

CAS SCIFINDER DISCOVERY PLATFORM™

反应检索策略及典型案例



陈开乾 博士

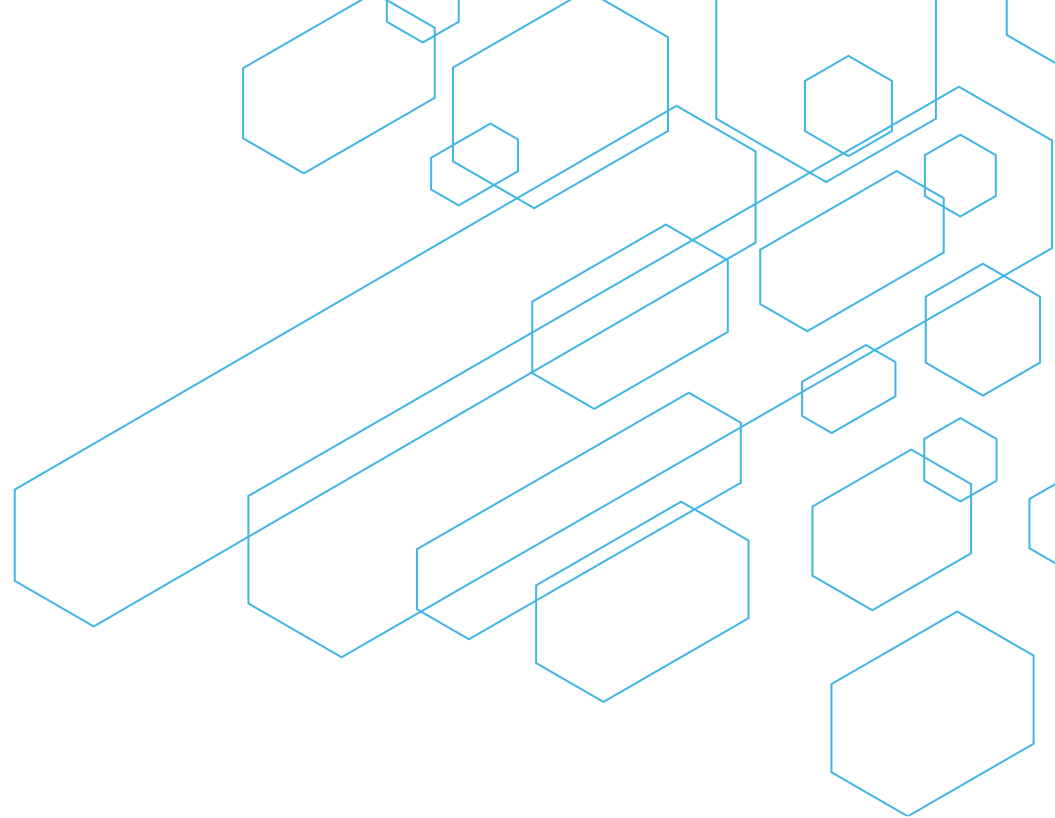
China@acs-i.org

美国化学文摘社北京代表处

5/23/2025

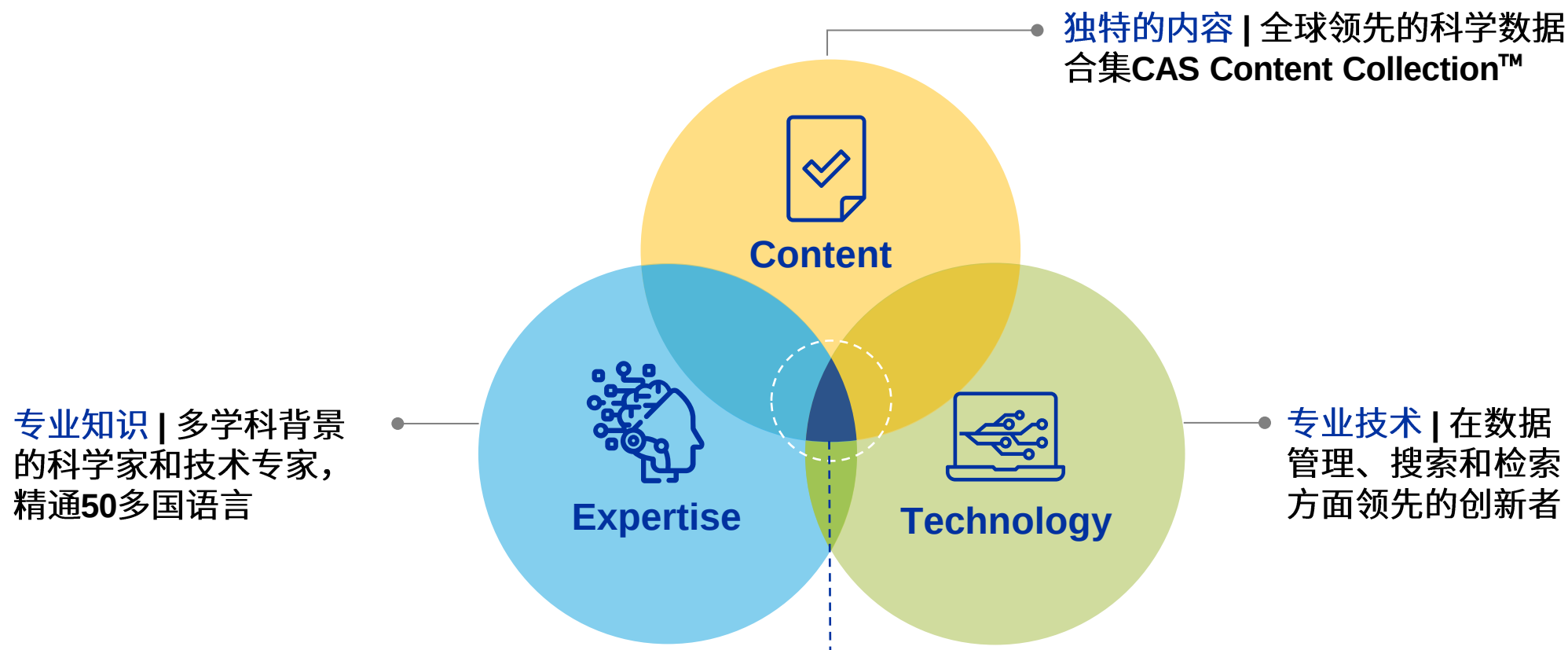
提纲

- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
 - 反应检索策略
 - 典型反应检索案例
- Q&A



关于 CAS

CAS 从专业知识、内容和技术三方面为全球创新保驾护航



我们在全球出版的科学数据间建立关联，
将科学数据转化为更好的洞察力

历经百年，CAS 始终如一 承担着连接全球科学知识的工作

协助科学家解决重大科学信息挑战



50K+

超过5万种科技期刊

50+

50多种语言

290+

超过2.9亿种物质

109

109家
专利授权机构

CAS 对文献的独特解读

以专利WO2018152134为例

改写的标准和摘要，尽可能揭示专利核心价值

丰富的增值标引信息：

19 Concepts

163 Substances

625 Reactions

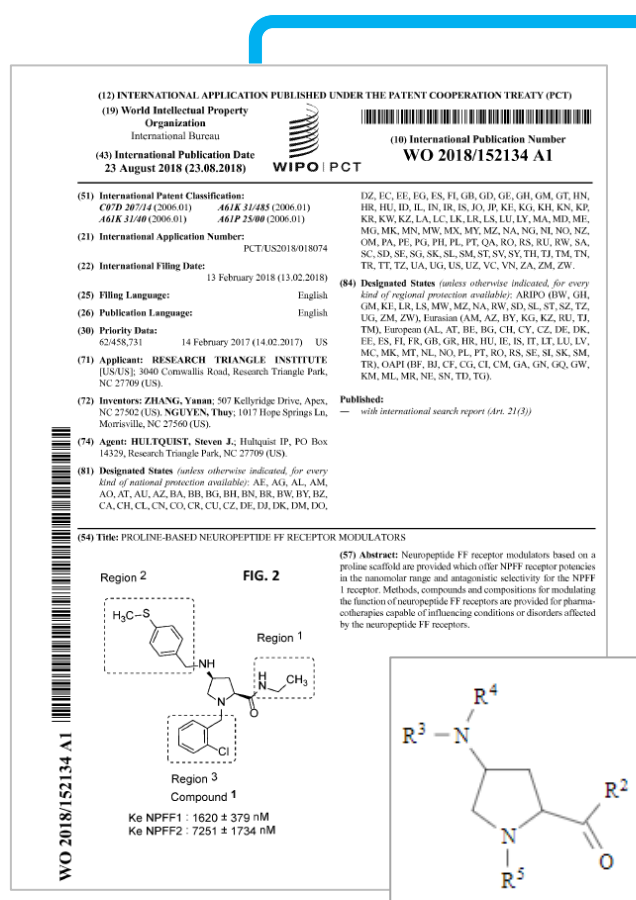
15 Patent Family Members

3 Formulations

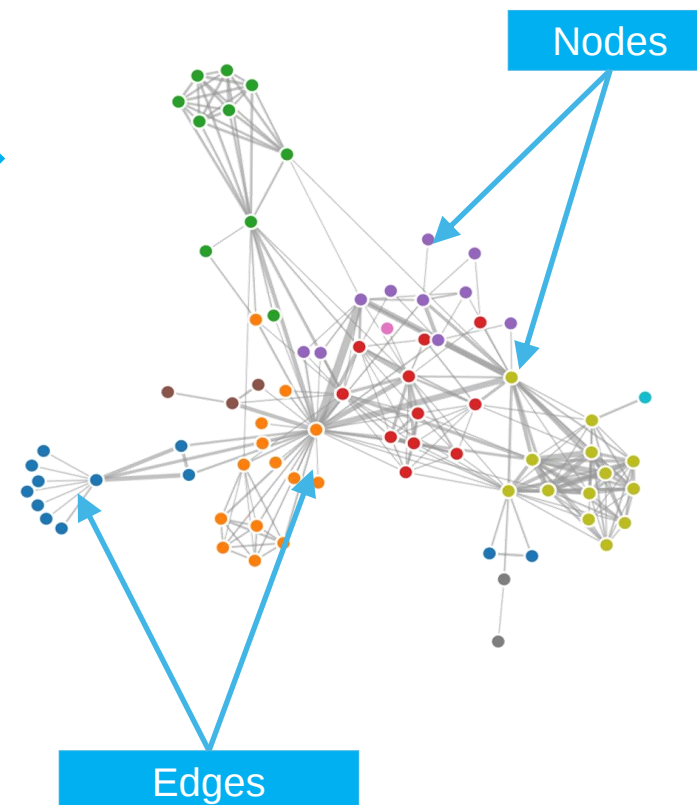
1 Markush structure

18 SAR data points

141 ADME data points



Click document to view on CAS SciFinder®



提纲

- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
 - 反应检索策略
 - 1.通过物质标识符、结构、自然语言等，直接检索反应
 - 2.通过相似反应拓展，物质/文献关联，间接检索反应
 - 3.通过逆合成路线分析获取反应路线
 - 典型反应检索案例
- Q&A

