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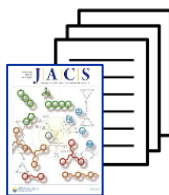
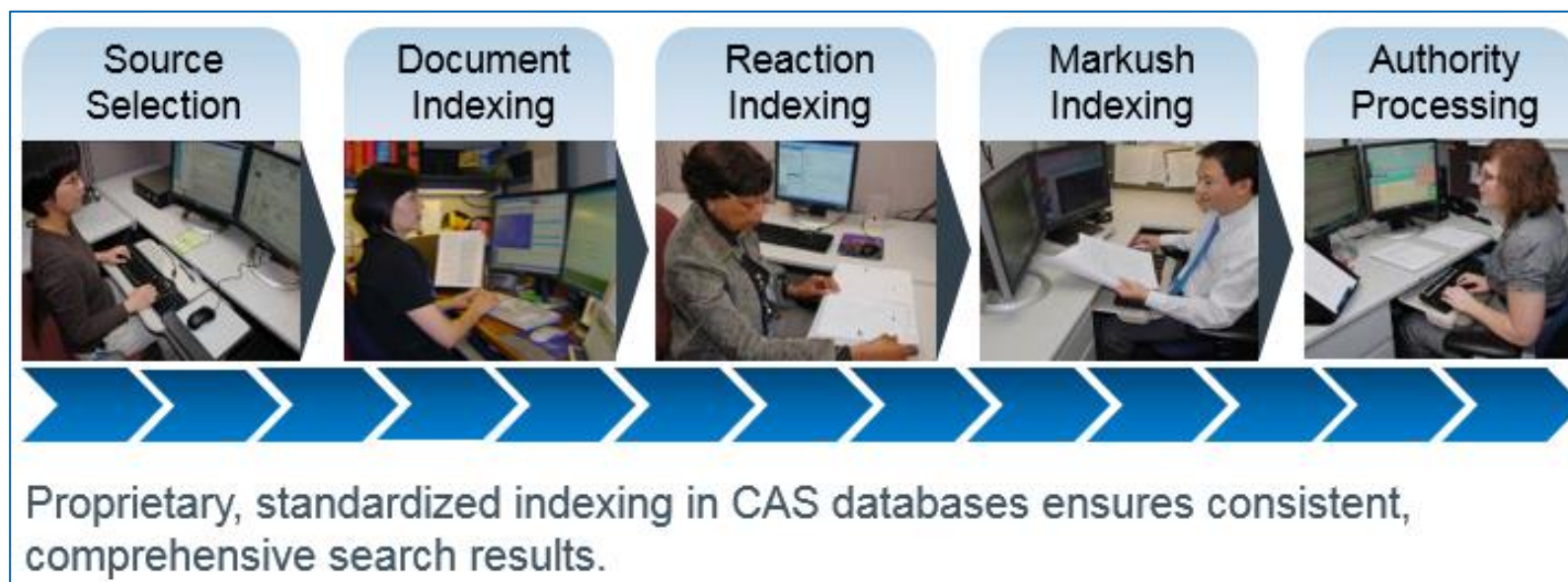
刘子露
ZLiu@acs-i.org
美国化学文摘社(CAS)北京代表处



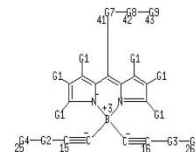
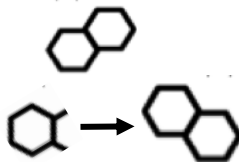
大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 序列检索*
- 常见问题及解答

CAS科学家的智力标引



1990
Smith, M.
anthracene



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

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Antitumor

AND Author Name Enter last name, first name middle name.

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February 8, 2023

References CSF-1R inhibitor (371K Results) 10:25 AM

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大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 生物序列检索*
- 常见问题及解答



文献检索

- 文献检索方法
 - 主题词的构建技巧
 - 利用高级检索项自定义组合检索
 - 间接检索：从物质、反应获得文献
- 检索策略推荐
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 - 关注物质有关的文献：先获得物质，再获得文献或文本+结构联合检索
 - 关注某科研人员的文献：作者名检索
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支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI

Searching for...

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

References

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

Seebeck

- Seebeck effect
- Seebeck coefficient
- Seebeck thermoelec. effect
- Seebeck thermoelectric effect
- Thermoelectric Seebeck effect
- Thermoelectric Seebeck coefficient

References

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seabeck

- Seebeck effect
- Seebeck coefficient
- Seebeck thermoelec. effect
- Seebeck thermoelectric effect
- Thermoelectric Seebeck effect
- Thermoelectric Seebeck coefficient

- 充分利用自动提示检索词
- 充分利用自动纠错功能
- 基于科学家创建的叙词表

使用布尔逻辑运算符，精准构建检索主题

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

The screenshot displays the 'References' search interface in CAS SciFinder-n. On the left, a sidebar titled 'Searching for...' lists various search categories: All, Substances, Reactions, References (highlighted in blue), Suppliers, Sequences, and Retrosynthesis. The main search area is titled 'References' and includes a search bar with the text 'Seebeck effect and "coordination polymer"'. Below the search bar, there is a dropdown menu set to 'AND' and an 'Author Name' field with the placeholder text 'Enter last name, first name middle name.' and an example 'Schubert, J A'. A '+ Add Advanced Search Field' button is visible below the author field. At the bottom, there is a 'Launch CAS Lexicon' button and a text box explaining that CAS Lexicon enables users to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.

CAS SciFinder-n Help

使用布尔逻辑运算符，精准构建检索主题

“crude oil” and “catalytic cracking” not “thermal cracking”
检索：原油裂解，排除热解

References search for ""crude oil" and catalytic cracking not "thermal cracking""

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior: Filter by Exclude

Document Type: Journal (675), Patent (542), Review (83), Conference (60), Report (3)

Language: English (434), Chinese (411), Undetermined (212), German (92), Russian (40)

Publication Year: 1930 to 2023

1,276 Results Sort: Relevance View: Partial Abstract

1
Catalytic cracking of crude oil to light olefins and naphtha: Experimental and kinetic modeling
By: Usman, Abdulhafiz; Siddiqui, M. Abdul Bari; Hussain, Abdelrahman; Aitani, Abdullah; Al-Khattaf, Sulaiman
Chemical Engineering Research and Design (2017), 120, 121-137 | Language: English, Database: CPlus

The direct **catalytic cracking** of three light **crude oils** have been evaluated over an equilibrated **FCC catalyst** (E-Cat) blended with MFI zeolite in a microactivity test unit at 550 °C and catalyst/oil ratio between 1 to 4. At 60% conversion, the Super Light (ASL) **crude oil** yielded about 10 weight% C₂-C₄ olefins and 60 weight% naphtha over E-Cat. Extra Light (AXL) **crude oil** yielded 13 weight% light olefins and 52 weight% naphtha, while for Arab Light (AL) **crude oil**, light olefins and naphtha produced were 12 and 51 weight%, resp. The addition of MFI with varying Si/Al molar ratio (Z30, Z280 and Z...

Full Text Substances (2) Reactions (0) Citing (47) Citation Map

2
Catalytic Cracking of Arab Super Light Crude Oil to Light Olefins: An Experimental and Kinetic Study
By: Al-Khattaf, Sulaiman S.; Ali, Syed A.
Energy & Fuels (2018), 32(2), 2234-2244 | Language: English, Database: CPlus

Catalytic cracking of Arab Super Light (ASL) **crude oil** (containing 46.1 wt % naphtha-range fraction) was studied over zeolite Y- and MFI-based (Z-Cat) catalysts at 500-575 °C. Experiments were conducted in a riser simulator by varying the residence times from 1 to 10 s. ASL **crude oil** and the cracked products were divided into heavy fraction, naphtha, and C₂-C₄ gases. Exptl. results showed that

(Nickel or Ni) and "crude oil" and "catalytic cracking"
检索：与镍、及原油裂解相关

References search for "(nickel or Ni) and "crude oil" and "catalytic cracking""

Substances Reactions Citing Knowledge Graph Save and Alert

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
Learn about result relevance.
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88 Results Sort: Relevance View: Partial Abstract

1
Microwave-assisted nickel and vanadium removal from crude oil
By: Shang, Hui; Liu, Yu; Shi, Jin-Chun; Shi, Quan; Zhang, Wen-Hui
Fuel Processing Technology (2016), 142, 250-257 | Language: English, Database: CPlus

Most **crude oils** contain traces of metal complexes, among which vanadium (V) and **nickel (Ni)** compounds are the most harmful poisons to the **catalysts** of **fluid catalytic cracking** (FCC) and hydrogenation units. These metals are proven to be extremely hard to remove, since they exist in **crude oil** as stable oil-soluble complexes. The microwave technol. provides a new way for **Ni/V** removal, their removal efficiency using chem. reagents and the mechanism of microwave-assisted demetallization were studied in this paper. It was concluded that the demetallization efficiency can be highly enhanced under mi...

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Full Text Substances (7) Reactions (0) Citing (39) Citation Map

2
Fluid catalytic cracking: recent developments on the grand old lady of zeolite catalysis
By: Vogt, E. T. C.; Weckhuysen, B. M.
Chemical Society Reviews (2015), 44(20), 7342-7370 | Language: English, Database: CPlus and MEDLINE

A review. **Fluid catalytic cracking** (FCC) is one of the major conversion technologies in the oil refinery industry. FCC currently produces the majority of the world's gasoline, as well as an important fraction of propylene for the polymer industry. In this critical review, we give an overview of the latest trends in this field of research. These trends include ways to make it possible to process either very heavy or very light **crude oil** fractions as well as to

高级检索—高效实现多项自定义组合检索

The screenshot shows the CAS search interface. On the left, there is a sidebar with search categories: All, Substances, Reactions, References (highlighted), Suppliers, Sequences, and Retrosynthesis. The main search area is titled 'References' and contains a search bar with the query: "crude oil" and "catalytic cracking" not "thermal cracking". Below the search bar, there is a dropdown menu for 'Publication Name' with a search input field containing 'ACS Ca'. A list of suggestions is shown, including 'ACS Catalysis', 'ACS case reviews in surgery', 'ACS Case Rev Surg', 'ACS Catal.', 'ACS Applied Materials & Interfaces', 'ACS Nano', and 'Abstracts of Papers, 221st ACS National Meeting, San Diego, CA, United St...'. The interface also includes logical operators (AND, OR, NOT) and a 'Draw' button.

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* 检索方法可单独使用，也可联用

CAS Lexicon—利用词库选词启发检索

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers
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- Retrosynthesis

References

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

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- Narrower Terms
- Broader Terms
- Related Terms

Search CAS Lexicon

Seebeck effect Your Query

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

^ Preferred Term

- Seebeck effect

This will search synonyms: Seebeck coefficient; Seebeck thermoelec. effect; Seebeck thermoelectric effect; Thermoelectric Seebeck coefficient; Thermoelectric Seebeck effect

[View fewer synonyms](#)

^ Broader Terms (1)

- Thermoelectricity

^ Related Terms (3)

- joule effect
- Peltier effect
- Thermocouples

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

Seebeck effect

Seebeck effect - Related Terms (3 Concepts)

Thermoelectricity

文献结果集—排序与筛选

- 聚类筛选项一目了然
- 直接勾选高效定位所需信息
- 无需逐步二次检索和限定

文献类型
文献语言
研究发展趋势
作者
发表机构
发表年份
CAS标引的技术术语
CAS标引的学科研究方向

二次检索
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References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph Save and Alert

687 Results 知识图谱 Sort: Relevance View: Partial Abstract

1

High-Performance Flexible All-Solid-State Supercapacitor from Layered PEDOT/PSS Films
By: Liu, Yuqing; Weng, Bo; Razal, Joselito M.; Xu, Qun; Zhao, Chen; Hou, Yuyang; Seyedin, G.; Chen, Jun
Scientific Reports (2015), 5, 17045 | Language: English, Database: CAPlus and MEDLINE

Although great attention has been paid to **wearable electronic devices** in recent years, flexible lightweight batteries or supercapacitors with high performance are still not readily available due to the limitations of the flexible electrode inventory. In this work, highly flexible, bendable and conductive rGO-**PEDOT**/PSS films were prepared using a simple bar-coating method. The assembled device using rGO-**PEDOT**/PSS electrode could be bent and rolled up without any decrease in electrochem. performance. A relatively high areal capacitance of 448 mF cm⁻² was achieved at a scan rate of 10 mV s⁻¹ usin...

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Full Text Substances (13) Reactions (0) Citing (173) Citation Map

2

Highly stretchable multilayer electronic circuits using biphasic gallium-indium
By: Liu, Shanliangzi; Shah, Dylan S.; Kramer-Bottiglio, Rebecca
Nature Materials (2021), 20(6), 851-858 | Language: English, Database: CAPlus and MEDLINE

Stretchable electronic circuits are critical for soft robots, **wearable technologies** and biomedical applications. Development of sophisticated stretchable circuits requires new materials with stable conductivity over large strains, and low-resistance interfaces between soft and conventional (rigid) electronic components. To address this need, we introduce biphasic Ga-In, a printable conductor with high conductivity (2.06 x 10⁶ S m⁻¹), extreme stretchability (>1,000%), negligible resistance change when strained, cyclic stability (consistent performance over 1,500 cycles) and a reliable interf...

