

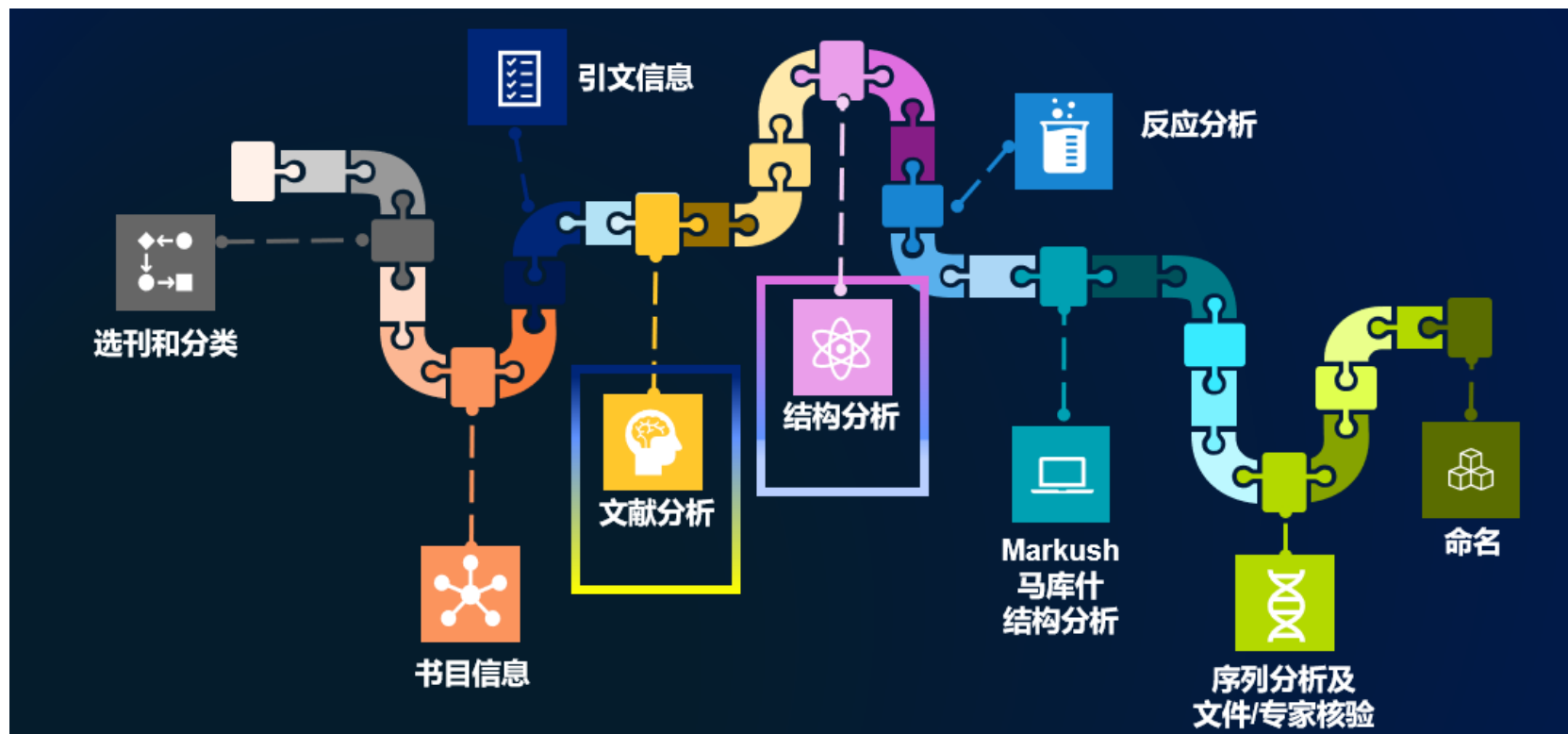
CAS SCIFINDER DISCOVERY PLATFORM™

结构绘制面板及案例详解

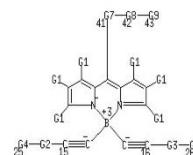
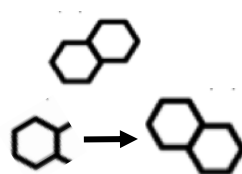


刘子露
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美国化学文摘社(CAS)北京代表处

CAS 科学家的智力标引



1990
Smith, M.
anthracene



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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS独特的内容合集



来源：

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

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

提纲

CAS SciFinder Discovery Platform 结构绘制面板及案例详解

- 结构的绘制、导入及保存
- 案例详解

CAS Draw 结构绘制面板

The image shows the CAS Draw software interface with various toolbars and callouts explaining their functions:

- Top Bar:** CAS Draw, 导入和导出结构文件 (Import and Export Structure Files), 输入 CAS 登记号、SMILES, 或 InChI 以创建结构 (Enter CAS Registry Number, SMILES, or InChI to create structure).
- Left Toolbar:** 套索|选框工具 (Lasso/Select tool), 绘制原子和化学键|橡皮擦 (Draw atoms and bonds/Eraser), 元素周期表|常见官能团和保护基 (Periodic table/Common functional groups and protecting groups), 可变基团定义工具|R基团定义工具 (Variable group definition tool/R-group definition tool), 片段结构定义工具|从模板中选择结构 (Fragment structure definition tool/Select structure from template), 添加正电荷|添加负电荷 (Add positive charge/Add negative charge), 重复结构单元工具|碳链工具 (Repeat structure unit tool/Carbon chain tool), 可变位置定义工具|环锁定工具 (Variable position definition tool/Ring locking tool), 原子锁定工具|旋转/翻转片段 (Atom locking tool/Rotate/Flip fragment), 反应角色定义工具|反应原子标记工具 (Reaction role definition tool/Reaction atom marking tool), 化学键标记工具|反应箭头绘制工具 (Chemical bond marking tool/Reaction arrow drawing tool).
- Right Toolbar:** 杂原子和氢同位素绘制 (Heteroatoms and hydrogen isotopes drawing), 绘制环 (Draw rings), 调整窗口大小 (Adjust window size).
- Callouts:**
 - 了解键盘快捷键 (例如, 快捷绘制杂原子) (Learn keyboard shortcuts (e.g., quick drawing of heteroatoms))
 - 绘制化学键, 带有 ▲ 符号说明有其他展开选项 (Draw chemical bonds, with ▲ symbol indicating other expandable options)
 - 输入要绘制的元素符号 (Enter the element symbol to be drawn)
- Bottom Bar:** Zoom: 90%, OK, Cancel.

快速导入物质结构

CAS Draw

1. 导入结构文件

2. 从模板中选择结构

3. 输入 CAS 登记号、SMILES, 或 InChI 以创建结构

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

Import

Molecular Formula: C₄₇H₅₁NO₁₄ (853.92)

Zoom: 100%

Cancel OK

CAS Registry Number
33069-62-4

CAS Name
Benzenepropanoic acid, β -(benzoyl amino)- α -hydroxy-, (2*a**R*,4*S*,4*a**S*,6*R*,9*S*,11*S*,12*S*,12...

Get Substance Details

Get Life Science Data

Get Reactions (12K)

Synthesize (10K)

Start Retrosynthetic Analysis

Get References (77K)

Get Suppliers (121)

