

CAS SciFinder[®]

反应信息的获取

程小燕博士
2022年3月15日



ACS
International



A division of the
American Chemical Society

2022年CAS SciFinderⁿ论坛直播日程表

	日期	主题	主讲人
基础 培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder ⁿ 顺利开题、进行文献综述	钱欣
检索 策略 详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构设计与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间:

18:00 – 19:00

关注公众号：**ACS美国化学会**
随时观看回放，了解直播信息



提纲

- CAS和CAS SciFinderⁿ简介
- CAS SciFinderⁿ 反应检索方法
- 反应案例分享
- 在线演示以及Q&A



CAS具有最全面的学科连接内容合集



Over
55K
scientific journals
and documents

Over
263
million
substances

Over
50
languages
translated

64
patent offices
worldwide

CAS SciFinderⁿ中覆盖的内容合集



来源:

<https://www.cas.org/cas-data>

<https://www.cas.org/about/cas-content>

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International

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American Chemical Society



提纲

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- CAS SciFinderⁿ 反应检索方法
- 反应案例分享
- 在线演示以及Q&A



反应检索方法——直接检索

Searching for...

- All
- Substances
- Reactions**
- References
- Suppliers
- Biosequences
- Retrosynthesis

Reactions 根据反应式/结构式、物质标识符、文献号检索反应

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Edit

Retrosynthesis 根据一个具体的结构进行逆合成反应路线设计

Draw or import a structure to perform a retrosynthetic analysis. [Learn more about Retrosynthesis searching.](#)

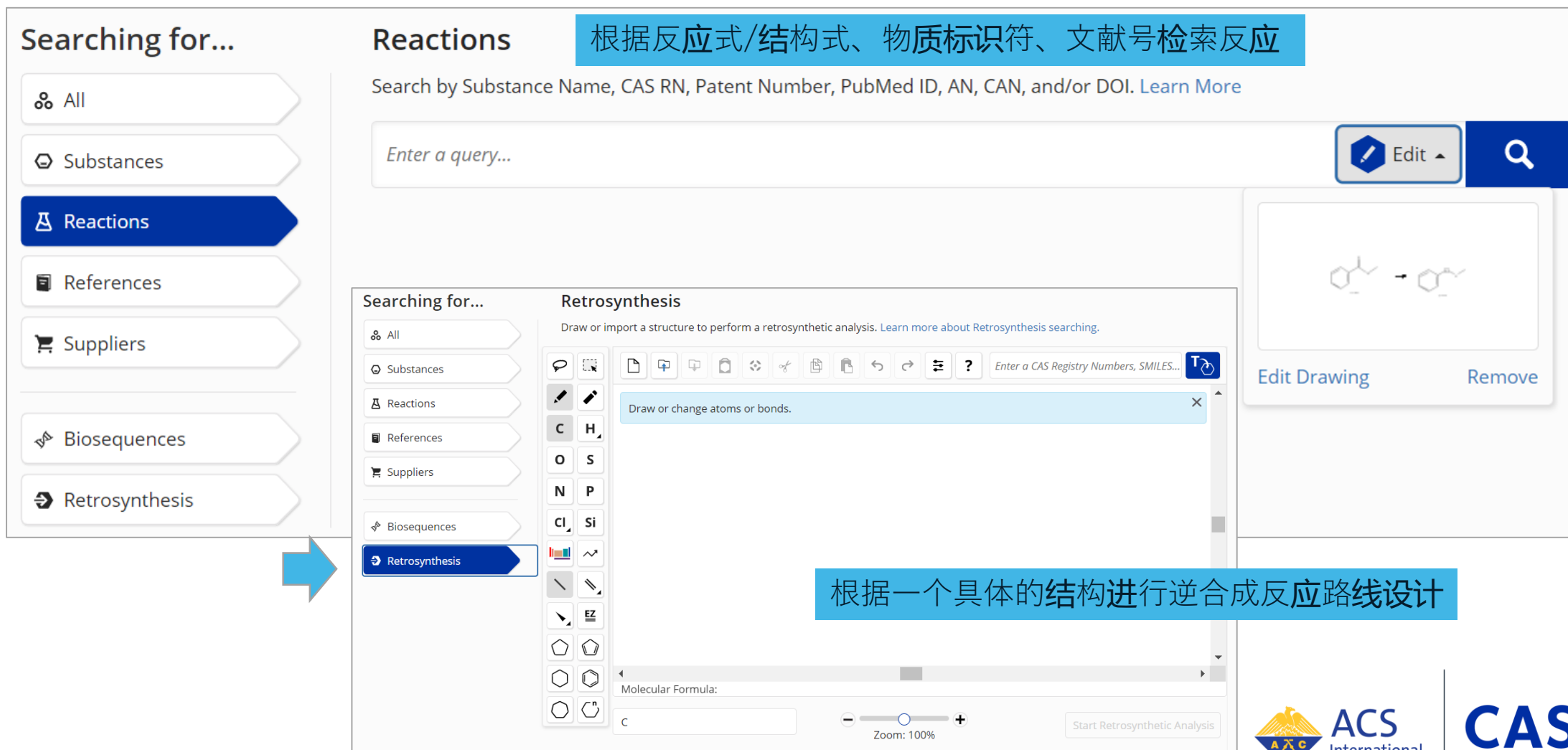
Enter a CAS Registry Numbers, SMILES...

Draw or change atoms or bonds.

Molecular Formula: c

Zoom: 100%

Start Retrosynthetic Analysis



反应检索方法——间接检索

Searching for...

- All
- Substances
- Reactions
- References**
- Suppliers
- Biosequences
- Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Draw Q

Author Name X

Example: Schubert, J A

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

通过文献结果获取反应信息

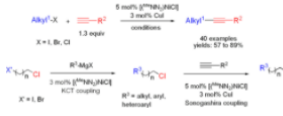
References (11) Sort: Relevance View: Partial Abstract

Substances **Reactions** Citing

1

Ni-Catalyzed Sonogashira Coupling of Nonactivated Alkyl Halides: Orthogonal Functionalization of Alkyl Iodides, Bromides, and Chlorides

By: Vechorkin, Oleg; Barmaz, Delphine; Proust, Valerie; Hu, Xile
Journal of the American Chemical Society (2009), 131(34), 12078-12079 | Language: English, Database: CPlus and MEDLINE



Ni-catalyzed Sonogashira **coupling** of nonactivated, β -H-containing alkyl halides, including chlorides, is reported. The **coupling** is tolerant to a wide range of functional groups, including ether, ester, amide, nitrile, keto, heterocycle, acetal, and aryl halide, in both **coupling** partners. The **coupling** can be selective for a specific C-X bond (X = I, Br, Cl) and allows for orthogonal functionalization of alkyl halides with multiple reactive sites.

Full Text

Substances (110) **Reactions (64)** Citing (183) Citation Map

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Draw Q

Molecular Formula X

Examples: C6H6 | (C8H8)x | C22H26CuN2O5.C2H3N

+ Add Advanced Search Field [Learn more about SciFinder[®] Advanced Search.](#)

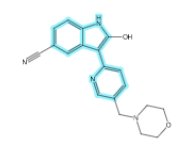
通过物质结果获取反应信息

Substances (9,750) Sort: Number of

References **Reactions** Suppliers

1

612487-72-6

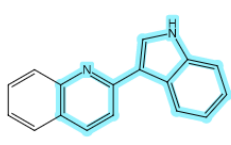


C₁₉H₁₈N₄O₂
2-Hydroxy-3-[5-[(morpholin-4-yl)methyl]pyridin-2-yl]-1H-indole-5-carbonitrile

69 References **24 Reactions** 51 Suppliers

2

5552-65-8



C₁₇H₁₂N₂
2-(1H-Indol-3-yl)quinoline

37 References 72 Reactions 6 Suppliers

反应检索方法汇总

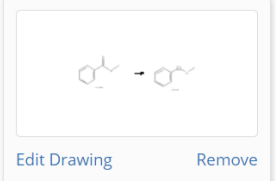
Searching for...

Reactions

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query...

Edit



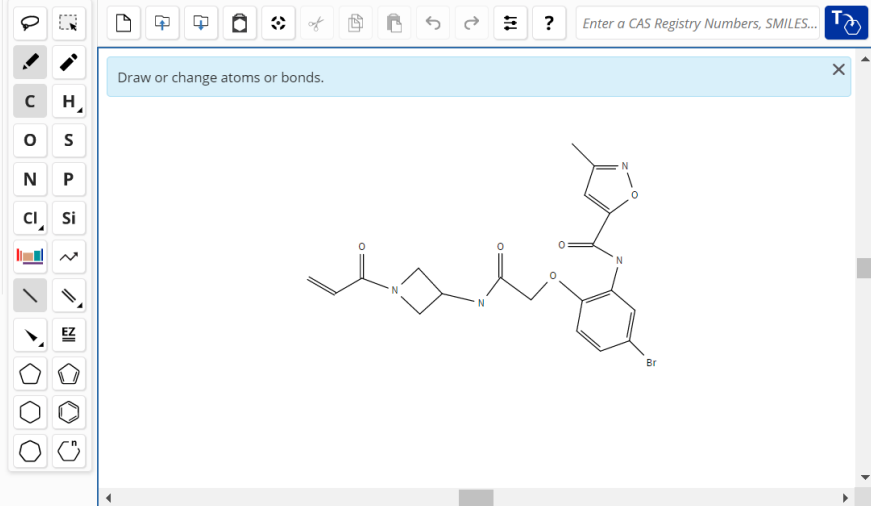
Searching for...

Retrosynthesis

Draw or import a structure to perform a retrosynthetic analysis. [Learn more about Retrosynthesis searching.](#)

Enter a CAS Registry Numbers, SMILES...

Draw or change atoms or bonds.



Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

Start Retrosynthetic Analysis

1. 直接进行Reaction检索

2. 通过Retrosynthesis Plan

获取逆合成反应路线

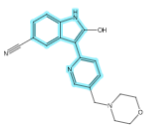
3. 通过物质获取反应

4. 通过文献获取反应

Substances (9,750) Sort: Number of

References Reactions Suppliers

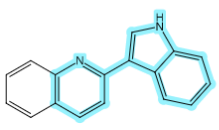
1 612487-72-6



C₁₉H₁₈N₄O₂
2-Hydroxy-3-[5-[(morpholin-4-yl)methyl]pyridin-2-yl]-1H-indole-5-carbonitrile

24 Reactions

2 5552-65-8



C₁₇H₁₂N₂
2-(1H-Indol-3-yl)quinoline

72 Reactions

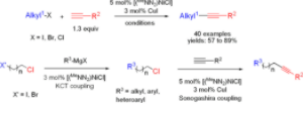
References (11) Sort: Relevance View: Partial Abstract

Substances Reactions Citing

1

Ni-Catalyzed Sonogashira **Coupling** of Nonactivated Alkyl Halides: Orthogonal Functionalization of Alkyl Iodides, Bromides, and Chlorides

By: Vechorkin, Oleg; Barmaz, Delphine; Proust, Valerie; Hu, Xile
Journal of the American Chemical Society (2009), 131(34), 12078-12079 | Language: English, Database: CPlus and MEDLINE



Ni-catalyzed Sonogashira **coupling** of nonactivated, β-H-containing alkyl halides, including chlorides, is reported. The **coupling** is tolerant to a wide range of functional groups, including ether, ester, amide, nitrile, keto, heterocycle, acetal, and aryl halide, in both **coupling** partners. The **coupling** can be selective for a specific C-X bond (X = I, Br, Cl) and allows for orthogonal functionalization of alkyl halides with multiple reactive sites.