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Full Text Substances (17) Reactions (0) Citing (91) Citation Map

3

A self-powered skin-patch electrochromic biosensor
By: Santiago-Malagon, Sara; Rio-Colin, Diego; Azizkhani, Haniyeh; Aller-Pellitero, Miguel; Guirado, Gonzalo; del Campo, F. Javier
Biosensors & Bioelectronics (2021), 175, 112879 | Language: English, Database: CAPlus and MEDLINE
| Analytical Methods

One of the limitations of many skin-patch wearable sensors today is their dependence on silicon-based electronics, increasing their complexity and unit cost. Self-powered sensors, in combination with electrochromic materials, allow simplifying the construction of

排序方式：
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CAS标引的学科研究方向

CA Section 通过CA Section 纵览并定位学科研究方向 ×

By Count **Alphanumeric**

6 Selected

<input type="checkbox"/> Electrochemical, Radiational, and Thermal Energy Technology (210)	<input type="checkbox"/> Inorganic Analytical Chemistry (5)	<input type="checkbox"/> Physical Organic Chemistry (2)
<input checked="" type="checkbox"/> Electric Phenomena (169)	<input type="checkbox"/> Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes (5)	<input type="checkbox"/> Thermodynamics, Thermochemistry, and Thermal Properties (2)
<input checked="" type="checkbox"/> Biochemical Methods (83)	<input checked="" type="checkbox"/> Surface Chemistry and Colloids (5)	<input type="checkbox"/> Unit Operations and Processes (2)
<input type="checkbox"/> Textiles and Fibers (55)	<input type="checkbox"/> Synthetic Elastomers and Natural Rubber (4)	<input type="checkbox"/> Apparatus and Plant Equipment (1)
<input type="checkbox"/> Plastics Fabrication and Uses (52)	<input type="checkbox"/> Air Pollution and Industrial Hygiene (3)	<input type="checkbox"/> Cement, Concrete, and Related Building Materials (1)
<input checked="" type="checkbox"/> Pharmaceuticals (22)	<input type="checkbox"/> Chemistry of Synthetic High Polymers (3)	<input type="checkbox"/> Food and Feed Chemistry (1)
<input type="checkbox"/> Plastics Manufacture and Processing (20)	<input checked="" type="checkbox"/> Magnetic Phenomena (3)	<input type="checkbox"/> Nonferrous Metals and Alloys (1)
<input type="checkbox"/> Optical, Electron, and Mass Spectroscopy and Other Related Properties (18)	<input type="checkbox"/> Coatings, Inks, and Related Products (2)	<input type="checkbox"/> Pharmacology (1)
<input type="checkbox"/> Unavailable (8)		<input type="checkbox"/> Toxicology (1)
<input checked="" type="checkbox"/> Electrochemistry (7)		<input type="checkbox"/> Water (1)

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文献结果集—聚类筛选Concept

Concept **通过Concept纵览并精准定位核心研究点**

Top Count Alphanumeric Search

7 Selected

<input type="checkbox"/> Wearable devices (501)	<input checked="" type="checkbox"/> Current density (50)	<input checked="" type="checkbox"/> Coating materials (30)
<input type="checkbox"/> Fluoropolymers (343)	<input checked="" type="checkbox"/> Hydrogels (50)	<input type="checkbox"/> Electrolytes (29)
<input type="checkbox"/> Electric conductivity (155)	<input type="checkbox"/> Humans (48)	<input type="checkbox"/> Sheet resistance (29)
<input type="checkbox"/> Electrodes (128)	<input type="checkbox"/> Polymers (48)	<input type="checkbox"/> Surface area (29)
<input checked="" type="checkbox"/> Surface structure (124)	<input type="checkbox"/> Carbon black (47)	<input checked="" type="checkbox"/> Skin (28)
<input type="checkbox"/> Homo sapiens (117)	<input type="checkbox"/> Electronics (47)	<input type="checkbox"/> Supercapacitor electrodes (28)
<input type="checkbox"/> Human (117)	<input checked="" type="checkbox"/> Nanowires (47)	<input type="checkbox"/> Cyclic voltammetry (27)
<input type="checkbox"/> Nanofibers (101)	<input type="checkbox"/> Electric capacitance (45)	<input type="checkbox"/> Dielectric loss (26)
<input type="checkbox"/> Electric current-potential relationship (100)	<input type="checkbox"/> Piezoelectric materials (44)	<input type="checkbox"/> Energy storage systems (26)
<input type="checkbox"/> Polyesters (92)	<input type="checkbox"/> Electric potential (41)	<input type="checkbox"/> Lithium-ion secondary batteries (26)
<input type="checkbox"/> Carbon nanotubes (86)	<input type="checkbox"/> Electronic device fabrication (40)	<input type="checkbox"/> Plastic films (26)
<input checked="" type="checkbox"/> Flexibility (84)	<input type="checkbox"/> Electronic device fabrication (40)	<input type="checkbox"/> Strain (26)
<input type="checkbox"/> Stress-strain relationship (83)	<input type="checkbox"/> Triboelectric nanogenerators (40)	<input type="checkbox"/> Surface roughness (26)
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Concept **通过Search精准定位感兴趣的核心研究点**

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Concept Name

nano* Search

17 Selected

<input checked="" type="checkbox"/> Carbon nanofibers (14)	<input type="checkbox"/> Nanofibril (2)	<input checked="" type="checkbox"/> Nanosheets (23)
<input type="checkbox"/> Carbon nanotube fibers (4)	<input checked="" type="checkbox"/> Nanofilms (6)	<input checked="" type="checkbox"/> Nanospheres (1)
<input checked="" type="checkbox"/> Carbon nanotubes (86)	<input type="checkbox"/> Nanofilters (1)	<input type="checkbox"/> Nanostructured materials (9)
<input type="checkbox"/> Cellulosic nanofibers (1)	<input checked="" type="checkbox"/> Nanoflakes (2)	<input type="checkbox"/> Nanostructures (18)
<input checked="" type="checkbox"/> Core-shell nanoparticles (1)	<input type="checkbox"/> Nanoflowers (2)	<input type="checkbox"/> Nanotechnology (4)
<input type="checkbox"/> Electric nanogenerators (24)	<input type="checkbox"/> Nanohorns (1)	<input type="checkbox"/> Nanotubes (12)
<input checked="" type="checkbox"/> Metal Nanoparticles (3)	<input type="checkbox"/> Nanoimprint lithography (1)	<input type="checkbox"/> Nanotubes, Carbon (11)
<input type="checkbox"/> Nanoantennas (1)	<input type="checkbox"/> Nanoparticles (53)	<input checked="" type="checkbox"/> Nanowires (47)
<input type="checkbox"/> Nanocoils (2)	<input type="checkbox"/> Nanoparticle size distribution (2)	<input type="checkbox"/> Pharmaceutical nanocarriers (1)
<input checked="" type="checkbox"/> Nanocomposites (63)	<input type="checkbox"/> Nanoplatelets (3)	<input type="checkbox"/> Pharmaceutical nanocomposites (2)
<input type="checkbox"/> Nanocrystals (4)		

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文献结果集—保存及下载

References search for "(PVDF or PEDOT) and "wearable device""

Substances Reactions Citing Knowledge Graph

Filtering: Concept: Hydrogels X
Excluding: Search Within Results: dop* X

41 Results Sort: Relevance View: Partial Abstract

1

Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE
By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun
ACS Applied Materials & Interfaces (2022), 14(40), 45853-45868 | Language: English, Database: CAlplus and MEDLINE

Conductive hydrogels have attracted attention because of their wide application in wearable devices. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluori...

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Full Text Substances (7) Reaction (1) Citing (1) Citation Map

2

Antifreeze and moisturizing high conductivity PEDOT/PVA hydrogels for wearable motion sensor
By: Peng, Yinjie; Yan, Bin; Li, Yueshan; Lan, Ji; Shi, Lingying; Ran, Rong
Journal of Materials Science (2020), 55(3), 1280-1291 | Language: English, Database: CAlplus

Conductive hydrogel has shown significant promise in the field of wearable devices. However, the mediocre antifreezing property and relatively low strain sensitivity limit the application of these gels. Herein, we developed a multifunctional hydrogel sensor based on a polyvinyl alc. substrate with poly(3,4-ethylenedioxythiophene) as the conductive filler and a glycerin/water component solvent as the dispersion medium. The resulting optimal sample exhibits attractive combination of high tensile stress (~ 1.0 MPa), large elongation (> 400%), reasonable conductivity (~ 3.5 S m⁻¹), while the el...

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Full Text Substances (5) Reaction (1) Citing (40) Citation Map

3

High-Stretchability, Ultralow-Hysteresis ConductingPolymer Hydrogel Strain Sensors for Soft Machines
By: Shen, Zegun; Zhang, Zhilin; Zhang, Ningbin; Li, Jinhao; Zhou, Peiwei; Hu, Fagui; Peng, Yur; Lu, Baoyang; Gu, Guoqing

Save Results and Create Alert

Name: EGFR

Save Options:
 Query Only
 Selected Answers
 All Answers (Up to 20,000)

Alert Frequency:
 No Alerts
 As Available
 Weekly
 Monthly

Add Existing Tags (Optional): No tags defined

New Tag (Optional): Pharm Tag Color: Light Green

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Enhancing Strain-Sensing Properties of the Conductive Hydrogel by Introducing PVDF-TrFE

Substances (7) Reaction (1) Citing (1) Citation Map

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ACS Applied Materials & Interfaces
Volume: 14
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Pages: 45853-45868
Journal: Article
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CODEN: AAMICK
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Database Information
AN: 2022:2510278
CAN: 180:208379
PubMed ID: 36170495
CAPUS and MEDLINE

Company/Organization
School of Materials Science and Engineering
North University of China
Taiyuan 030051
China

Publisher
American Chemical Society

Language
English

By: Hu, Zhirui; Li, Jie; Wei, Xiaotong; Wang, Chen; Cao, Yang; Gao, Zhiqiang; Han, Jing; Li, Yingchun

Conductive hydrogels have attracted attention because of their wide application in **wearable devices**. However, it is still a challenge to achieve conductive hydrogels with high sensitivity and wide frequency band response for smart wearable strain sensors. Here, we report a composite hydrogel with piezoresistive and piezoelec. sensing for flexible strain sensors. The composite hydrogel consists of cross-linked chitosan quaternary ammonium salt (CHACC) as the hydrogel matrix, poly(3,4-ethylenedioxythiophene);poly(styrenesulfonate) (PEDOT: PSS) as the conductive filler, and poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) as the piezoelec. filler. A one-pot thermoforming and solution exchange method was used to synthesize the CHACC/PEDOT: PSS/PVDF-TrFE hydrogel. The hydrogel-based strain sensor exhibits high sensitivity (GF: 19.3), fast response (response time: 63.2 ms), and wide frequency range (response frequency: 5-25 Hz), while maintaining excellent mech. properties (elongation at break up to 293%). It can be concluded that enhanced strain-sensing properties of the hydrogel are contributed to both greater change in the relative resistance under stress and wider response to dynamic and static stimulus by adding PVDF-TrFE. This has a broad application in monitoring human motion, detecting subtle movements, and identifying object contours and a hydrogel-based array sensor. This work provides an insight into the design of composite hydrogels based on piezoelec. and piezoresistive sensing with applications for wearable sensors.



Keywords: conductive hydrogel wearable strain piezoelec sensor; composite hydrogels; fast response; high sensitivity; piezoresistive and piezoelectric sensation; wearable sensors

View Source Full Text

Expand All | Collapse All

- Concepts
- Substances**
- Cited Documents

CAS科学家提供的标准技术术语

Electric resistance	Polythiophenes Role: Properties; Technical or Engineered Material Use
Elongation at break	Strain sensors
Hydrogels	Stress-strain relationship
Open circuit potential	Tensile strength
Piezoelectric sensors	Wearable devices

原文中重点研究的物质信息

Substances (7)

2839834-68-1

106602-18-0
Image Not Available



(C₃H₅ClO.Unspecified)_x

Role: Properties, Synthetic Preparation, Preparation

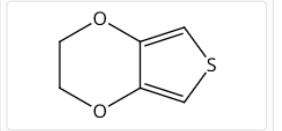
1219717-04-0

Image Not Available

Unspecified
Clevios PH 570

Role: Properties, Technical or Engineered Material Use, Uses

126213-51-2



(C₆H₆O₂S)_x
Poly(3,4-ethylenedioxythiophene)

Role: Properties, Technical or Engineered Material Use, Uses

Notes: polystyrenesulfonate-doped

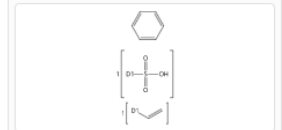
106602-18-0

Image Not Available

Unspecified
N-[2-Hydroxy-3-(trimethyl ammonium)propyl]chitosan chloride

Role: Reactant, Reactant or Reagent

50851-57-5

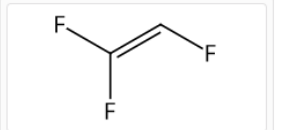


(C₈H₈O₃S)_x
Poly(styrenesulfonic acid)