View in CAS BioFinder

Edit Structure

Reset

Download

4. 获取感兴趣的物质时, 可将结构发送到结构编辑器

从模板中选择结构

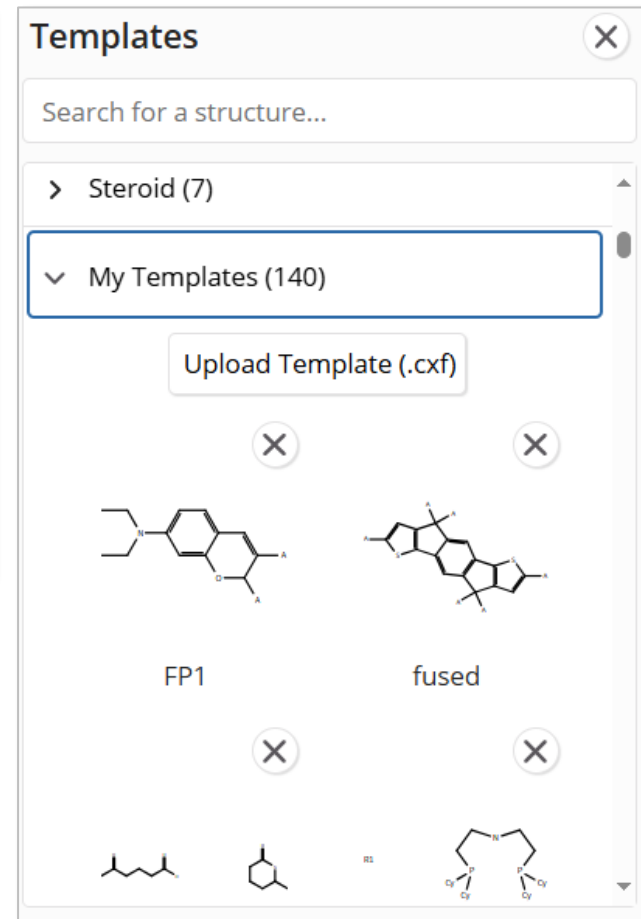
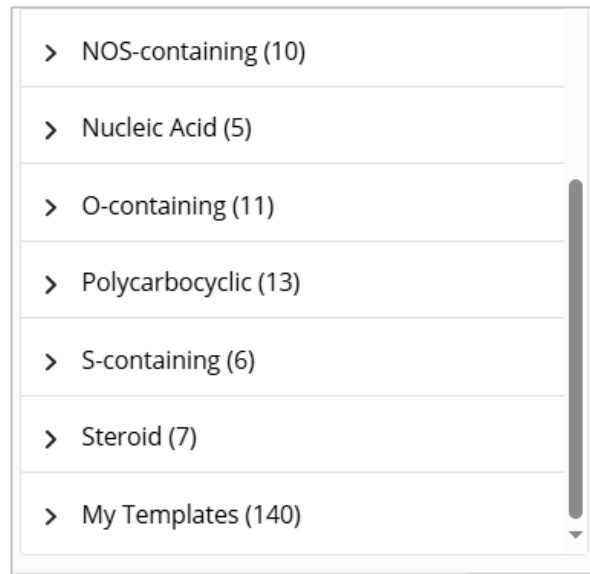
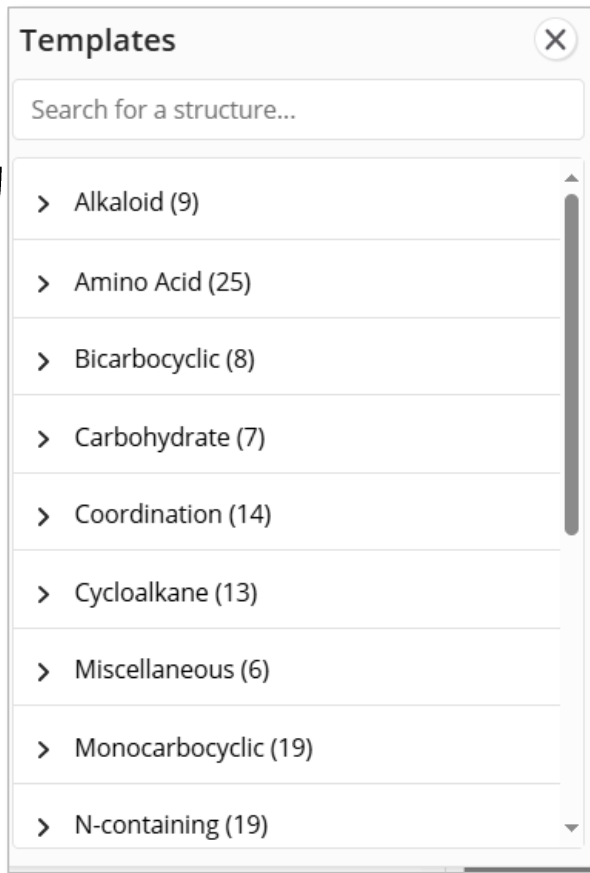


从模板中选择结构



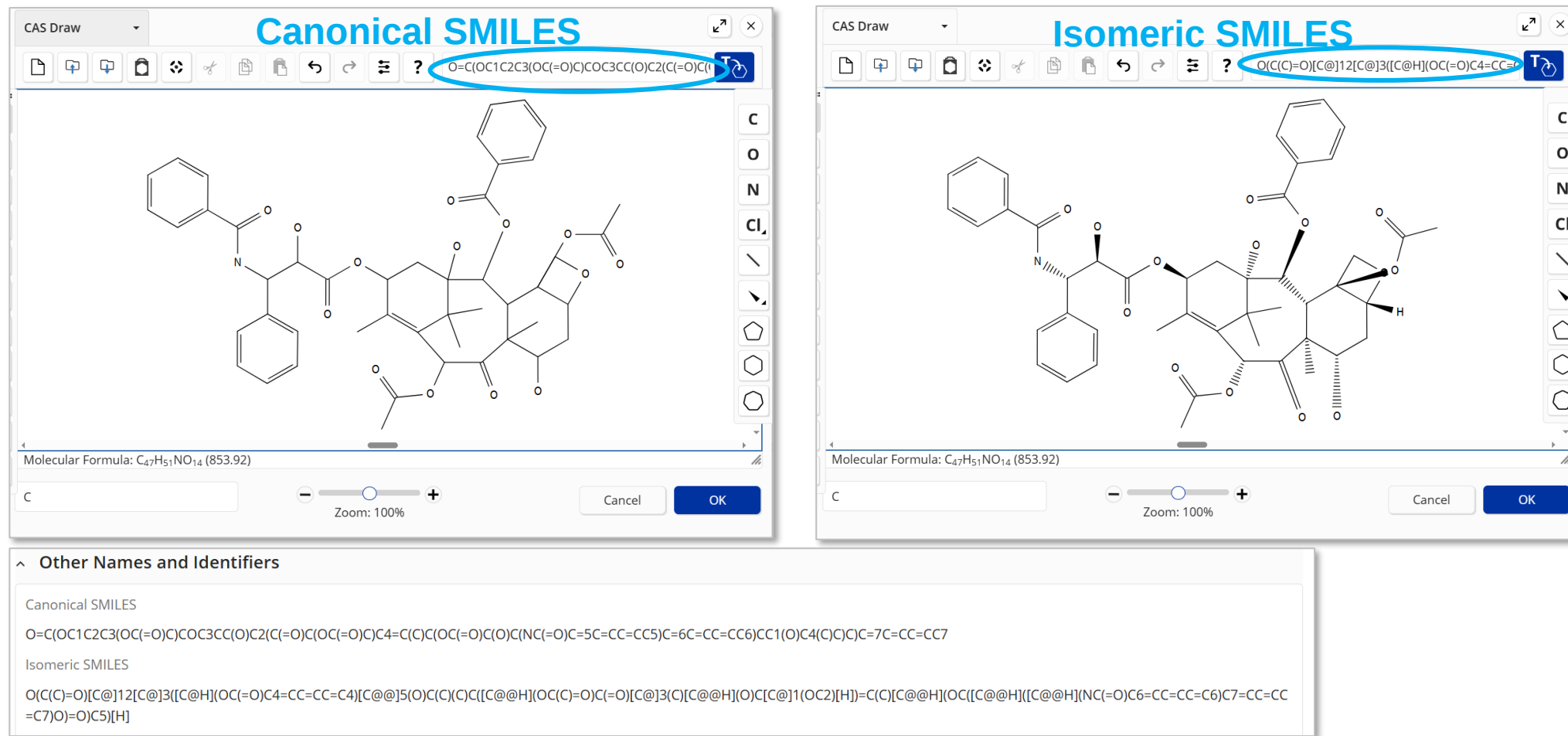
Save as
Template

将结构存入模板



利用SMILES导入手性结构

如需导入含立体化学和同位素的结构，请使用Isomeric SMILES



手性物质

CAS SciFinder Substances search for drawn structure

References Reactions Suppliers

Stereochemistry

- ☒ Absolute Stereo Match (54)
- ☐ Absolute Stereo Mirror Image (69)
- ☐ Stereo that Doesn't Match Query (6)
- ☐ No Stereo in Answer Structure (12)

Isotopes Metals Experimental Property Experimental Spectrum GHS Hazard Statements Regulatory Data by Country/Region Regulatory Data by List

Filtering: Stereochemistry: Absolute Stereo

54 Results

1 2 3

3082-62-0

Absolute stereochemistry shown, Rotation (-)

$C_{12}H_{13}N$
2-Naphthalenemethanamine, α -methyl-, (αS)-

403 References 420 Reactions 75 Suppliers

1422958-42-6

Absolute stereochemistry shown

$C_{12}H_{12}DN$
2-Naphthalenemethan- α -d-amine, α -methyl-, (αS)-

1 Reference 1 Reaction 0 Suppliers

2642176-79-0

Absolute stereochemistry shown, Rotation (-)