Full Text

Substances (110) Reactions (64) Citing (183) Citation Map

反应检索场景及检索方法建议

1. 直接进行Reaction检索——根据反应式/结构式、物质标识符、文献号检索反应
 - ✓ 已知反应式，或者反应物/产物/反应试剂的结构式
 - ✓ 已知物质标识符（包括名称、CAS RN等）
 - ✓ 已知文献号或专利号等
2. 通过Retrosynthesis Plan获取逆合成反应路线——依据一个确定结构的物质进行设计
 - ✓ 有报道且结构明确的物质，无论是否有反应信息报道
 - ✓ 未有报道且结构明确的物质
3. 通过物质获取反应——先检索物质，再通过物质结果获取反应信息
 - ✓ 需要先对物质结果进行结构、属性或反应角色等筛选，然后再看反应
 - ✓ 某些物质（手性分子、多片段结构组成的物质）和盐类化合物、聚合物等多组分物质的反应
4. 通过文献获取反应——先检索文献，再通过文献结果获取反应
 - ✓ 通过结构检索没有得到反应结果
 - ✓ 需要通过关键词精炼感兴趣的反应信息

反应绘制工具介绍

反应绘制工具注释



反应箭头



反应角色标记



原子标记



化学键标记

CAS Draw

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

Draw or change atoms or bonds.

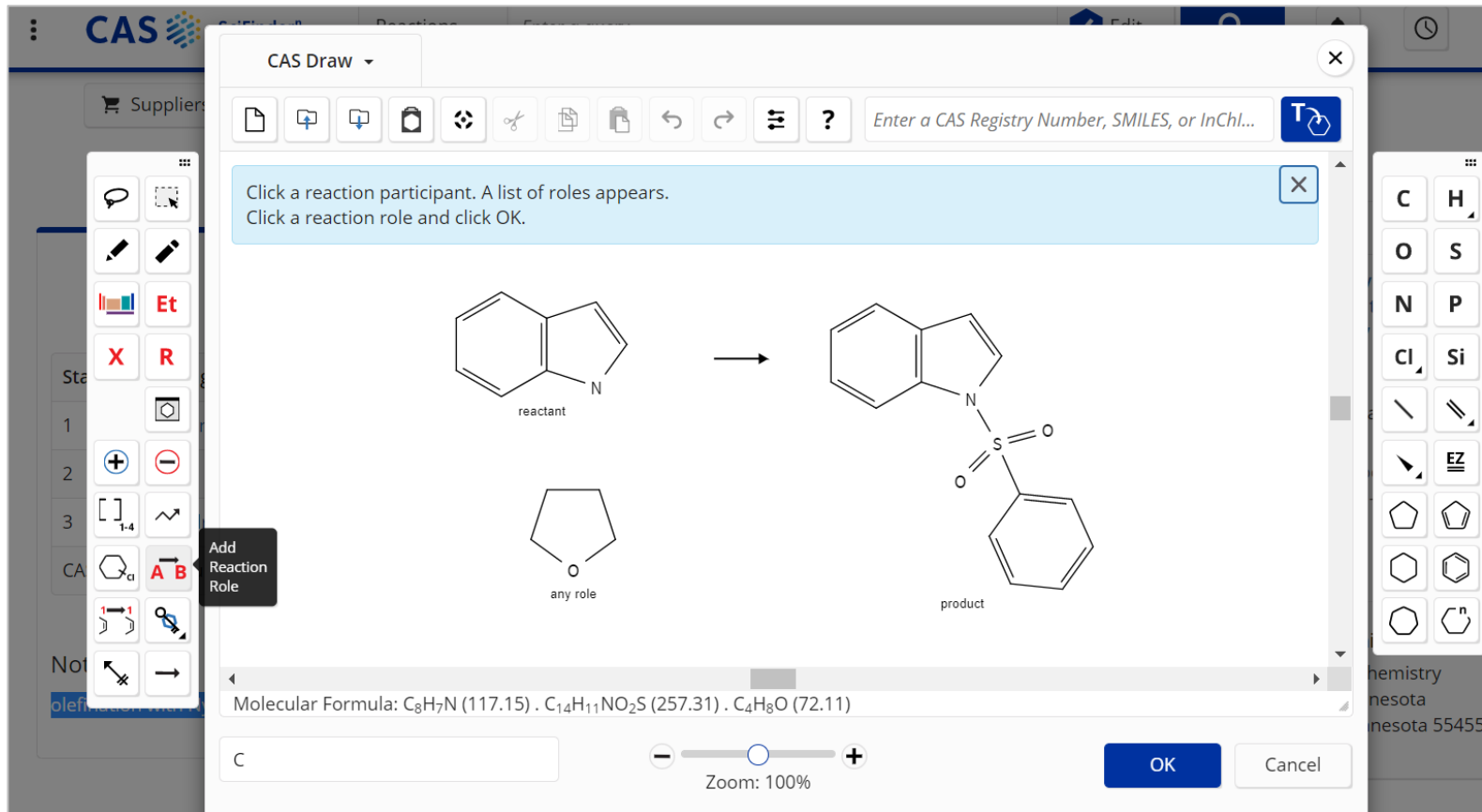
Molecular Formula:

C

Zoom: 100%

OK Cancel

反应箭头和反应角色标记



反应箭头



反应角色标记

Reaction Roles

Select a role for the structure fragment.

- Product
- Reactant
- Reagent
- Reactant/Reagent
- Any Role

OK Cancel

Reagent：参与反应，但不构成产物的碳原子

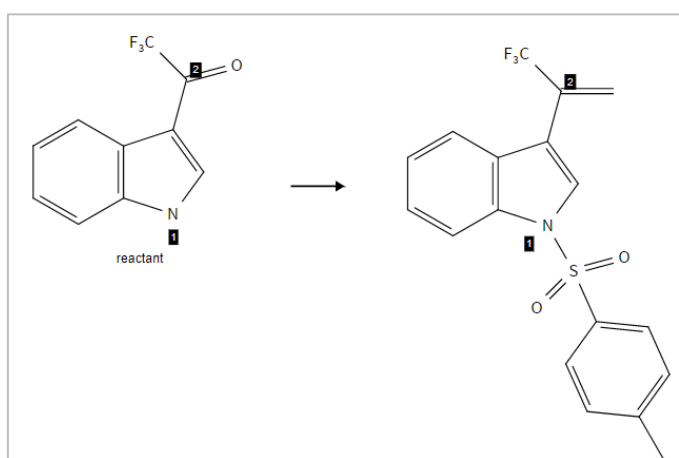
Any Role: 指reactant、reagent或product中的一种

原子标记

原子标记



标记反应物和产物中的同一个原子



CAS SciFinder® Reactions Enter a query... Edit Search

Return to Home

Structure Match: As Drawn (1), Substructure (10), Similarity (2)

Filter Behavior: Filter by Exclude

Yield: 90-100% (7), 50-69% (2), 30-49% (1)

Number of Steps: 1 (10)

Non-Participating Functional Groups: Alkyl halide (10), Alkene (9), Cyclic alkene (9), Halide (9), Carboxylic ester (8)

Reactions (10)

References

Edit Drawing Remove Save And Alerts

Start Retrosynthetic Analysis

1

Stereoselective Synthesis of Terminal Monofluoroalkenes from Trifluoromethylated Alkenes

By: Poutrel, Pauline; Pannecoucke, Xavier; Jubault, Philippe; Poisson, Thomas
Organic Letters (2020), 22(12), 4858-4863 | Language: English, Database: CAplus and MEDLINE

Full Text

Suppliers (75) Suppliers (75) Suppliers (92)

2

Asymmetric Synthesis of CF₃- and Indole-Containing Thiochromanes via a Squaramide-Catalyzed Michael-Aldol Reaction

By: Zhu, Yuanyuan; Dong, Zhenghao; Cheng, Xin; Zhong, Xiaoling; Liu, Xiaolin; et al
Organic Letters (2016), 18(15), 3546-3549 | Language: English, Database: CAplus and MEDLINE

Full Text

Supplier (1) Suppliers (62)

Double bond geometry shown

Reaction Summary Steps: 1 Yield: 59%

1.1 Solvents: [Dimethylformamide](#), [Tetrahydrofuran](#); 0 °C; 80 °C; 80 °C → rt

1.2 Reagents: [Ammonium chloride](#)
Solvents: [Water](#)

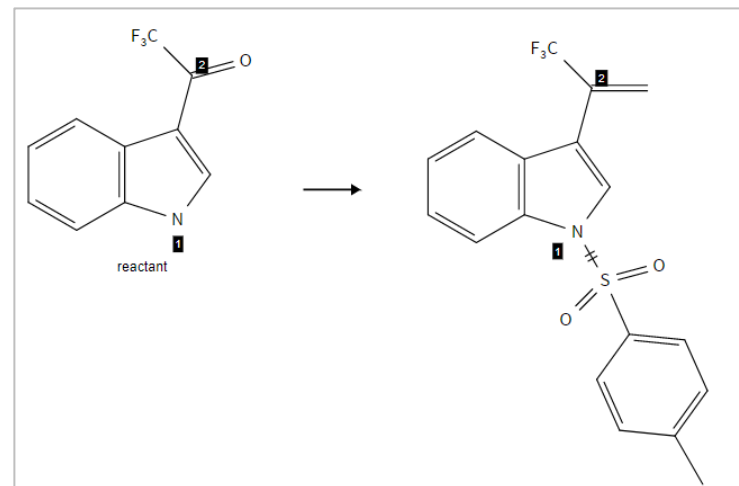
[View Reaction Detail](#) | [Experimental Protocols](#)

