View Details](#)



(±)-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

 Formulation Designer

Formulation Designer

[Clear All Selections](#)

Industry

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


Purpose


Cosmetics and Personal care products
Skin conditioners
Sunscreens
Hair dyes
Hair preparations
Antiperspirants
Cleaning compositions
Skin-lightening cosmetics
Skin cleansers
Oral hygiene products
Skin care products
[- View More Purposes -](#)


Physical Form

Emulsions
Cream preparations
Cosmetic lotions
Cosmetic packs
Gels
Liquids
Solutions
Nanospheres
Pastes
Capsules
[- View More Physical Forms -](#)

Add up to 5 Ingredients

Vitamin A 

Polyethylene glycol 

 [Add Another Ingredient](#)

Create Template

设计配方

Formulation Designer Clear All Selections

| Industry | Purpose | Physical Form | Active or Featured Ingredient |
|---------------------------|--------------------|---------------|----------------------------------|
| Cosmetics & Personal Care | Skin care products | Gels | Vitamin A Polyethylene glycol |

Edit Selections Download

Your Template

| Function | Ingredient | Regulatory | Top Alternatives | Amounts |
|--------------------------------|-----------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|
| Active or Featured Ingredient: | Vitamin A | ANMAT; NMPA | - | Amount not available |
| Active or Featured Ingredient: | Polyethylene glycol | ANMAT; Cosing; Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database | - | Amount not available |
| Function: Carriers | Ethylene glycol View More Alternatives | Cosing; Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database | Water; Polyethylene glycol | |
| Function: Skin conditioners | Ethylene glycol View More Alternatives | Cosing; Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; FDA Inactive Ingredients Database | Glycerol; Allantoin; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated | Approximate Range: 2 - 14% |

- 原料详情
- 原料管制信息
- 可替代的原料选项

Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

| | | |
|-----------------|--------------------------------------|-----------------------------|
| Allantoin | Tricaprin | hydrogenated |
| Ethylene glycol | Palm-oil glycerides, monoglycerides, | Glyceryl polyacrylate |
| 1,2-Octanediol | diglycerides and triglycerides, | N-(2-Hydroxyethyl)acetamide |

文献关联的配方

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 "encapsulat* and resistant starch"

Substances - Reactions - Citing - Knowledge Graph

857 Results Sort: Relevance - View: Partial Abstract -

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

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organ
- Public

CAS Solutions

- Formulus (37)
- Analytical Methods (4)

Resistant starch from high-amylose maize increases insulin sensitivity in overweight and obese men
By: Maki, Kevin C.; Pelkman, Christine L.; Finocchiaro, E. Terry; Kelley, Kathleen M.; Lawless, Andrea L.; Schild, Arianne L.; Ra
Journal of Nutrition (2012), 142(4), 717-723 | Language: English, Database: CAlplus and MEDLINE

This study evaluated the effects of 2 levels of intake of high-amylose maize type 2 resistant starch (HAM-RS2) on insulin S₁ in participants with waist circumference ≥89 (women) or ≥102 cm (men). Participants received 0 (control starch), 15, or 30 (double-blind) of HAM-RS2 in random order for 4-wk periods separated by 3-wk washouts. Minimal model S₁ was assessed at the end of each period using the insulin-modified i.v. glucose tolerance test. The efficacy evaluable sample included 11 men and 11 women (mean ± SEM age 49.5 ± 1.6 y, with a BMI of 30.6 ± 0.5 kg/m² and waist circ...

View More

Full Text - Substances (9) Reactions (0) Citing (131) Citat

Conserved and variable responses of the gut microbiome to resistant starch type 2
By: Bendiks, Zachary A.; Knudsen, Knud E. B.; Keenan, Michael J.; Marco, Maria L.
Microbiome (2020), 8(1), 1-12 | Language: English, Database: CAlplus and MEDLINE

Resistant starch type 2 (RS2), a dietary fiber comprised solely of glucose, has been extensively studied in clinical trials for its ability to improve metabolic and systemic health. Because the health modulatory effects of RS2 are thought to occur through modification of the gut microbiome, those studies frequently include assessments of the gut microbial composition and function. In this review, we identify the conserved responses