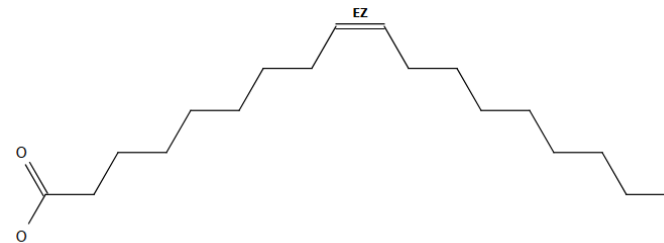
$C_{12}H_{13}N.H$
Components: 2
Component RN: 3082-62-0

1 Reference 0 Reactions 0 Suppliers



- Absolute Stereo Match
- Absolute Stereo Mirror Image
- Stereo that Doesn't Match Query
- No Stereo in Answer Structure

顺反异构体



CAS SciFinder

Substances search for drawn structure

References Reactions Suppliers

Filtering: Stereochemistry: Double Bond Geometry As D... X

3,819 Results

Stereochemistry

- ☒ Double Bond Geometry As Drawn (3,819)
- ☐ Stereo that Doesn't Match Query (145)
- ☐ No Stereo in Answer Structure (94)

Isotopes

Metals

Experimental Property

Experimental Spectrum

GHS Hazard Statements

112-80-1

Double bond geometry shown

$C_{18}H_{34}O_2$
9-Octadecenoic acid (9Z)-

195K References 9,272 Reactions 168 Suppliers

115-06-0

Double bond geometry shown

$C_{18}H_{33}O_2$
9-Octadecenoic acid (9Z)-, ion(1-)

422 References 5 Reactions 5 Suppliers

7049-68-5

Double bond geometry shown

$(C_{18}H_{34}O_2)_2$
9-Octadecenoic acid (9Z)-, dimer

277 References 57 Reactions 2 Suppliers

Edit Drawing Remove

Search Patent Markush

Clear All Filters

Sort: Relevance View: Partial



碳链工具

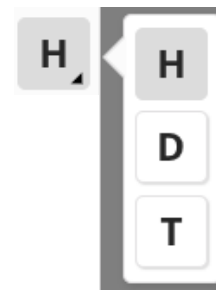
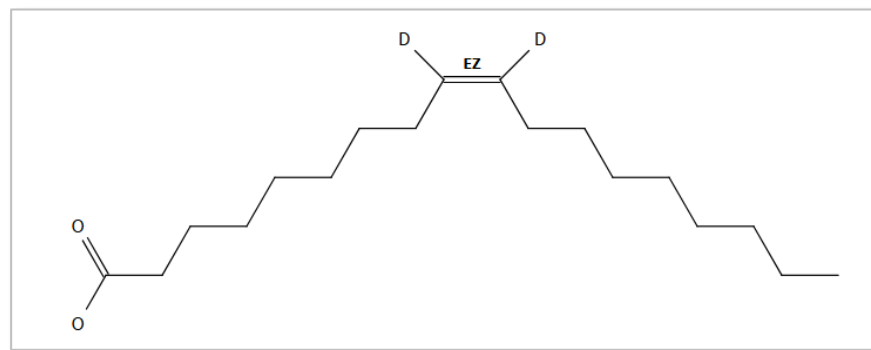


EZ锁定

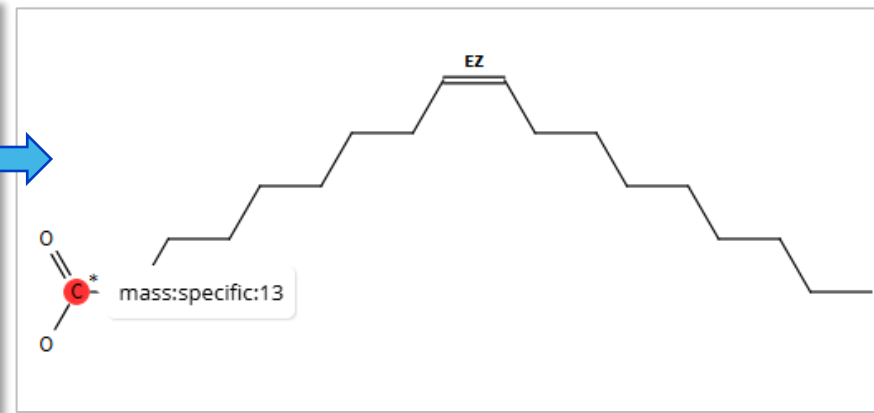
同位素

鼠标右键点击某原子，在弹出窗口中进行设置：

- Any：获取所有的同位素标记物和非同位素标记物
- Abnormal：获取所有的同位素标记物；
- Specific：精准检索特定同位素质量数的标记物



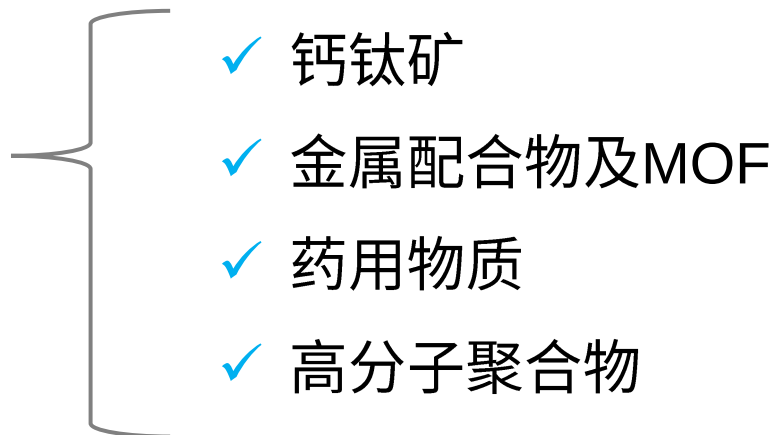
氢同位素



提纲

— 案例详解

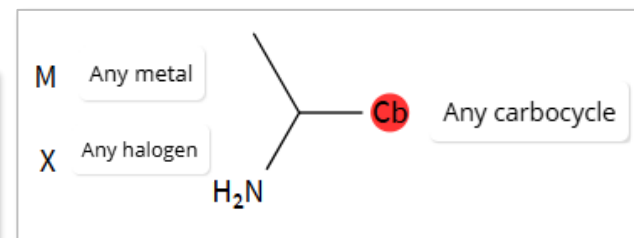
- 物质检索
- 反应检索



案例1：钙钛矿

同时识别关键词与结构式

The screenshot shows the CAS SciFinder interface. At the top, the search bar contains 'perovskite and chiral'. Below the search bar, there are tabs for 'Substances', 'Reactions', 'Citing', and 'Knowledge Graph'. The 'Structure Match' section is highlighted with a blue circle. The search results show 39 results. The first result is 'Chiral 2D Perovskites with a High Degree of Circularly Polarized Photoluminescence' by Ma, Jiaqi; Fang, Chen; Chen, Chao; Jin, Long; Wang, Jiaqi; Wang, Shuai; Tang, Jiang; Li, Dehui. The second result is 'Chiral 2D-Perovskite Nanowires for Stokes Photodetectors' by Zhao, Yingjie; Qiu, Yuchen; Feng, Jiangang; Zhao, Jiahui; Chen, Gaosong; Gao, Hanfei; Zhao, Yuyan; Jiang, Lei; Wu, Yuchen. The interface also includes a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons, and a 'Publication Year' histogram.



可变基团

Variables list showing search criteria for different atom types:

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- Ak Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

定题追踪：研究领域中的最新进展

文献、物质、反应和Markush检索结果集皆可设置提醒

References search for "perovskite and chiral" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (39)

Substructure (45)

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CA Section

Publication Year

39 Results

1

Chiral 2D Perovskites with a High De

By: Ma, Jiaqi; Fang, Chen; Chen, Chao; Jin, Long; V

ACS Nano (2019), 13(3), 3659-3665 | Language: E

Chiral n

spintrom

increasin

chirality

studies o

Intensity (a.u.)