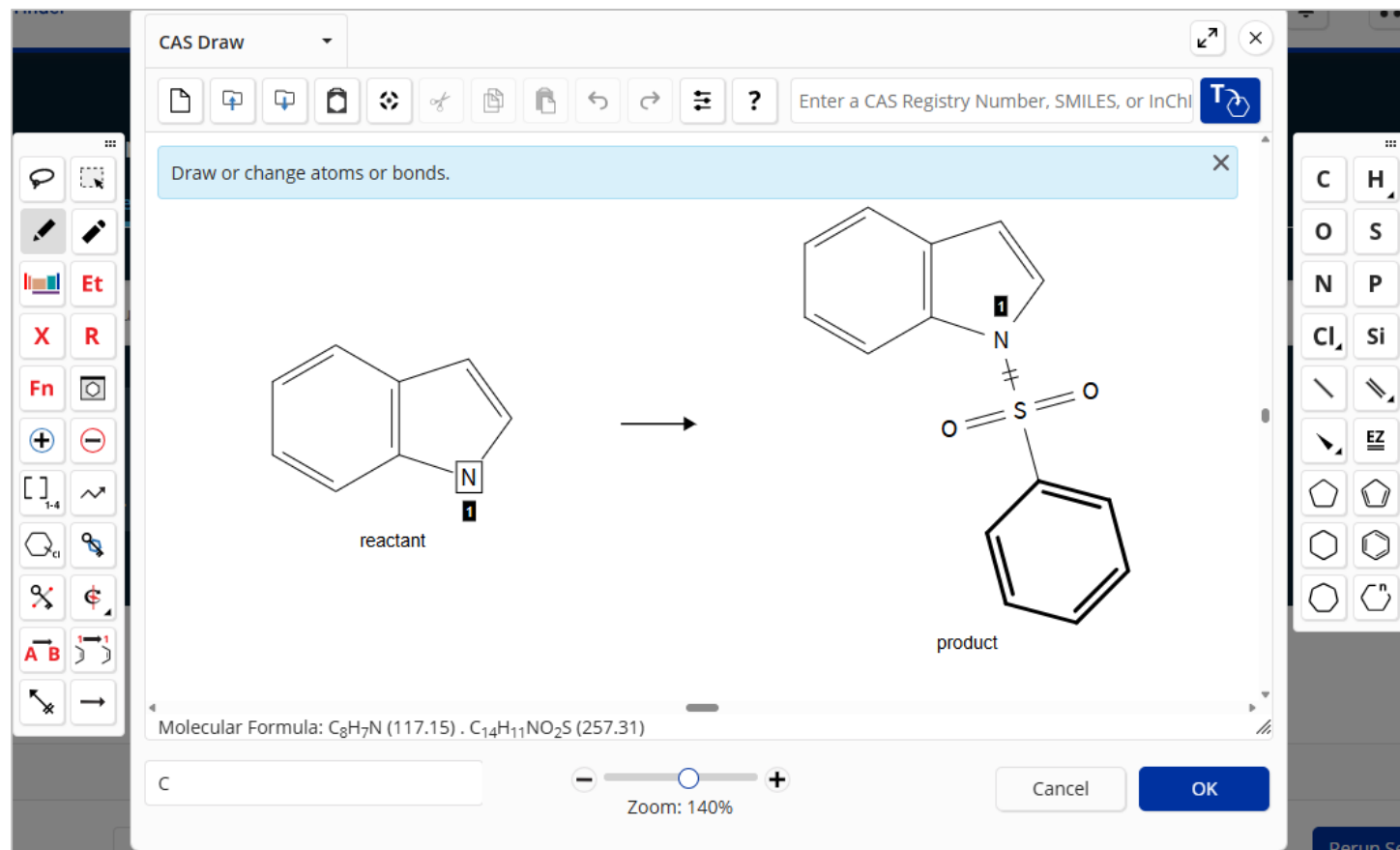
1. 反应的检索方法——直接检索

根据CAS反应方法号、反应式/结构式、物质标识符、文献号、自然语言检索反应

The screenshot displays the CAS Reactions search interface. At the top, there is a navigation bar with tabs for 'All', 'Substances', 'Reactions' (selected), 'References', and 'Suppliers'. A 'For You' button with a 'NEW' tag is also present. Below the navigation bar is a search bar with the placeholder text: 'Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' To the right of the search bar is an 'Edit' button with a dropdown arrow. Below the search bar, a 'CAS Draw' window is open. This window contains a toolbar with various drawing tools, a text input field for 'Enter a CAS Registry Number, SMILES, or InChI.', and a 'Molecular Formula' section with a 'C' input field. To the right of the 'CAS Draw' window, a 'Edit Drawing' button is visible, which is highlighted by a yellow arrow pointing from the 'Edit' button in the search bar. The 'Edit Drawing' button shows a chemical reaction scheme and a 'Remove' button.

(续) 1. 反应的检索方法——直接检索

使用绘制反应式、底物或产物检索反应



反应绘制工具注释:



反应角色定义工具



反应原子标记工具



化学键标记工具



反应箭头



环锁定工具



原子锁定工具

Reaction Roles

Select a role for the structure fragment.

☐ Product

☒ Reactant

☐ Reagent

☐ Reactant/Reagent

☐ Any Role

OK Cancel

(续) 1. 反应的检索方法——直接检索

利用自然语言, 检索某一类反应

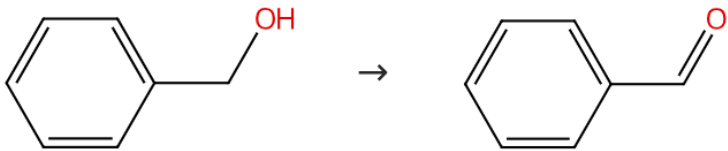
Reactions search for "synthesis of aldehyde catalyzed by Palladium diacetate"

References

乙酸钯催化合成醛类化合物

111,878 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (63 Reactions) Steps: 1 Yield: 100%



Suppliers (168) Suppliers (81)

31-480-CAS-15515097 Steps: 1 Yield: 100%

1.1 Reagents: [Oxygen](#)
Catalysts: [Pyridine](#), [Palladium diacetate](#)
Solvents: [Acetic acid](#); 2 h, 1 atm, 60 °C

Highly selective oxidation of allylic alcohols catalyzed by monodisperse 8-shell Pd nanoclusters in the presence of molecular oxygen
By: Choi, Kwang-Min; et al
New Journal of Chemistry (2003), 27(2), 324-328

Full Text

Filter Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

Catalyst

- ☐ Palladium diacetate (111K)
- ☐ Grubbs second generation catalyst (56K)
- ☐ Grubbs' catalyst (53K)
- ☐ Monopotassium monosodium tartrate tetrahydrate (53K)
- ☐ Water (27K)

产物:
synthesis/preparation
/manufacture of
反应物: from
溶剂: in
催化剂: catalyzed by
试剂: mediated by

2. 反应的检索方法——间接检索

获取相似反应，拓展实验设计思路

Scheme 4 (15 Reactions) Steps: 1 Yield: 60%

Absolute stereochemistry shown Absolute stereochemistry shown, Rotation (-)

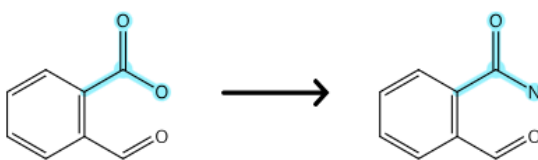
Suppliers (120) Suppliers (75)

31-614-CAS-42267257 Steps: 1 Method and system for the

1.1 Solvents: [Methanol](#), [Water](#); 2.4 MPa, 179 °C; 183.8 °C

Get Similar Reactions

Set Reaction Similarity



☐ Broad (34,980) Reaction centers only ☒ Medium (4,709) Reaction centers plus adjacent atoms and bonds ☐ Narrow (596) Reaction centers plus extended atoms and bonds

Cancel Get Reactions

Reactions similar to 31-614-CAS-42267257

References

Filter Behavior Filter by Exclude

Search Within Results Yield Number of Steps Non-Participating Functional Groups Reaction Mapping Reaction Scale Experimental Protocols Reaction Type Stereochemistry Reagent Catalyst Solvent Commercial Availability Reaction Notes

4,709 Results Group: By Scheme Sort: Publication Date: Newest View: Expanded

Scheme 1 (3 Reactions) Steps: 1 Yield: 78%

Suppliers (83) Suppliers (63)

31-614-CAS-42231899 Steps: 1 Yield: 78% Pyrrolidinone urea fpr2 agonists treating atherosclerosis Assignee: Bristol-Myers Squibb Company World Intellectual Property Organization, WO2024220482 A1 2024-10-24 PatentPak Full Text

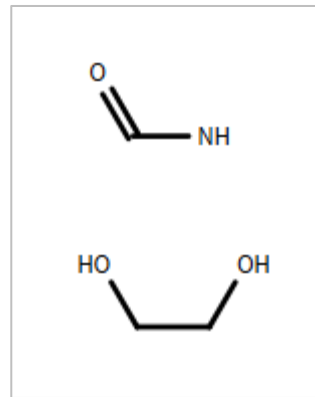
31-367-CAS-21603883 Steps: 1 Yield: 78% Preparation of phenylpyrrolidinone formyl peptide 2 receptor agonists Assignee: Bristol-Myers Squibb Company United States, US20190270704 A1 2019-09-05 PatentPak Full Text

31-367-CAS-19142997 Steps: 1 Preparation of sulfonamides compound as cccDNA inhibitor for treating hepatitis B Assignees: Chia Tai Tianqing Pharmaceutical Group Co., Ltd.; Medshine Discovery Inc.