Role: Properties, Technical or Engineered Material Use, Uses

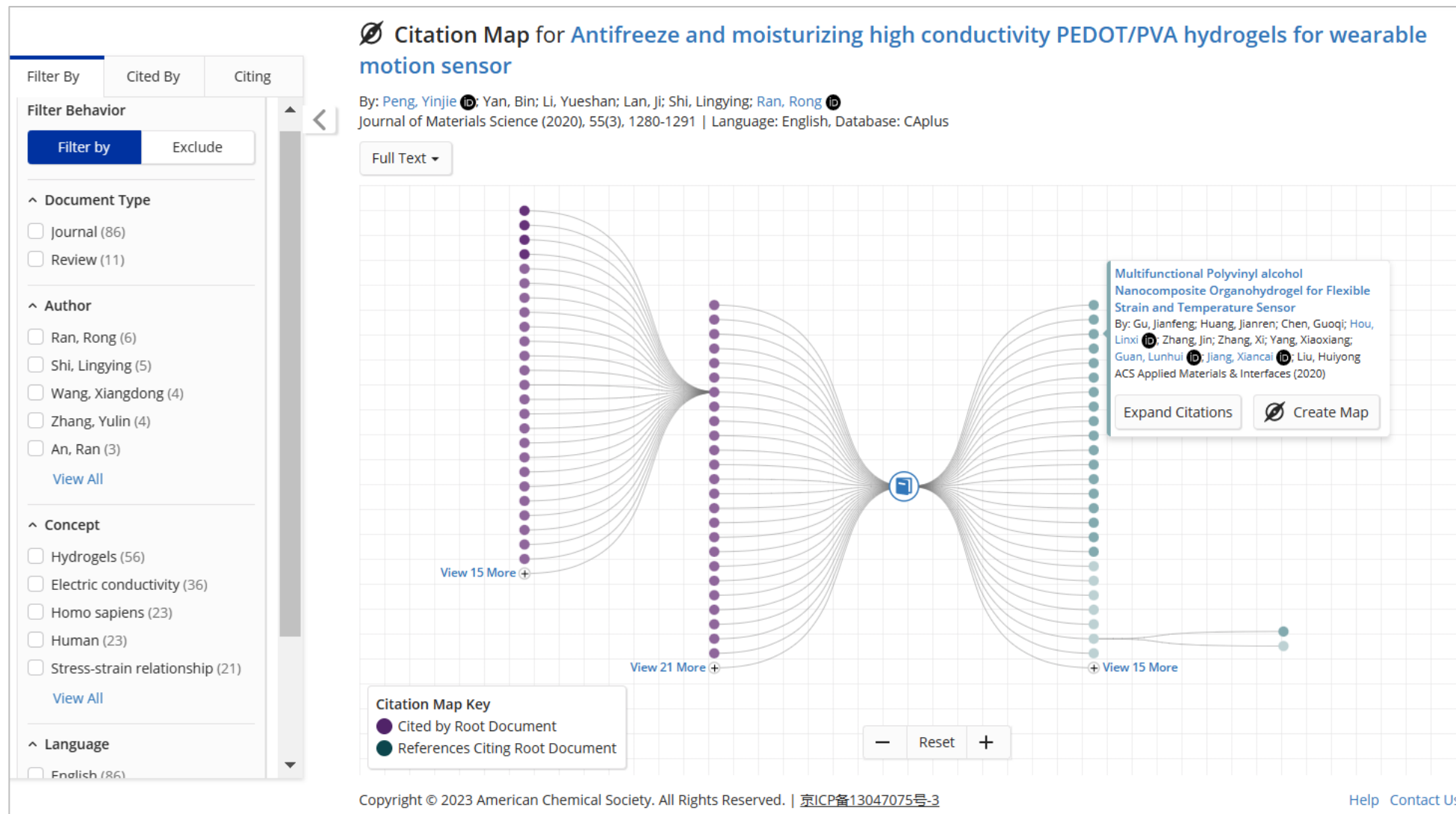
Notes: PEDOT dopant

28960-88-5



物质角色

文献详情—引文地图



引文地图：

- 获取前向引文
- 获取后向引文
- 可通过聚类选项筛选引文

文献检索—主题词+结构联合检索

The screenshot shows the CAS SciFinder interface. At the top, the search query is "petroleum and fluid catalytic cracking". A chemical structure of benzene is overlaid on the search bar. The left sidebar shows "Structure Match" with "As Drawn (130)" selected. Below it, "Filter Behavior" has "Filter by" selected. Under "Document Type", "Journal (74)", "Patent (56)", and "Review (2)" are listed. The "Substance Role" filter is expanded, showing "Preparation (53)", "Uses (42)", "Process (28)", and "Properties (16)". The main results area shows 130 results, sorted by "Publication Date: Newest". The first result is "Conversion of light cycle oil to benzene and alkylated monoaromatics over monometallic and bimetallic CoMo catalysts in the presence of hydrogen donor" by Ramteke, Akshata Vijay; Bhatia, Divesh; Pant, K. K. (2023). The abstract mentions "fluid catalytic cracking".

物质在文献中的研究角色

The "Substance Role" dialog box is shown, allowing selection of roles for the search results. The "By Count" tab is active. The following roles are selected:

- Process (28)
- Industrial Manufacture (27)
- Synthetic Preparation (19)
- Analyte (8)

The following roles are not selected:

- Preparation (53)
- Uses (42)
- Physical, Engineering, or Chemical Process (28)
- Other Use, Unclassified (21)
- Technical or Engineered Material Use (18)
- Properties (16)
- Formation, Non-preparative (13)
- Formation, Unclassified (11)
- Analytical Study (9)
- Occurrence (9)
- Purification or Recovery (8)
- Reactant (8)

Buttons for "Apply" and "Cancel" are at the bottom.

查看Chemzent 来源的文献

- ChemZent是最古老的德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案
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References search for "enzyme and reduction" + drawn structure

Substances Reactions Citing Knowledge Graph Save and Alert

Structure Match: As Drawn (0), Substructure (8,881)

Filter Behavior: Filter by Exclude

Document Type Language Publication Year Available at My Institution Author Publication Name Concept

Database: CAPus (8,605), MEDLINE (6,814), **CHEMZENT (31)**

Search Within Results

Filter Content Report: Download filter data from this result set

Filtering: Database: CHEMZENT 31 Results Sort: Relevance View: Partial Abstract

1

Fabric change of CARB azole in rats and rabbit
By: Johns, S. R.; Wright, S. E.
Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

Machine Translated: After administration of carbazoles is 3-hydroxy carbazole, conjugate with glucuronic acid in the urine separated Hauptstoffwechselprod. in rats and rabbits. The hydroxylation in 3-position is in accordance with the etching oxidizing **enzymes** at the position of greatest electron density. For the investigation of werden carbazole-14 C is used. Experiments: 14C-carbazole (I), Melting Point 242-244 ° (from benzene) by diazotization and **reduction** of 14C-aniline to 14C-phenylhydrazine (240-245 ° F.) with cyclohexanone in 14C-tetrahydrocarbazole is converted. Dehydrogenation to Pd-C gives I. Respect m...

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ChemZent Full Text Substances (14) Reactions (0) Citing (0) Citation Map

2

Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors
By: Ghambeer, R. K.; Blakley, R. L.
Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

Machine Translated: Hysic. Res. common. 20 (1965) 20. — the content of ribo nucleoside triphosphate reductase (I) in extracts of L. leichmanii depends on the age of the culture. During the linear growth if I-Geh. with increasing age up to the end of the linear phase on and falls then. Extracts from stationary cells exhibit no significant I-Aktivität. The rapid I-Synth. during the linear growth by chloramphenicol and ActinomycinD inhibited. The decrease of I-Geh. after completion of the linear growth is based not on the presence one increased amount protobact. **Enzymes** nor on incomplete release of said **enzymes**. The

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ChemZent Full Text Substances (3) Reactions (0) Citing (0) Citation Map

3

Nr. 5-1559 E-6. Pharmakologie, Therapie, Toxikologie, Hygiene 1966

68-74, 1963; Washington, D.C., George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninanalogen Purin-antimetaboliten 4-Aminopyrazolopyrimidin (I) verursachte bei Mäusen einen Anstieg der Gesamtleberlipide innerhalb 24 Std. auf das 3-4fache. Hierin waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid-(III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von ¹⁴C₁₁-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. ¹⁴C₁₁-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von ¹⁴C₁₁-Orotosäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von ¹⁴C₁₁-Glycin in Leber- u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. VI. schließt aus den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber bemmt. H. Zöllner 4607

1559 Stoffwechsel des Carbazols in Ratten und Kaninchen. S. R. Johns und S. E. Wright. (J. med. Chem. 7, 158-161, 1964; Sydney, Univ. of Sydney, Dep. of Pharmacy; engl.) — Nach Gabe von Carbazol 25 3-Hydroxycarbazol, konjugiert mit Glucuronsäure, das im Harn verschiedene Hauptstoffwechselprod. bei Ratten u. Kaninchen. Die Hydroxylierung in 3-Stellung ist in Übereinstimmung mit dem Angriff oxydierender Enzyme an der Stellung mit der größten Elektronendichte. Für die Unters. wurde Carbazol-¹⁴C verwendet.

Versuche: ¹⁴C-Carbazol (I), F. 242-244° (aus Bel.) durch Diazotierung u. Red. von ¹⁴C-Anilin zu ¹⁴C-Phenylhydrazinhydrochlorid (F. 240-245°), das mit Cyclohexanon in ¹⁴C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellte Bezugs-substanzen: 1-Hydroxycarbazol, F. 160-162° durch Cyclisierung von Cyclohexan-1,2-dionmonophenylhydrazon (F. 183-185°) in äthanol. Essigsäure über 1.2.3.4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. 3-Hydroxycarbazol (II), F. 260-261° über folgende Stufen: p-Methoxyphenylhydrazinhydrochlorid (III), F. 198-200° (aus A.) durch Diazotierung u. Red. von p-Anisidin. — 6-Methoxy-1,2,3,4-tetrahydrocarbazol (IV), C₁₃H₁₇NO, F. 94-95° (aus A.), durch Rk. von III mit Cyclohexanon in wss. Essigsäure (50%ig) bei Ggw. von Natriumacetat. 3-Methoxycarbazol (V) C₁₃H₁₇NO,

N-Butyl-, Äthobromid, DL₅₀ 38.4, Curarisierungswirk., 30,7, cholinolyt. Aktivität, 0,04; N-Cyclohexyl-, Äthobromid, 33,5/28/0,02; N-Phenyl-, Äthobromid, 17,5/20/0,09; N-Phenyl-, Benzylbromid, 11/13/0,14; N-β-Phenäthyl-, Äthobromid, 21/22/0,1, N-Octyl-, Äthobromid, 6,8/6,7/1,5; Lauryl-, Äthobromid, 21,5/12,6/16; N-Butyl-, Hydrochlorid, 115/-/0,02; N-Cyclohexyl-, HCl, 75/-/0,02; N-Phenyl-, HCl, 47,5/-/cholinerg.; N-β-Phenäthyl-, HCl, 60/-/0,03; N-Octyl-, HCl, 47/-/0,5; N-Lauryl-, HCl, 37,5/-/1,5; N,N-dialkylcarbaminsäure-β-diäthylaminoäthylester, Äthobromide: diäthyl-, DL₅₀ 26, Curarisierungswirk., 26, spasmolyt. Aktivität, 50 (Papaverin = 100), 0,05 (I = 100), Antihistaminaktivität, — (Promethazin = 100); dibutyl-, 8/11/2100/6/4,3; dicyclohexyl-, 2,2/4,8/2300/2,4/0,05; Diphenyl-, 9,5/11,6/310/0,13/0,03; Di-[β-phenäthyl]-, 6,5/6,5/570/0,38/0,07; Dibutyl-, Benzylbromid, 7,5/5,5/200/0,11/-; Carbazol(II), Äthobromid, 3,3/4,6/730/0,28/0,20; Acridin (III), Äthobromid, 5,8/4,5/770/0,6/0,20; Phenozasin (IV), Äthobromid, 4,0/5,3/1400/1,3/0,5; Phenothiazin (V), Äthobromid, 3,0/4,6/6000/8,0/5,0; Hydrochloride: Dibutyl-, 38/-/1000/3,0/3,0; Dicyclohexyl-, 22/-/1130/2,4/0,1; Diphenyl-, 42,5/-/770/4,5/0,1; Di-[β-phenäthyl]-, 10,3/-/400/0,14/0,2; II, 20/-/280/0,1/0,3; III, 35/-/1800/1/1; IV, 24,5/-/770/0,8/1; V, 25/-/12 000/16/30.

K. Maier 4607

1561 Wirkung von Chlorcyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen. Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therapeut. 148, 192-98, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — VI. untersuchten verschiedene Substanzen mit bekannter Wirkg. auf die Lebermikrosomen-Enzymsyst. auf deren Wirkg. auf die Toxizität einiger Organophosphatsektizide an Mäusen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit Chlorcyclizin (I), Phenobarbital (II), SKF-525A (α,α-Diphenyl-α-propyl-essigsäure-β-diäthylaminoäthylester - HCl; III) oder Cyclizin zeigte einen deutlichen Schutz gegen die Toxizität von Malathion, Parathion (IV) u. EPN (p-Nitrophenylthionbenzolphosphordureäthylester). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL₅₀ von Paraoxon (V), TEPPE (Tetraäthylpyrophosphat) u. Physostigmin. Eine s.c.-Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-Paraoxonase (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI. I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um

专利文献详情

PatentPak:

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References search for "petroleum and "fluid catalytic cracking"" + drawn structure

Substances | Reactions | Citing | Knowledge Graph

Structure Match: As Drawn (130), Substructure (440)

Filtering: Document Type: Patent, Language: English

29 Results | Sort: Relevance | View: Partial Abstract

Method for the conversion of feedstock containing naphtha to low carbon olefins and aromatics

By: Zhao, Yinfeng; Ye, Mao; Liu, Zhongmin; Tang, Hailong; Wang, Jing; Zhang, Jinling; Zhang, Tao; Al-Shammari, Talal Khaled
World Intellectual Property Organization, WO2020157540 A1 2020-08-06 | Language: English, Database: CAplus

Disclosed is a method for producing low carbon olefins and/or aromatics from feedstock comprising naphtha. The method can include the following steps: a) feeding feedstock comprising naphtha into a fast fluidized bed reactor; b) contacting the feedstock with a catalyst under conditions to produce a gas product and spent catalyst; c) separating the gas product to produce a stream comprising primarily one or more low carbon olefins and/or one or more aromatics; d) transporting the spent catalyst to a regenerator; e) regenerating the spent catalyst in the regenerator to form regenerated catalyst;...

PatentPak | Full Text | Substances (5) | Reactions (0) | Citing (0) | Citation Map

Patent	Language	Kind Code	PatentPak Options
WO2020157540	English	A1	PDF PDF+ Viewer
CN113366089	Chinese	A	PDF
US20220119717	English	A1	PDF

CAS PatentPak

Key Substances in Patent

- CAS RN 74-85-1
- CAS RN 115-07-1
- CAS RN 106-99-0
- CAS RN 71-43-2
- CAS RN 108-88-3

separating, by the stripper, the effluent into the spent catalyst and the gas product; flowing the gas product into a separation system to obtain a stream comprising one or more low carbon olefins and/or one or more aromatics; transporting the spent catalyst into the stripper; transporting the spent catalyst from the fluidized bed reactor through a stripper to a stripper inclined pipe and then to a regenerator riser; lifting, by gas, the spent catalyst through the regenerator riser into the regenerator; and returning the regenerated catalyst to the fast-fluidized bed reactor via a stripping section of the regenerator and a regenerator inclined pipe.

13. The method of any of claims 1 to 12, wherein, in the gas product, yield of low carbon olefins is in a range of 38 to 47 wt. %, yield of aromatics is in a range of 15 to 20 wt. % and yield of methane is in a range of 7 wt. % to 8 wt. %.

16

WO 2020/157540 | PCT/IB2019/050689

14. The method of any of claims 1 to 13, wherein the one or more low carbon olefins is a selection of the list consisting of: ethylene, propylene, and butadiene.