化学键标记

化学键标记



标记反应中发生变化的键（断裂、生成或键级变化）



小结：

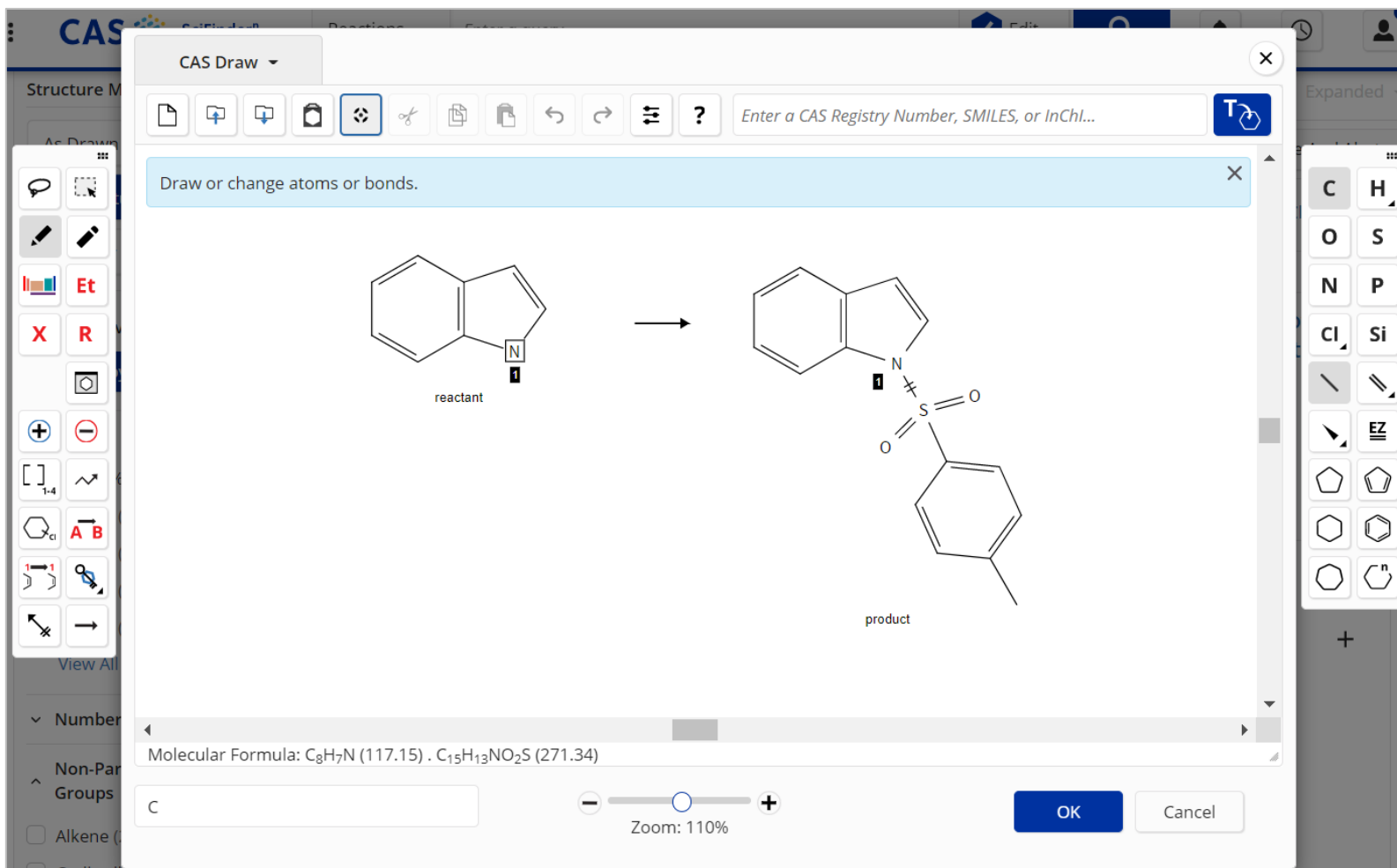
- **反应检索方法**：直接检索（Reaction Search, Retrosynthesis），间接获取反应（通过物质或文献获取）
- **反应检索场景及检索方法建议**：基于四种检索方法下的多个应用场景，考虑检索前已知哪些信息，检索中的具体需求
- **反应绘制工具介绍**：反应箭头、反应角色标记、原子标记和化学键的标记
- **数据关联支持灵活检索**：文献、物质和反应数据已经CAS科学家进行深度关联

提纲

- CAS和CAS SciFinderⁿ简介
- CAS SciFinderⁿ 反应检索方法
- 反应案例分享**
- 在线演示以及Q&A



例1：直接通过反应式检索反应



反应结果分析与精炼

产率
步数
不参与反应官能团
实验详情
反应类型
试剂
催化剂
溶剂
供应商信息
反应分类
二次结构检索
文献类型
语言
发表年份
刊物名
CA学科领域

- Reaction Type
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results
Search for up to 3 structures within the result set.
- Source Reference
- Document Type
- Language
- Publication Year

No Min to No Max
[View Larger](#)
- Publication Name
- CA Section

CAS SciFinder® Reactions

[Return to Home](#)

Structure Match

- As Drawn (88)**
- Substructure (2,740)
- Similarity (150)

Filter Behavior

Filter by

Yield

- 90-100% (37)
- 80-89% (11)
- 70-79% (8)
- 30-49% (5)
- No Yield Available (27)

Number of Steps

Non-Participating Functional Groups

- Alkene (87)
- Cyclic alkene (87)

Reaction Mapping

Experimental Protocols

- Synthetic Methods (32)
- Experimental Procedure (9)

Reactions (88)

Group: By Scheme View: Expanded

Scheme 1 (84 Reactions) Steps: 1 Yield: 100%

Reaction Summary Steps: 1 Yield: 100%
1.1 Reagents: [Diisopropylethylamine](#); 24 h, rt
By: Li, Jianqi; et al
China, CN103420898 A 2013-12-04

Reaction Summary Steps: 1 Yield: 100%
1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt
By: MacKenzie, Ian A.; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80

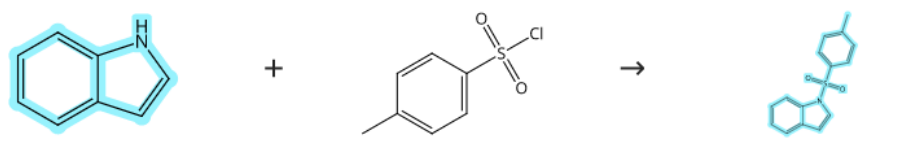
Reaction Summary Steps: 1 Yield: 100%
1.1 Reagents: [Sodium hydroxide](#), [Tetrabutylammonium hydrogen sulfate](#)
[Quinols as Novel Therapeutic Agents. 2. 4-\(1-Arylsulfonylindol-2-yl\)-4-hydroxycyclohexa-2,5-dien-1-ones and Related Agents as Potent and Selective Antitumor Agents](#)

Group by Scheme/Document : 选择反应结果的呈现方式

Reactions (88) Group: By Scheme View: Expanded

References

Scheme 1 (84 Reactions) Steps: 1 Yield: 100%



Suppliers (97) Suppliers (75) Suppliers (34)

Reaction Summary Steps: 1 Yield: 100% **Diaryl piperidine derivatives and applications as multi-targeting antidepressants**

1.1 Reagents: [Diisopropylethylamine](#); 24 h, rt

By: Li, Jianqi; et al
China, CN103420898 A 2013-12-04

View Reaction Detail PatentPak Full Text

Reaction Summary Steps: 1 Yield: 100% **Discovery and characterization of an acridine radical photoreductant**

1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt

By: MacKenzie, Ian A.; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80

View Reaction Detail | Experimental Protocols Full Text

Reaction Summary Steps: 1 Yield: 100% **Quinolins as Novel Therapeutic Agents. 2. 4-(1-Arylsulfonylindol-2-yl)-4-hydroxycyclohexa-2,5-dien-1-ones and Related Agents as Potent and Selective Antitumor Agents**

1.1 Reagents: [Sodium hydroxide](#), [Tetrabutylammonium hydrogen sulfate](#)
Solvents: [Toluene](#), [Water](#); 0 °C; 16 h, rt

By: Berry, Jane M.; et al
Journal of Medicinal Chemistry (2005), 48(2), 639-644

Reactions (88) Group: By Document View: Expanded

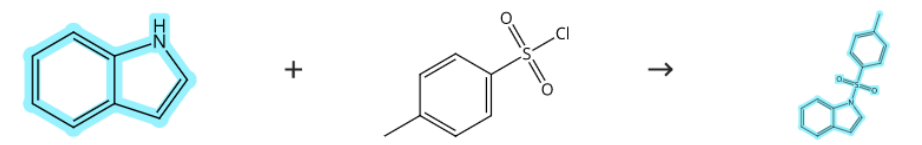
References

1

Discovery and characterization of an acridine radical photoreductant

By: MacKenzie, Ian A.; Wang, Leifeng; Onuska, Nicholas P. R.; Williams, Olivia F.; Begam, Khadiza; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80 | Language: English, Database: CAplus and MEDLINE

Full Text



Suppliers (97) Suppliers (75) Suppliers (34)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt

View Reaction Detail | Experimental Protocols

Non-participating Functional Group: 浏览 或筛选不参与反应官能团

CAS SciFinder® Reactions Enter a query... Edit Search Alerts Clock Profile

Return to Home

Structure Match

- As Drawn (88)
- Substructure (2,740)**
- Similarity (150)

Filter Behavior

Filter by Exclude

- Yield
- Number of Steps
- Non-Participating Functional Groups**
 - Alkene (2,480)
 - Cyclic alkene (2,480)
 - Halide (1,076)
 - Ether (434)
 - Amine (416)
 - Secondary amine (52)
 - View All
- Reaction Mapping
- Experimental Protocols
 - Synthetic Methods (27)
 - Experimental Procedure (6)

Reactions (52) Group: By Document View: Expanded

References

Filtering: Non-Participating Functional Groups: Secondary amine X Clear All Filters

1

ZnO-mediated regioselective C-arylsulfonylation of indoles: a facile solvent-free synthesis of 2- and 3-sulfonylindoles and preliminary evaluation of their activity against drug-resistant mutant HIV-1 reverse transcriptases (RTs)

By: Tocco, Graziella; Begala, Michela; Esposito, Francesca; Caboni, Pierluigi; Cannas, Valeria; et al
Tetrahedron Letters (2013), 54(46), 6237-6241 | Language: English, Database: CAplus

Full Text View 11 Related Reactions

Suppliers (89) Suppliers (106)

Reaction Summary Steps: 1 Yield: 78%

出现在反应前后，但未发生变化的官能团

同时考虑分子间和分子内的官能团

6

γ -Regioselective Functionalization of 3-Alkenylindoles via 1,6-Addition to Extended Alkylidene indolenine Intermediates

By: Bertuzzi, Giulio; Lenti, Lucia; Giorgiana Bisag, Denisa; Fochi, Mariafrancesca; Petrini, Marino; et al
Advanced Synthesis & Catalysis (2018), 360(6), 1296-1302 | Language: English, Database: CAplus

Full Text View 5 Related Reactions

Double bond geometry shown Suppliers (6) Suppliers (99) Suppliers (75)

Double bond geometry shown

Reaction Summary Steps: 1 Yield: 66%

1.1 Catalysts: [Zinc triflate](#)
Solvents: [Acetonitrile](#); 4 h, rt; rt \rightarrow 0 °C

1.2 Reagents: [Potassium hydroxide](#)
Catalysts: [Tetrabutylammonium hydrogen sulfate](#)
Solvents: [Water](#); 1 h, 0 °C

使用Exclude, 一键排除不感兴趣的反应

The screenshot displays the CAS SciFinder Reactions search results page. On the left sidebar, the 'Filter Behavior' section has the 'Exclude' button highlighted with a red box. Below it, the 'Solvent' filter is expanded, with 'Tetrahydrofuran (975)' selected, also highlighted with a red box. The main content area shows a list of reactions. The first reaction, titled 'Discovery and characterization of an acridine radical photoreductant', is selected. Its chemical reaction is shown with acridine reacting with a sulfonyl chloride derivative to form a sulfonamide. Below the reaction, the reagents are listed as 'Pyridine; 0 °C; 2 - 3 h, rt'. The reaction summary indicates 'Steps: 1 Yield: 100%'. The second reaction, 'Diaryl piperidine derivatives and applications as multi-targeting antidepressants', is partially visible below.