(续) 2. 反应的检索方法——间接检索

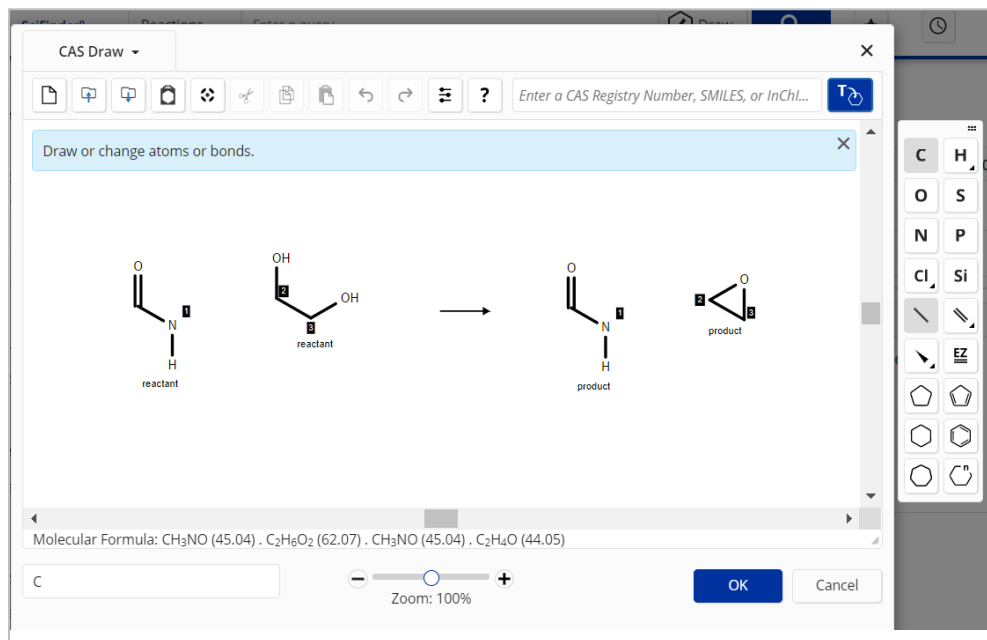
先从结构出发进行物质检索，再获取反应

The screenshot displays the CAS SciFinder web interface. On the left, a sidebar offers various filters: Number of Components (1 (21K) selected), Molecular Weight, LogP, Stereochemistry, Element, Functional Group, Aromatic Rings, and Substance Class (Organic/Inorganic Small Molecule (21K) selected). The main search area is titled 'Substances search for drawn structure'. A dropdown menu 'Get Reactions for Substances' is open, showing 'All Results' and 'Selected Results' options. Below this, search results are displayed in a grid. Each result card shows a chemical structure, a CAS number, a chemical name, and a summary of references, reactions, and suppliers. For example, result 1 shows a chemical structure with CAS number 54393-33-8, identified as Glyceramide ($C_3H_7NO_3$), with 38 references, 14 reactions, and 5 suppliers.



(续) 2. 反应的检索方法——间接检索

Search Within Results: 精炼产物结构



使用原子标记工具精准定位原料和产物中的同一原子

Reactions from Substances

References

Filter Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit

Substance Role

Product (34)

Reactant (178)

Yield

Number of Steps

Non-Participating Functional Groups

Filtering: Search Within Results: Drawn Structure Substance Role: Reactant Clear All Filters

178 Results

Group: By Scheme Sort: Relevance View: Expanded

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

Absolute stereochemistry shown

31-614-CAS-32103514 Steps: 1 Yield: 100%

1.1 Reagents: Sodium hydride; 15 h, 0 °C

1.2 Reagents: Tosyl chloride; 90 min, 0 °C; 90 min, rt; 0 °C

1.3 Reagents: Ammonium chloride

Solvents: Water

Preparation of 2,3-dihydrofuro[2,3-c]pyridine derivatives as anti-viral agents

Assignee: Enanta Pharmaceuticals, Inc.

United States, US20220119398 A1 2022-04-21

PatentPak Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 99%

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (+)

Suppliers (11)

(续) 2. 反应的检索方法——间接检索

主题词与结构联用检索

联用检索提高检索效率

Search interface for "Friedel-Crafts acylation" with a drawn structure of indole. The interface shows the search results for "References search for 'Friedel-Crafts acylation' + drawn structure". The results are filtered by "Structure Match" (As Drawn, 1,280) and "Substructure" (2,827). The search results are sorted by Relevance and viewed as Partial Abstract. The results show a list of references, including a highlighted entry: "ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole". The entry includes the authors (Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad), the journal (Journal of Organic Chemistry, 2011, 76(11), 4753-4758), and the language (English). The abstract describes an efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides in the presence of ZrCl₄. The results are displayed in a table with columns for Substances (40), Reactions (21), Citing (103), and Citation Map.

Search results for "Friedel-Crafts acylation" showing four reaction schemes (Scheme 1 to Scheme 4) with chemical structures and associated suppliers.

- Scheme 1 (1 Reaction):** Steps: 1 Yield: 82% ***
Reactants: 1,2-dichloro-4-methylbenzene + Indole
Product: 1,2-dichloro-4-methyl-3-(indol-1-yl)benzene
Suppliers: (85), (117), (14)
- Scheme 2 (1 Reaction):** Steps: 1 Yield: 78% ***
Reactants: 1-methyl-2-(2-chlorophenyl)indole + Benzoyl chloride
Product: 1-methyl-2-(2-benzoylphenyl)indole
Suppliers: (104), (89), (9)
- Scheme 3 (1 Reaction):** Steps: 1 Yield: 77% ***
Reactants: Indole + 4-methoxybenzoyl chloride
Product: 3-(4-methoxybenzoyl)indole
Suppliers: (117), (73), (23)
- Scheme 4 (1 Reaction):** Steps: 1 Yield: 77% ***
Reactants: 2-chloro-2-methylpropanoic acid + 1-methyl-2-(2-chlorophenyl)indole
Product: 1-methyl-2-(2-(2-methylpropanoyl)phenyl)indole
Suppliers: (46), (104), (33)

3. 反应的检索方法——Retrosynthetic Analysis

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知或未知分子设计合成路线



Retrosynthetic Analysis

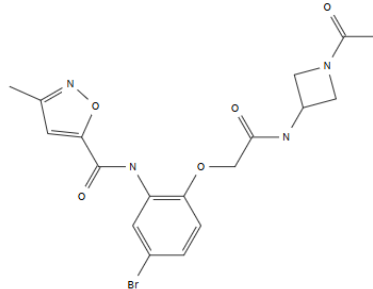
Make reaction plans with conditions, yields, catalysts, and experimental procedures.



Retrosynthetic Analysis

Draw or import a structure.

Enter a CAS Registry



Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

C

Zoom: 100%

Cancel

Start Retrosynthetic Analysis

Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions

☒ Common

☐ Uncommon (includes common rules)

☐ Rare (includes common and uncommon rules)

反应规则的常见

Set Starting Materials Cost Limit

100

USD/mol

起始原料价

☐ Email me when my plan is complete

Continue to Retrosynthesis Plan

Break and Protect Bonds (Optional)

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. [Learn more](#)

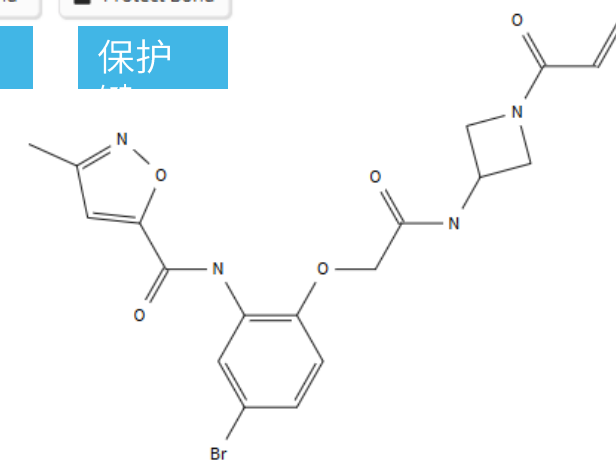
Break Bond

断裂

Protect Bond

保护

Clear All Bond Selections



14

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CAS
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American Chemical Society

(续) 3. 反应的检索方法——Retrosynthetic Analysis

可查看每步反应的文献支持与详细条件

Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

Key: Experimental Steps Predicted Steps Edit Plan Options View Excluded Options Save