CAS RN 106-99-0

CAS Name 1,3-Butadiene

C=CC=C

Get Substance Details | Get Bioactivity Data | Get Reactions (25K) | Synthesize (3,153) | Start Retrosynthetic Analysis | Get References (61K) | Get Suppliers (71)

Edit Structure | Reset

文献检索小结

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

物质检索

- 物质检索方法
 - 物质标识符、文献标识符检索
 - 分子式、物性参数、谱图数据检索
 - 结构式检索
- 检索策略推荐
 - 有机化合物，金属配合物，天然产物：结构检索
 - 无机物，合金：分子式检索
 - 高分子化合物：分子式检索和结构检索

物质检索

- 通过物质标识符、文献标识符检索物质

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Sequences
- 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

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- 使用结构绘制面板进行结构检索

- 高级检索

物质检索—物质名称、CAS RN、代码

The screenshot displays the CAS SciFinder search results page. At the top, the search bar contains 'Paxlovid 2628280-40-8'. Below the search bar, there are tabs for 'References', 'Reactions', and 'Suppliers'. The left sidebar shows filter options under 'Filter Behavior', including 'Reaction Role' (Product, Reactant), 'Reference Role' (Adverse Effect, Analyte, Analytical Study, Biological Study), 'Commercial Availability', 'Number of Components', and 'Molecular Weight'. The main content area shows two results. The first result is for CAS RN 2628280-40-8, with a chemical structure and the text 'Absolute stereochemistry shown'. Below the structure, the formula $C_{23}H_{32}F_3N_5O_4$ and the name '3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...]' are visible. At the bottom of this result, there are buttons for '319 References', '106 Reactions', and '39 Suppliers'. The second result is for CAS RN 2803933-60-8, also with a chemical structure and 'Absolute stereochemistry shown'. Below it, the formula $C_{37}H_{48}N_6O_5S_2 \cdot C_{23}H_{32}F_3N_5O_4$ and the name 'Components: 2 Paxlovid' are visible. At the bottom of this result, there are buttons for '39 References', '0 Reactions', and '0 Suppliers'.

- 物质检索框中可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开（<2000个字符）

物质检索—文献标识符及结果集排序

Substances search for "10.1126/science.abl4784"

Filter Behavior: Filter by, Exclude

Reaction Role: Product (9), Reactant (7), Reagent (4), Catalyst (2), Solvent (2)

Reference Role: Biological Study (10), Biological Study, Unclassified (10), Pharmacokinetics (10), Pharmacological Activity (10), Preparation (10)

Bioactivity Data: View All

Commercial Availability: Available (6), Not Available (4)

10 Results

Sort: Molecular Formula: Ascending | View: Partial

Result ID	Chemical Name	References	Reactions	Suppliers
147-85-3	L-Proline	117K	48K	164
61-90-5	L-Leucine	125K	6,092	154
2628280-40-8	3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-[[[(1S)-1-cyano-2-[[[(3S)-2-oxo-3-pyrroli...			
870153-29-0	1H-Indole-2-carboxamide, N-[(1S)-1-[[[(1S)-3-hydroxy-2-oxo-1-[[[(3S)-2-oxo-3-pyrroli...			
2757763-45-2	3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-2-(2-benzothiazolyl)-2-oxo-1-[[...			

使用文献标识符，迅速获得关注文献中的物质信息

不同物质排序：

- 相关度
- CAS RN
- 分子式
- 分子量
- 文献量
- 供应商数量

物质检索—分子式

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Co.Fe.Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性 **Na₂SO₄: H₂O₄S.2Na**

Searching for...

All

Substances

Reactions

References

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

Molecular Formula CH₂O₃

Searching for...

All

Substances

Reactions

References

Substances

Search by Substance Name, CAS RN, Patent Number

Enter a query...

Molecular Formula Co.Fe.Ni

适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物

物质检索—Advanced Search

Searching for...

All

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Reactions

References

Suppliers

Sequences

Retrosynthesis

Substances

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

Enter a query...

Draw

Molecular Formula

Molecular Formula

CAS Registry Number >

Chemical Identifier >

Document Identifier

Patent Identifier

Experimental Spectra >

Biological >

Chemical Properties >

Density >

Electrical >

Lipinski >

Magnetic >

Mechanical >

Optical and Scattering >

Structure Related >

Thermal >

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

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Recent Search History

February 13, 2023

Substances 157119-63-6 (1 Result) 2:05 PM

[View All Search History](#)

Rerun Search

Edit Search

高级检索字段：

- CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号
- 实验谱图：¹H, ¹³C, ¹⁵N, ¹⁹F, ³¹P NMR
- 化学标识符：化学名称、InChI key
- 生物：生物富集因子、LD50
- 化学：Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压
- 密度属性：密度、摩尔体积
- 电学：电导/电导率、电阻/电阻率
- Lipinski：自由旋转键、H受体/供体
- 磁：磁力矩
- 机械属性：拉伸强度
- 光散射：旋光性、折射率
- 结构：极性表面积
- 热学：熔点、沸点、闪电、玻璃转化温度、蒸发焓

物质检索—联用检索(1)

查找满足以下属性要求的合金：

1. 密度 $<7\text{g/cm}^3$
2. 拉伸强度 $>1000\text{MPa}$
3. 熔点 >600

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Element

Substance Class

- Alloy (12)
- Element (2)
- Manual Registration (2)
- Organic/Inorganic Small Molecule (1)

Isotopes

Metals

Experimental Property

- Density (12)
- Melting Point (12)
- Tensile Strength (12)
- Glass Transition Temperature (11)

Filtering: Substance Class: Alloy X

12 Results

1

56802-58-5

Image Not Available

Unspecified

Aluminum alloy, base, (Duralumin)

2

252664-07-6

Component	Percent
Zr	68
Cu	13
Ni	9.7
Nb	6.1
Al	3.5

Al.Cu.Nb.Ni.Zr

Components: 5

Zirconium alloy, base, Zr,Al,Cu,Nb,Ni (VIT 106)

2,476 References 1 Reaction 0 Suppliers

62 References 0 Reactions 0 Suppliers

4

857638-02-9

Component	Percent
Zr	59

5

253178-50-6

Component	Percent
Zr	66

物质类别中锁定合金Alloy

Substances

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

Enter a query...

Draw

Density (g/cm3) <7

Include predicted values. *Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2*

Search key property values only.

AND Tensile Strength (Mpa) 1000 to 2500

Search key property values only. *Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2*

AND Melting Point (°C) >600

Search key property values only. *Examples: 1.15 | <7.53 | >150 | 9.3 to 15 | 8.9e-2*

Zirconium alloy, base, Zr 59,Cu 39,Al 2.5 (9CI, ACI)

Key Physical Properties	Value	Condition
Melting Point (Experimental)	700-935 °C	-
Density (Experimental)	6.35 g/cm ³	Temp: Room temp; Press: 800 Torr

Experimental Properties

Property	Value	Condition	Source
Tensile Strength	1820 MPa (Yield) (approx)	-	(1) CAS
Tensile Strength	1600 MPa (Yield) (approx)	-	(1) CAS
Compressive Strength - 1 Source	See Full Text		(2) CAS
Hardness - 1 Source	See Full Text		(3) CAS
Microhardness - 1 Source	See Full Text		(4) CAS

物质检索—联用检索(2)

- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

Searching for...

Substances

Enter a query...

Molecular Weight 220 to 280
Predicted values only. Examples: 46.07 | 125 to 350 | >300

AND pKa 1.3 to 1.8
Predicted values only. Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25

AND Carbon-13 NMR 114 to 171, 96, 11.5
Allowance of ± 2 ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field

Learn more about SciFinder[®] Advanced Search.

Substances search for 3 Advanced Fields

References Reactions Suppliers

Filtering: Bioactivity Data: 3 Selected

15 Results Sort: Molecular Formula: Ascending View: Partial

1 296262-16-3

2 723-46-6

3 1631737-39-7

4 442571-27-9

5 1927010-88-5

6 697787-29-4

Filter Behavior

Filter by Exclude

Reaction Role

- Product (15)
- Reactant (11)
- Reagent (1)
- Catalyst (1)

Reference Role

- Preparation (15)
- Synthetic Preparation (15)
- Biological Study (14)
- Pharmacological Activity (14)
- Uses (14)

Bioactivity Data

- Structure Activity Relationships (15)
- Toxicity (2)
- Absorption, Distribution, Metabolism, Excretion (1)

Commercial Availability

Number of Components

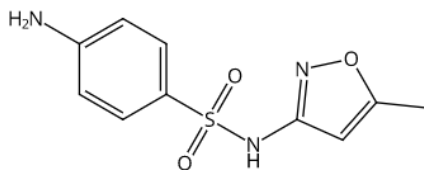
Molecular Weight

Stereochemistry

物质详情

CAS Registry Number: 723-46-6

References (24K) Reactions (961) Suppliers (120)



C₁₀H₁₁N₃O₃S

Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.1±55.0 °C	Press: 760 Torr
Density (Experimental)	1.4895 g/cm ³	-
pKa (Predicted)	5.81±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names and Identifiers

Experimental Properties

Experimental Spectra

Structure Activity Relationships



Absorption, Distribution, Metabolism, and Excretion Data



Toxicity



Predicted Properties

Predicted Spectra

折叠菜单显示物质各类信息

Bioactivity Indicators

Target Indicators

Experimental Spectra

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible
Source						
View Proton NMR Spectrum	(1) LC					
View Proton NMR Spectrum	(2) ENAMINE					
View Proton NMR Spectrum	(2) ENAMINE					
View Proton NMR Spectrum	(3) CAS					
View Proton NMR Spectrum	(4) CAS					
View Proton NMR Spectrum	(5) CAS					
View Proton NMR Spectrum	(6) BIORAD					
View Proton NMR Spectrum	(6) BIORAD					
View Proton NMR Spectrum	(7) AIST					
Proton NMR Spectrum - 4 Sources						(8-11) CAS

Sources

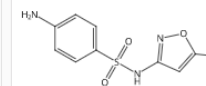
(1) Spectral data were obtained from Life Chemicals

(2) Spectral data were obtained from Enamine Ltd.

(3) Ham, Won Seok; Angewandte Chemie, International Edition, (2019), 58(2), 532-536, CAplus

Proton NMR Spectrum for 723-46-6

723-46-6



C₁₀H₁₁N₃O₃S

CAS Name
Sulfamethoxazole

Conditions

Working Frequency

400 MHz

Solvent

[Dimethyl sulfoxide \(67-68-5\)](#)

[Carbon tetrachloride \(56-23-5\)](#)

Temperature

20 °C

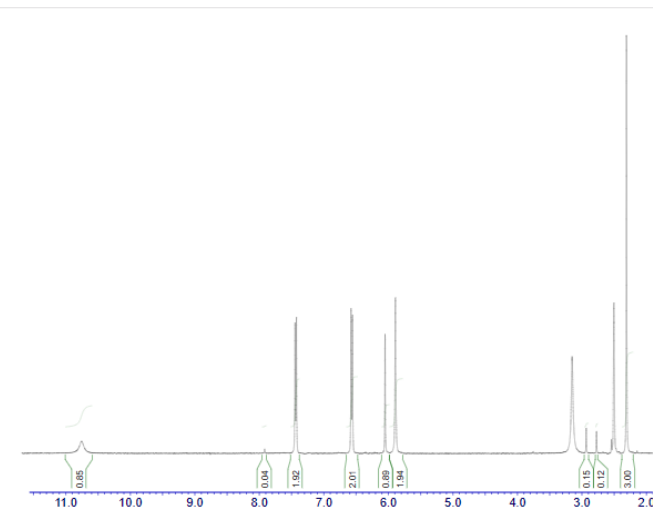
Spectrum Summary

Spectrum ID

F0175-0013

Source

Spectral data were obtained from Life Chemicals



物质详情

Structure Activity Relationships

Filter Disease

- Bacterial infection (273)
- Microbial infection (206)
- Oxidative stress (76)
- Toxoplasmosis (46)
- Bacterial infections

Target	Function	Parameter	Disease	Organism	Assay	Source
1132187-M	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
207419-N	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
226605-F	Inhibitor	Drug ren	-	-	View Detail	(1) CAS
A. baumannii	Inhibitor	MIC	-	-	View Detail	(2) CAS
Acanthamoeba	Inhibitor	IC50	Microbial infections	-	View Detail	(3) CAS
Acanthamoeba	Inhibitor	IC50	Acanthamoeba keratitis	-	View Detail	(3) CAS
Acanthamoeba	Inhibitor	IC50	Acanthamoeba keratitis	0.8 ug/mL	View Detail	(3) CAS

Absorption, Distribution, Metabolism, and Excretion Data

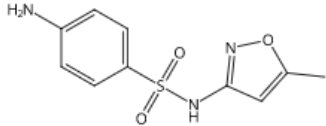
Filter Parameter

- Drug concentration (7)
- Cell uptake (2)
- Serum concentration (2)
- fAUC(0-24 h) (2)
- fCmax (2)
- t1/2 (2)

Target	Function	Value	Disease	Organism	Assay	Source
Methicillin-resistant Staphylococcus aureus	-	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	13 mg/L	Bacterial infections	-	View Detail	(1) CAS
Methicillin-resistant Staphylococcus aureus	-	10 h	Bacterial infections	-	View Detail	(1) CAS
Methicillin-sensitive Staphylococcus aureus	-	217.5 mg x h/L	Bacterial infections	-	View Detail	(1) CAS