定位配方或制剂的功能目标

Formulation Purpose

By Count Alphanumeric

4 Selected

- Food (7)
- Antidiabetic agents (6)
- Dietary supplements (5)
- Diet (3)
- Drug delivery systems (3)
- Antimicrobial agents (2)
- Antibacterial agents (1)
- Antihypertensives (1)
- Antioxidants (1)
- Antitumor agents (1)
- Bakery products (1)
- Beverages (1)

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文献关联的配方

Concepts

MEDLINE® Medical Subject Headings

Substances

Formulations

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

| Component | 成分 | Function | 功能 | Amount Reported | 用量 |
|------------------------------------------------------|----|--------------------|----|-----------------|----|
| Group: bioactive component-loaded microparticle core | | model active agent | | - | |
| 5-Aminosalicylic acid | | - | | 20 % | |
| Cellulose | | additives | | Ratio: 3 | |
| Starch | | excipients | | Ratio: 1 | |
| Group: RS3-based aqueous coating dispersion | | coating materials | | - | |

Resistant Starch (RS 3)Film-Coated Microparticles: Drug Delivery Systems--Controlled Release Drug Delivery Systems

[View CAS Formulus® Detail](#)

Location: SI Page 3 Article Page 2 Figure 15

Purpose: Drug delivery systems

Target: 5-aminosalicylic acid

Resistant Starch Film-Coated Microparticles for an Oral Colon-Specific Polypeptide Delivery System and Its Release Behaviors

Substances (3) Reactions (0) Citing (42) Citation Map

JOURNAL

Source

Journal of Agricultural and Food Chemistry

Volume: 62

Issue: 16

Pages: 3599-3609

Journal: Evaluation Study; Article;

Research Support, Non-U.S. Gov't

2014

DOI:

[10.1021/jf500472b](https://doi.org/10.1021/jf500472b)

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CAPUS and MEDLINE

Company/Organization

Ministry of Education Engineering

Research Centre of Starch and

Protein Processing, Guangdong

Province Key Laboratory for Green

Processing of Natural Products

and Product Safety

South China University of

Technology

Guangzhou 510640

China

Publisher

American Chemical Society

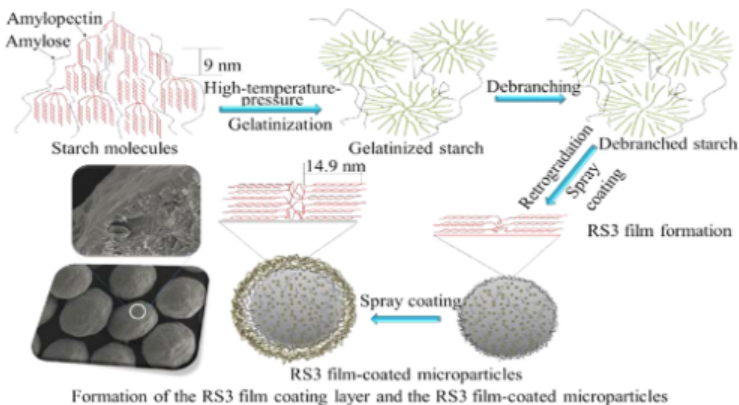
Language

English

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®](#).

By: Situ, Wenbei; Chen, Ling; Wang, Xueyu; Li, Xiaoxi

For the delivery of bioactive components to the colon, an oral colon-specific controlled release system coated with a resistant starch-based film through aqueous dispersion coating process was developed. Starch was modified by a high-temperature-pressure reaction, enzymic debranching, and retrogradation, resulting in a dramatic increase in the resistibility against enzymic digestion (meaning the formation of resistant starch, specifically RS3). This increase could be associated with an increase in the relative crystallinity, a greater amount of starch mol. aggregation structure, and the formation of a compact mass fractal structure, resulting from the treatment. The microparticles coated with this RS3 film showed an excellent controlled release property. In streptozotocin (STZ)-induced type II diabetic rats, the RS3 film-coated insulin-loaded microparticles exhibited the ability to steadily decrease the plasma glucose level initially and then maintain the plasma glucose level within the normal range for total 14-22 h with different insulin dosages after oral administration; no hypoglycemia or glycemic fluctuation was observed. Therefore, the potential of this new RS3 film-coated microparticle system has been demonstrated for the accurate delivery of bioactive polypeptides or protein to the colon.