Experimental Protocols 获取反应详情

^ Experimental Protocols

- Synthetic Methods (32)
- Experimental Procedure (9)

^ Reaction Type

- Full (32)

^ Reagent

- Sodium hydride (10)
- Sodium hydroxide (9)
- Potassium hydroxide (4)
- Pyridine (4)
- Ammonium chloride (3)

[View All](#)

^ Catalyst

- Benzyltriethylammonium chloride (4)
- Tetrabutylammonium hydrogen sulfate (4)
- 4-(Dimethylamino)pyridine (2)
- 1,8-Diazabicyclo[5.4.0]undec-7-ene (1)
- Sodium (1)

^ Solvent

^ Commercial Availability

^ Reaction Notes

1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt

[View Reaction Detail](#) | [Experimental Protocols](#)

2

Marine-natural-products for biocides development: first discovery of meridianin alkaloids as antiviral and anti-phytopathogenic-fungus agents

By: Dong, Ji; Huang, Shi-sheng; Hao, Ya-nan; Wang, Zi-wen; Liu, Yu-xiu; et al
Pest Management Science (2020), 76(10), 3369-3376 | Language: English, Database: CAPlus and MEDLINE

[Full Text](#) ▾

[Suppliers \(97\)](#) [Suppliers \(75\)](#) [Suppliers \(34\)](#)

Reaction Summary Steps: 1 Yield: 99%

1.1 Reagents: [Potassium hydroxide](#)
Catalysts: [Tetrabutylammonium hydrogen sulfate](#)
Solvents: [Toluene](#), [Water](#); 15 min, rt

1.2 Solvents: [Toluene](#); 0 °C; 2 h, rt

[View Reaction Detail](#) | [Experimental Protocols](#)

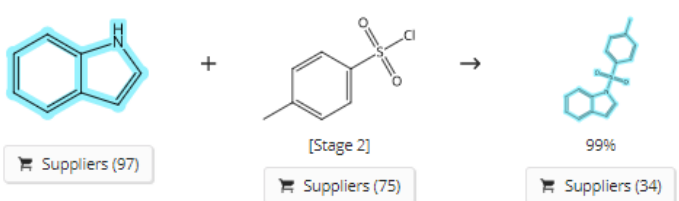
Synthetic Methods 获取增值的反应详情

[Return to Results](#)

Reaction Detail (Document 2, Reaction 1 of 1)

[Prev](#) [Next](#) [Save](#)

Steps: 1
Yield: 99%



Suppliers (97) [Stage 2] Suppliers (75) 99% Suppliers (34)

Step 1

[Alternative Steps \(83\)](#)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Potassium hydroxide	Tetrabutylammonium hydrogen sulfate	Toluene Water	15 min, rt
2	-	-	Toluene	0 °C; 2 h, rt

CAS Reaction Number: 31-081-CAS-22650181

Experimental Protocols

Synthetic Methods

Products	1-[(4-Methylphenyl)sulfonyl]-1H-indole, Yield: 99%
Reactants	Indole Tosyl chloride
Reagents	Potassium hydroxide
Catalysts	Tetrabutylammonium hydrogen sulfate
Solvents	Toluene Water

JOURNAL

Marine-natural-products for biocides development: first discovery of meridianin alkaloids as antiviral and anti-phytopat hogenic-fungus agents

By: Dong, Ji; et al
[View All](#)

Pest Management Science (2020), 76(10), 3369-3376

[Full Text](#)

Company/Organization

Tianjin Key Laboratory of Structure and Performance for Functional Molecules, MOE Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry, College of Chemistry Tianjin Normal University Tianjin China

Procedure

1. Add tetrabutylammonium hydrogen sulfate (0.95 g, 3 mmol) and 50% KOH aqueous solution (50 mL) to a solution of substituted indole (40 mmol) in toluene (50 mL).
2. Stir the reaction mixture at room temperature for 15 minutes.
3. Add TsCl (9.2 g) in toluene (100 mL) at 0 °C.
4. Stir the reaction at room temperature for 2 hours.
5. After completion of the reaction, extract the mixture with ethyl acetate (200 mL×3).
6. Wash the combined organic phase with brine (200 mL).
7. Dry the combined organic phase over anhydrous Na₂SO₄.
8. Concentrate the combined organic phase.

Transformation

Sulfonation of Aromatic Compounds
Formation of Sulfonamides

Scale

milligram

Characterization Data

1-[(4-Methylphenyl)sulfonyl]-1H-indole

Proton NMR Spectrum	(400 MHz, CDCl ₃) δ 7.99 (d, <i>J</i> = 8.4 Hz, 1H, Ar-H), 7.75 (d, <i>J</i> = 8.3 Hz, 2H, Ar-H), 7.55 (d, <i>J</i> = 3.6 Hz, 1H, Ar-H), 7.51 (d, <i>J</i> = 7.8 Hz, 1H, Ar-H), 7.30 (t, <i>J</i> = 7.6 Hz, 1H, Ar-H), 7.24-7.20 (m, 1H, Ar-H), 7.17 (d, <i>J</i> = 8.4 Hz, 2H, Ar-H), 6.63 (d, <i>J</i> = 3.6 Hz, 1H, Ar-H), 2.29 (s, 3H, CH ₃).
Carbon-13 NMR	(100 MHz, CDCl ₃) δ 145.0, 135.3, 134.8, 130.8, 129.9, 126.8, 126.4, 124.6, 123.3, 121.4, 113.6, 109.1, 21.8.
Melting Point	77-78 °C.
State	white solid.

CAS Method Number 3-081-CAS-22650181

CAS PatentPak : 高效获取专利详情

Source Reference

Document Type

- Journal (1,611)
- Patent (1,091)
- Conference (4)
- Dissertation (26)
- Preprint (8)

Language

Publication Year

No Min to No Max Apply View Larger

Publication Name

- World Intellectual Property Organization (745)
- Journal of Organic Chemistry (132)
- Organic Letters (132)
- Bioorganic & Medicinal Chemistry Letters (113)
- China (109)

View All

Heterocyclic Compounds (More Than One Hetero Atom) (446)

Optical, Electron, and Mass Spectroscopy and Other Related Properties (22)

Pharmacology (15)

Preparation of 4-[1-(sulfonyl)-1H-indol-2-yl]-4-(hydroxy)-cyclohexa-2,5-dienone compounds and analogs thereof as therapeutic agents

By: Stevens, Malcolm Francis Graham; Westwell, Andrew David; Poole, Tracey Dawn; Wells, Geoffrey; Berry, Jane Marie
World Intellectual Property Organization, WO2004056361 A1 2004-07-08 | Language: English, Database: CPlus

PatentPak Full Text View 4 Related Reactions

Patent	Language	Kind Code	PatentPak Options
WO2004056361	English	A1	PDF PDF+ Viewer
CN1717233	Chinese	A	PDF

Download filter data from this result set.

Suppliers (97) Suppliers (75) Suppliers (34)

Reaction Summary Steps: 1 Yield: 91%

1.1 Reagents: [Sodium hydroxide](#)
Catalysts: [Tetrabutylammonium hydrogen sulfate](#)
Solvents: [Toluene](#), [Water](#); 0 °C; 16 h, rt

[View Reaction Detail](#)

CAS PatentPak : 一键定位专利中重要的物质

CAS PatentPak

PAGE 103 / 141 ZOOM DOWNLOAD PDF PDF+

Key Substances in Patent

Analyst Markup Locations (1)
Page 102

CAS RN 935-50-2

Analyst Markup Locations (1)
Page 102

CAS RN 40899-71-6

Analyst Markup Locations (1)
Page 103

CAS RN

WO 2004/056361 PCT/GB2002/005842

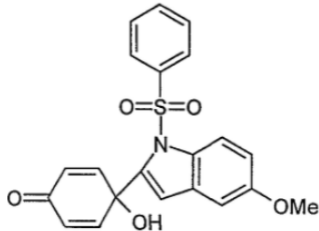
- 101 -

The title compound was prepared from 4,4-dimethoxy-cyclohexa-2,5-dienone and 1-benzenesulfonyl-1H-indole (available commercially), according to Method C, described above. Yield 18%; mp 170-172 °C; ¹H NMR (CDCl₃) δ 8.0 (d, J = 8 Hz, 1H), 7.87 (d, J = 8 Hz, 2H), 7.51-7.60 (m, 3H), 7.30-7.46 (m, 3H), 7.18-7.27 (m, 2H), 6.80 (s, 1H), 6.32 (d, J = 10 Hz, 2H), 5.50 (s, 1H); ¹³C NMR (CDCl₃) δ 185.3, 147.9, 141.2, 138.6, 137.8, 134.7, 129.7, 128.7, 128.1, 127.0, 126.6, 125.0, 122.1, 115.6, 114.1, 67.9.

5

Example 11

10 4-(1-benzenesulfonyl-5-methoxy-1H-indol-2-yl)-4-hydroxy-cyclohexa-2,5-dienone



小结：

- 直接通过反应式检索反应：绘制反应式，并根据需要使用原子标记或化学键标记工具等
- 反应结果聚类分析工具：Filter by/Exclude——Yield、Steps、Reagent、Catalyst、Solvent、Commercial Availability、Non-participating Functional Groups、Reaction Note、Experimental Protocols、Search Within Results、Source Reference
- 反应结果分组：Group by Scheme/Document
- 反应详情的查看：Experimental Protocols——Synthetic Methods、Experimental Procedures, CAS PatentPak

例2：直接通过物质标识符检索反应

CAS SciFinder[®] Reactions 7647-10-1

Filter Behavior: Filter by Exclude

Substance Role: Product (21), Reagent (7,567), Catalyst (49K)

Yield: 90-100% (9,784), 80-89% (10K), 70-79% (8,998), 50-69% (11K), 30-49% (5,065)

Number of Steps: 1 (57K)

Non-Participating Functional Groups

Experimental Protocols: Synthetic Methods (25K), Experimental Procedure

Reactions (57,215) Group: By Document View: Expanded

Preparation of Recyclable and Versatile Porous Poly(aryl thioether)s by Reversible Pd-Catalyzed C-S/C-S Metathesis

By: Rivero-Crespo, Miguel A.; Toupalas, Georgios; Morandi, Bill
Journal of the American Chemical Society (2021), 143(50), 21331-21339 | Language: English, Database: CPlus and MEDLINE

Full Text View 4 Related Reactions

Reaction Summary: Steps: 1 Yield: 100%

1.1 Reagents: Diisopropylethylamine
Catalysts: Triphenylphosphine, Palladium chloride
Solvents: Toluene; 18 h, 100 °C

Substance Role：浏览物质在反应中的角色

CAS SciFinder[®] Reactions PA 66

Filter Behavior: Filter by Exclude

Substance Role: Product (416), Reactant (372), Reagent (50), Catalyst (4)

Yield: 90-100% (5), 80-89% (5), 70-79% (5), 50-69% (2), 30-49% (3)

Number of Steps: 1 (732), 2 (54), 3 (18), 4 (14), 5 (7), 6-10 (1)

Reactions (838) Group: By Document View: Expanded

Methods for production of polyamides using ionic liquid solvents

By: Whiston, Keith; Langrick, Charles Richard; Seddon, Kenneth R.; Puga, Alberto V.
World Intellectual Property Organization, WO2011004138 A1 2011-01-13 | Language: English, Database: CPlus

PatentPak Full Text

Reaction Summary: Suppliers (20)

例3：通过Retrosynthesis工具设计逆合成反应路线，获得更多启发

CAS SciFinder[®] Saved and Alerts History Account

CAS Analytical Methods[®] is available as part of your CAS SciFinder[®] experience. [Identify and compare](#) the latest published analytical methods, featuring step-by-step instructions, in pharmacology, HPLC, food analysis, natural product isolation analysis, water analysis and more.

Searching for... All Substances Reactions References Suppliers Biosequences **Retrosynthesis**

Retrosynthesis
Draw or import a structure to perform a retrosynthetic analysis. [Learn more about Retrosynthesis searching.](#)

Enter a CAS Registry Numbers, SMILES...

Draw or change atoms or bonds.