Assay Data

Ligand 723-46-6



C10H11N3O3S
Sulfamethoxazole

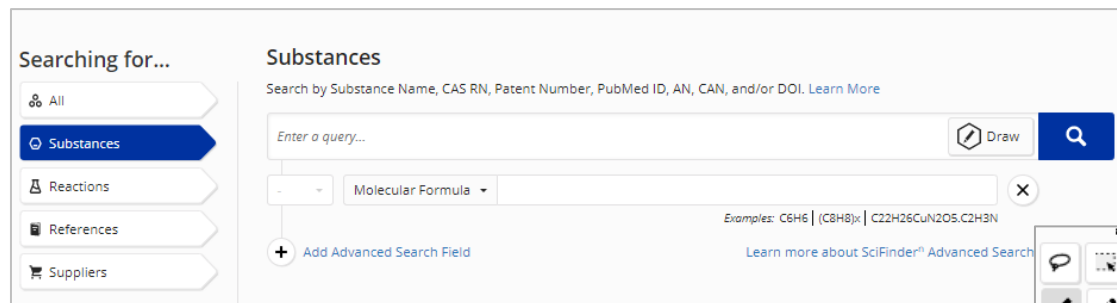
Target	207419-N
Assay Name	-
Assay Type	Functional
Procedure	Laccase degradation assay
Function	Inhibitor
Parameter	Drug removal
Value	0.00 %
Ligand Dose	-
Disease	-
Biological System	in vitro
Source	Evaluation of bezafibrate, gemfibrozil, indomethacin, sulfamethoxazole, and diclofenac removal by ligninolytic enzymes By: Camarillo Ravelo, Dante; Loera Corral, Octavio; Gonzalez-Martinez, Ignacio; Chan Cupul, Wilberth; Rodriguez Nava, Celestino Odin Preparative Biochemistry & Biotechnology (2020), 50(6), 592-597 Language: English, Database: CPlus and MEDLINE

Toxicity

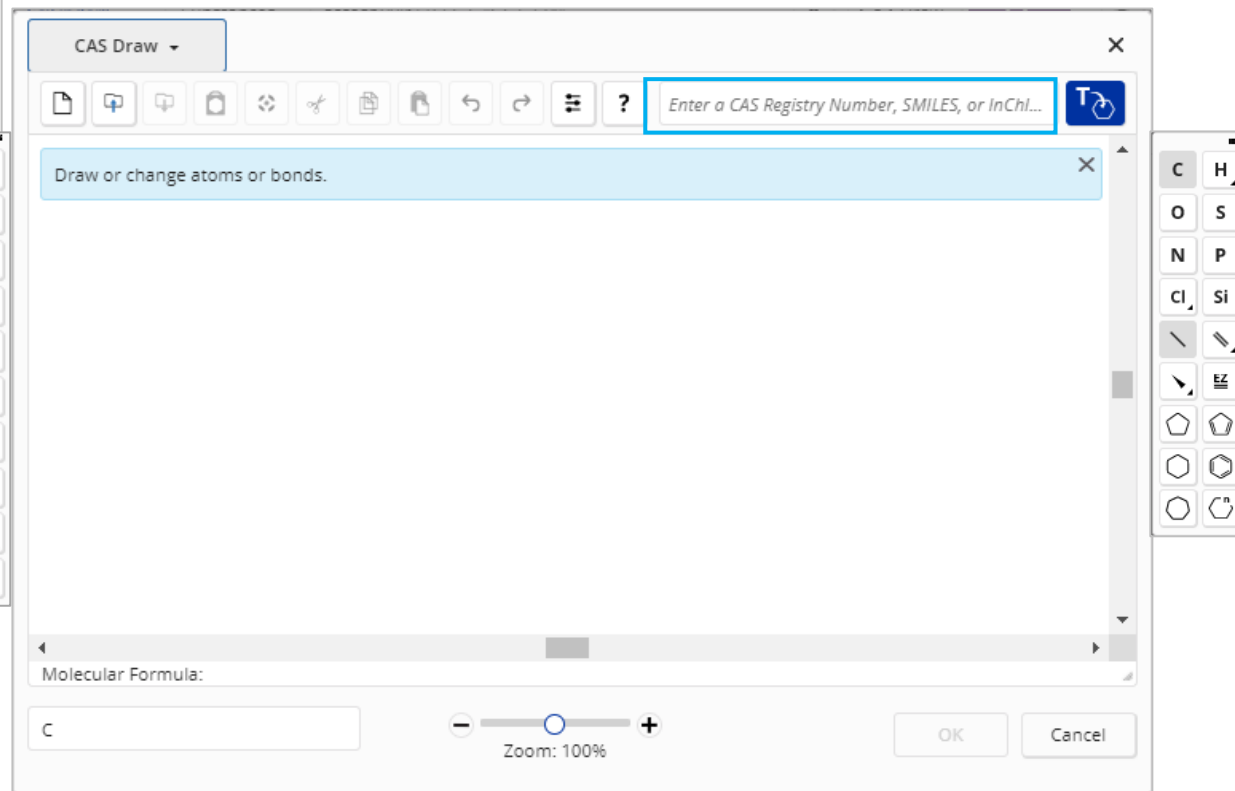
Target	Function	Parameter	Value	Disease	Organism	Assay	Source
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS
-	-	EC50	1.917 µM	-	-	View Detail	(1) CAS
-	-	EC50	>12.500 µM	-	-	View Detail	(1) CAS

(1) Plouffe, David M.; Cell Host & Microbe (2016), 19(1), 114-126, CPlus and MEDLINE

物质检索—结构检索



-  选择可变基团
-  取代位点可变
-  自定义R基团
-  锁工具
-  重复片段工具
-  片段结构



CAS Draw和ChemDoodle的使用指南

https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm <https://www.cas.org/support/training/scifinder-n/structure-search>

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

物质检索—结构检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

CAS Draw

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

Draw or change atoms or bonds.

R1

Molecular Formula: Formula is not available

R1

Zoom: 100%

OK Cancel

R-Group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 >

R1: Ni, Cu, Co

Atoms

H																			He
Li	Be												B	C	N	O	F	Ne	
Na	Mg												Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	**																	
*Lanthanides		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
**Actinides		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			
Isotopes		D	T																

物质检索—检索结果集筛选

结构检索类别:

As Drawn

亚结构

相似结构

Chemscape分析

Filter by & Exclude

物质筛选类别:

反应角色

文献角色

立体化学

物质类别

同位素

金属包含

实验物性数据

二次检索.....

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

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

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Stereochemistry

Element

Substance Class

Isotopes

Metals

Experimental Property

Bioactivity Indicator

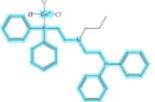
Search Within Results

732 Results

Sort: Relevance View: Partial

1

685504-28-3

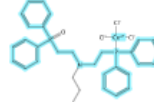


$C_{31}H_{35}Cl_3CoNP_2$
(T-4)-Trichloro[N-[2-(diphenylphosphino- κ P)ethyl]-N-[2-(diphenylphosphino)ethyl]...]

References Reactions Suppliers

2

807307-30-8

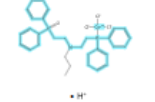


$C_{31}H_{35}Cl_3CoNOP_2$
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κ P)ethyl]-N-[2-(diphenylphosphino)ethyl]...

References Reactions Suppliers

3

635299-07-9

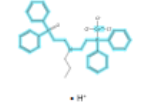


$C_{31}H_{35}Cl_3CoNOP_2 \cdot H^+$
Components: 2
Component RN: 807307-30-8
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κ P)ethyl]-N-[2-(diphenylphosphino)ethyl]...

References Reactions Suppliers

4

635299-08-0

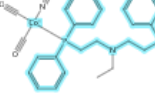


$C_{31}H_{35}Cl_3CoNOP_2 \cdot 2/5 C_2H_6O \dots$
Components: 3
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino- κ P)ethyl]-N-[2-(diphenylphosphino)ethyl]...

References Reactions Suppliers

5

16827-53-5

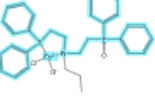


$C_{34}H_{33}Co_2N_3O_6P_2$
Cobalt, [μ -[2,2'-bis(diphenylphosphino)triethylamine]]tetracarboxyldinitrosyl(d...

References Reactions Suppliers

6

635299-09-1



$C_{31}H_{35}Cl_2CoNOP_2$
(T-4)-Dichloro[N-[2-(diphenylphosphino- κ P)ethyl]-N-[2-(diphenylphosphino)ethyl]...

References Reactions Suppliers

物质检索—结构检索

结构检索类别：

- As Drawn

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

- Substructure 亚结构

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

- Similarity 相似结构

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

注：如果关注相似结构检索结果，请不要绘制通式结构

物质检索-检索结果集筛选: Reaction Role

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match: As Drawn (0), Substructure (732), Similarity (9), 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

Reaction Role: Catalyst (36)

Product (216), Reactant (53), Reagent (3)

Reference Role, Commercial Availability, Number of Components, Molecular Weight

Filtering: Reaction Role: Catalyst X Clear All Filters

36 Results Sort: Relevance View: Partial

1879110-74-3 C ₃₃ H ₃₉ Cl ₂ CoNP ₂ (T-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-1-pentanamine]dichlorocobalt 1 Reference, 2 Reactions, 0 Suppliers	2332371-33-0 C ₃₀ H ₃₃ Cl ₂ CoNP ₂ (T-4)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]-N-ethyl... 1 Reference, 3 Reactions, 0 Suppliers	1879110-75-4 C ₃₁ H ₃₅ Cl ₂ CoNP ₂ (T-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-2-propanamine]dichlorocobalt 1 Reference, 2 Reactions, 0 Suppliers
1087216-22-5 C ₂₈ H ₂₉ Cl ₂ CoNP ₂ Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN... 8 References, 105 Reactions, 0 Suppliers	2170923-58-5 C ₂₈ H ₂₉ Cl ₂ CoNP ₂ (T-5-13)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]eth... 1 Reference, 32 Reactions, 0 Suppliers	1846596-28-8 C ₂₈ H ₅₃ Cl ₂ CoNP ₂ (T-5-13)-Dichloro[2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]eth... 7 References, 13 Reactions, 0 Suppliers

利用物质在反应中的角色精准定位相应的物质

物质检索—检索结果集筛选：Reference Role

利用物质的研究角色精准定位相应的物质

Reference Role

By Count | Alphanumeric

5 Selected

<input type="checkbox"/> Preparation (489)	<input checked="" type="checkbox"/> Process (32)	<input checked="" type="checkbox"/> Biological Study (4)
<input checked="" type="checkbox"/> Synthetic Preparation (488)	<input type="checkbox"/> Physical, Engineering, or Chemical Process (31)	<input type="checkbox"/> Pharmacological Activity (4)
<input type="checkbox"/> Properties (245)	<input checked="" type="checkbox"/> Industrial Manufacture (9)	<input type="checkbox"/> Therapeutic Use (4)
<input type="checkbox"/> Reactant (98)	<input type="checkbox"/> Technical or Engineered Material Use (8)	<input type="checkbox"/> Analytical Reagent Use (1)
<input type="checkbox"/> Reactant or Reagent (98)	<input type="checkbox"/> Formation, Non-preparative (6)	<input type="checkbox"/> Analytical Study (1)
<input type="checkbox"/> Uses (88)	<input type="checkbox"/> Formation, Unclassified (1)	
<input checked="" type="checkbox"/> Catalyst Use (77)		

Apply | Cancel

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscrape Analysis

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

Create Chemscrape Analysis

Filter Behavior

Filter by | Exclude

Reaction Role

Reference Role

Preparation (489)

Synthetic Preparation (488)

Properties (245)

Reactant (98)

Reactant or Reagent (98)

Industrial Manufacture (9)

[View All](#)

Commercial Availability

Not Available (9)

Filtering: Reference Role: Industrial Manufacture X

Clear All Filters

9 Results

Sort: Relevance View: Partial

1

1087216-22-5

$C_{28}H_{29}Cl_2CoNP_2$
Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethana mine-κN...

8 References | 105 Reactions | 0 Suppliers

2

1395056-63-9

$C_{28}H_{29}Cl_3CoNP_2.H$
Components: 2
Component RN: 1395144-60-1
Cobaltate(1-), trichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)eth...

3 References | 8 Reactions | 0 Suppliers

3

579490-65-6

$C_{40}H_{37}NNiP_2$
(SP-4-1)-Butyl[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl] benzen...

6 References | 20 Reactions | 0 Suppliers

4

579490-58-7

$C_{37}H_{31}NNiP_2$
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen amina...

7 References | 22 Reactions | 0 Suppliers

5

579490-62-3

$C_{38}H_{33}NNiP_2$
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen amina...

6 References | 21 Reactions | 0 Suppliers

6

579490-55-4

$C_{36}H_{28}CINNIP_2$
(SP-4-3)-Chloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl] benze...

8 References | 52 Reactions | 0 Suppliers

物质检索—检索结果集的保存

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

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

文献信息 反应信息 供应商信息

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Element

Filtering: Search Within Results: Drawn Structure X

109 Results

Sort: Relevance View: Partial

1 1698881-12-7

C58H56N2NiP4S4
Nickel(1+), [N,N-bis[2-(diphenylphosphino)ethyl]carbamodithioato-kS,kS'] nickel

2 65120-45-8

C34H43N2NiP2S
Nickel(1+), [N,N-bis[2-(diphenylphosphino)ethyl]-N',N'-diethyl-1,2-ethanediamine...

3 65120-39-0

C35H45N2NiP2S
Nickel(1+), [N,N-bis[2-(diphenylphosphino)ethyl]-N',N'-diethyl-1,2-ethanediamine...

6 1698881-15-0

C87H84CoN3P6S6
(OC-6-11)-Tris[N,N-bis[2-(diphenylphosphino)ethyl]carbamodithioato-kS,kS'] cobalt

1698881-21-8

C58H56Au4Cl4N2NiP4S4
Bis[μ₃-[N,N-bis[2-(diphenylphosphino)ethyl]carbamodithioato-kS,kS']]tetrakis (...)

References Reactions Suppliers

Save Results and Create Alert

Name

PNP-S

Save Options

Query Only

Selected Answers

All Answers (Up to 20,000)

Alert Frequency

No Alerts

As Available

Weekly

Monthly

Add Existing Tags (Optional)

catalyst

Other fields

Task

Try

New Tag (Optional)

Tag Color

Save Cancel

Download Substance Results

File Type

PDF

Select Quantity

All Results

Selected Results

Range (ex. 2 to 20)

Display

Structures Only

Result Summary

Result Details

File Name

Substance_20221121_1345

Include

Task History

Substance Identifiers

Experimental Spectra

Predicted Spectra

Regulatory Information

Experimental Properties

Predicted Properties

Bioactivity Indicators

Target Indicators

Download Cancel

Learn more about downloads.