Keywords: starch film coated microparticle colon polypeptide delivery insulin

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Concepts

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
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|-------|--------------------------------------------------------|
| 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 |



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2023 年 9 月 — 12 月

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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

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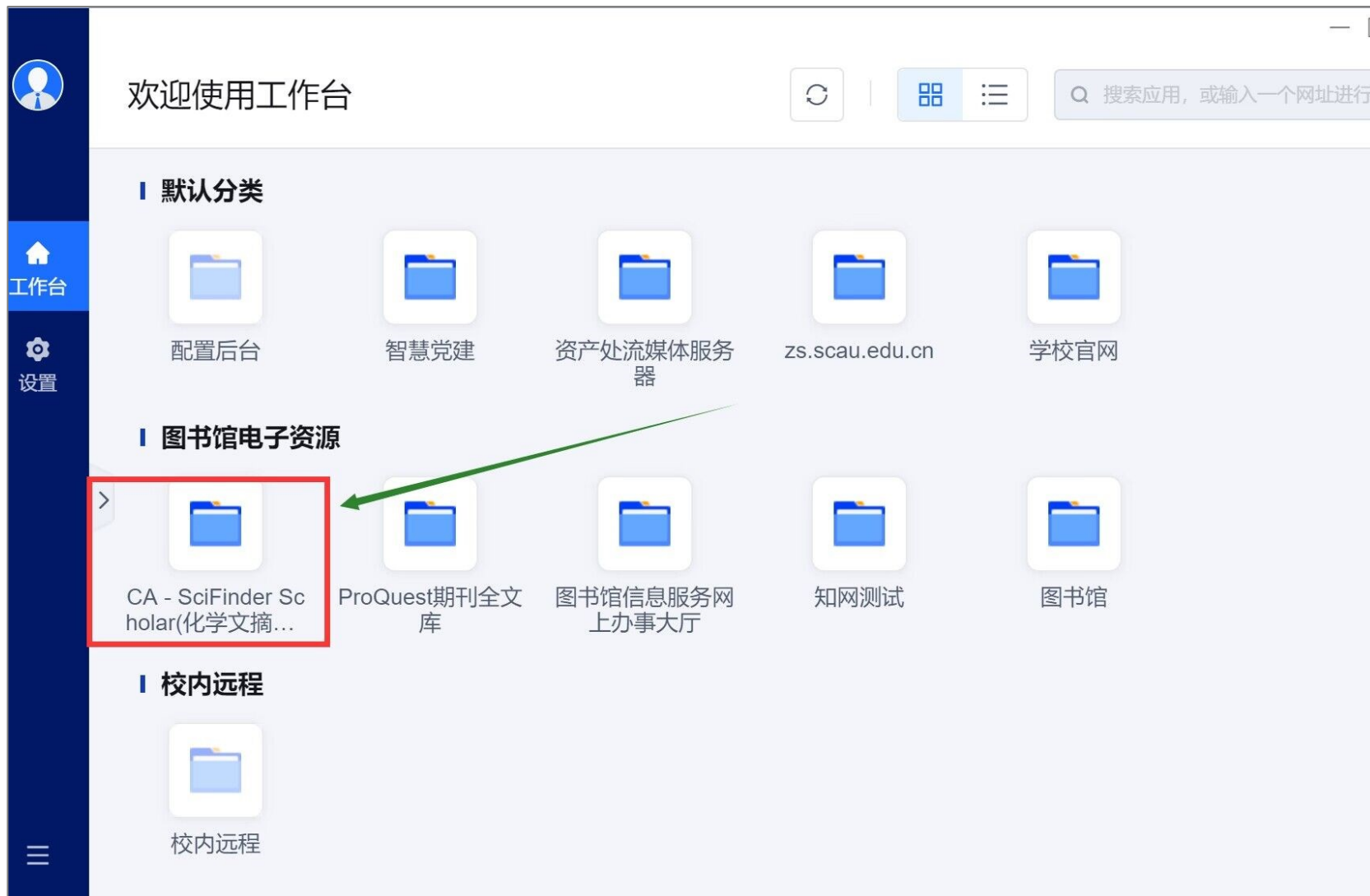
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