Wavelength (nm)

Responsivity (A/W)

Wavelength (nm)

View More

Full Text

2

Chiral 2D-Perovskite Nanowires for S

By: Zhao, Yingjie; Qiu, Yuchen; Feng, Jiangang; Zh

Journal of the American Chemical Society (2021),

Set Citing Alert

Name

Please provide a name for your search

Add Existing Tags (Optional)

☐ CO2

☐ Fermentation

☐ Flow chemistry

☐ Formula

☐ Higgs

☐ High Entropy

New Tag (Optional)

Add tag name

Tag Color

Light Blue

Alerts

Frequency

As Available

Add Email(s)

china@acs-i.org xxx@163.com

Cancel Save

Save and Alert

Share Results

Copy Search to Clipboard

多篇文献中的手性钙钛矿材料

References search for "perovskite and chiral" + drawn structure

Substances Reactions

Get Substances from References

All Results Selected Results

Substructure (42)

Substances from References

References Reactions Suppliers

Filtering: Functional Group: Amine X Stereochemistry: Stereo in Answer Structur... X Metals: Containing Metals X Clear All Filters

48 Results

Sort: Number of References: Descending View: Partial

1 2 3

935739-36-9

2748667-79-8

935739-32-5

Functional Group

- ☒ Amine (48)
- ☐ Halide (48)
- ☐ Metal halide (48)
- ☐ Primary amine (48)
- ☐ Phenyl halide (3)

View All

Number of Components

Commercial Availability

Molecular Weight

Stereochemistry

- ☒ Stereo in Answer Structure (48)
- ☐ No Stereo in Answer Structure (13)

Isotopes

Metals

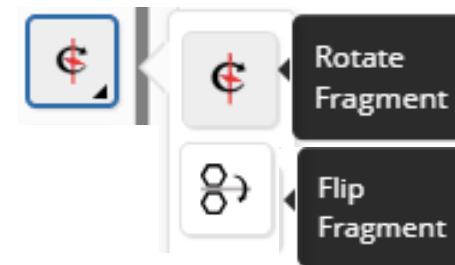
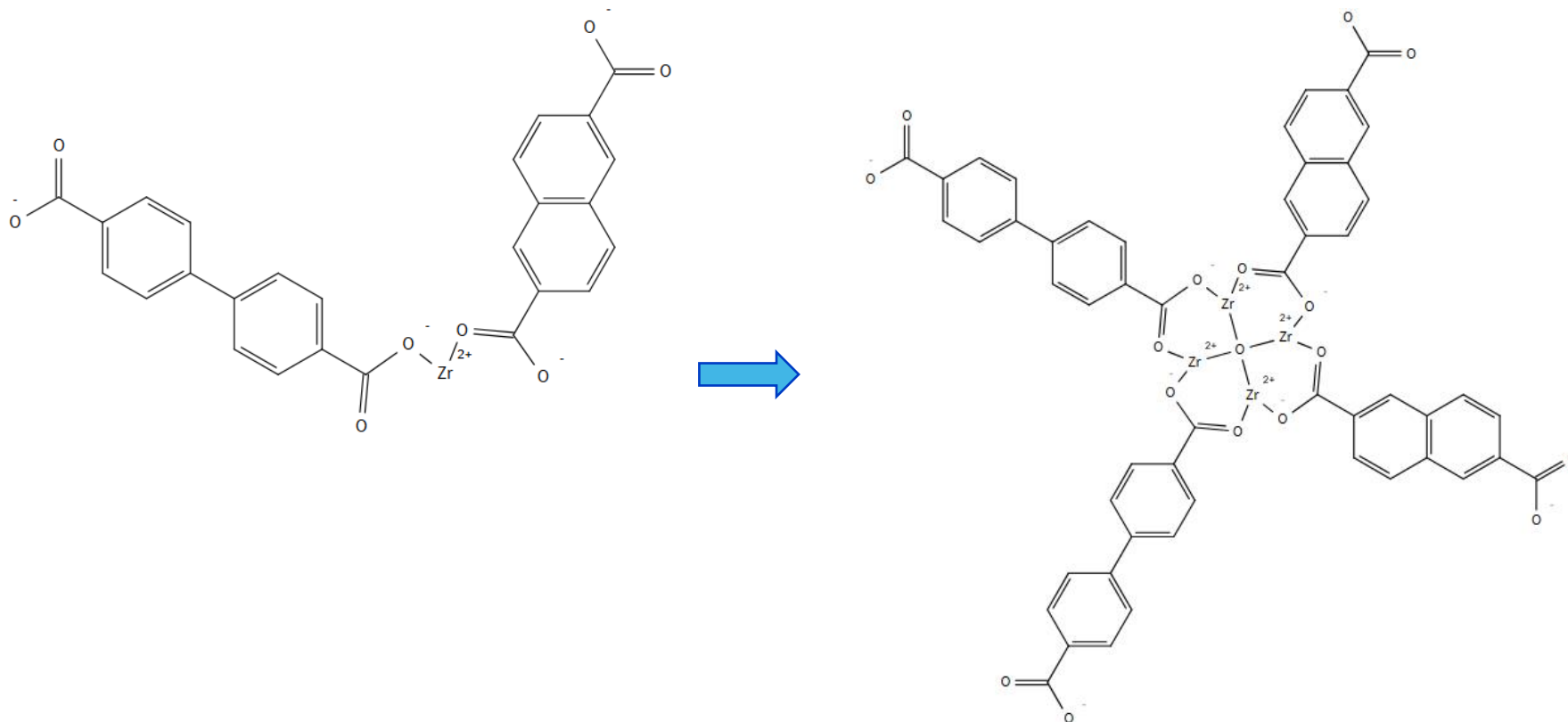
- ☒ Containing Metals (48)
- ☐ Not Containing Metals (76)

Chemical structures and data for three results:

- 935739-36-9**: $C_8H_{11}N \cdot \frac{1}{2}H \cdot \frac{1}{4}I_4Pb$, Components: 3, Plumbate(2-), tetraiodo-, (T-4)-, hydrogen, compd. with (αS)-α-methylbenzenemeth...
- 2748667-79-8**: $C_8H_{11}N \cdot \frac{1}{2}H \cdot \frac{1}{4}I_4Pb$, Components: 3, Plumbate(2-), tetraiodo-, (T-4)-, hydrogen, compd. with (αR)-α-methylbenzenemeth...
- 935739-32-5**: $C_8H_{11}N \cdot H \cdot I_3Pb$, Components: 3, Plumbate(1-), triiodo-, hydrogen, compd. with (αS)-α-methylbenzenemethanamine (1...

基于数据关联，获取文献中“包含金属、胺基、立体结构的物质”

案例2：金属有机配合物及MOF



旋转/翻转片段

金属有机配合物

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (6)

Substructure (98)

Similarity (105K)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

6 Results

1

1673512-68-9

C₉₆H₇₆O₃₂Zr₆
Zirconium, hexakis[μ-[2,2'-dimethyl[1,1'-biphenyl]-4,4'-dicarboxylato(2-)-κO⁴:κO...

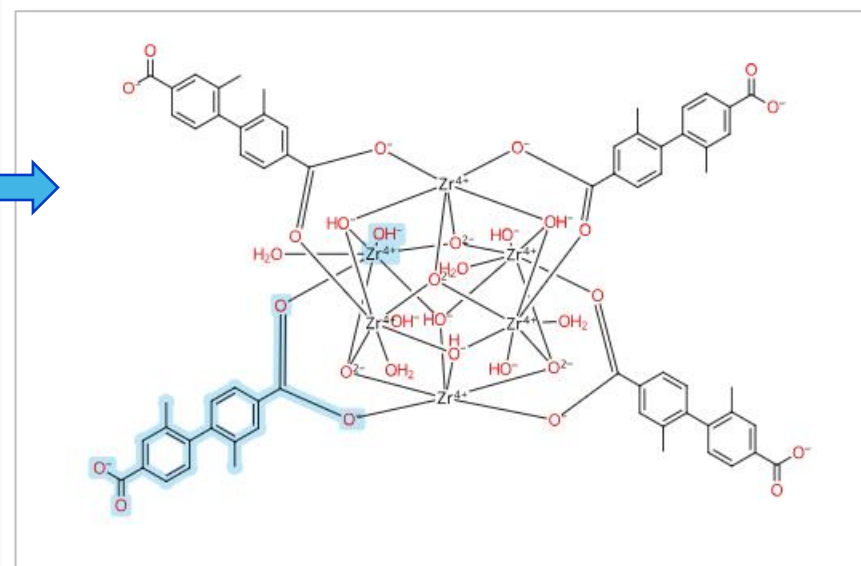
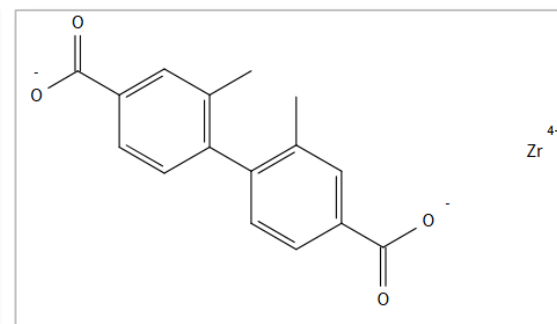
4 References 3 Reactions 0 Suppliers

2

1667709-07-0

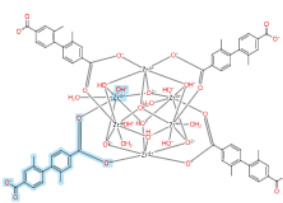
C₆₄H₆₄O₃₂Zr₆
Zirconium, tetraaquatetrakis[μ-[2,2'-dimethyl[1,1'-biphenyl]-4,4'-dicarboxylato(2-)-κO⁴:κO...