Molecular Formula: C₁₄H₂₂ClN₃O₃ (315.80)

Start Retrosynthetic Analysis

Retrosynthesis Tool：可用于未知化合物或已知化合物和的逆合成路线设计

预设参数

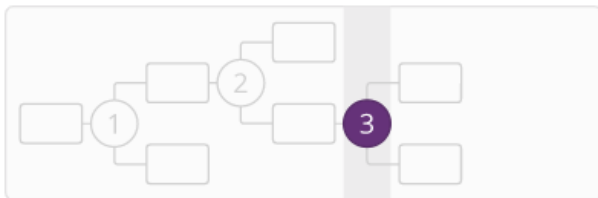
Retrosynthesis Plan Options

Powered by ChemPlanner®

Select Synthetic Depth

[Learn more.](#)

- 1
 2
 3
 4



Set Rules Supporting Predicted Reactions

[Learn more.](#)

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

Set Starting Materials Cost Limit

[Learn more.](#)

10 USD/mol

USD/mol

USD/mol

USD/g

Email me when my plan is complete

[Create Retrosynthesis Plan](#)

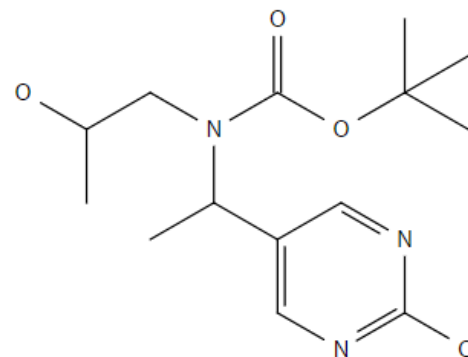
Break and Protect Bonds

[Learn more.](#)

Break Bond

Protect Bond

[Clear All Bond Selections](#)



结果查看

The screenshot displays the CAS SciFinder Retrosynthesis interface. The main window shows the 'Retrosynthesis' section with a 'Predicted Results' toggle set to 'OFF'. A search history entry for 'Retrosynthesis' on March 14, 2022, is highlighted. A detailed view of this entry shows a chemical structure and search parameters: Synthetic Depth: 3, Predicted Rules: Common, Break & Protect Bonds: No, Starting Material Cost Limit: \$10.00/mol. The plan expires on Jun 12, 2022. A 'Retrosynthesis Step Key' is visible at the bottom.

Plan Options
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$10.00/mol
Edit Plan Options

Profile scoring is available when Experimental and Predicted results have loaded.

Scoring Profiles
Complexity Reduction
Convergence
Evidence
Cost

Retrosynthesis Step Key

Recent Search History
View All Search History
March 14, 2022
Retrosynthesis 8:16 AM
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$10.00/mol
Retrosynthesis Plan will expire on Jun 12, 2022.
Open Plan
Edit Search
Complete

Your retrosynthesis query produced no experimental results. Predicted steps will continue to be generated unless they have already completed. Your plan's status is available on the Home page and in your Search History.

Filter by
Result Type
All (365)
Blosequences (116)
Patent Markush (382)
Prior Art Analysis (32)
Reactions (992)
References (5,146)
Retrosynthesis (344)
Substances (3,245)
Suppliers (95)
Date

Your Search History
10,717 Searches
March 14, 2022
Retrosynthesis 8:16 AM
Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$10.00/mol
Retrosynthesis Plan will expire on Jun 12, 2022.
Open Plan
Edit Search
Complete

逆合成路线的第一步没有Experimental报道；
预测路线正在运算，等Predicted Steps: ON，
可看到预测路线

获得逆合成反应路线结果

Retrosynthesis Powered by ChemPlanner®

Overview Steps **Predicted Results** ON Predicted Steps: ON, 才可看到预测路线

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C + D
Average Yield: 65%
Evidence (1,178)
Alternative Steps (13)

B ⇒ E Stereoselective
Maximum Yield: 50%
Evidence (1,238)
Alternative Steps (13)

C ⇒ F + G
Maximum Yield: 97%
Evidence (18)
Alternative Steps (7)

D ⇒ H
Maximum Yield: 100%
Evidence (92,407)
Alternative Steps (38)

Retrosynthesis Step Key
Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

- ⇒ Experimental Steps
- ⋯ Predicted Steps

Experimental Steps: 实验报道路线 (紫色)
Predicted Steps: 预测路线 (绿色)

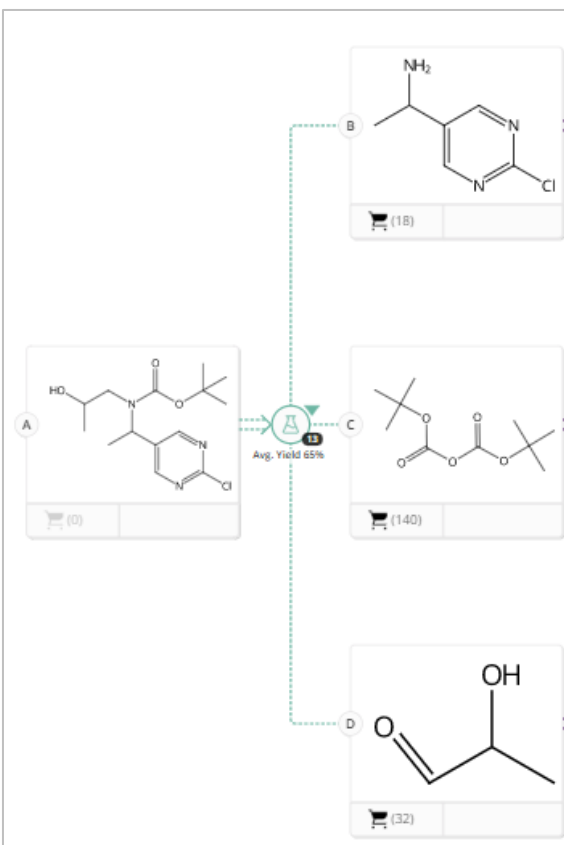
Predicted steps

A ⇒ B + C + D

Average Yield: 65%

Evidence (1,178)

Alternative Steps (13)



Filter Behavior

Filter by Exclude

Yield

- 90-100% (97)
- 80-89% (117)
- 70-79% (147)
- 50-69% (201)
- 30-49% (106)

View All

Number of Steps

- 1 (1,178)

Non-Participating Functional Groups

Experimental Protocols

- Synthetic Methods (262)
- Experimental Procedure (320)

Reaction Type

Stereochemistry

Reagent

Reactions (1,178)

Group: By Document View: Expanded

References

A ⇒ B + C + D 的证据



1

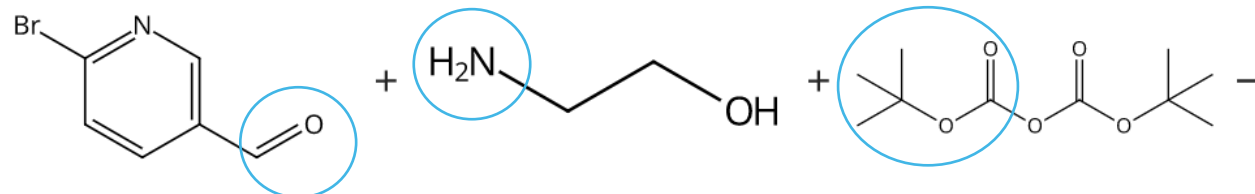
Preparation of substituted thiophene-2-hydroxamic acids as histone deacetylase inhibitors useful against disorders involving increased cell proliferation

By: Dyke, Hazel Joan; Price, Stephen; Van den Heuvel, Marco; Sutton, Jonathan Mark; Mackenzie, Robert Edward; et al
World Intellectual Property Organization, WO2005014588 A1 2005-02-17 | Language: English, Database: CPlus

PatentPak

Full Text

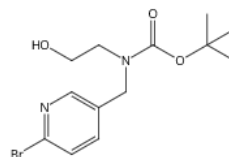
View 5 Related Reactions



Suppliers (110)

Suppliers (119)

Suppliers (140)



参考实验详情

Reaction Detail (Document 1, Reaction 1 of 5)

← Prev Next →

Download Email Save

Steps: 1
Yield: 90%

Suppliers (106) Suppliers (62) [Stage 4] Suppliers (140) 90% Suppliers (2)

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (+)

Absolute stereochemistry shown, Rotation (+)

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Methanol	2 h, rt; rt → 0 °C
2	Sodium borohydride	-	-	0 °C; 1 h, 0 °C → rt; rt → 0 °C
3	Ammonium chloride	-	Water	-
4	Triethylamine	-	Tetrahydrofuran	16 h, rt
5	Hydrochloric acid	-	Water	-

CAS Reaction Number: 31-313-CAS-16424766

Experimental Protocols

Synthetic Methods

Products	1,1-Dimethylethyl N-[(1S)-2-hydroxy-1-methylethyl]-N-(phenylmethyl)carbamate, Yield: 90%
Reactants	Benzaldehyde L-Alaninol Di-tert-butyl dicarbonate
Reagents	Sodium borohydride Ammonium chloride Triethylamine Hydrochloric acid

JOURNAL

Substrate-Controlled Diastereoselectivity Reversal in NHC-Catalyzed Cross-Benzoin Reactions Using N-Boc-N-Bn-Protected α -Amino Aldehydes

By: Haghshenas, Pouyan; et al
View All

Journal of Organic Chemistry (2016), 81(24), 12075-12083

Full Text

Company/Organization
Department of Chemistry
University of Saskatchewan
Saskatoon, Saskatchewan S7N 5C9
Canada

Solvents	Methanol Water Tetrahydrofuran						
Procedure	<ol style="list-style-type: none">1. Add freshly distilled benzaldehyde (1 equivalent) to a solution of the α-amino alcohol (1 equivalent) in dry MeOH (0.25M) at room temperature.2. Stir the resulting solution for 2 hours.3. Cool the resulting solution to 0 °C using an ice bath.4. Add NaBH₄ (5 equivalents) slowly to the mixture in three portions.5. Warm the resulting suspension to room temperature.6. Stir the resulting suspension for 1 hour.7. Cool the suspension once again to 0 °C.8. Quench the suspension with the addition of saturated NH₄Cl (aqueous).9. Extract the reaction mixture with EtOAc (×3).10. Dry the combined organic layers over MgSO₄.11. Reduce the crude mixture in vacuo.12. Add triethylamine (1 equivalent) to a solution of N-Bn-amino alcohol (1 equivalent) in THF (0.3M) at room temperature.13. Add di-tert-butyl dicarbonate (Boc₂O) (1.1 equivalents) to the solution.14. Stir the solution at ambient temperature for 16 hours.15. Quench the reaction mixture by addition of HCl (1M).16. Extract reaction mixture with Et₂O (×3).17. Wash the combined organic layers with brine.18. Dry the combined organic over MgSO₄.19. Purify the crude product by column chromatography.						
Transformation	Reductive Alkylation of Ammonia or Amines Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates						
Characterization Data	<p>1,1-Dimethylethyl N-[(1S)-2-hydroxy-1-methylethyl]-N-(phenylmethyl)carbamate</p> <table border="1"><tbody><tr><td>Proton NMR Spectrum</td><td>(500 MHz, CDCl₃) δ 7.35-7.26 (m, 4H), 7.26-7.22 (m, 1H), 4.39 (br s, 2H), 4.05-3.90 (m, 1H), 3.73-2.85 (m, 1H), 2.93 (br s, 1H), 1.43 (s, 9H), 1.14 (br d, J= 4.9 Hz, 3H).</td></tr><tr><td>R_f</td><td>0.21 (25% EtOAc in hexane).</td></tr><tr><td>State</td><td>clear colorless oil.</td></tr></tbody></table>	Proton NMR Spectrum	(500 MHz, CDCl ₃) δ 7.35-7.26 (m, 4H), 7.26-7.22 (m, 1H), 4.39 (br s, 2H), 4.05-3.90 (m, 1H), 3.73-2.85 (m, 1H), 2.93 (br s, 1H), 1.43 (s, 9H), 1.14 (br d, J = 4.9 Hz, 3H).	R _f	0.21 (25% EtOAc in hexane).	State	clear colorless oil.
Proton NMR Spectrum	(500 MHz, CDCl ₃) δ 7.35-7.26 (m, 4H), 7.26-7.22 (m, 1H), 4.39 (br s, 2H), 4.05-3.90 (m, 1H), 3.73-2.85 (m, 1H), 2.93 (br s, 1H), 1.43 (s, 9H), 1.14 (br d, J = 4.9 Hz, 3H).						
R _f	0.21 (25% EtOAc in hexane).						
State	clear colorless oil.						