已知反应 预测反应

可自由拖动、缩放的路线图

反应中心一致，周边化学结构相似的反应方法

支持的反应 可替换的反应

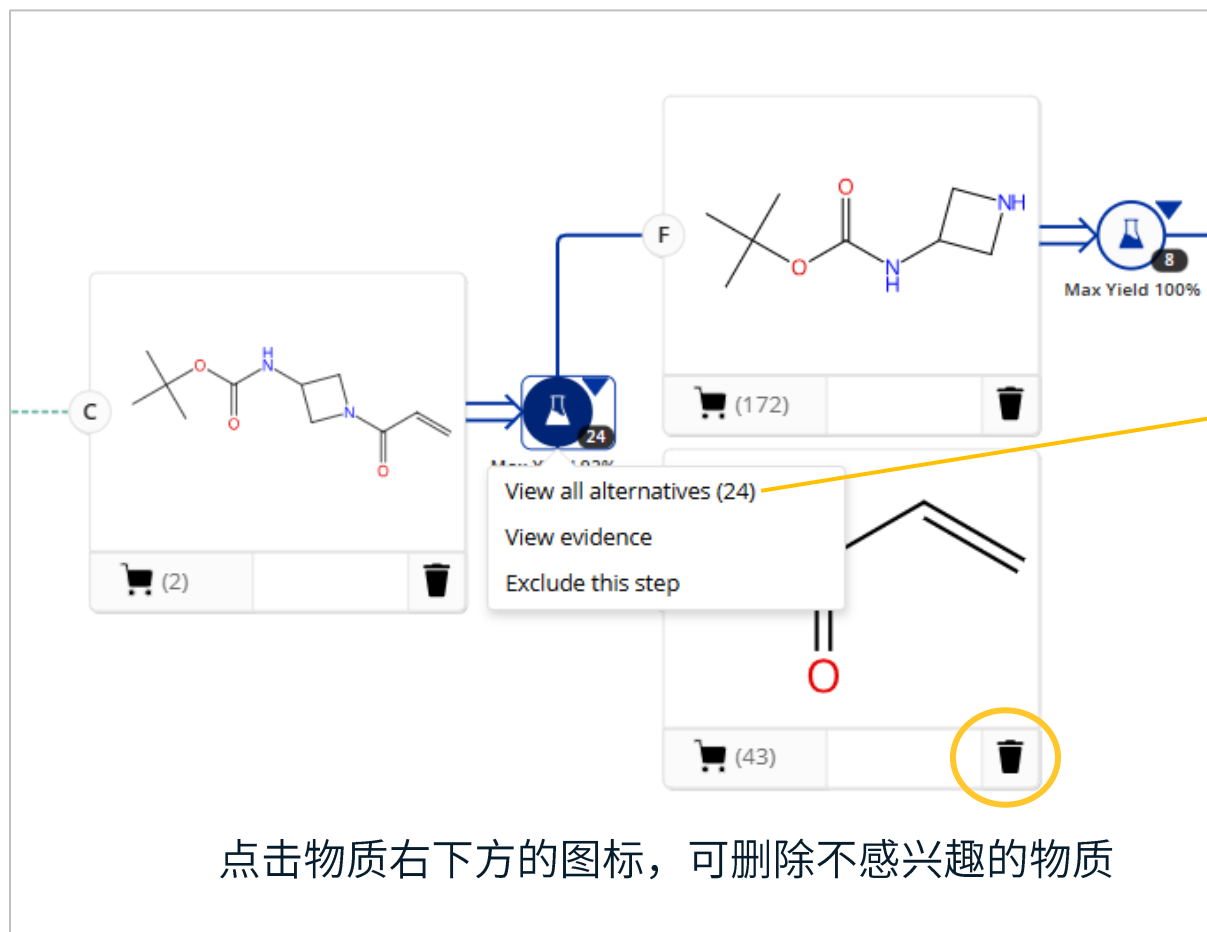
反应条件

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Step	Evidence
A ⇒ B + C	1.1 Reagents: Trifluoroacetic acid Average Yield: 66% Solvents: Dichloromethane Evidence Alternative steps (69)
B ⇒ D + E	1.1 Reagents: Hydrogen Average Yield: 63% Catalysts: Palladium Solvents: Methanol; 4 h, 4 atm, 53 °C Evidence Alternative steps (67) Experimental Protocols
C ⇒ F + G	1.1 Reagents: Sodium bicarbonate Maximum Yield: 92% Solvents: Tetrahydrofuran, Water; 0 °C; 30 min, 5 °C Evidence Alternative steps (25)
D ⇒ I	1.1 Reagents: Potassium carbonate Solvents: Dimethylformamide; 30 min, 5 °C Evidence Alternative steps (15)
E ⇒ J	1.1 Solvents: Acetone, Water; 0 °C; overnight, 0 °C Maximum Yield: 100% Evidence Alternative steps (15)

(续) 3. 反应的检索方法——Retrosynthetic Analysis

反应路线的拓展与优化



C ⇒ F + G Alternative Steps (24)

Filter by

- Alternative Step Type
 - ☐ Experimental (2)
 - ☐ Predicted (22)
- Experimental Stereochemistry
 - ☐ Non-Selective (2)

1 of 11 Experimental Step

Selected View 5 similar Alternatives View evidence Maximum yield: 92%

2 of 11 Predicted Step

Select View 1 similar Alternative View evidence Average yield: 68%

3 of 11 Predicted Step

View All Alternatives: 查看所有的替代反应路线

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

小结

1. 反应的直接检索：

- ✓ 通过反应式，或者反应物/产物/反应试剂的结构式，进行反应检索。
- ✓ 通过物质标识符（包括名称、CAS RN等）、文献号或专利号等，进行反应检索。
- ✓ 通过自然语言进行反应信息检索。

2. 反应的间接检索：

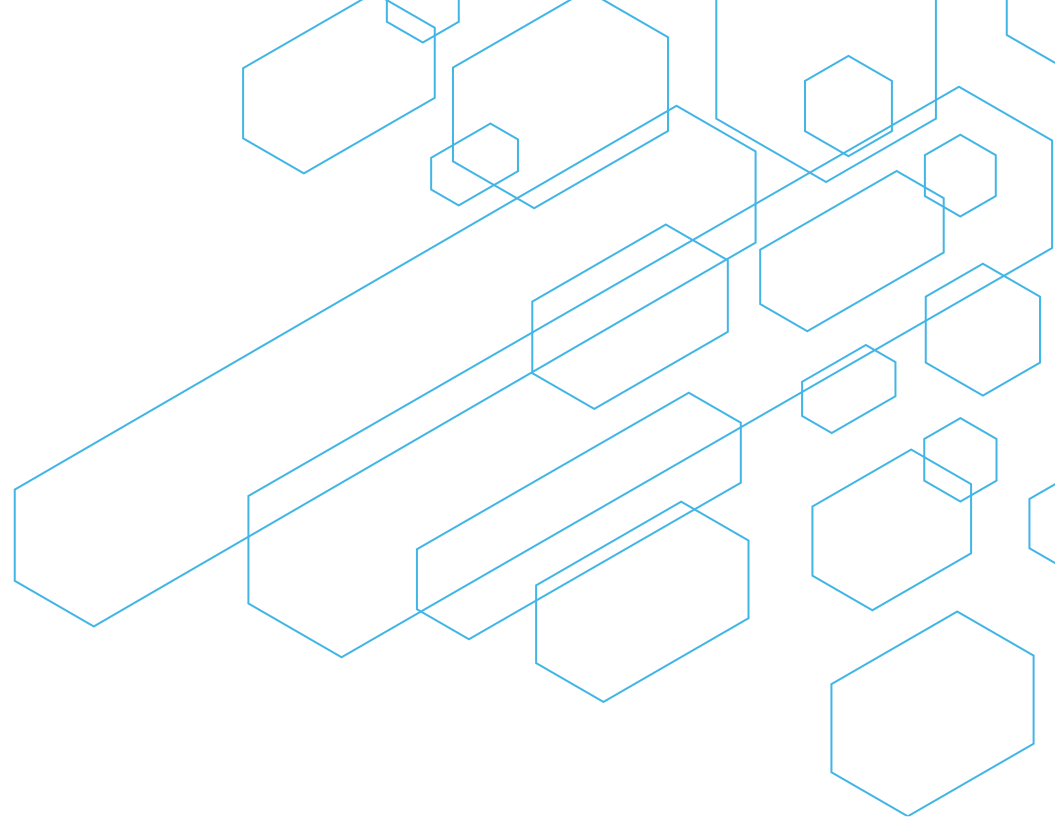
- ✓ 通过相似反应拓展，获取更多相似反应路线支持。
- ✓ 针对某类关注物质，进行结构、属性或反应角色等筛选，再关联到相关反应。
- ✓ 通过关键词或关键词与结构联用，精炼感兴趣的文献信息，并获取相关反应。

3. 通过Retrosynthetic Analysis获取逆合成反应路线

- ✓ 利用AI技术和CAS科学家标引的反应信息，提供已知或未知结构的已有或预测合成路线。

提纲

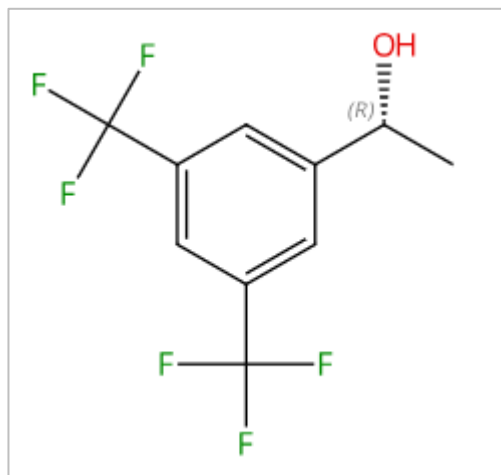
- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
 - 反应检索策略
 - 典型反应检索案例
 - 1. 目标化合物的合成工艺调研
 - 2. 手性化合物的制备与拆分
 - 3. 聚合物材料改性研究
 - 4. 生物转化与生物发酵反应检索
- Q&A



案例1：目标化合物的合成工艺调研

示例：

含氟中间体(R)-1-[3,5-二(三氟甲基)苯基]乙醇的合成工艺



- 通过物质结构、名称或其他物质标识符检索物质
- 一键链接到相关反应

(续) 案例1: 目标化合物的合成工艺调研

示例:

含氟中间体(R)-1-[3,5-二(三氟甲基)苯基]乙醇的合成工艺

- 限定物质角色为产物, 通过产率筛选较优的反应条件
- 可进一步筛选反应规模、实验详情等

关注放大反应

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

☒ Product (51)

☐ Reactant (17)

Yield

☒ 90-100% (51)

☐ 80-89% (10)

☐ 70-79% (5)

☐ 50-69% (5)

☐ 30-49% (5)

View All

Number of Steps

☐ 1 (51)

Reaction Scale

☐ Milligram (12)

☒ Gram (6)

☒ Kilogram (1)

No Scale Provided (32)

Experimental Protocols

☒ Synthetic Methods (26)

☐ Experimental Procedure (7)

Reactions for 127852-28-2

References

Filtering: Substance Role: Product X Yield: 90-100% X Clear All Filters

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

Scheme 1 (49 Reactions) Steps: 1 Yield: 100%



Absolute stereochemistry shown, Rotation (+)

Suppliers (86) Suppliers (90)

31-614-CAS-28848381 Steps: 1 Yield: 100% Sequence of reductase LX05 gene and method for construction of Escherichia coli expressing reductase LX05

1.1 Solvents: Isopropanol, Acetone, Water; 12 h, pH 7.4, 30 °C

Assignee: Hunan University of Science & Technology China, CN113388627 A 2021-09-14

PatentPak Full Text

31-513-CAS-17773066 Steps: 1 Yield: 100% Base-Free Asymmetric Transfer Hydrogenation of 1,2-Di- and Monoketones Catalyzed by a (NH)₂P₂-Macrocyclic Iron(II) Hydride