24 References 73 Reactions 0 Suppliers



金属有机配合物的制备方法

1667709-07-0



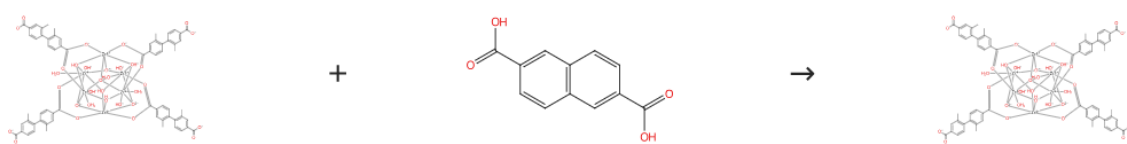
$C_{64}H_{64}O_{32}Zr_6$
Zirconium, tetraaquatetrakis[μ-
[2,2'-dimethyl[1,1'-biphenyl]-
4,4'-dicarboxylato(...

24 References 73 Reactions 0 Suppliers

Filtering: Experimental Protocols: Synthetic Methods X Substance Role: Product X Clear All Filters

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 98%



post-treated with H_2NDC

Suppliers (79)

31-614-CAS-29297272 Steps: 1 Yield: 98% Flexible Zirconium Metal-Organic Frameworks as Bioinspired Switchable Catalysts
By: Yuan, Shuai; et al
Angewandte Chemie, International Edition (2016), 55(36), 10776-10780
Full Text

1.1 Solvents: [Dimethylformamide](#); 24 h, 75 °C
[Experimental Protocols](#)

Collapse Scheme

Experimental Protocols

- Reagent
- Solvent
- Experimental Protocols
 - ☒ Synthetic Methods (32)
 - ☐ Experimental Procedure (3)
- Non-Participating Functional Groups
 - ☐ Carboxylic acid (9)
- Substance Role
 - ☒ Product (32)
 - ☐ Reactant (27)
 - ☐ Catalyst (2)
- Reaction Mapping
- Stereochemistry
- Reaction Type

金属有机配合物的制备方法

Experimental Protocols

Synthetic Methods

Products [Tetraaquatetrakis\[μ-\[2,2'-dimethyl\[1,1'-biphenyl\]-4,4'-dicarboxylato\(2-\)-κO⁴:κO⁴\]\]tetra-μ₃-hydroxytetrahydroxytetra-μ₃-oxohexazirconium](#), Yield: 98%
(post-treated with H₂NDC)

Reactants [2,6-Naphthalenedicarboxylic acid](#)
[Tetraaquatetrakis\[μ-\[2,2'-dimethyl\[1,1'-biphenyl\]-4,4'-dicarboxylato\(2-\)-κO⁴:κO⁴\]\]tetra-μ₃-hydroxytetrahydroxytetra-μ₃-oxohexazirconium](#)

Solvents [Dimethylformamide](#)

Procedure

1. Charge PCN-700-Me₂ (100 mg), H₂NDC (250 mg) and DMF (40 mL) in a Pyrex vial.
2. Heat the mixture in 75 °C oven for 24 h.
3. Collect the crystals of PCN-700-NDC by filtration and wash with fresh DMF 3 times.

Scale milligram

Characterization Data

^ Tetraaquatetrakis[μ-[2,2'-dimethyl[1,1'-biphenyl]-4,4'-dicarboxylato(2-)-κO⁴:κO⁴]]tetra-μ₃-hydroxytetrahydroxytetra-μ₃-oxohexazirconium

Crystal Structure Data Crystal Data : Formula Zr₆ C₇₆ H₅₄ O₃₂, [Zr₆ O₁₂] [C₁₆ H₁₂ O₄]₄ [C₁₂ H₆ O₄], Formula weight 2026.51, Crystal system Tetragonal, Space group *P*4₂/*mmc*, *a* (Å) 23.679 (8), *b* (Å) 23.679, *c* (Å) 16.816 (6), α (°) 90.00, β (°) 90.00, γ (°) 90.00, *V* (Å³) 9428 (4), *Z* 2

^ Experimental Protocols

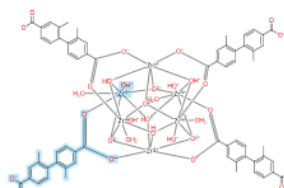
☒ Synthetic Methods (32)

☐ Experimental Procedure (3)

金属有机配合物的催化应用

2

1667709-07-0



C₆₄H₆₄O₃₂Zr₆

Zirconium, tetraaquatetrakis[μ-[2,2'-dimethyl[1,1'-biphenyl]-4,4'-dicarboxylato(...

24

References

73

Reactions



Reactions for 1667709-07-0

References

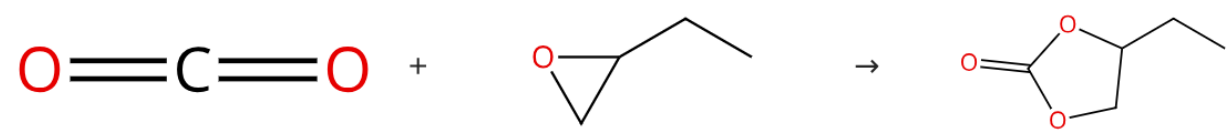
Filtering: Substance Role: Catalyst X

Clear All Filters

6 Results

Group: By Scheme Sort: Publication Date: Newest View: Collapsed

Scheme 1 (1 Reaction) Steps: 1



Suppliers (17)

Suppliers (42)

Suppliers (47)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1



Suppliers (17)

Suppliers (89)

Suppliers (39)

20

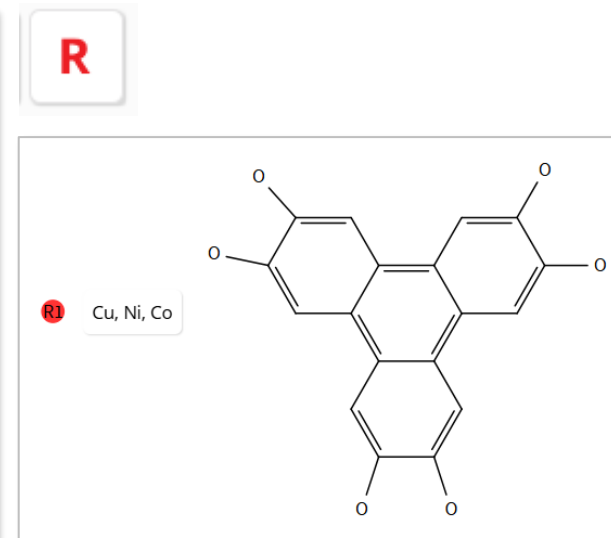
© 2025 American Chemical Society. All rights reserved.