CAS Method Number 3-313-CAS-16424766

精炼反应物结构

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Type

Reagent

Solvent

Commercial Availability

Search Within Results

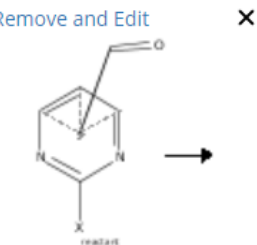
Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit



Reactions (1)

Group: By Document View: Expanded

References

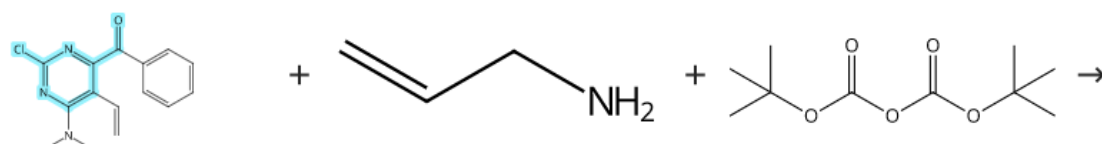
Filtering: Search Within Results: Drawn Structure X Clear All Filters

1

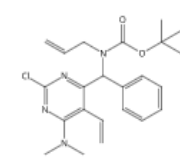
Synthesis of pyrimido[4,5-c]azepine- and pyrimido[4,5-c]oxepine-based γ -secretase modulators

By: Wu, Yong-Jin; Zhang, Yunhui; Toyn, Jeremy H.; Macor, John E.; Thompson, Lorin A.
Bioorganic & Medicinal Chemistry Letters (2016), 26(6), 1554-1557 | Language: English, Database: CAplus and MEDLINE

Full Text



Supplier (1) Suppliers (40) Suppliers (140)



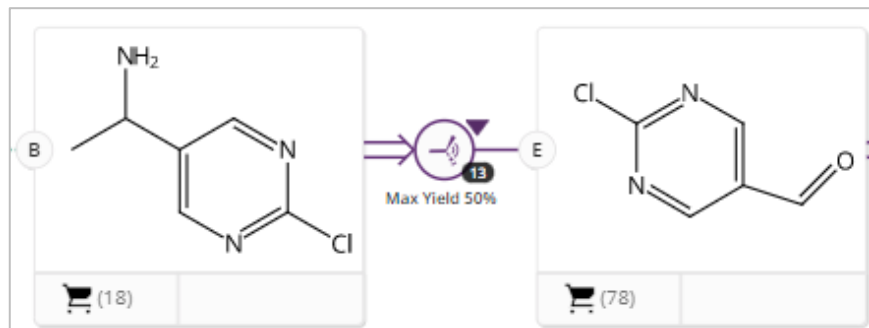
Reaction Summary Steps: 1 Yield: 78%

1.1 Reagents: [Titanium tetrachloride](#); rt

1.2 Reagents: [Acetic acid](#), [Sodium cyanoborohydride](#)

通过Search Within Results, 二次限定参考文献 (Evidence) 中最相关的原料结构

Experimental Steps



Overview **Steps**

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C + D

Average Yield: 65%
Evidence (1,178)
Alternative Steps (13)

B ⇒ E Stereoselective

Maximum Yield: 50%
Evidence (1,238)
Alternative Steps (13)



Reactions (1,238) Group: By Document View: Expanded

References

1

Diastereo and enantioselective preparation of N-carboxamidopyrazoline derivatives as P2X3 receptor antagonists

By: Cheng, Yunfeng; Zhu, Xinqiang
China, CN111892585 A 2020-11-06 | Language: Chinese, Database: CAplus

PatentPak [View 10 Related Reactions](#)

Absolute stereochemistry shown

Reaction Summary Steps: 1

- 1.1 Reagents: [Copper sulfate](#), [\(S\)-2-Methyl-2-propanesulfonamide](#)
Solvents: [Dichloromethane](#); 18 - 20 h, 50 °C
- 1.2 Solvents: [Dichloromethane](#), [Tetrahydrofuran](#); 2.5 h, -78 - -70 °C; -70 °C → -40 °C; 2 h, -40 °C
- 1.3 Reagents: [Ammonium chloride](#)
Solvents: [Water](#); 10 min, rt
- 1.4 Reagents: [Hydrochloric acid](#)
Solvents: [Methanol](#), [1,4-Dioxane](#); rt; 1 h, rt
- 1.5 Reagents: [Potassium carbonate](#)
Solvents: [Water](#)

[View Reaction Detail](#)

2

Preparation of N-biphenylmethylindole modulators of PPARG for treatment of osteoporosis

By: Griffin, Patrick R.; Kamenecka, Theodore Mark; Lecka-Czernik, Beata
World Intellectual Property Organization, WO2015161108 A1 2015-10-22 | Language: English, Database: CAplus

PatentPak [View 36 Related Reactions](#)

Filter Behavior

Yield

- 90-100% (34)
- 80-89% (37)
- 70-79% (135)
- 50-69% (343)
- 30-49% (268)

[View All](#)

Number of Steps

- 1 (1,238)

Non-Participating Functional Groups

- Alkene (568)
- Cyclic alkene (568)
- Ether (561)
- Diene (469)
- Halide (348)

[View All](#)

Experimental Protocols

- Synthetic Methods (29)
- Experimental Procedure (596)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

浏览Alternative Steps, 获取其他合成方法

Alternative Steps (13)

Filter by

- Alternative Step Type
 - Predicted (13)
- Stereochemistry
 - Non-Selective (13)

7 of 13

Select 🚩 Predicted Step Evidence (5,625) Average Yield: 74%

8 of 13

Select 🚩 Predicted Step Evidence (3,409) Average Yield: 76%

9 of 13

获得新的逆合成路线

Retrosynthesis

Overview Steps Predicted Results

View step specific evidence and alternate steps below or select the node between the steps on the plan.

A ⇒ B + C
Average Yield: 76%
Evidence (3,409)
Alternative Steps (13)

B ⇒ D + E
Average Yield: 54%
Evidence (19,780)
Alternative Steps (27)

C ⇒ F + G
Maximum Yield: 97%
Evidence (18)
Alternative Steps (7)

D ⇒ H + I
Maximum Yield: 49%
Evidence (4)
Alternative Steps (23)

Plan Information

Estimated Yield: 20%
Overall Price: \$1,227.22
(USD per 100 grams)

Commercially Available:
C, D, E, F, G, H, I, J, K

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$10.00/mol
[Edit Plan Options](#)

Retrosynthesis Step Key

Chemical structures shown in the diagram include: A (a complex molecule with a hydroxyl group and a chlorine atom), B (a molecule with a hydroxyl group and a benzene ring), C (a molecule with a hydroxyl group and a chlorine atom), D (a molecule with a chlorine atom and a benzene ring), E (a molecule with a hydroxyl group and a benzene ring), F (a molecule with a hydroxyl group and a benzene ring), G (a molecule with a hydroxyl group and a benzene ring), H (a molecule with a chlorine atom and a benzene ring), I (a molecule with a chlorine atom and a benzene ring), J (a molecule with a benzene ring and an amino group), K (a molecule with a benzene ring and an amino group).

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通过Scoring Profiles重新调整逆合成路线

Retrosynthesis Powered by ChemPlanner®

Overview Steps Predicted Results

Edit Plan Options

Scoring Profiles

- Complexity Reduction
- Convergence
- Evidence
- Cost
- Yield
- Atom Efficiency

Apply Reset Scoring

Retrosynthesis Step Key

Retrosynthesis reaction scheme showing the breakdown of a complex starting material (A) into various reagents (B, C, D, E, F, G, H, I) with associated yields and costs.

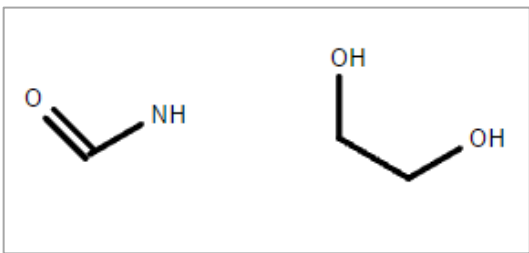
- A: Starting material (0 cost)
- B: Reagent (18 cost, Max Yield 50%)
- C: Reagent (140 cost, Avg. Yield 65%)
- D: Reagent (32 cost, Max Yield 100%)
- E: Reagent (78 cost, Max Yield 80%)
- F: Reagent (265 cost)
- G: Reagent (265 cost)
- H: Reagent (284 cost)
- I: Reagent (69 cost)



小结：

- 逆合成反应路线支持的物质：有具体且单一结构的未知化合物或已知化合物
- 预设参数：Synthetic Depth、Set Rules、Starting Material Cost、Break/Protect Bond
- 结果查看：执行逆合成路线设计的当前界面、主界面上的Recent Search History处、检索历史界面
- 预测路线/实验路线：Predicted Steps（绿色），Experimental Steps（紫色）
- 查看相关反应和替代反应：Evidence, Alternative Steps
- 精炼相关反应结果：利用Synthetic Methods和Search within Results从反应详情和反应物的结构来精炼Evidence中提供的支持反应
- 评分介绍Scoring Profile：Complexity Reduction, Convergence, Evidence, Cost, Yield, Atom Efficiency

例4: 通过片段结构信息获取反应



片段结构的反应检索：先从结构出发进行物质检索，再通过物质获取反应

- Number of Components
 - 1 (18K)
- Substance Class
 - Organic/Inorganic Small Molecule (18K)
 - Protein/Peptide Sequence (1,581)
 - Polymer (199)
 - Incompletely Defined Substance (124)
 - Coordination Compound (24)

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CAS SciFinder Substances (18,210)

Structure Match: As Drawn (0), **Substructure (313K)**, Similarity (178)

Chemscapes Analysis: Visually explore structure similarity with a powerful new tool. Learn more about Chemscapes. **Create Chemscapes Analysis**

Filter Behavior: **Filter by** Exclude

Commercial Availability: Available (2,240), Not Available (15K)

Reaction Role: Product (95K), **Reactant (18K)**, Reagent (86)

Filtering: Reaction Role: Reactant, Number of Components: 1, Substance Class: Organic/Inorganic Small Molecule

ID	Chemical Structure	Formula	References	Reactions	Suppliers
2761217-93-8		$C_{12}H_{20}N_2O_8$	2	4	0
2761182-56-1		$C_{26}H_{24}F_4N_2O_5$	1	12	0
2760904-89-8		$C_{63}H_{78}N_4O_20$	1	5	0
2760527-70-4		$C_{25}H_{34}N_6O_6$	1	5	0
2759169-78-1		$C_{25}H_{35}ClN_6O_6$	1	5	0
2759154-25-9		$C_{25}H_{35}ClN_6O_6$	1	5	0