1.1 Reagents: Isopropanol Catalysts: 2128314-37-2; 0.2 h, 50 °C

By: De Luca, Lorena; et al

Angewandte Chemie, International Edition (2017), 56(39), 11949-11953

Experimental Protocols Full Text

筛选不参与反应官能团

Synthetic Methods——CAS科学家增值标引的合成制备详情

易于阅读的实验操作流程

产物表征数据

反应转化类型

反应注释

(续) 案例1: 目标化合物的合成工艺调研

关注反应转化类型与反应注释

Reactions for 127852-28-2

References

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

☒ Product (215)

☐ Reactant (121)

Yield

☐ 90-100% (51)

☐ 80-89% (10)

☐ 70-79% (5)

☐ 50-69% (5)

☐ 30-49% (5)

[View All](#)

Number of Steps

☐ 1 (172)

☐ 2 (28)

☐ 3 (6)

☐ 4 (2)

Non-Participating Functional Groups

☐ Alkyl halide (172)

☐ Halide (172)

Filtering: Substance Role: Product X

215 Results

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

1

Reduction of Aldehydes and Ketones to Alcohols

[View 158 Related Reactions](#)

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}^1 \longrightarrow \text{R}-\text{CH}(\text{OH})-\text{R}^1$$

2

Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters

[View 6 Related Reactions](#)

$$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{Y}-\text{R}^1 \xrightarrow[\text{H}_2]{\text{H}_2\text{O}} \text{R}-\text{COOH}$$

$$\text{Y} = \text{O}, \text{S}$$

Reaction Notes

By Count Alphanumeric

2 Selected

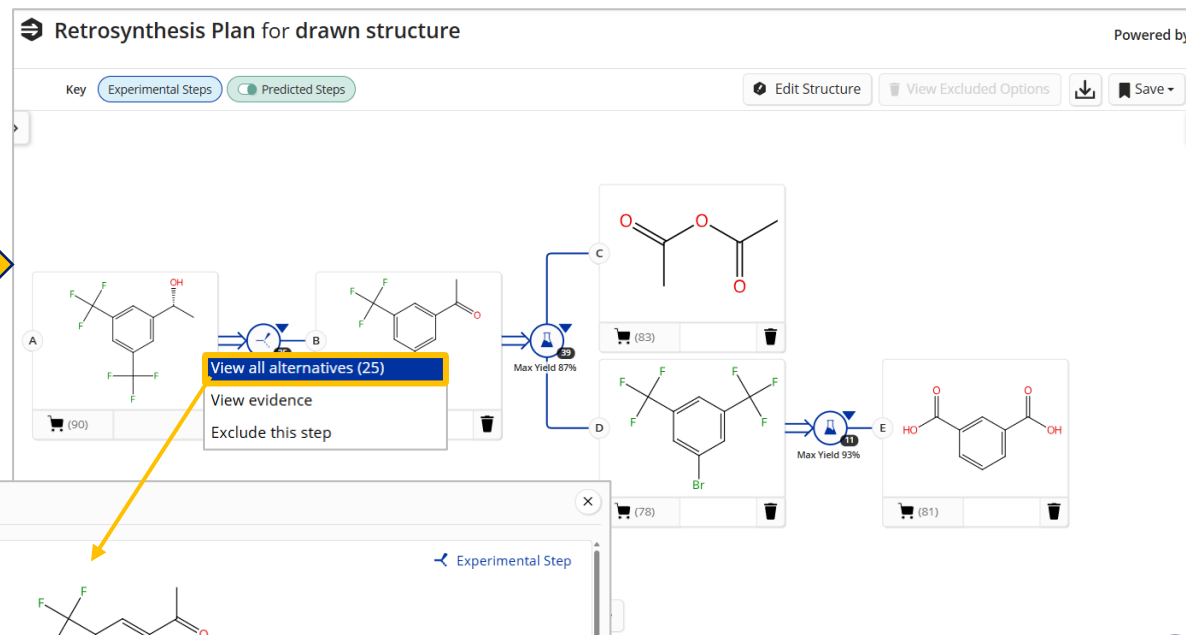
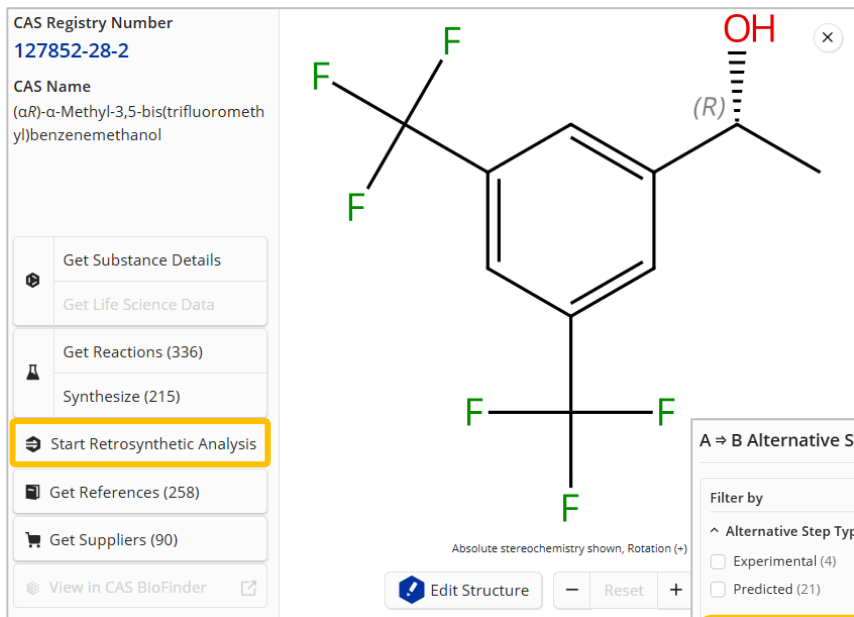
☐ Stereoselective (189)	☐ Photochemical (7)	☐ Green Chemistry-Reagent (1)
☐ Biotransformation (53)	☐ Prophetic Reaction (4)	☐ In The Dark (1)
☐ Enzymic (42)	☐ Solid-Supported Catalyst (4)	☐ Solid State (1)
☐ High Pressure (25)	☐ Regioselective (3)	☐ Solid-Supported Reaction (1)
☒ Green Chemistry (7)	☐ Chemoselective (2)	
☒ Green Chemistry-Catalyst (7)	☐ Thermal (2)	

通过反应注释，精炼筛选感兴趣的反应，如：绿色化学

Cancel Apply

(续) 案例1: 目标化合物的合成工艺调研

逆合成路线分析



A ⇒ B Alternative Steps (25)

Filter by

Alternative Step Type

- ☐ Experimental (4)
- ☐ Predicted (21)

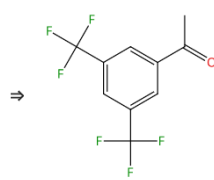
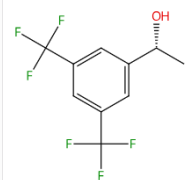
Experimental Stereochemistry

- ☐ Selective (2)
- ☐ Non-Selective (2)

Predicted Stereochemistry

- ☐ Non-Selective (11)
- ☐ Exact (9)
- ☐ Enantiomeric (2)

1 of 10 Stereoselective

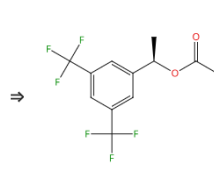
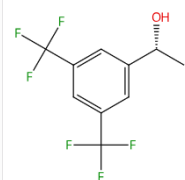


Selected

View evidence

Maximum yield: 100%

2 of 10



Select

View evidence

Maximum yield: 89%

立体化学筛选项

(续) 案例1: 目标化合物的合成工艺调研

获取目标化合物的合成工艺报道文献

- 对结构进行文献检索
- 对物质角色进行筛选
- 对核心研究点进行筛选
- 深入查看感兴趣的文献

The screenshot displays the CAS SciFinder interface. At the top, there's a search bar with "Enter a query..." and a "References" dropdown. Below the search bar, a chemical structure is shown with "Edit Drawing" and "Remove" buttons. The main search results area shows "References search for drawn structure" with 384 results. The left sidebar contains filters for "Structure Match", "Filter Behavior", "Search Within Results", "Document Type", "Substance Role", "Language", "Publication Year", "Author", "Organization", "Publication Name", and "Concept". The "Substance Role" filter is expanded, showing a list of roles with checkboxes. The "Concept" filter is also expanded, showing a list of concepts with checkboxes. Two panels are overlaid on the right side of the interface: "Substance Role" (物质角色) and "Concept" (核心研究点). The "Substance Role" panel shows a list of roles with checkboxes, including "Preparation (284)", "Synthetic Preparation (183)", "Reactant (139)", "Reactant or Reagent (139)", "Biological Study (102)", "Biosynthetic Preparation (79)", "Industrial Manufacture (27)", "Bioindustrial Manufacture (20)", "Purification or Recovery (19)", "Properties (17)", "Biological Study, Unclassified (15)", "Process (9)", "Physical, Engineering, or Chemical Process (6)", "Uses (5)", "Analytical Study (4)", "Analyte (3)", "Biochemical Process (3)", "Byproduct (3)", "Therapeutic Use (3)", "Technical or Engineered Material Use (2)", "Agricultural Use (1)", "Analytical Role, Unclassified (1)", "Catalyst Use (1)", "Formation, Non-preparative (1)", "Formation, Unclassified (1)", and "Prophetic Synthesis or Use (1)". The "Concept" panel shows a list of concepts with checkboxes, including "Process scale-up (2)" and "Spin drying process (1)".