CAS Markush检索

(19) 中华人民共和国国家知识产权局

(12) 发明专利申请

(10) 申请公布号 CN 104945470 A
(43) 申请公布日 2015.09.30

(21) 申请号 201410122313.4
(22) 申请日 2014.03.30
(71) 申请人 浙江大学
地址 310027 浙江省杭州市西湖区浙大路38号
申请人 中国科学院上海药物研究所
(72) 发明人 南永洲 李佳 刘滔 张建康
周宇波 杨波 何俏军 许磊 南小蓓
(74) 专利代理机构 杭州求是专利事务所有限公司 33200
代理人 张法高 赵杭丽

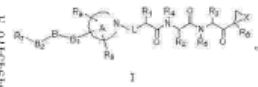
(51) Int. Cl.
C07K 1/16(2006.01)
C07K 1/06(2006.01)
A61K 38/06(2006.01)
A61P 35/00(2006.01)
A61P 35/02(2006.01)
A61P 25/28(2006.01)
A61P 37/02(2006.01)

权利要求书3页 说明书24页 附图4页

(54) 发明名称
杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要
本发明提供一种杂环构建的三肽环氧酮类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性,是有前景的蛋白酶体抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式 I 的结构通式:

CN 104945470 A



具体物质[Specific Substance]:

以具体化学结构陈述的特定物质, 会被分配CAS RN

具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明,以下实施例仅是说明本发明,而不是以任何方式限制本发明。

[0027] 制备实施例 1、4-(吡嗪-2-基氨基酰基)哌啶-1-甲酸叔丁酯(1a, 1b)

将 1-(叔丁氧羰基)哌啶-4-甲酸(2.75g, 12mmol)置于 50mL 三颈瓶中, N₂ 保护下加入 25mL 无水 CH₂Cl₂, 然后缓缓滴入吡啶(2.5mL, 30mmol)和二氯亚砷(1.1mL, 14mmol), 该反应液置于室温反应半小时。随后, 2-氨基吡嗪(0.95g, 10mmol)和三乙胺(5.7mL, 40mmol)溶于 15mL CH₂Cl₂ 后缓缓滴入上述反应液, 室温反应 6 小时。反应液加 30mL 饱和食盐水稀释, 分出有机层, 水层 CH₂Cl₂ 提取(15mL×3), 合并有机层, 无水硫酸钠干燥后减压除去溶剂, 柱层析分离得白色固体 2.3g, 收率 74%。m.p.: 134-136°C; ¹H NMR (500MHz, CDCl₃): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH₂), 2.81 (m, 2H, CH₂), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH₂), 1.76 (m, 2H, CH₂), 1.47 (s, 9H, CH₃) ppm; ESI-MS: m/z = 307 [M+H]⁺。

[0028] 制备实施例 2、4-(吡嗪-2-酰基)哌啶-1-甲酸叔丁酯(1c, 1d)

吡嗪-2-羧酸(1.5g, 12mmol)置于 50mL 反应瓶中, 加入 35mL 无水 CH₂Cl₂ 溶解, 随即加入 1-羟基苯并三氮唑(1.6g, 12mmol)和 N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐(3.5g, 18mmol), 室温反应半小时。随后, 哌啶-1-甲酸叔丁酯(1.9g, 10mmol)加入反应液中, 室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释, 分出有机层, 饱和食盐

CAS Markush检索

预测性物质[Prophetic Substance]:

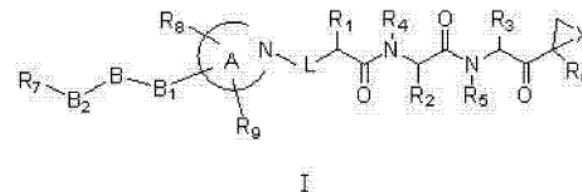
- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



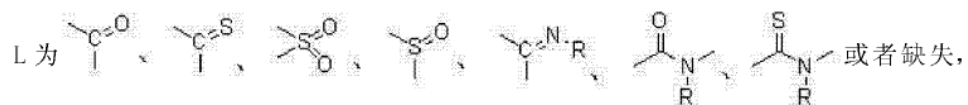
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_9)$ (R_9) 或缺失， R_9, R_9 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、 $C(O)O-C_{1-6}$ 烷基、 $C(O)NH-C_{1-6}$ 烷基、芳烷基；

X 为 O、S、NH、 $N-C_{1-6}$ 烷基或 N- 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

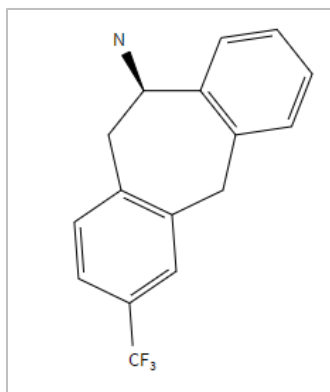
环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基 -D、芳基、杂环芳基、环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

2 Results

Sort: Number of R

1 146364-17-2

C₁₇H₁₄F₃N
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-3-(trifluoromethyl)-

1 Reference 1 Reaction 0 Suppliers

2 146364-18-3

C₁₈H₁₆F₃N
10,5-(Iminomethano)-5H-dibenzo[a,d]cycloheptene, 10,11-dihydro-12-methyl-3-(trifluoromethyl)-

1 Reference 1 Reaction 0 Suppliers

Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Similarity

- 85-89 (1)
- 80-84 (2)
- 75-79 (20)
- 70-74 (140)
- 65-69 (958)
- 60-64 (4,211)

Reaction Role

Reference Role

Filtering: Number of Components: 1 X Clear All Filters

5,332 Results

Sort: Number of References: Descending View: Partial

1 61

1210-33-9

C₁₅H₁₃Cl
5-Chlorodibenzosuberene

143 References 130 Reactions 61 Suppliers

2 64

1057277-76-5

C₁₆H₁₄F₃N
1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline

90 References 121 Reactions 2 Suppliers

3 68

7005-53-0

C₁₅H₁₅N
IEM 2115

58 References 78 Reactions 14 Suppliers

4 60

3436-04-2

C₁₈H₁₇Br
5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene

5 62

1729-63-1

C₁₆H₁₃N
10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile

6 64

35764-73-9

C₂₁H₂₄F₃N
Fluotracen

Relative stereochemistry shown

Feedback

CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

- 直观呈现检索结构与专利原文中Markush匹配部分的结构；
- 标引其在专利中出现的位置；
- 详细的结构取代信息描述

The screenshot displays the CAS SciFinder interface for a Patent Markush search. At the top, there is a search bar with the text "Enter a query..." and a search button. Below the search bar, the page title is "Patent Markush search for drawn structure". A chemical structure is shown in a box, with options to "Edit Drawing", "Remove", and "Search Patent Markush". The search results are displayed in a list format, showing 4 results. The first result is WO2011025969, and the second is EP502788. The interface includes a "Filter Behavior" section with "Filter by" and "Exclude" buttons, and a "Filter Content Report" section with a "Download filter data from this result set" button. The results table has columns for Patent, Language, Kind Code, and PatentPak Options.

Patent	Language	Kind Code	PatentPak Options
WO2011025969	English	A1	PDF PDF+ Viewer
CN102595894	Chinese	A	PDF
US20120196882	English	A1	PDF PDF+ Viewer
US9375424	English	B2	PDF
US20160303103	English	A1	PDF

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索

物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用CAS Markush检索尽可能全面的获得结构的公开信息

反应检索

- 反应检索方法
 - 物质或文献标识符
 - 结构式
 - 关键词与结构联用
- 常用获取方法推荐
 - 已知物质：由物质获取反应
 - 已知文献：从文献中获取反应
 - 精确结构反应检索
 - 亚结构反应检索

反应检索

通过物质或文献标识符进行检索

CAS SciFinder[®] Reactions Semaglutide

Return to Home

Reactions search for "Semaglutide"

References - Save and Alert

Filter Behavior

- Filter by
- Exclude

Substance Role

- Product (222)
- Reactant (10)

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (2)
- 10-29% (1)

View All

Number of Steps

Reaction Mapping

Experimental Protocols

- Synthetic Methods (11)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

228 Results Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (1 Reaction) Steps: 7

910463-68-2 Image Not Available Suppliers (28)

Absolute stereochemistry shown, Rotation (+)

Suppliers (98)

Expand Scheme

Scheme 2 (5 Reactions) Steps: 5-7

910463-68-2 Image Not Available Suppliers (28)

Suppliers (79)

Suppliers (37)

Expand Scheme

Scheme 3 (2 Reactions) Steps: 3-7

910463-68-2 Image Not Available Suppliers (28)

Absolute stereochemistry shown, Rotation (-)

Suppliers (93)

Suppliers (132)

CAS SciFinder[®] Reactions 175:621496

Return to Home

Reactions search for "175:621496"

References - Save and Alert

Filter Behavior

- Filter by
- Exclude

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (3)
- No Yield Available (120)

Number of Steps

- 1 (25)
- 2 (29)
- 3 (27)
- 4 (21)
- 5 (16)
- 6-10 (15)

Non-Participating Functional Groups

- Amide (10)
- Carboxylic ester (10)
- Carboxylic acid (9)
- Ether (5)
- Amine (3)

View All

Reaction Mapping

Experimental Protocols

- Synthetic Methods (132)

Reaction Type

Stereochemistry

133 Results Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (2 Reactions) Steps: 7-8

204656-20-2 Image Not Available Suppliers (37)

Suppliers (145)

Suppliers (77)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 8

204656-20-2 Image Not Available Suppliers (37)

Absolute stereochemistry shown

Suppliers (136)

Expand Scheme

Scheme 3 (1 Reaction) Steps: 7

204656-20-2 Image Not Available Suppliers (37)

Absolute stereochemistry shown

Suppliers (32)

Supplier (1)

反应检索

Searching for...

Reactions

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

Enter a query...

Draw

通过结构式进行检索

CAS Draw

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

Draw or change atoms or bonds.

reactant

product

Molecular Formula: Formula is not available

C

Zoom: 100%

OK Cancel

C H
O S
N P
Cl Si
/ \
EZ
Cyclopentane, Cyclohexane, Cycloheptane

反应检索—结果集的分组与排序

As drawn结果为32

Reactions search for drawn structure

References

Structure Match

- As Drawn (32)
- Substructure (8,521)
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

- Synthetic Methods (3)
- Experimental Procedure (12)

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Filtering: Reaction Mapping: Mapping Data Available

16 Results

Group: By Scheme

Sort: Yield

View: Collapsed

Scheme 1 (5 Reactions)

Suppliers (85)

Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 76%

Suppliers (51)

Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76%

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelbaugh, Todd M.; et al
World Intellectual Property Organization, WO2009091874 A1
2009-07-23

PatentPak Full Text

Experimental Protocols

反应分组：
按类型分组
按文献分组

反应排序：
相关度
公布时间
产率
步数

反应检索—结果集筛选

Substructure结果8521

As Drawn反应检索
亚结构反应检索
相似反应检索

反应筛选类别：
产率、反应步数
不参与反应的官能团
实验步骤
反应类型
立体化学
试剂、催化剂、溶剂
商品信息……

文献筛选类别：
文献类型、语言
出版年份、刊物名

The screenshot shows a search interface with a left sidebar and a main results area. The sidebar includes filters for 'Yield', 'Number of Steps', 'Non-Participating Functional Groups', 'Reaction Mapping', 'Experimental Protocols', 'Reaction Type', 'Stereochemistry', 'Reagent', 'Catalyst', 'Solvent', 'Commercial Availability', 'Reaction Notes', and 'Search Within Results'. The main area displays 8,521 results, with the first three highlighted:

- 1** Acylation of Nitrogen Nucleophiles by Carboxylic Acids
R-C(=O)OH + R1-NH-R1 -> R-C(=O)-N(R1)2
- 2** Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters
R-C(=O)YR1 + H2O / H2 -> R-C(=O)OH + R1-YH / R1-H
- 3** Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs
R-C(=Y)X + R1-NH-R1 -> R-C(=Y)-N(R1)2

The screenshot shows a search interface with 2 results. The results are displayed as reaction schemes:

- Scheme 1 (1 Reaction)**: Shows a reaction between a substituted benzamide derivative and a substituted benzamide derivative, resulting in a product. Suppliers are listed as 39, 63, and 78.
- Scheme 2 (1 Reaction)**: Shows a similar reaction to Scheme 1, but with a different product. Suppliers are listed as 39, 63, and 61.