CAS
A division of the
American Chemical Society

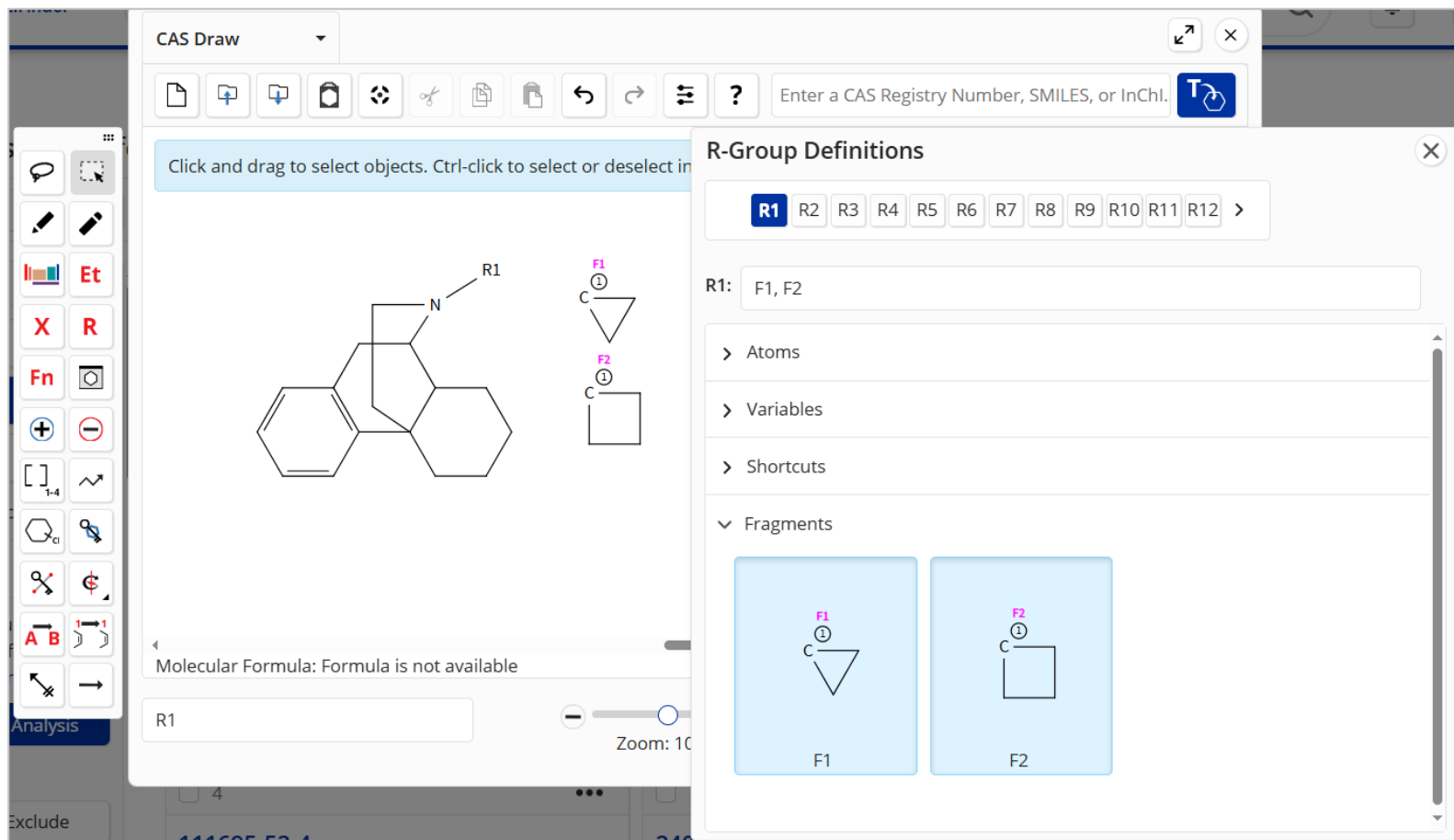
MOF的表征信息

文本结构联合检索：研究了目标MOF结构X射线光电子能谱 (XPS) 的文献

The screenshot shows the CAS SciFinder web interface. At the top, there's a search bar with 'X-ray photoelectron spectra' entered. Below the search bar, there are tabs for 'Substances', 'Reactions', 'Citing', and 'Knowledge Graph'. On the left side, there's a 'Structure Match' section with 'As Drawn (27)' selected. Below that, there's a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. The main search results area shows 27 results. The first result is titled 'Conductive Two-Dimensional Phthalocyanine-based Metal-Organic Framework Nanosheets for Efficient Electroreduction of CO₂'. The authors listed are Yi, Jun-Dong; Si, Duan-Hui; Xie, Ruikuan; Yin, Qi; Zhang, Meng-Di; Wu, Qiao; Chai, Guo-Liang; Huang, Yuan-Biao; and Cao, Rong. The journal is 'Angewandte Chemie, International Edition' (2021), 60(31), 17108-17114. The abstract mentions the electrocatalytic conversion of CO₂ into value-added chemicals and the use of metal-organic frameworks (MOFs) for CO₂ electroreduction.



案例3：药用物质



Fn

片段结构标记

R

自定义R基团



Draw 3-15 Sided Ring

Enter the number of
carbons for your ring:

7

OK

Cancel

药用物质

CAS SciFinder

Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Reference Role

- ☐ Preparation (19)
- ☐ Synthetic Preparation (19)
- ☐ Biological Study (13)
- ☒ Pharmacological Activity (12)
- ☒ Therapeutic Use (12)
- ☐ Uses (12)
- ☐ Reactant (11)
- ☐ Reactant or Reagent (11)
- ☐ Properties (2)
- ☐ Prophetic Synthesis or Use (1)

Filtering: Reference Role: 2 Selected X

12 Results

1

2355249-58-8

Absolute stereochemistry shown

$C_{20}H_{24}FNO_2$
Morphinan, 17-cyclopropyl-4,5-epoxy-6-fluoro-3-methoxy-, (5 β ,9 α ,13 α ,14 α)-

1 Reference 0 Reactions 0 Suppliers

2

1041639-72-8

Absolute stereochemistry shown

$C_{20}H_{24}N_2O_4$
Morphinan-3-carboxamide, 17-cyclopropyl-4,14-dihydroxy-6-oxo-

1 Reference 0 Reactions 0 Suppliers

3

1041639-71-7

Absolute stereochemistry shown

$C_{20}H_{22}N_2O_4$
Morphinan-3-carboxamide, 17-cyclopropyl-4,5-epoxy-14-hydroxy-6-oxo-, (5 α)-

1 Reference 0 Reactions 0 Suppliers

Edit Drawing Remove

Search Patent Markush

Clear All Filters

Sort: Relevance View: Partial

药用物质

CAS SciFinder

Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (158)

Similarity (53K)

Analyze Structure Precision

Chemscap Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscap.

Create Chemscap Analysis

158 Results

1

2005463-58-9

Absolute stereochemistry shown

$C_{28}H_{34}N_4O_3$

3H-Pyrazol-3-one, 4-[[[(1S,3aR,5aS,6R,11bR,11cS)-14-(cyclopropylmethyl)-1,2,3a,4,...

4 References 18 Reactions 0 Suppliers

2

32392-32-8

Absolute stereochemistry shown

$C_{32}H_{33}N_3O_3$

6,14-Ethenomorphinan-3-ol, 17-(cyclopropylmethyl)-4,5-epoxy-6-methoxy-7-(1-phenyl...

3 References 2 Reactions 0 Suppliers

2005463-71-6

Absolute stereochemistry shown

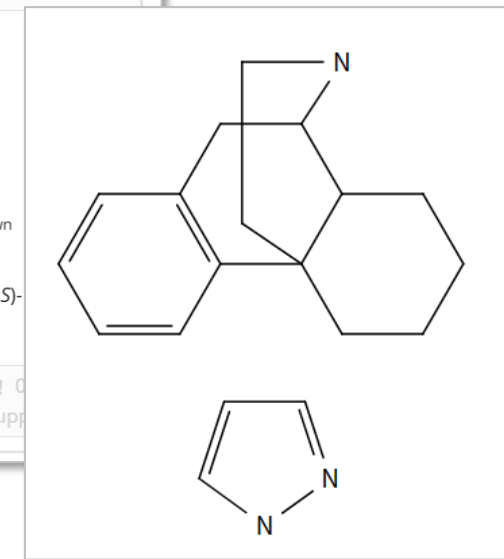
$C_{29}H_{36}N_4O_3$

Methanone, [(1S,3aR,5aS,6R,11bR,11cS)-opylmethyl)-1,2,3a,4,5,6,7,11c-...

3 References 18 Reactions 0 Suppliers

Edit Drawing Remove Descending View: Partial

Search Patent Markush



药用物质

CAS SciFinder

Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (39)

Similarity (53K)

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

39 Results

1

2043656-43-3

Absolute stereochemistry shown

$C_{20}H_{25}N_3$

Morphinan, 17-methyl-3-(1H-pyrazol-4-yl)-

1 Reference 3 Reactions 0 Suppliers

2

2043656-44-4

Absolute stereochemistry shown

$C_{20}H_{25}N_3 \cdot x HCl$

Components: 2

Component RN: 2043656-43-3

Morphinan, 17-methyl-3-(1H-pyrazol-4-yl)-, hydrochloride (1:?)