Substance Role (物质角色)

By Count | Alphanumeric

5 Selected

- ☒ Preparation (284)
- ☒ Synthetic Preparation (183)
- ☐ Reactant (139)
- ☐ Reactant or Reagent (139)
- ☐ Biological Study (102)
- ☒ Biosynthetic Preparation (79)
- ☒ Industrial Manufacture (27)
- ☒ Bioindustrial Manufacture (20)
- ☐ Purification or Recovery (19)
- ☐ Properties (17)
- ☐ Biological Study, Unclassified (15)
- ☐ Process (9)
- ☐ Physical, Engineering, or Chemical Process (6)
- ☐ Uses (5)
- ☐ Analytical Study (4)
- ☐ Analyte (3)
- ☐ Biochemical Process (3)
- ☐ Byproduct (3)
- ☐ Therapeutic Use (3)
- ☐ Technical or Engineered Material Use (2)
- ☐ Agricultural Use (1)
- ☐ Analytical Role, Unclassified (1)
- ☐ Catalyst Use (1)
- ☐ Formation, Non-preparative (1)
- ☐ Formation, Unclassified (1)
- ☐ Prophetic Synthesis or Use (1)

Concept (核心研究点)

Top Count | Alphanumeric | Search

Concept Name

process

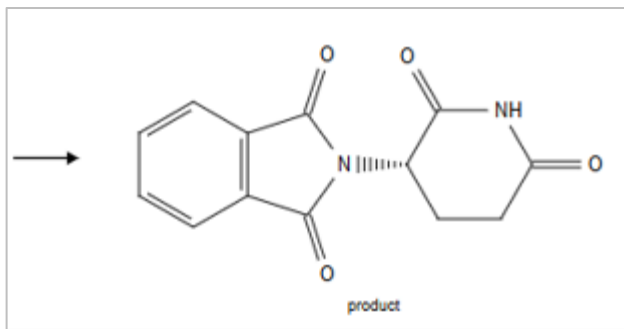
Search

1 Selected

- ☒ Process scale-up (2)
- ☐ Spin drying process (1)

案例2：手性化合物的制备与拆分

直接绘制包含立体结构的反应式进行检索



^ Stereochemistry

- ☒ Absolute Stereo Match (51)
- ☒ Absolute Stereo Mirror Image (24)
- ☐ Stereo that Doesn't Match Query (61)
- ☐ No Stereo in Answer Structure (173)

Reactions search for drawn structure

References

Structure Match

- As Drawn (297)
- Substructure (294K)

Filter Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Filtering: Stereochemistry: 2 Selected X

- ☒ Absolute Stereo Match
- ☒ Absolute Stereo Mirror Image

63 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (2 Reactions) Steps: 1 Yield: 75-90%

Absolute stereochemistry shown

Absolute stereochemistry shown, Rotation (-)

Suppliers (40)

Suppliers (49)

31-367-CAS-622921 Steps: 1 Yield: 90%

1.1 Reagents: [1,1'-Carbonyldiimidazole](#), [4-\(Dimethylamino\)pyridine](#)

Solvents: [Tetrahydrofuran](#)

Preparation of non-polypeptide imides as inhibitors of TNF α

Assignee: Celgene Corporation

United States, US5463063 A 1995-10-31

PatentPak Full Text

31-367-CAS-4058441 Steps: 1 Yield: 75%

1.1 Reagents: [1,1'-Carbonyldiimidazole](#)

Catalysts: [4-\(Dimethylamino\)pyridine](#)

Solvents: [Tetrahydrofuran](#); 20 h, reflux

Synthesis of conjugate of thalidomide and folic acid

By: Wang, Shu-yan; et al

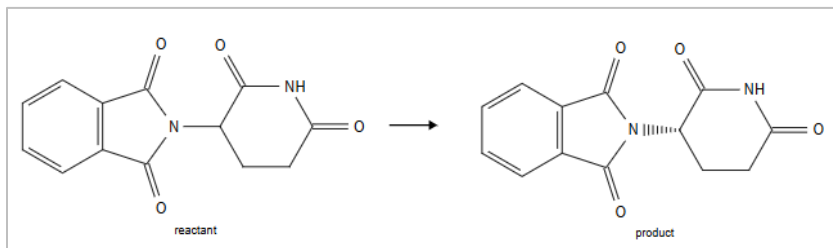
Huaxue Yanjiu Yu Yingyong (2012), 24(3), 469-473

Full Text

Collapse Scheme

(续) 案例2: 手性化合物的制备与拆分

快速获取各类手性拆分反应



直接绘制反应式，检索手性拆分反应

Reactions search for drawn structure

References

Structure Match

- As Drawn (12)
- Substructure (83K)
- Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Source Reference

Document Type

12 Results

Group: By Document Sort: Relevance View: Expanded

根据文献分组

1

Synthesis and configurational stability of (S)- and (R)-deuteriothalidomides

By: Yamamoto, Takeshi; Tokunaga, Etsuko; Nakamura, Shuichi; Shibata, Norio; Toru, Takeshi

Chemical & Pharmaceutical Bulletin (2010), 58(1), 110-112 | Language: English, Database: CApius and MEDLINE

Full Text View 3 Related Reactions

Absolute stereochemistry shown

31-614-CAS-26840098

Steps: 1 Yield: 95%

1.1

Reagents: Sodium periodate

Catalysts: Ruthenium dioxide

Solvents: Dichloromethane, Ethyl acetate, Water; overnight, 40 °C

2

Preparation of chiral ligand H3L with C3 symmetry containing amide bond and application thereof

Assignee: Hefei University of Technology

China, CN113354556 A 2021-09-07 | Language: Chinese, Database: CApius

PatentPak Full Text View 2 Related Reactions

Patent	Language	Kind Code	PatentPak Options
CN113354556	Chinese	A	PDF PDF+ Viewer
CN113354556	Chinese	B	PDF

Absolute stereochemistry shown, Rotation (-)

Suppliers (101)

Suppliers (49)

高效定位专利中重点物质信息——CAS PatentPak

CAS PatentPak:

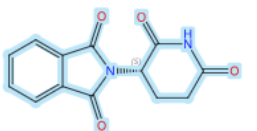
- 快速理解专利
- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

(续) 案例2: 手性化合物的制备与拆分

先检索产物，再链接到反应，并限定底物

1

841-67-8



Absolute stereochemistry shown, Rotation (-)

$C_{13}H_{10}N_2O_4$
(-)-Thalidomide

207 References 51 Reactions 49 Suppliers

在二次检索中，
绘制底物结构

Search Within Results

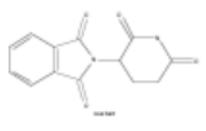
Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit



Substance Role

☒ Product (8)

☐ Reactant (7)

Collapse Scheme ^

Scheme 2 (1 Reaction) Steps: 1



Suppliers (99)

Suppliers (49)

31-614-CAS-24041285 Steps: 1

1.1 Catalysts:
[Tetracosaaquaotakis\[\(N,N'-\(1,3,5-benzenetriyltricarboxyl\)tris\(L-phenylalana...](#)

Solvents: [Acetone](#); 8 h, rt

1.2 -

Preparation of chiral ligand H3L with C3 symmetry containing amide bond and application thereof

Assignee: Hefei University of Technology
China, CN113354556 A 2021-09-07

PatentPak Full Text

Collapse Scheme ^

(续) 案例2: 手性化合物的制备与拆分

使用CAS Analytical Methods获取手性化合物拆分方法: <https://methods.cas.org/>

分析物

方法类别

CAS Analytical Methods 841-67-8

Results for 841-67-8

Filter By

- ^ Analyte
 - ☒ (-)-Thalidomide (24)
 - ☐ (+)-Thalidomide (23)
 - ☐ (+)-Etozolin (8)
 - ☐ (+)-Temazepam (8)
 - ☐ (-)-Etozolin (8)
 - [View All](#)
- ^ Matrix
 - ^ Method Category
 - ☒ Chiral Separation (24)
 - ☐ Active Pharmaceutical Ingredient and Metabolite Analysis (6)
 - ^ Technique
 - ^ Validation
 - ^ Year

24 Results Sort: Relevance Group: By Method

1

Analysis of (-)-Thalidomide by Affinity chromatography JOURNAL

By: Rosengren, Jenny P.; Karlsson, Jesper G.; Nicholls, Ian A.
Enantioselective synthetic thalidomide receptors based upon DNA binding motifs
Organic & Biomolecular Chemistry (2004), 2 (22), 3374-3378. Royal Society of Chemistry

Analyte (-)-Thalidomide

Other Materials Reagent: Acetone; Methacrylic acid; Acetonitrile; 9-(2-Hydroxyethyl)adenine; Methacryloyl chloride; Ethylene glycol dimethacrylate; Chloroform; Sodium hydride; Azobisisobutyronitrile; Dimethylformamide
Material: Sieve (63 μ m); Stainless steel HPLC column (250 x 4.6 mm); Molecularly imprinted polymer (MIP);
[View All](#)

Method Category Chiral Separation

Technique Absorption spectroscopy; Affinity chromatography

Equipment Used Plunger pump; HPLC system; LC pump; Programmable absorbance detector

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

2

Analysis of (+)-Thalidomide in Thalidomide by HPLC JOURNAL

By: Zhang, Tong; Kientzy, Christophe; Franco, Pilar; Ohnishi, Atsushi; Kagamihara, Yasuhiro; Kurosawa, Hidehiro
Solvent versatility of immobilized 3,5-dimethylphenylcarbamate of amylose in enantiomeric separations by HPLC
Journal of Chromatography A (2005), 1075 (1-2), 65-75. Elsevier B.V.

(续) 案例2: 手性化合物的制备与拆分

分析方法详情页

CAS Method Number 1-116-CAS-18769		Method Category Chiral Separation		Technique UV-visible spectroscopy; HPLC	
Analyte (-)-Thalidomide (+)-Thalidomide 分析物	Matrix Thalidomide 基质	Material Chiralpak IA 所用材料	Reagent -	Biological Reagent -	
Equipment Used HPLC system, D-7000, Merck Hitachi Auto-sampler, L- 7200, Merck Hitachi Pump, L-7100, Merck Hitachi Ultraviolet detector, L-7400, Merck Hitachi Column oven, L-7300, Merck Hitachi HPLC system, 1100, Agilent Quaternary pump, Agilent Vacuum degasser, Agilent Column oven, Agilent Multiple wavelength UV detector, Agilent Auto-sampler, Agilent 所用仪器		Instructions High performance liquid chromatography - UV detection procedure using methyl <i>t</i> -butyl ether (MtBE)/1,4-dioxane 90/10 v/v as mobile phase 1. Analyze the sample using HPLC unit Agilent 1100 series apparatus equipped with a quaternary pump, a vacuum degasser, a column oven, a multiple wavelength UV detector, an auto-sampler and a HP Chemstation software. 2. Perform separation on analytical CHIRALPAK IA column (250 mm x 4.6 mm (I.D.)) by Daicel Chemical Industries Ltd. (Japan). 3. Use methyl <i>t</i>-butyl ether (MtBE)/1,4-dioxane 90/10 v/v as mobile phase. 4. Set the flow rate at 1.0 mL/min. 5. Maintain the temperature at 25 °C. 6. Perform detection at a wavelength of 300 nm. 实验步骤			
Validation Separation Factor 1.65, (+)-Thalidomide/(-)-Thalidomide 数据验证					

Conditions 仪器测试条件

Instrument

Mobile phase - methyl *t*-butyl ether (MtBE)/1,4-dioxane 90/10 v/v; flow rate - 1.0 mL/min; temperature - 25 °C

Detection wavelength - 300 nm

Source 文献来源

JOURNAL

Solvent versatility of immobilized 3,5-dimethylphenylcarbamate of amylose in enantiomeric separations by HPLC

Zhang, Tong; Kientzy, Christophe; Franco, Pilar; Ohnishi, Atsushi; Kagamihara, Yasuhiro; Kurosawa, Hidehiro

Journal of Chromatography A (2005), 1075 (1-2), 65 - 75. Elsevier B.V.