Search Within Results : 精炼产物结构

Filter Behavior

Filter by Exclude

Substance Role

- Product (53)
- Reactant (135)

Yield

Number of Steps

Non-Participating Functional Groups

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Searching for... Clear All

Remove and Edit

Reactions (135)

Group: By Document View: Expanded

References

Filtering: Substance Role: Reactant Search Within Results: Drawn Structure

1

Highly stereoselective asymmetric aldol routes to tert-butyl-2-(3,5-difluorophenyl)-1-oxiran-2-yl) ethyl)carbamates: Building blocks for novel protease inhibitors

By: Ghosh, Arun K.; Cardenas, Emilio L.; Brindisi, Margherita
Tetrahedron Letters (2017), 58(43), 4062-4065 | Language: English, Database: CAplus and MEDLINE

Full Text View 2 Related Reactions

Absolute stereochemistry shown, Rotation (+)

Suppliers (11)

Reaction Summary Steps: 1 Yield: 99%

1.1 Reagents: [Tosyl chloride](#), [Triethylamine](#)
Catalysts: [Dibutyltin oxide](#)
Solvents: [Dichloromethane](#); 4 h, 23 °C

1.2 Reagents: [Potassium carbonate](#)
Solvents: [Methanol](#); 23 °C → 0 °C; 0 °C → 23 °C; 1 h, 23 °C

View Reaction Detail | Experimental Protocols

2

A new synthetic method for the preparation of α,β -didehydroamino acid derivatives by means of a Wittig-type reaction. Syntheses of (2S, 4S)- and (2R, 4R)-4-hydroxyprolines

By: Kimura, Rumi; Nagano, Tanemasa; Kinoshita, Hideki
Bulletin of the Chemical Society of Japan (2002), 75(11), 2517-2525 | Language: English, Database: CAplus

Full Text

CAS Draw

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

Draw or change atoms or bonds.

reactant reactant product product

Molecular Formula: CH₃NO (45.04) · C₂H₆O₂ (62.07) · CH₃NO (45.04) · C₂H₄O (44.05)

Zoom: 100%

OK Cancel

使用原子标记工具精准定位原料和产物中的同一原子

例5：通过多组分物质的结构信息获取反应

CAS SciFinder Substances Edit Search Alerts Clock User

Structure Match

- As Drawn (151)**
- Substructure (174K)
- Similarity (2,584)

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

Commercial Availability

Reaction Role

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

Substances (2)

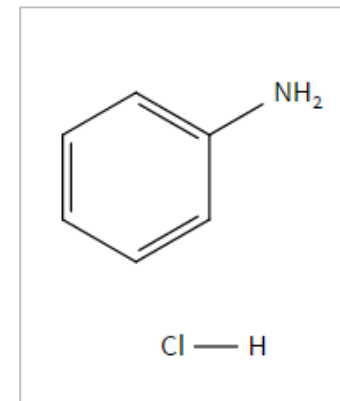
References Reactions Suppliers

Filtering: Number of Components: 2 Substance Class Isotopes: Not Containing Isotopes

Descending View: Partial Save And Alerts Clear All Filters

1 919288-94-1 C6H7N.2ClH
Components: 2
Component RN: 62-53-3
Benzenamine, hydrochloride (1:2)
1 Reference 0 Reactions 0 Suppliers

2 142-04-1 C6H7N.ClH
Components: 2
Component RN: 62-53-3
Benzenamine hydrochloride (1:1)
4,258 References **2,014 Reactions** 54 Suppliers



可提前精炼组分数、物质类型、排除同位素标记物等，再通过物质获取反应

获得多组分物质参与的各种角色的反应

CAS SciFinder[®] Reactions 142-04-1

Return to Home

Filter Behavior

Filter by Exclude

Substance Role

- Product (241)
- Reactant (1,399)
- Reagent (201)
- Catalyst (171)
- Solvent (2)

Yield

- 90-100% (159)
- 80-89% (167)
- 70-79% (165)
- 50-69% (256)
- 30-49% (196)

View All

Number of Steps

- 1 (1,876)
- 2 (27)
- 3 (11)
- 4 (38)

Reactions (2,014) Group: By Document View: Expanded

References

1

Solvent-free N-Boc deprotection by ex situ generation of hydrogen chloride gas

By: Verschuere, Rik H.; Gilles, Philippe; Van Mileghem, Seger; De Borggraeve, Wim M.
Organic & Biomolecular Chemistry (2021), 19(26), 5782-5787 | Language: English, Database: CAPLUS and MEDLINE

Full Text View 2 Related Reactions

CC(C)(C)OC(=O)Nc1ccccc1>>Nc1ccccc1.Cl

Suppliers (64) Suppliers (54)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: [Sodium chloride](#), [Sulfuric acid](#); 1 h, rt; > 1 min, rt

View Reaction Detail

通过Substance Role, 浏览
或筛选此物质参与的反应角色

对比直接通过多组分物质的结构信息获取反应

Structure Match

As Drawn (19K)

Substructure (418K)

Filter Behavior

Filter by Exclude

Yield

- 90-100% (1,547)
- 80-89% (1,722)
- 70-79% (1,682)
- 50-69% (2,169)
- 30-49% (1,282)

View All

Number of Steps

- 1 (19K)

Non-Participating Functional Groups

- Alkene (3,042)
- Halide (2,627)
- Cyclic alkene (2,289)

Reactions (19,217)

References

1

Quantitative detection of reducing sugars

By: Kleinnijhuis, Anne
World Intellectual Property Organization, WO2022015162 A1 2022-01-20 | Language: English, Database: CAplus

PatentPak Full Text

Suppliers (18) Suppliers (76) Supplier (1)

Reaction Summary

Steps: 1 Yield: 100%

1.1 Reagents: Hydroxyamine hydrochloride, Hydrochloric acid, Sodium sulfate
Solvents: Water; reflux

View Reaction Detail

各种As Drawn的结果都会出现，包括同位素标记物等

多组分物质中的多个组分会出现在不同的物质中

例6：通过文献获取反应

CAS SciFinder[®] References reduction and nitrile and catalyst and (nickel or Ni) Draw

← Return to Home

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

- Journal (273)
- Patent (166)
- Review (4)
- Conference (2)
- Preprint (1)

Substance Role

- Uses (178)
- Preparation (42)
- Properties (20)
- Nanoscale (18)
- Reactant or Reagent (15)

[View All](#)

References (441) Sort: Publication Date: Newest View: Partial Abstract

Substances Reactions Citing [Download](#) [Email](#) [Save And Alerts](#)

1

Ultrafine and well-dispersed Pd-Ni bimetallic catalyst stabilized by dendrimer-grafted magnetic graphene oxide for selective reduction of toxic nitroarenes under mild conditions
By: Niakan, Mahsa; Masteri-Farahani, Majid
Journal of Hazardous Materials (2022), 424(Part_D), 127717 | Language: English, Database: CPlus and MEDLINE

A facile and efficient strategy is introduced for growing a dendrimer structure on the surface of magnetic graphene oxide by using thiol-ene click reaction. The as-synthesized dendrimer-grafted magnetic graphene oxide was used as a suitable support for bimetallic Pd-Ni nanoparticles. The prepared nanocomposite was utilized for the reduction of toxic nitroarenes to aminoarenes by using sodium borohydride in aqueous medium at room temperature. Various nitroarenes with functional groups like nitrile, halogen, carbonyl, hydroxyl, acid, and heterocycles were converted to their corresponding anilines...

[View More](#)

[Full Text](#) Substances (7) Reactions (0) Citing (0) [Citation Map](#)

2

Ni-Catalyzed enantioselective reductive arylocyanation/cyclization of N-(2-iodo-aryl) acrylamide
By: Wang, Guangzhu; Shen, Chaoren; Ren, Xinyi; Dong, Kaiwu
Chemical Communications (Cambridge, United Kingdom) (2022), 58(8), 1135-1138 | Language: English, Database: CPlus and MEDLINE

A Ni/(S,S)-BDPP-catalyzed intramol. Heck cyclization of N-(2-iodo-aryl)acrylamides with 2-methyl-2-phenylmalononitrile was developed to give oxindoles with good enantioselectivities. By utilizing such an electrophilic cyanation reagent could tackle the deleterious effect of the coordinative cyanide ion in the asym. alkene arylocyanation.

- 主题词：reduction and nitrile and catalyst and (nickel or Ni)
- Substance Role & Concept 精炼
- 通过文献获取反应

Substance Role : 精炼检索主题中的物质在文献中最相关的研究角色 ; Concept : 纵览并精炼文献核心研究点

Substance Role

By Count | Alphanumeric

1 Selected

<input type="checkbox"/> Uses (178)	<input type="checkbox"/> Physical, Engineering, or Chemical Process (14)	<input type="checkbox"/> Formation, Non-preparative (2)
<input checked="" type="checkbox"/> Catalyst Use (163)	<input type="checkbox"/> Process (14)	<input type="checkbox"/> Formation, Unclassified (2)
<input type="checkbox"/> Preparation (42)	<input type="checkbox"/> Reactant (13)	<input type="checkbox"/> Reagent (2)
<input type="checkbox"/> Synthetic Preparation (32)	<input type="checkbox"/> Industrial Manufacture (11)	<input type="checkbox"/> Analytical Role, Unclassified (1)
<input type="checkbox"/> Properties (20)	<input type="checkbox"/> Purification or Recovery (6)	<input type="checkbox"/> Biological Study (1)
<input type="checkbox"/> Nanoscale (18)	<input type="checkbox"/> Technical or Engineered Material Use (6)	<input type="checkbox"/> Biological Study, Unclassified (1)
<input type="checkbox"/> Reactant or Reagent (15)	<input type="checkbox"/> Analytical Study (2)	<input type="checkbox"/> Modifier or Additive Use (1)

Apply | Cancel

Concept

Top Count | Alphanumeric | Search

4 Selected

<input type="checkbox"/> Nitriles (83)	<input type="checkbox"/> Aromatic nitro compounds (7)	<input type="checkbox"/> Esterification (4)
<input checked="" type="checkbox"/> Hydrogenation catalysts (75)	<input type="checkbox"/> Drying process (7)	<input type="checkbox"/> Fischer-Tropsch catalysts (4)
<input type="checkbox"/> Reduction (52)	<input type="checkbox"/> Group 8-10 elements (7)	<input type="checkbox"/> Fischer-Tropsch reaction (4)
<input type="checkbox"/> Amines (48)	<input type="checkbox"/> Hydrolysis (7)	<input type="checkbox"/> Green chemistry (4)
<input type="checkbox"/> Hydrogenation (45)	<input type="checkbox"/> Oxidation (7)	<input type="checkbox"/> Group 11 element compounds (4)
<input checked="" type="checkbox"/> Reduction catalysts (31)	<input type="checkbox"/> Oxidation catalysts (7)	<input type="checkbox"/> Group 12 element compounds (4)
<input type="checkbox"/> Alkenes (16)	<input type="checkbox"/> Recycling (7)	<input type="checkbox"/> Group 13 element compounds (4)
<input checked="" type="checkbox"/> Catalyst supports (16)	<input type="checkbox"/> Secondary amines (7)	<input type="checkbox"/> Group 15 element compounds (4)
<input type="checkbox"/> Alcohols (15)	<input type="checkbox"/> Diamines (6)	<input type="checkbox"/> Group 3 element compounds (4)
<input type="checkbox"/> Aldehydes (15)	<input type="checkbox"/> Nitriles, dinitriles (6)	<input type="checkbox"/> Group 8-10 element
<input type="checkbox"/> Nanoparticles (13)	<input type="checkbox"/> Reducing agents (6)	
<input checked="" type="checkbox"/> Catalysts (12)	<input type="checkbox"/> Aliphatic nitriles (5)	
<input type="checkbox"/> Imines (12)	<input type="checkbox"/> Alkali metal compounds (5)	