1 Reference 1 Reaction 0 Suppliers

2991240-22-1

Absolute stereochemistry shown

$C_{21}H_{27}N_3O$

Morphinan, 3-methoxy-17-methyl-2-(1H-pyrazol-1-yl)-, (9a,13a,14a)-

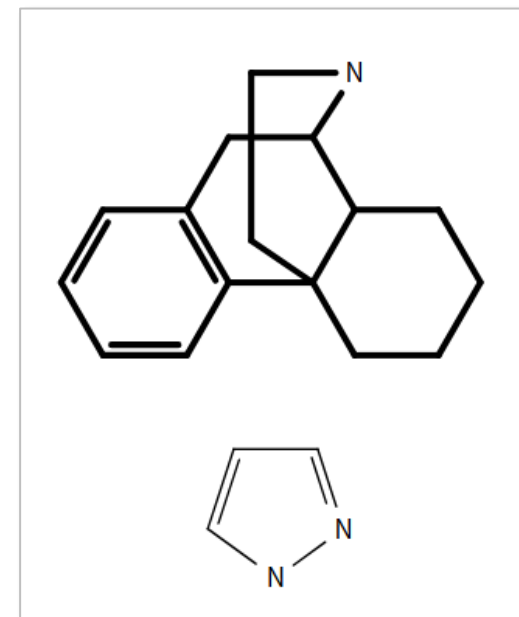
1 Reference 2 Reactions 0 Suppliers

Edit Drawing Remove

Search Patent Markush



环锁定工具



快速获取生命科学数据

CAS SciFinder Substances Enter a query...

References Reactions Suppliers

Filtering: Life Science Data: 2 Selected

16 Results

1 2043656-43-3 C20H25N3
Morphinan, 17-methyl-3-(1H-pyrazol-4-yl)-
Absolute stereochemistry shown

2 2043656-44-4 C20H25N3.XClH
Absolute stereochemistry shown

3 2043657-41-4 C24H33N3O2
Morphinan, 17-[2-(2-methoxyethoxy)ethyl]-3-(1H-pyrazol-4-yl)-
Absolute stereochemistry shown

Pharmacological Data

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Mu-type opioid receptor	Inhibitor	IC50	0.055 μM	-	Homo sapiens	View Detail	(1) CAS

(1) Anand, Neel; World Intellectual Property Organization, WO2016182840 A1 2016-11-17, CAplus

案例4：含特定结构的高分子

CAS SciFinder

Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers

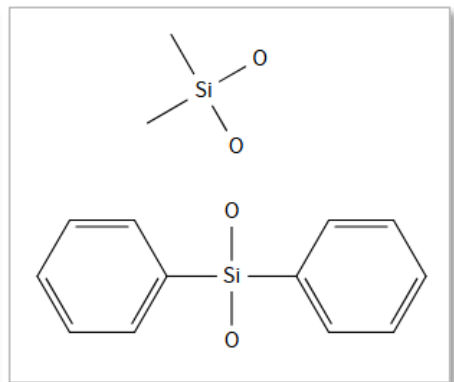
Filtering: Polymer Class: Polyamic acid X

38 Results

- Polyether (376)
- Polyvinyl (113)
- Polyether (103)
- Polyether only (100)
- Polyacrylic (83)
- ☒ Polyamic acid (38) View All

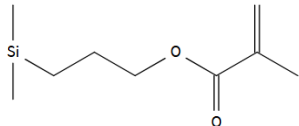
Number of Components Commercial Availability Molecular Weight Isotopes Metals Reference Availability

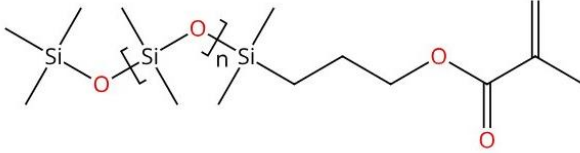
ID	Chemical Structure	Formula	Description	References	Reactions	Suppliers
2377179-26-3		(C ₁₆ H ₆ O ₆ .C ₁₂ H ₁₂ O ₂ Si.C ₆ H ₁₄ N ₂) _n	[5,5'-Biisobenzofuran]-1,1',3,3'-tetrone, polymer with cyclohexanediamine, 1,1-dimethylsilane	2	2	0
2377179-23-0		(C ₁₂ H ₁₂ N ₂ O.C ₁₂ H ₁₂ O ₂ Si.C ₁₀ H ₈) _n	1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, polymer with 1,1-dimethylsilane	2	2	0
2377179-24-1		(C ₁₄ H ₁₆ N ₂ .C ₁₂ H ₁₂ O ₂ Si.C ₁₀ H ₈) _n	1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, hexahydro-, polymer with 2,2'-bis(4-amino-1-methylphenyl)-1,1'-dimethylsilane	2	2	0



特定端基和特定类别高分子







CAS SciFinder

Substances

Substance Class

☐ Organic/Inorganic Small Molecule (190)

☒ Polymer (148)

Functional Group

Polymer Class

Number of Components

☒ 1 (148)

☐ 2 (623)

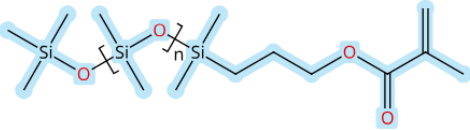
☐ 3 (1,263)

☐ 4 (1,312)

Filtering: Substance Class: Polymer X Number of Components: 1 X

148 Results

123109-42-2



$(C_2H_6OSi)_n C_{12}H_{26}O_3Si_2$
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]pr...

655
References

847
Reactions

0
Suppliers

Functional Group

Polymer Class

☐ Polyacrylic (1,253)

☐ Polyvinyl (169)

☐ Polyether (148)

☐ Polyether (120)

☒ Polystyrene (110)

[View All](#)

Number of Components

☐ 2 (52)

☒ 3 (110)

☐ 4 (123)

☐ 5 or more (509)

Commercial Availability

Molecular Weight

Stereochemistry

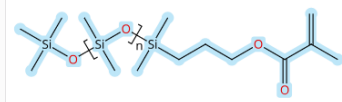
Isotopes

Metals

Filtering: Polymer Class: Polystyrene X Number of Components: 3 X

110 Results

181798-33-4



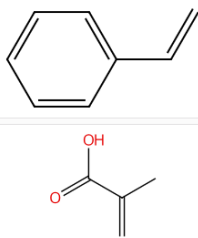
$(C_8H_8.C_5H_8O_2.(C_2H_6OSi)_n C_1...$
Components: 3
2-Propenoic acid, 2-methyl-, methyl ester, polymer with α-[dimethyl[3-[(2-methyl...

8
References

1
Reaction

0
Suppliers

1451148-82-5



$(C_8H_8.C_4H_6O_2.(C_2H_6OSi)_n C_1...$
Components: 3
2-Propenoic acid, 2-methyl-, polymer with α-methylsilyl)-ω-[[dimethyl[3-...

8
References

5
Reactions

0
Suppliers

高分子的配方应用

CAS Formulus

Formulations 123109-42-2

Formulations search for "123109-42-2"

Get Additional References

Filter by

- Industry
 - Coating materials (124)
 - ☒ Antifouling coating materials (44)
 - Adhesives (43)
 - Cosmetics and Personal care products (32)
 - Transparent coating materials (28)
- Purpose
 - Coating materials (124)
 - ☒ Antifouling coating materials (44)
 - Adhesives (43)
 - Cosmetics and Personal care products (32)
 - Transparent coating materials (28)
- Information Included
 - Component Amount (44)
 - ☒ Experimental Activity (44)
 - Process (44)

44 Results

Sort: Relevance Group: By Family

1

Antifouling Coating Composition: Antifouling Coating Materials

Location: Table 1, 3, 10, Example 24
Purpose: Antifouling coating materials
Target: Carriers

Component	Function	Amount Reported
Group: Resins	-	87.17 mass parts
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]propyl)silyl]-ω-[[trimethylsilyl]oxy]-	-	15 mass parts

Compare

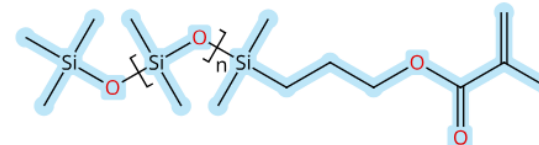
PATENT

Preparation of coating composition and coating film, composite coating film, ship and underwater structure

Assignee : Nippon Paint Marine Coating Co., Ltd.
JP7324379
Language: Japanese

Patent PDF View in CAS SciFinder

123109-42-2



$(C_2H_6OSi)_nC_{12}H_{26}O_3Si_2$
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]propyl)silyl]-ω-[[trimethylsilyl]oxy]-