Below the schemes, there is a list of reagents and solvents for a specific reaction:

- 31-313-CAS-18612019 Steps: 1 Benzamide compounds as ROR gamma modulators and their preparation
- 1.1 Reagents: Titanium isopropoxide, (R)-2-Methylpropane-2-sulfonamide; Solvents: Tetrahydrofuran; 18 h, 70 °C
- 1.2 Reagents: Sodium borohydride; 3 h, rt
- 1.3 Reagents: Methanol; 0 °C
- 1.4 Reagents: Hydrochloric acid; Solvents: Diethyl ether, 1,4-Dioxane; 1 h, 0 °C

折叠菜单显示：相同反应类型的反应在同一菜单里，方便阅读和筛选

反应检索—结果集筛选：不参与反应官能团

Reactions search for drawn structure

References

Structure Match

- As Drawn (32)
- Substructure (8,521)
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Halide (290)
- Phenyl halide (286)
- Carboximidine (109)
- Alkene (84)
- Cyclic alkene (80)
- [View All](#)

Reaction Mapping

Experimental Protocols

Reaction Type

Stereochemistry

Filtering: Non-Participating Functional Groups: Halide

290 Results

Group: By Scheme Sort: Relevance View: Collapsed

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

Suppliers (107)

Expand Scheme

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

Expand Scheme

Scheme 3 (1 Reaction) Steps: 1 Yield: 100%

不参与反应官能团：
出现在反应前后，但未发生变化的官能团

Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

<input checked="" type="checkbox"/> Halide (282)	<input type="checkbox"/> Diene (45)	<input type="checkbox"/> Acetal (3)
<input type="checkbox"/> Phenyl halide (278)	<input type="checkbox"/> Ether (40)	<input type="checkbox"/> Acyclic alkene (3)
<input type="checkbox"/> Carboximidine (101)	<input type="checkbox"/> Cyclic ketone (29)	<input type="checkbox"/> Carbamate (3)
<input type="checkbox"/> Alkene (84)	<input type="checkbox"/> Urea (16)	<input type="checkbox"/> Carboxylic acid (3)
<input type="checkbox"/> Cyclic alkene (80)	<input type="checkbox"/> Tertiary amine (9)	<input type="checkbox"/> Alcohol (2)
<input type="checkbox"/> Amide (69)	<input type="checkbox"/> Imine (8)	<input type="checkbox"/> Primary alcohol (2)
<input type="checkbox"/> Amine (59)	<input type="checkbox"/> Thiocarbonyl (7)	<input type="checkbox"/> Unsaturated ester (2)
<input type="checkbox"/> Carboxylic ester (53)	<input type="checkbox"/> Acyclic ketone (5)	<input type="checkbox"/> Nitro (1)
<input type="checkbox"/> Secondary amine (50)	<input type="checkbox"/> Alkyl halide (4)	<input type="checkbox"/> Primary amine (1)
<input type="checkbox"/> Ketone (48)	<input type="checkbox"/> Nitrile (4)	<input type="checkbox"/> Unsaturated ketone (1)

Apply Cancel

反应检索—结果集筛选: Synthetic Methods™

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

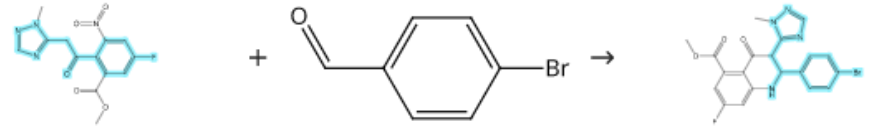
Source Reference

Filtering: Non-Participating Functional Groups: Halide X Clear All Filters

Experimental Protocols: Synthetic Methods X

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

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



Suppliers (15) Suppliers (89)

31-614-CAS-24450288 Steps: 1 Yield: 98%

1.1 Reagents: [Hydrochloric acid](#), [Titanium chloride \(TiCl₃\)](#)
Solvents: [Methanol](#), [Tetrahydrofuran](#), [Water](#); rt; 30 min, rt; 2 h, 30 - 50 °C

1.2 Reagents: [Water](#)

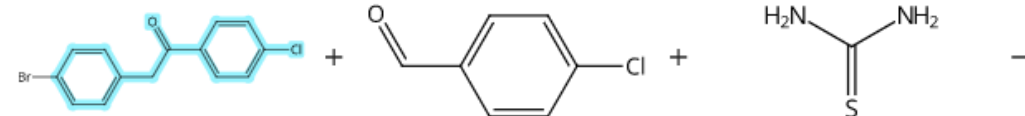
DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: Bowden, Gregory D. et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

Experimental Protocols Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 96%

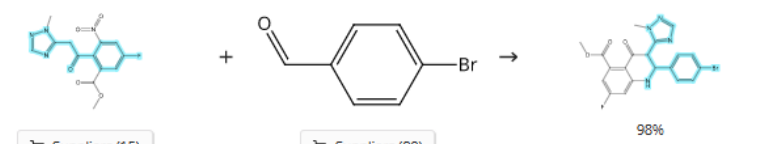


Suppliers (9) Suppliers (97) Suppliers (91)

反应检索—结果集筛选: Synthetic Methods™

Synthetic Methods™: 查看文献详情, 分类显示详尽信息, 方便操作

CAS Reaction Number: 31-614-CAS-24450288



Suppliers (15) Suppliers (89) 98%

Reaction Overview
Steps: 1 Yield: 98%

JOURNAL
DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer
By: Bowden, Gregory D.; et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701
View PDF Full Text

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

Step 1

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

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

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

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

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

Procedure

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

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

Scale
gram

Characterization Data
5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-, methyl ester
State: yellow amorphous solid

Transformations

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

CAS Method Number 3-315-CAS-33168860

联合检索—结构与关键词

联用检索提高检索效率

Searching for...
References

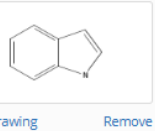
Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Friedel-crafts acylation

AND Author Name Enter last name, first name middle name.

+ Add Advanced Search Field [Learn more about Sci](#)

Launch CAS Lexicon CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms.



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

Substances Reactions Citing Knowledge Graph

1,100 Results Sort: Relevance View: Partial Abstract

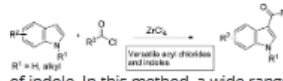
As Drawn (1,100)
Substructure (2,270)

Filter Behavior Filter by Exclude

Document Type Journal (996) Patent (68) Review (31) Conference (27) Dissertation (1) Preprint (8)

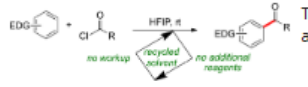
Substance Role Reactant or Reagent (1,067) Process (34) Properties (29)

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



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

Hexafluoro-2-propanol-Promoted Intermolecular Friedel-Crafts Acylation Reaction
By: Valeriya, Rakesh H.; Aube, Jeffrey
Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: CAlup and MEDLINE



Full Text Substances (50) Reactions (24) Citing (82) Citation Map



Reactions for AN 2011:601374

References

Filter Behavior Filter by Exclude

Yield 80-89% (1) 70-79% (8) 50-69% (12)

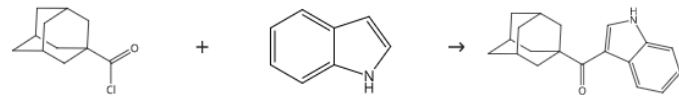
Number of Steps 1 (21)

Non-Participating Functional Groups Alkene (21) Amine (21) Cyclic alkene (21) Secondary amine (14) Tertiary amine (7) [View All](#)

Reaction Mapping

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

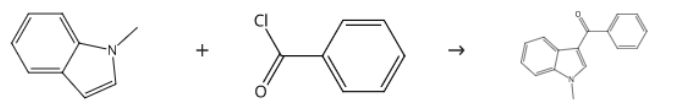
Scheme 1 (1 Reaction) Steps: 1 Yield: 82%



Suppliers (84) Suppliers (100) Suppliers (11)

Expand Scheme

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



Suppliers (90) Suppliers (63) Suppliers (10)

Expand Scheme

反应检索小结

1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 利用Synthetic Methods™查看文献中合成方法详情
4. 关键词与反应式的联合检索

大纲

- CAS Retrosynthesis Tool的使用
 - 获得已知化合物的逆合成反应路线
 - 获得未知化合物的逆合成反应路线



CAS Retrosynthesis Tool—由物质获得

获得已知化合物的逆合成路线（1）：

点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

1

2628280-40-8

Absolute stereochemistry shown

$C_{23}H_{32}F_3N_5O_4$
3-Azabicyclo[3.1.0]hexane-2-carboxamide, *N*-[(1*S*)-1-cyano-2-[(3*S*)-2-oxo-3-pyrroli...

236 References 53 Reactions 39 Suppliers

CAS RN
2628280-40-8

CAS Name
3-Azabicyclo[3.1.0]hexane-2-carboxamide, *N*-[(1*S*)-1-cyano-2-[(3*S*)-2-oxo-3-pyrroli...

Substance Detail

Reactions (53)

Synthesize (52)

Start Retrosynthetic Analysis

References (236)

Suppliers (39)

Absolute stereochemistry shown

Edit Structure - Reset + Download

CAS Retrosynthesis Tool:

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线

CAS Retrosynthesis Tool—直接绘制

获得已知化合物的逆合成路线（2）：

点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线

The screenshot shows the CAS Retrosynthesis Tool interface. On the left, under 'Searching for...', there is a list of categories: All, Substances, Reactions, References, Suppliers, Biosequences, and Retrosynthesis (which is highlighted in blue). The main area is titled 'Retrosynthesis' and contains a drawing board. The drawing board has a toolbar at the top with various icons for drawing and editing. Below the toolbar is a text input field with the placeholder 'Draw or change atoms or bonds.' and a 'T' icon. The drawing board itself shows a chemical structure of a bicyclic compound with a nitrogen atom and a carbonyl group. Below the drawing board, the molecular formula is displayed as 'Molecular Formula: C₈H₁₃NO₂ (155.20)'. At the bottom, there is a zoom control set to 100% and a 'Start Retrosynthetic Analysis' button.

CAS Retrosynthesis Tool—预设参数

预设反应路线参数：

反应深度

反应规则常见性

起始原料费用

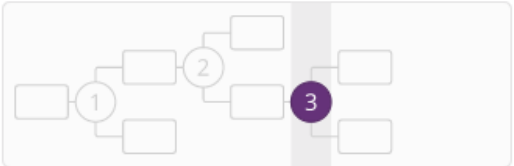
设置断裂键或保护键

Retrosynthesis Plan Options for drawn structure Powered by ChemPlanner®

[Learn more.](#)

Select Synthetic Depth

1 2 3 4



[Learn more.](#)

Set Rules Supporting Predicted Reactions

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

[Learn more.](#)

Set Starting Materials Cost Limit

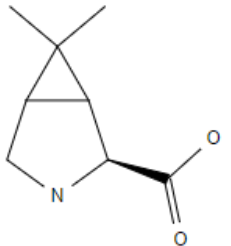
100 USD/mol

Email me when my plan is complete

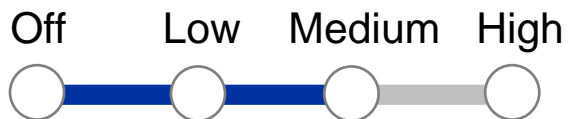
[Create Retrosynthesis Plan](#)

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

[Clear All Bond Selections](#)



CAS Retrosynthesis Tool—路线概览



Scoring Profiles:

降低每步原料结构的复杂性

逆合成路线中前体的数量

支持预测路线的文献数量多少

预测路线大概成本

每步的产率

每步的原子转化效率

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Overview Steps Predicted Results

[View Excluded Options](#) [Download](#) [Email](#) [Save](#)

Plan Information 路线概览

Estimated Yield: 49%
Overall Price: \$96.82
(USD per 100 grams)

Commercially Available: A, B, C

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$100.00/mol
[Edit Plan Options](#)

Scoring Profiles 调节参数

Complexity Reduction

Convergence

Evidence

Cost

Yield

Retrosynthesis Step Key

Feedback

CAS Retrosynthesis Tool—路线详情

Reactions (1,181) Group: By Scheme View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Supplier (1) Suppliers (3) Suppliers (103)

Reaction Summary Steps: 1

1.1 Reagents: 1-Ethyl-3-(2-dimethylamino)propylcarbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine
Solvents: Dichloromethane; overnight, rt

1.2 Reagents: Zinc
Solvents: Acetic acid; 30 min, rt

1.3 Reagents: 4-Methylmorpholine, O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate
Solvents: Dimethylformamide; 16 h, rt

Preparation of N-(heteroaryl)amino acid amide compounds useful as matrix metalloproteinase 13 (MMP-13) inhibitors
By: Farrow, Neil Alexander; et al
World Intellectual Property Organization, WO2010056585 A2
2010-05-20

PatentPak Full Text

View Reaction Detail Experimental Protocols

Collapse Scheme

Retrosynthesis Predicted Results ON

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: 37%
Evidence (1,181)
Alternative Steps (85)

B ⇒ E
Maximum Yield: 80%
Evidence (180,876)
Alternative Steps (20)

C ⇒ F + G
Maximum Yield: -
Evidence (1)
Alternative Steps (15)

E ⇒ H + I
Maximum Yield: -
Evidence (1)
Alternative Steps (24)

View All Alternatives (14)
View Evidence (4,737)
Exclude This Step

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

Experimental Steps
Predicted Steps

Reset

- 快速获取最优的逆合成路线
- 可获取预测逆合成路线
- 可查看每步路线的详细条件
- 可自定义选择替代路线

CAS Retrosynthesis Tool—路线详情

点击Alternative Steps查看并选择替换路线，得到自定义的合成路线

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Overview **Steps** Predicted Results

[View Excluded Options](#) [Download](#) [Email](#) [Save](#)

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

- A ⇒ B + C + D**
Average Yield: 41%
Evidence (1,209)
Alternative Steps (93)
- B ⇒ E**
Maximum Yield: 80%
Evidence (199,213)
Alternative Steps (15)
- C ⇒ F + G**
Maximum Yield: -
Evidence (1)
Alternative Steps (13)
- D ⇒ H**
Maximum Yield: -
Evidence (1)
Alternative Steps (58)
- E ⇒ I + J**
Maximum Yield: 92%
Evidence (22,464)
Alternative Steps (24)

Retrosynthesis Step Key

获取替代路线

A ⇒ B + C + D Alternative Steps (93)

Filter by

- Alternative Step Type
 - Predicted (93)
- Stereochemistry
 - Non-Selective (93)

1 of 34 Predicted Step

Selected [View 1 similar Alternative](#) [View Evidence \(1,209\)](#) Average Yield: 41%

2 of 34 Predicted Step

Select [View 7 similar Alternatives](#) [View Evidence \(277\)](#) Average Yield: 59%

3 of 34 Predicted Step

Reaction network diagram showing the synthesis of a target molecule from starting material A through various alternative steps (B, C, D, E, F, G, H, I, J, K). The diagram illustrates the flow of the reaction sequence, including the selection of a specific alternative step (2 of 34) and the resulting products (B, C, D, E, F, G, H, I, J, K). The network includes yield information (e.g., Avg. Yield 59%, Max Yield 80%, Max Yield 92%) and a shopping cart icon for each step.

逆合成路线小结

1. 通过物质结构获取已知化合物的逆合成路线
2. 获取预测的逆合成路线
3. 反应路线参数的预先设定与调节
4. 查看反应路线详情和文献支持，自定义选择替代路线

大纲

- CAS SciFinderⁿ中的序列检索
 - BLAST
 - CDR
 - Motif

视频链接:

https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000

[下一节：反应检索](#)

Sequences Search™ — Blast检索

Searching for...

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

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

Enter a query or upload a file...