CODEN : JCRAEY | ISSN : 00219673 | DOI : 10.1016/j.chroma.2005.03.116

View Abstract ▾

Full Text ▾

(续) 案例2: 手性化合物的制备与拆分

通过CAS Analytical Methods浏览分析方法类别，获取手性拆分分析方法实验



Explore Methods
Search methods using criteria like method categories and subcategories.

Explore Methods

Category

- 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

Category Name

- Active Pharmaceutical Ingredient
- Chiral Separation**
- Natural Product Isolation Analysis
- Organic Compound Analysis

Include Keywords (Optional)

841-67-8

+ Add Another Keyword

Search Methods

案例3：聚合物材料改性研究

通过单体结构、重复结构单元、分子式、属性等，多角度检索聚合物信息

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

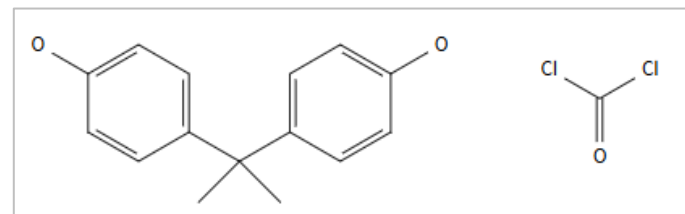
AND - Tensile Strength (Mpa) >50

Search key property values only.

Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2

+ Add Advanced Search Field

拉伸强度大于50Mpa



Search by Substance Name, Functional Group, CAS RN, Patent Number, PubMed ID, AN, C

Molecular Formula (C15H16O2.CCl2O)x

(C₂H₄O)_nC₄H₈O: 括号中是重复结构单元，括号外为n

(C₁₅H₁₆O₂.CCl₂O)_x: 括号中是单体，括号外为x

Substances search for 1 Advanced Field + drawn structure

References Reactions Suppliers

Structure Match

As Drawn (7)

Substructure (8)

Similarity (59)

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

7 Results

Sort: Relevance View: Partial

Results shown:

- 25971-63-5: (C₁₅H₁₆O₂.CCl₂O)_x Components: 2 Carbonic dichloride, polymer with 4,4'-(1-methylethylidene)bis[phenol]
- 103598-77-2: (C₁₅H₁₆O₂.CCl₂O)_x.XC₁₀H₁₄... Components: 3 Carbonic dichloride, polymer with 4,4'-(1-methylethylidene)bis[phenol], 4-(1,1-d...
- 81669-21-8: (C₁₅H₁₆O₂.C₅H₈O₂.CCl₂O)_x Components: 3 2-Propenoic acid, 2-methyl-, methyl ester, polymer with carbonic dichloride and ...

(续) 案例3: 聚合物材料改性研究

从聚碳酸酯物质出发, 获取改性反应

Reactions for 25971-63-5

References

Filter Behavior

Filter by Exclude

Search Within Results

Substance Role

- ☐ Product (50)
- ☒ Reactant (48)
- ☐ Reagent (1)
- ☐ Solvent (1)

Yield

Number of Steps

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Low Pressure (3)

Solid State (3)

Thermal (3)

Green Chemistry (2)

Filtering: Substance Role: Reactant X

48 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Reaction scheme showing the reaction of a polycarbonate resin (HO-(C₆H₄)_n-O-CO-O-(C₆H₄)_n-OH) with a dihydroxy compound (HO-C₆H₄-C(CH₃)₂-C₆H₄-OH) and a reagent (Cl-CO-Cl) to form a modified polycarbonate resin (HO-(C₆H₄)_n-O-CO-O-C(CH₃)₂-C₆H₄-C(CH₃)₂-C₆H₄-O-CO-O-(C₆H₄)_n-OH).

Absolute stereochemistry shown, Rotation (+)

Suppliers (7)

31-614-CAS-38277926 Steps: 1

1.1 Reagents: Triethylamine, Sodium hydroxide
Solvents: Dichloromethane, Water; 1 h, rt

1.2 Reagents: Triethylamine
Solvents: Water; 1 h, rt

Preparation method of eco-friendly polycarbonate resin composition with excellent impact strength and molded products
Assignee: Samyang Holdings Corp.
Korea, Republic of, KR2023097871 A 2023-07-03

PatentPak Full Text

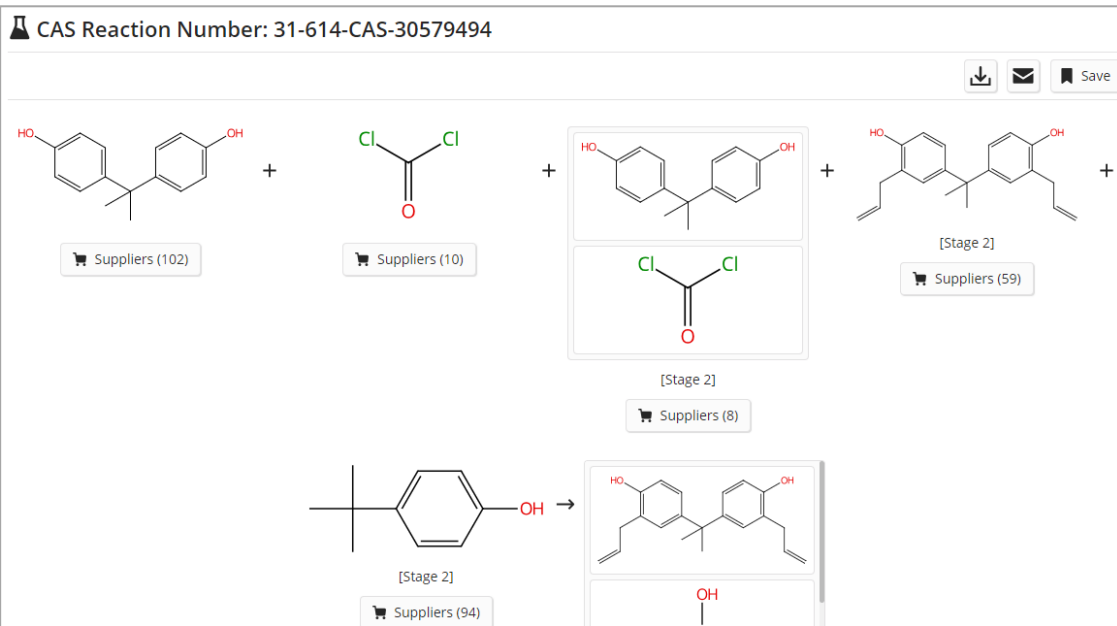
Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1

Reaction scheme showing the reaction of a polycarbonate resin (HO-(C₆H₄)_n-O-CO-O-(C₆H₄)_n-OH) with a dihydroxy compound (HO-C₆H₄-C(CH₃)₂-C₆H₄-OH) and a reagent (Cl-CO-Cl) to form a modified polycarbonate resin (HO-(C₆H₄)_n-O-CO-O-C(CH₃)₂-C₆H₄-C(CH₃)₂-C₆H₄-O-CO-O-(C₆H₄)_n-OH).

(续) 案例3: 聚合物材料改性研究

改性反应详情



Step 1				
Stage	Reagents	Catalysts	Solvents	Conditions
1	Sodium hydroxide	-	Dichloromethane Water	rt; 30 min, rt
2	Triethylamine Sodium hydroxide	-	Dichloromethane	3 h, rt
3	Triethylamine Sodium hydroxide	-	Dichloromethane Water	3 h, rt
4	Hydrochloric acid	-	Water	neutralized

Synthetic Methods	Experimental Procedure
Products	Carbonic dichloride, polymer with 1,1-dimethylsilanediol, 4,4'-(1-methylethylidene)bis[phenol] and 4,4'-(1-methylethylidene)bis[2-(2-propen-1-yl)phenol], graft
Reactants	Phosgene 2,2-Bis(4-hydroxyphenyl)propane 4-tert-Butylphenol o,o'-Diallylbisphenol A Carbonic dichloride, polymer with 4,4'-(1-methylethylidene)bis[phenol]
Reagents	Sodium hydroxide Triethylamine Hydrochloric acid
Solvents	Dichloromethane Water
Procedure	1. Add bisphenol A (114 g) and 5.4 wt% aqueous NaOH solution (44.8 g, 1.12 mol) to a 3 L of three-necked round bottomed flask that is filled with a nitrogen inlet and ice jacket. 2. Add phosgene (64.35 g) dissolved in 950 mL of methylene chloride slowly to the solution. 3. Stir the mixture for 30 minutes. 4. Separate the methylene chloride and water layers. 5. Place 50 mL of methylene chloride layer (bischloroformate 0.061 mol, 95 mol%) and 75 mL of aqueous layer in a 500 mL of three necked round bottomed flask. 6. Add 30 μL of triethylamine (15%, w/v), 0.988 g of diallyl bisphenol A (0.00321 mol, 5 mol%) dissolved in a 10 mL of NaOH solution (0.32 g, 8 mmol) and 0.2516 g of p-tert-butyl phenol (1.68 mmol), which is also dissolved in a 10 mL of NaOH solution (0.08 g, 2 mmol) to the reaction mixture. 7. Use p-tert-butyl phenol as a molecular weight controller. 8. Stir the reaction mixture for 3 hours at room temperature by using a mechanical stirrer (stirring speed 500 r.p.m). 9. Separate the methylene chloride layer. 10. Add 37 μL of triethylamine, 10 mL of methylene chloride and 2.05 g of NaOH in 15 mL of distilled water to the separated methylene chloride solution. 11. Stir the mixture for 3 hours at room temperature. 12. Wash the polymer solution with distilled water. 13. Neutralize the polymer solution with HCl. 14. Precipitate the polymer solution into a mixture of acetone and distilled water (50:50, v/v).
Scale	gram