655 References 847 Reactions 0 Suppliers

高分子的配方详情

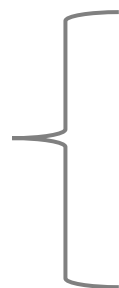
Component	Function	Amount Reported	Optionality
Group: Resins	-	87.17 mass parts	Mandatory
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]propyl]silyl]-ω-[[trimethylsilyl]oxy]-	-	15 mass parts	Mandatory
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]propyl]silyl]-ω-[[trimethylsilyl]oxy]-	-	10 mass parts	Mandatory
Poly[oxy(dimethylsilylene)], α-[dimethyl[3-[(2-methyl-1-oxo-2-propen-1-yl)oxy]propyl]silyl]-ω-[[trimethylsilyl]oxy]-	-	15 mass parts	Mandatory
Xylene	Solvents	50 mass parts	Mandatory
Tris(1-methylethyl)silyl 2-methyl-2-propenoate	-	5 mass parts	Mandatory
tert-Butyl methacrylate	-	5 mass parts	Mandatory
2-Propenoic acid, 2-methyl-, methyl ester	-	27 mass parts	Mandatory
tert-Butyl peroxy-2-ethylhexanoate	Polymerization catalysts	1.0 mass parts	Mandatory
Butyl acrylate	-	6 mass parts	Mandatory
Acrylic acid	-	17 mass parts	Mandatory
Naphthenic acids	-	33.0 mass parts	Mandatory

Process		
coating compositions were prepared by mixing the resin compositions and the other components using a high-speed dispenser.		
Experimental Activity		
Descriptor	Notes	Details
dynamic antifouling property	the antifouling coating compositions were applied to a blast plate previously coated with an antirust paint so that the dry film thickness was 300 μm, and the plate was left to dry for two days and nights indoors to obtain a test plate having an antifouling coating film at 6 months	5
dynamic antifouling property	the antifouling coating compositions were applied to a blast plate previously coated with an antirust paint so that the dry film thickness was 300 μm, and the plate was left to dry for two days and nights indoors to obtain a test plate having an antifouling coating film at 12 months	5
dynamic antifouling property	the antifouling coating compositions were applied to a blast plate previously coated with an antirust paint so that the dry film thickness was 300 μm, and the plate was left to dry for two days and nights indoors to obtain a test plate having an antifouling coating film at 18 months	5
dynamic antifouling property	the antifouling coating compositions were applied to a blast plate previously coated with an antirust paint so that the dry film thickness was 300 μm, and the plate was left to dry for two days and nights indoors to obtain a test plate having an antifouling coating film at 24 months	4
stationary stain resistance	the obtained test plate was attached to the side of a rotating cylinder, and a test was conducted for 24 months in which the test plate surface was rotated in natural seawater at about 10 knots per hour, and the adhesion area of marine organisms was determined and evaluated at 6 months	Adhesion area of marine organisms is 0% or more and less than 5%

提纲

— 案例详解

- 物质检索
- 反应检索



- ✓ 区域选择性的环内烯烃氧化反应
- ✓ 光催化的C-H 键氧化胺化

案例1：区域选择性反应

以烯烃的环氧化为例，精准筛选特定的区域选择性的环内烯烃氧化反应

CAS SciFinder Reactions Epoxidation of Alkene

Reactions search for "Epoxidation of Alkene" 1. 利用自然语言便捷检索“烯烃的环氧化”反应

References

We are displaying the most relevant results. Learn about result relevance. Load All Results

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Stereoselective (34K)

Solid-Supported Catalyst (6,078)

Regioselective (3,857)

Green Chemistry (3,176)

Chemoselective (2,757)

View All

Filtering: Reaction Notes: Regioselective X

3,857 Results

Group: By Scheme Sort: Yield View: Collapsed

Scheme 1 (38 Reactions) Steps: 1 Yield: 99-100%

Double bond geometry shown

Relative stereochemistry shown

Suppliers (110)

Suppliers (4)

Expand Scheme

Scheme 2 (7 Reactions) Steps: 1 Yield: 86-100%

Suppliers (58)

Suppliers (65)

2. 利用Reaction Notes 筛选区域选择性的反应结果

结构的二次筛选

3. 利用Search Within Results 二次筛选结构

Filtering: Search Within Results: Drawn Structure X Reaction Notes: Regioselective X Clear All Filters

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

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

Absolute stereochemistry shown

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 97%

Absolute stereochemistry shown, Rotation (-)

Expand Scheme

Search Within Results

Search for up to 3 structures within the result set.

Draw

Searching for... Clear All

Remove and Edit X

reactant



反应角色标记



不确定键

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: reactant、reagent或product中的一种

结构的二次筛选

精准筛选特定的区域选择性的环内烯烃氧化反应

CAS SciFinder Reactions Epoxidation of Alkene

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

Scheme 2 (1 Reaction)

Steps: 1 Yield: 96%

Absolute stereochemistry shown, Rotation (+)
Double bond geometry shown

Suppliers (14)

Expand Scheme

Scheme 3 (1 Reaction)

Relative stereochemistry shown

Expand Scheme



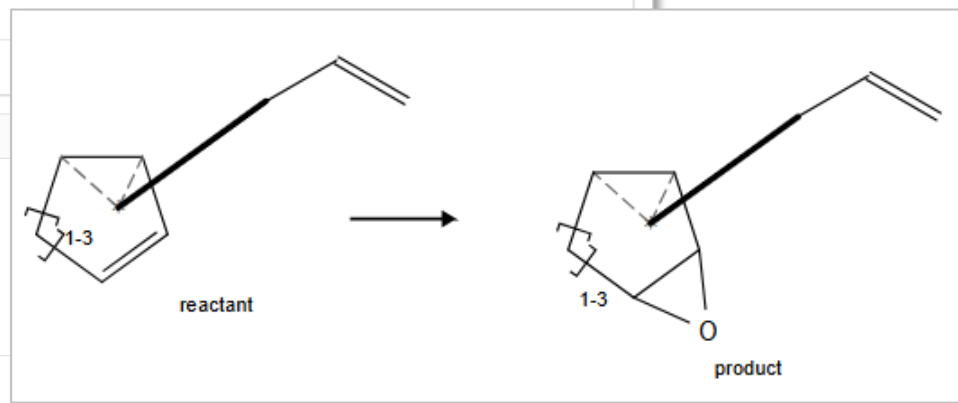
重复片段



取代位点可变



反应箭头



案例2：光催化的C-H 键氧化胺化

Reactions search for drawn structure

References

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

- ☐ Solid-Supported Catalyst (72)
- ☐ Green Chemistry-Catalyst (30)
- ☐ Green Chemistry (24)
- ☒ Photochemical (22)
- ☐ Regioselective (16)

View All

Number of Steps

Catalyst

Experimental Protocols

Non-Participating Functional Groups

Filtering: Reaction Notes: Photochemical X Reaction Mapping: Mapping Data Available X

22 Results Group: By Scheme Sort: Relevance

Scheme 1 (1 Reaction)

Chemical reaction scheme showing the synthesis of a tricyclic product from a benzylamine derivative and a pyridine derivative.

Suppliers (76) Suppliers (88) Suppliers (3)

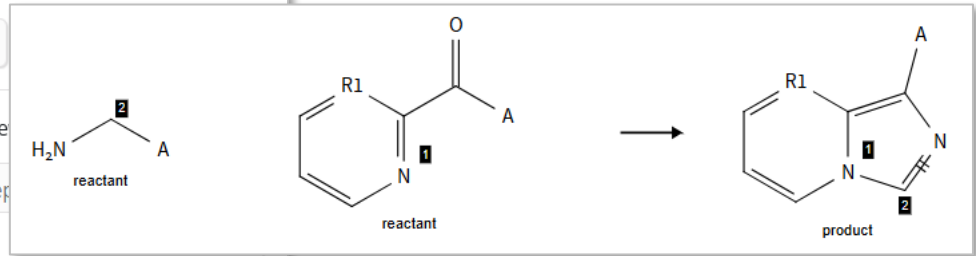
Expand Scheme

Scheme 2 (1 Reaction)

Chemical reaction scheme showing the synthesis of a tricyclic product from a pyridine derivative and a benzylamine derivative.

Suppliers (72) Suppliers (76)

Steps: 1 Yield: 94%



化学键标记



原子标记

总结

CAS SciFinder Discovery Platform 结构绘制面板及案例详解

结构绘制、导入及保存

- 多途径导入：快速上传文件、输入SMILES/InchI等字符串，或点击获得的物质结构导入
- 灵活绘制：从复杂的精确分子到片段、通式结构，省时省力开展各类物质/材料的调研
- 便捷保存：从模板存储到多格式的结构保存，轻松检索并获取论文配图

物质检索

- 精准定位：利用结构或文本-结构联合，灵活检索和筛选各类物质/材料
- 关联数据：一键高效获取物质的属性、谱学、生物学数据，相关的合成反应和文献

反应检索

- 便捷检索&灵活筛选：利用结构或自然语言检索反应，灵活锁定特定的反应类型

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

谢谢!

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