Sequence Type:
Nucleotide Protein

Search Within:
 Nucleotides Proteins
 Include NCBI Sequences

Start Sequence Search

Advanced Sequence Search

可选择是否包含NCBI中的序列

支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

高级检索—设置相关参数

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA

Sequence Type:
 Nucleotide Protein

Search Within:
 Nucleotides Proteins
 Include NCBI Sequences

[Start Sequence Search](#)

Advanced Sequence Search Adjust Parameters for Short Sequences | Reset All

Alignment Identity %

Match with Gaps? Yes No

Gap Costs

Query Coverage %

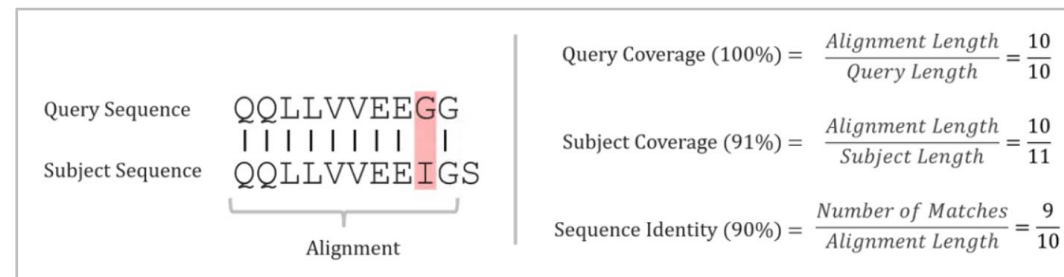
Word Size

Reward for Match Penalty for Mismatch

BLAST Algorithm

E-Value

Exclude Low Complexity Regions Yes No



Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA	View Results Edit Options Searching...
-----------------------	--	---	--

Results will expire on Mar 15, 2023.

Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACTTGA	View Results Edit Search Complete
-----------------------	--	---	---

Results will expire on Mar 15, 2023.

BLAST检索结果

6 Alignment Identity: 100%

Query 1 39

Subject 1 1,060

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

CAS Registry Number: [785872-37-9](#)
Length: 1,060 nt

Sequence

```

1  CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC ACACTTGAAC CGTGCCCGC
81  AGCGGAGGGA GCTTGACGG GCCAACGCAC ACATAACACA AGTCGTCGT CGATGGCGCG GTGGGCTGCG GTGCTGGCGC
161 TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGGCGGG CGGCACATG AACCGGACA AGACGGAGTG CGCGGACCA
241 CTGTGGGCC TGGCCCGTG CCTGCAGTAC GTGCAGGGG AGGCCCGCG GCCCGGCC GACTGTGCG GCGGCCTGCG
321 CCAGTGCTG GGAAGAGCC CCAAGTGCCT GTGCGTGCTC GTCAAGGACA AGGACGACCC CAACCTGGGC ATCAAGATCA
    
```

Alignment Subject References

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS J.; ZHOU, YIHUA; KOVALIC, DAVID K.; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS G.; HARDEMAN, KRISTINE J.; EDGERTON, MICHAEL D.; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY W.
US20120216318 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS; ZHOU, YIHUA; KOVALIC, DAVID; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS; HARDEMAN, KRISTINE; EDGERTON, MICHAEL; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY
US20040214272 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants

Substance Detail

Reference (1) Reactions (0) Suppliers (0)

CAS Registry Number
785872-37-9

Image Not Available

Unspecified
DNA (Zea mays clone MRT4577_11549C.1 protein fragment-specifying cDNA) (9CI)

Nucleic Acid Sequence
Sequence Length: 1060
204 a, 336 c, 311 g, 209 t

Sequence Details

Sequence: DNA: linear

1	cattgggtac	ctcgagbccg	gccgggagct	cgcaactca	cactcacaag
51	tcacacagcc	acacttgaac	cgctgccgc	agcggagga	gcttgacgg
101	gccaacgac	acataacaca	agctcgtgt	cgatggcgc	gtggctgctg
151	gtgtggcgc	tggccgggc	cacggccatc	gctgtgggt	ccgtggcgg
201	cgcgacatg	aacgggaca	agacggagt	cgcgaccag	ctgtggccc
251	tggcgctg	cctgcagta	gtcaggggc	agcccgcgc	gcccgcgcc
301	gactgctgc	gcccctcgc	ccaggtcgt	gggaagacc	ccaagtctt
351	gtcgtgctc	gtcaaggaca	aggacgacc	caactgggc	atcaagatca
401	agccaccct	cgctcgcgc	ctcccaacg	cctgggggc	caccgcgcc
451	aacgtctcc	actgcctca	gctcctgat	atcccccgg	gctccaaaga
501	cgccgcgtc	ttcagtcgg	gcagcacia	gggtccact	gctcctcag
551	ccaaggaaa	ctcagcggc	acgaccgact	ccgcgcgct	gacgggacc
601	accggacgc	gctgtcctc	ctcggcggc	accggggtg	ctgcaactca

Other Names and Synonyms

1 Other Name for this Substance
1999: PN: US20040214272





Patent Annotations

Source: Zea mays
Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

序列详情及相关的专利文献结果

References from your sequence

Substances Reactions Citing Knowledge Graph    

Filter Behavior 38 Results Sort: Publication Date: Newest View: Full Abstract

1

Expressing Arabidopsis thaliana genes in plants for low low-nitrogen tolerance
By: Nadzan, Gregory; Schneeberger, Richard; Kim, Han Suk; Dang, David Van-Dinh; Feldmann, Kenneth A.; Pennell, Roger; Kwok, Shing; Zhang, Hongyu; Christensen, Cory; Okamura, Jack; et al
United States, US10815494 B2 2020-10-27 | Language: English, Database: CAplus

Methods and materials for modulating low-nitrogen tolerance levels in plants are disclosed. For example, nucleic acids encoding low nitrogen tolerance-modulating polypeptides are disclosed as well as methods for using such nucleic acids to transform plant cells. Also disclosed are plants having increased_{RLCL21} low-nitrogen tolerance levels and plant products produced from plants having increased low-nitrogen tolerance levels.

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

2

Functionally-defined, sequence-determined DNA fragments and their use in genetic engineering of plants
By: Alexandrov, Nikolai; Brover, Vyacheslav; Feldmann, Kenneth A.; Makarov, Vladimir; Swaller, Timothy J.; Nadzan, Gregory; Mascia, Peter; Troukhan, Maxim; Rarang, Joel; Burns, James; et al
United States, US20170037422 A1 2017-02-09 | Language: English, Database: CAplus

Libraries of plant genomic fragments that are functionally-defined and sequenced, included identification of open reading frames and gene products, are described for use in plant improvement. Members of the library contain extensive and 5'- and 3'-UTRs that will allow expression in a plant host. The DNA mols. are useful for specifying a gene product in cells, either as a promoter or as a protein coding sequence or as an UTR or as a 3' termination sequence, and are also useful in controlling the behavior of a gene in the chromosome, in controlling the expression of a gene or as tools for genetic mapping, recognizing or isolating identical or related DNA fragments, or identification of a particular individual organism, or for clustering of a group of organisms with a common trait.

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

Patent	Language	Kind Code	PatentPak Options
US20170037422	English	A1	PDF PDF+ Viewer
US20060107345	English	A1	PDF
US20120159672	English	A1	PDF
US20060150283	English	A1	PDF
US20060048240	English	A1	PDF
US20060168696	English	A1	PDF PDF+ Viewer

low nitrogen tolerance levels in plants
h; Feldmann, Kenneth A.; Pennell, Roger; Kwok,
plus
r example, nucleic acids encoding low nitrogen
ch nucleic acids to transform plant cells. Also
ducts produced from plants having increased low-

Sequences Search™—Motif检索

Motif中有可变部分，可借助符号来表示：

“[]” 中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个

“{ }” 大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号开，{2, 6} 表示在大括号左边紧密相连的氨基酸可重复2-6次

Searching for...

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

Sequences

Enter a protein or nucleotide string. [Learn more about Sequence Search.](#)

BLAST CDR **Motif** [Clear Search](#)

[SG]x{4}GK[DT]

- X代表未指定氨基酸，可以是常见氨基酸、不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

[Advanced Sequence Search](#) [Reset All](#)

Query Coverage % E-Value Combine Motif Results

Sequence Type:

Include NCBI Sequences

Motif检索结果

Motif Search Details

Sequence Type: Protein
NCBI Included: Yes
Query Coverage: 90%
E-Value: 10

Bioscape Analysis

Visually explore sequence similarity with a new tool.
[Learn more about Bioscape.](#)

[Create Bioscape Analysis](#)

Filter by

- E-Value
- Query Coverage %
- Subject Coverage %
- Alignment Identity %
- Sequence Length
- Organisms

Homo sapiens (248)
 synthetic construct (23)
 unidentified (2)
 Mus musculus (1)

Query Details [View More](#)

> Seq 1: 1 SXXXXGKD 8

248 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 75%

Query 1 8

Subject 1 114

Matches: 6
Mismatches: 2

[View Less](#)

Alignment Subject References

Alignment Data
BLAST Score: 77
E-Value: 0.00104148

```
Q 1 SXXXXGKD 8
   |||||++|
S 94 SXXXXXD 101
```

2 Alignment Identity: 75%

Query 1 8

Subject 1 643

Matches: 6
Mismatches: 2

[View Less](#)

Alignment Subject References

CAS Registry Number: -
Length: 643 aa
Organisms: Homo sapiens
Sequence

```
1 MEKSSSCESL GSQPAARPP SVDSLSSAST SHSENSVHTK SASVVSSDSI STSADNFSPD LRVLRNSNKL AEMEEPPLLP
```

Sequences Search™—CDR检索

CDR (complementarity—determining regions): 抗体或细胞中的互补决定区

Searching for...

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

Sequences

Enter a protein string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST **CDR** Motif [Clear Search](#)

Include NCBI Sequences

CDR1	RASQSVSGSRFTYMH	X
CDR2	YASILES	X
CDR3	QHSWEIPPWT	X

支持单个或多个CDR序列检索并用

CDR检索结果

Sequences search for your query

References

CDR Segments

Select a segment below to view individual or intersecting CDR results.

Apply

Reset Segments

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Create Bioscape Analysis

Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

Query Details [View Less](#)

> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

> CDR3
QHSWEIPPWT

21,934 Results Sort: Alignment Identity View: Expanded

Alignment Identity: 100%

Matches: 32
Mismatches: 0

View Less

Alignment Subject References

Alignment Data
BLAST Score: 84
E-Value: 7.45568461509489

CDR1	1	RASQSVSGSR	FTYMH	15
S	24	RASQSVSGSR	FTYMH	38
CDR2	1	YASILES		7
S	54	YASILES		60
CDR3	1	QHSWEIPPWT		10
S	93	QHSWEIPPWT		102

References

获取披露该序列的文献

CDR Segments

Select a segment below to view individual or intersecting CDR results.

Apply

Reset Segments

CDR Segments:

- 匹配到一个或者多个CDR的subject序列的序列数量
- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments:

- 重新选择查看匹配的序列结果

序列检索小结

- Sequences涵盖期刊、专利、NCBI当中的序列信息
- Sequences可以针对DNA/RNA的核苷酸序列、肽/蛋白的氨基酸序列进行检索
- 生物序列的获取方法：Sequences检索、物质名称/代码/结构式、关键词及文献-物质的数据关联
- Motif适合检索短序列，并支持可变部分输入
 - ✓ X代表未指定氨基酸，N代表未指定核苷酸
 - ✓ []表示出现在该位置的序列是括号里氨基酸/核苷酸中的任意一个
 - ✓ { } 代表氨基酸/核苷酸的重复次数，如重复次数是范围，用逗号将数字隔开，如{2, 6}

大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 生物序列检索*
- 常见问题及解答



如何获取CAS SciFinderⁿ账号

(登录贵校图书馆网站, 查看注册相关的链接和说明)

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: Tips

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: Why?

请注意:

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

Registration Already Complete

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

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

CAS SciFinderⁿ检索浏览器推荐

浏览器推荐：

- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- 不建议使用360浏览器，相关功能或插件会被自动拦截

使用注意事项

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

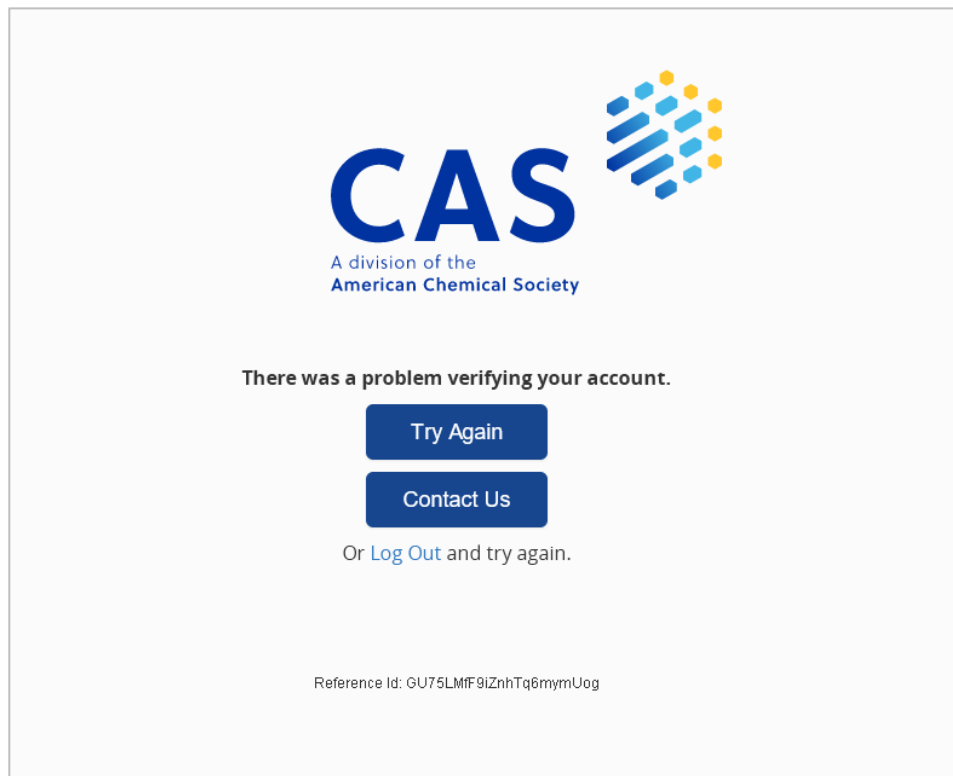
常见问题

Unauthorized IP Address

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

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

常见问题



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

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Thursday 11:06

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每次直播时间是18:00-19:00, 欢迎您带上问题, 我们将现场解答; 观看直播还有机会获得幸运纪念品!

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

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