反应中的重要物质及角色

详细的实验步骤、操作过程与表征信息

案例4：生物合成与生物转化反应检索

结构+关键词联用，精确查找与发酵/生物合成/生物转化相关，并涉及特定化合物结构的文献

CAS SciFinder

References biosynthe* or biotransformation or fermentation

Return to Home

References search for "biosynthe* or biotransformation or fermentation"

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (0)

Substructure (817)

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Substance Role

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Content

Life Science Data

817 Results

Sort: Relevance View: Partial Abstract

1

High-level semi-synthetic production of the potent antimalarial artemisinin

By: Paddon, C. J.; Westfall, P. J.; Pitera, D. J.; Benjamin, K.; Fisher, K.; McPhee, D.; Leavell, M. D.; Tal, A.; Main, A.; Eng, D.; et al
Nature (London, United Kingdom) (2013), 496(7446), 528-532 | Language: English, Database: CAPlus and MEDLINE

In 2010 there were more than 200 million cases of malaria, and at least 655,000 deaths. The World Health Organization has recommended artemisinin-based combination therapies (ACTs) for the treatment of uncomplicated malaria caused by the parasite *Plasmodium falciparum*. Artemisinin is a sesquiterpene endoperoxide with potent antimalarial properties, produced by the plant *Artemisia annua*. However, the supply of plant-derived artemisinin is unstable, resulting in shortages and price fluctuations, complicating production planning by ACT manufacturers. A stable source of affordable artemisinin is r...

View More

Full Text

Substances (25) Reactions (20) Citing (1,509) Citation Map

2

Biotransformation of artemisinin by fermentation of *Rhizopus chinensis* and *Cunninghamella elegans*

By: Zhan, Jixun; Guo, Hongzhu; Han, Jian; Zhang, Yuanxing; Guo, De'an
Zhongcaoyao (2002), 33(10), 869-872 | Language: English, Database: CAPlus

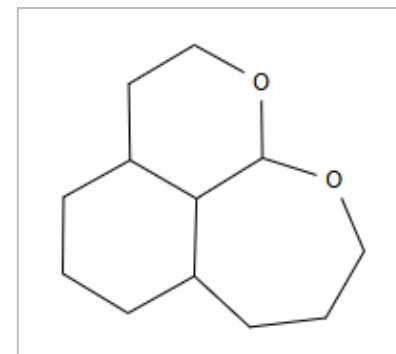
The microbial transformation of antimalarial drug artemisinin was studied. The **enzymes** secreted by **fermentation** of *Rhizopus chinensis* Saito CICC 3,043 and *Cunninghamella elegans* Lendn. AS 3,120 7 in the potato medium were used to transform artemisinin. Three products were obtained, among which deoxyartemisinin was also found in the controls without microorganisms, and the other two were identified as 3 α -hydroxydeoxyartemisinin (III) and 9 β -hydroxyartemisinin (IV, a new compound). Artemisinin could be transformed by the two strains, it was easy to release one O atom by breaking of peroxide brid...

View More

Full Text

Substances (5) Reactions (2) Citing (4) Citation Map

例：biosynthe* or biotransformation or fermentation



Substance Role

- ☐ Biological Study (187)
- ☐ Preparation (70)
- ☐ Uses (69)
- ☒ Biosynthetic Preparation (39)
- ☒ Bioindustrial Manufacture (23)
- ☒ Biochemical Process (15)

View All

Concept

- ☐ *Artemisia annua* (69)
- ☐ Antimalarials (44)
- ☐ Artemisinins (42)
- ☒ Fermentation (38)
- ☐ Plant tissue culture (30)
- ☒ Biotransformation (15)
- ☒ Biosynthetic Pathways (8)

View All

浏览CAS科学家标引的信息，聚焦物质在文献中的研究角色及文献核心研究点

(续) 案例4: 生物合成与生物转化反应检索

获取文献相关反应: 便捷筛选生物反应

Reactions from References

References

Filter Behavior: Filter by Exclude

Search Within Results: Search for up to 3 structures within the result set. Draw Search

Searching for... Clear All Remove and Edit

Yield Number of Steps Non-Participating Functional Groups Reaction Mapping

Filtering: Search Within Results: Drawn Structure Reaction Notes: 3 Selected

- ☒ Biotransformation
- ☒ Enzymic
- ☒ Fermentation

19 Results

Scheme 1 (1 Reaction) Steps: 1 Yield: 84%

Absolute stereochemistry shown, Rotation (+)

Supplier (1)

31-491-CAS-2809199 Steps: 1 Yield: 84% Hydroxylation of 10-Deoxoartemisinin by *Cunninghamella elegans*
By: Parshikov, Igor A.; et al
Journal of Natural Products (2004), 67(9), 1595-1597
Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 50%

Reaction Notes中
Biotransformation、Enzymic、
Fermentation等助力快速获取
生物转化类反应

获取反应步骤对应的科学家标引的注释和反应条件，助力快速了解生物转化过程

科学家标引的Notes帮助快速了解生物转化过程，包括：菌种、介质、代谢途径、酶等

(续) 案例4: 生物合成与生物转化反应检索

浏览&聚焦感兴趣的生物反应催化剂

Reactions search for drawn structure

References

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Stereoselective (4,529)

Regioselective (2,659)

Photochemical (1,246)

Biotransformation (1,152)

Enzymic (816)

Fermentation (42)

View All

Filtering: Reaction Mapping: Mapping Data Available X Reaction Notes: 3 Selected X Clear All Filters

1,152 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (10 Reactions) Steps: 1 Yield: 69-96%

Suppliers (123)

Suppliers (94)

31-614-CAS-42807637 Steps: 1 Yield: 96% Modularization of Immobilized Multienzyme Cascades Enantioselective C-H Amination By: Kong, Weixi; et al Angewandte Chemie, International Edition (2024), 63(37) Full Text

1.1 Reagents: Glucose Catalysts: Glucose oxidase (shell-bound to core-shell nanoparticle), Peroxygenase (core-bound to core-shell nanoparticle), Poly(dopamine), Silicic acid (H₂SiO₄), tetraethyl ester, polymer with 4,4,7,7-tetraethoxy-3,8-di... (surface amino-functionalized and activated with glutaraldehyde, Schiff...), Solvents: Dimethyl sulfoxide, Water; 6 h, pH 7, 30 °C Experimental Protocols

31-614-CAS-42021837 Steps: 1 Yield: 72% Chemoenzymatic Sequential Catalysis with Carbonic Anhydrase for the Synthesis of Chiral Alcohols from Alkanes, Alkenes, and Alkynes By: Li, Zhenzhong; et al ACS Catalysis (2024), 14(11), 8786-8793 Full Text

1.1 Reagents: Oxygen Catalysts: Acridinium, 10-methyl-9-(2,4,6-trimethylphenyl)-, perchlorate (1:1) Solvents: Acetonitrile; 6 h, rt 1.2 Reagents: Phenylsilane

Catalyst

Top Count Alphanumeric Search

3 Selected

☒ Cytochrome P450 (99)

☒ Peroxygenase (97)

☒ Streptavidin (56)

☐ Cytochrome CYP102 (46)

☐ Glucose 6-phosphate dehydrogenase (28)

☐ Alcohol dehydrogenase (26)

☐ Peroxidase (25)

☐ Triacylglycerol lipase (25)

☐ Monooxygenase (22)

☐ (Bis(diphenylphosphino)ethane)dichloronickel (8)

☐ Flavin mononucleotide (8)

☐ Tetrabutylammonium bromide (8)

☐ Toluene dioxygenase (8)

☐ Tris(2,2'-bipyridine)ruthenium (2+) bis(hexafluorophosphate) (8)

☐ Acridinium, 10-methyl-9-(2,4,6-trimethylphenyl)-, perchlorate (1:1) (7)

☐ Cytochrome P450 199A4 (7)

☐ Ruthenium, [(3aS,4S,6aR)-N-[4-[[[2-(amino-κN)ethyl]amino-κN]sulfonyl]phenyl]hexahydro-2-oxo-1H-thieno[3,4-d]imidazole-4-pentamido]-(η⁶-benzene)chloro- (4)

☐ Ruthenium, [(3aS,4S,6aR)-N-[4-[[[2-(amino-κN)ethyl]amino-κN]sulfonyl]phenyl]hexahydro-2-oxo-1H-thieno[3,4-d]imidazole-4-pentamido]chloro[(1,2,3,4,5,6-η)-1,2,4,5-tetramethylbenzene]- (4)

?

酶、菌、肽/蛋白、或其他化学催化剂

总结

反应检索策略

- 灵活通过物质标识符、文献号、构建结构式或反应式等多种策略，满足各种场景下的反应检索需求。
- 支持通过自然语言，高效便捷检索某种或某一类目标化合物的反应。
- 通过相似反应拓展，获取更多相似反应路线支持，助力获取最合适的反应。
- 利用数据关联，从物质或文献出发，灵活获取不同物质种类或不同研究领域的反应信息。
- 获取已知化合物或新化合物的逆合成路线，进行更多反应路线与合成工艺拓展。

反应结果分析策略

- 利用丰富的反应结果分组与聚类分析选项，可多维度查看反应结果，助力全方位纵览所有报道反应的技术全貌，并进行筛选聚焦。
- 通过CAS科学家标引的Synthetic Methods，无需阅读原文，直接获取实验步骤详情及产物表征等信息。
- 基于反应、物质、文献之间的深度关联，并通过CAS科学家标引的聚类分析选项，高效完成关注领域的信息检索。

Between problems
and progress **are**
connections that
matter

are connections
that matter

谢谢!

美国化学文摘社(CAS)北京代表处

China@acs-i.org

+86-10-6250 8026/7