Apply | Cancel

基于精炼后的文献获取反应信息

CAS SciFinder[®] | References | reduction and nitrile and catalyst and (nickel or Ni) | Draw | Search | Alerts | Clock | Profile

← Return to Home

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](#)

References (105) | Sort: Publication Date: Newest | View: Partial Abstract

Substances **Reactions** Citing

Filtering: Substance Role: Catalyst Use X | Concept: 4 Selected X | [Clear All Filters](#)

1

Method for preparing DL-menthol from dipentene using novel catalyst
By: Babani, Mahesh; Sharma, Sadanand
India, IN201911038842 A 2021-09-03 | Language: English, Database: CPlus

Title method comprises (a) hydrogenating dipentene to 3-para menthene using noble metal catalyst, wherein the noble metal is palladium/pt loaded on to the surface like alumina or carbon or Raney nickel catalyst with very good selectivity and yields; (b) carrying out the reaction at temperature varying from 100-230 °C, preferably 140-220 °C and most preferable 160-200°C; (c) epoxidizing 3-para menthene with peracetic acid generating insitu by addition of acetic anhydride, hydrogen peroxide and sodium carbonate and or via performic acid formed in situ using formic acid and hydrogen peroxide to g...

[View More](#)

2

Preparation method of Ni-Co bimetallic component catalyst, and application thereof in fixed bed continuous hydrogenation reaction of isophthalonitrile solution for producing m-xylylenediamine
By: Li, Peng; Tian, Zhijian; Ma, Huaijun; Qu, Wei; Liu, Hao; Pan, Zhendong; Wang, Congxin; Han, Jianqiang; Wang, Donge; Wang, Lin

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

Document Type: Journal (34) Patent (70) Conference (1)

Substance Role: Uses (110) **Catalyst Use (105)** Preparation (24) Process (12) Properties (9)

PatentPak | Full Text | Substances (35) | Reactions (0) | Citing (0) | Citation Map

进一步精炼反应结果

CAS SciFinder[®] Reactions Draw

Filter Behavior

Yield

- 90-100% (220)
- 80-89% (92)
- 70-79% (32)
- 50-69% (30)
- 30-49% (10)
- No Yield Available (649)

Number of Steps

- 1 (578)
- 2 (155)
- 3 (73)
- 4 (52)
- 5 (36)
- 6-10 (49)

Non-Participating Functional Groups

- Halide (102)
- Phenyl halide (83)
- Nitrile (80)

Reactions (1,033) Group: By Document View: Expanded

References

1

Fe₃O₄-SiO₂-P4VP pH-Sensitive Microgel for Immobilization of Nickel Nanoparticles: An Efficient Heterogeneous Catalyst for Nitrile Reduction in Water

By: Nabid, Mohammad Reza; Bide, Yasamin; Niknezhad, Mahvash
ChemCatChem (2014), 6(2), 538-546 | Language: English, Database: CAplus

Reaction Summary Steps: 1 Yield: 99%

1.1 Reagents: [Sodium borohydride](#)
Catalysts: [Nickel](#) (nanoparticle on silanized magnetite microgel)
Solvents: [Water](#); 2 h, pH 5.5, 25 °C

Filter Behavior

Yield

Number of Steps

Non-Participating Functional Groups

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Search for up to 3 structures within the result set.

Searching for...

Remove and Edit

Reaction Summary Steps: 1 Yield: 99%

1.1 Reagents: [Sodium borohydride](#)
Catalysts: [Nickel](#) (nanoparticle on silanized magnetite microgel)
Solvents: [Water](#); 2 h, pH 5.5, 25 °C

2

Nitrogen-Doped Carbon-Supported Nickel Nanoparticles: A Robust Catalyst to Bridge the Hydrogenation of Nitriles and the Reductive Amination of Carbonyl Compounds for the Synthesis of Primary Amines

By: Zhang, Yangmin; Yang, Hanmin; Chi, Quan; Zhang, Zehui
ChemSusChem (2019), 12(6), 1246-1255 | Language: English, Database: CAplus and MEDLINE

Source Reference

主题词与反应式联用检索

CAS SciFinder[®] References reduction and nitrile and catalyst and (nickel or Ni) Edit

Return to Home

Structure Match

As Drawn (0)

Substructure (112)

Filter Behavior

Filter by Exclude

Document Type

Journal (71)

Patent (40)

Preprint (1)

Substance Role

Uses (56)

Preparation (31)

Reactant or Reagent (15)

Properties (7)

Nanoscale (6)

View All

Language

References (112)

Substances Reactions Citing Edit Drawing Remove Save And Alerts

1

Ni-Catalyzed enantioselective **reductive** arylcyanation/cyclization of N-(2-iodo-aryl) acrylamide

By: Wang, Guangzhu; Shen, Chaoren; Ren, Xinyi; Dong, Kaiwu
Chemical Communications (Cambridge, United Kingdom) (2022), 58(8), 1135-1138 | Language: English, Database: CAplus and MEDLINE

A **Ni**/(S,S)-BDPP-**catalyzed** intramol. Heck cyclization of N-(2-iodo-aryl)acrylamides with 2-methyl-2-phenylmalononitrile was developed to give oxindoles with good enantioselectivities. By utilizing such an electrophilic cyanation reagent could tackle the deleterious effect of the coordinative cyanide ion in the asym. alkene arylcyanation.

Full Text Substances (174) **Reactions (322)** Citing (0) Citation Map

2

One-pot synthesis of pyrrolidone derivatives via reductive amination of levulinic acid/ester with nitriles over Pd/C catalyst

By: Liu, Yingxin; Zhang, Kaiyue; Zhang, Liang; Wang, Yun; Wei, Zuojun
Reaction Kinetics, Mechanisms and Catalysis (2021), 134(2), 777-792 | Language: English, Database: CAplus

The selective **reductive** amination of levulinic acid (LA) into pyrrolidone derivatives is regarded as one of the most promising reactions in the fields of biomass conversion into high value-added chems. Herein, we report a one-pot synthesis of N-substituted-5-methyl-2-pyrrolidones by **reductive** amination of LA/ester with **nitriles** over several com. **catalysts**. Among the **catalysts** tested, Pd/C was found to be the most efficient for the **reductive** amination of LA/ester with various **nitriles** to give high yields of pyrrolidones (up to 92%) under mild reaction conditions (80°C, 1.6 MPa H₂, THF solvent)...



Reference支持主题词和反应式联用检索，同时识别主题词和反应式

获得关联文献中的反应结果

CAS SciFinder[®] Reactions 2022:44786

← Return to Home

Filter Behavior

Filter by Exclude

Yield

- 90-100% (5)
- 80-89% (8)
- 70-79% (10)
- 50-69% (10)
- 10-29% (1)
- No Yield Available (288)

Number of Steps

- 1 (122)
- 2 (113)
- 3 (27)
- 4 (20)

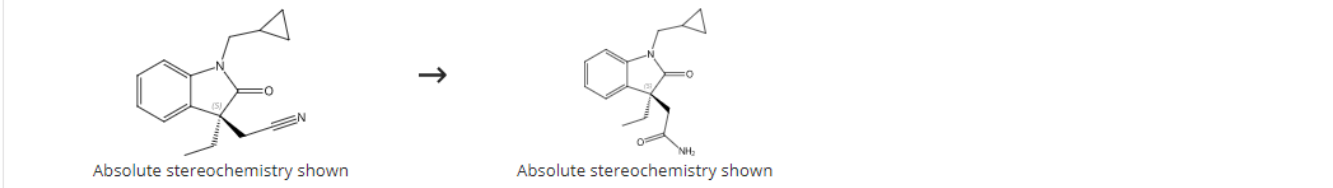
Non-Participating Functional Groups

Reactions (322) Group: By Scheme View: Expanded

References

Download Email Save And Alerts

Scheme 1 (1 Reaction) Steps: 1 Yield: 95%



Absolute stereochemistry shown

Reaction Summary Steps: 1 Yield: 95% **Ni-Catalyzed enantioselective reductive arylcyanation/cyclization of N-(2-iodo-aryl) acrylamide**

1.1 Reagents: [Potassium carbonate](#), [Hydrogen peroxide](#)
Solvents: [Dimethyl sulfoxide](#), [Water](#); 18 h, rt

By: Wang, Guangzhu; et al
Chemical Communications (Cambridge, United Kingdom)
(2022), 58(8), 1135-1138

View Reaction Detail Full Text

Collapse Scheme

小结：

- **通过文献获取反应**：基于需要检索的**反应**信息，形成**检索词**，并通过**逻辑符**构建**检索主题词**
- **Reference检索**：支持文献主题与**反应式联合检索反应文献**
- **文献结果精炼**：Substance Role**物质**在文献中的角色、Concept**核心研究点**
- **数据关联支持灵活获取信息**：通过**文献获取反应**
- **反应结果精炼**：可通过Search Within Results等工具**精炼反应结果**

总结：

- **反应信息的获取方法：**
 - ✓ 直接进行Reaction检、通过Retrosynthesis Plan获取逆合成反应路线、通过物质或文献获取反应。
 - ✓ 根据检索前掌握的信息和检索目的，灵活选择不同的检索方式。文献、物质和反应三者的数据已经CAS科学家进行高度关联。
- **反应结果聚类分析工具：** Filter by/Exclude
 - ✓ Yield, Steps, Reagent, Catalyst, Solvent, Commercial Availability
 - ✓ Non-participating Functional Groups, Reaction Note, Experimental Protocols, Search Within Results
 - ✓ Source Reference
- **反应详情的查看：** Experimental Protocols——Synthetic Methods、Experimental Procedures, CAS PatentPak
- **逆合成反应路线设计工具Retrosynthesis：** 预设参数、查看每一步的Evidence详情、浏览并根据需要调整 Alternative Steps、如有必要进一步使用Scoring Profile。

联系我们



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china@acs-i.org
010-62508026/7

记住本次讲座口令：

反应检索

30天内微信公众号回复讲座口令，获得PPT分享链接

学习资源

1. 关注“ACS美国化学会”微信公众号, 搜索**SciFinder-n**, 查看检索技巧、检索视频, 以及论坛回放视频



2. CAS SciFinderⁿ网络在线演示培训资料

<https://www.cas.org/about/events/scifinder-webinars>

3. CAS官网上的培训资料

<https://www.cas.org/support/training/scifinder-n>

4. CAS SciFinderⁿ Help使用指南

[https://scifinder-n.cas.org/help/#t=Searching in SciFinder-n%20Introduction to searching.htm](https://scifinder-n.cas.org/help/#t=Searching%20in%20SciFinder-n%20Introduction%20to%20searching.htm)

2022年CAS SciFinderⁿ论坛直播日程表

	日期	主题	主讲人
基础 培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder ⁿ 顺利开题、进行文献综述	钱欣
检索 策略 详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间：

18:00 – 19:00

扫描下方二维码
即可注册各期论坛：



谢谢关注!



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