

CAS SCIFINDER DISCOVERY PLATFORM™

零基础入门



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CAS SCIFINDER DISCOVERY PLATFORM

2025 春季专题论坛

您在日常科研与研发工作中，是否会遇到如下问题？

- 如何检索并持续追踪跨学科融合的前沿最新进展？
- 各领域特有的分子结构怎么画？
- 精心设计的分子有没有被他人报道过？
- 如何灵活绘制结构，分析目标化合物及相似结构在专利中的布局？
- 如何设计合成路线策略，优化绿色安全的制备工艺？
- 已制备的材料，如何实现应用上的突破？
- 如何高效管理和协作多个并行课题？

CAS SciFinder Discovery Platform 3 月至 5 月的六场专题论坛，直播时间为 **周五 14:00 - 15:00**。扫描二维码注册，观看直播有机会获得 **CAS定制纪念品**，欢迎在直播中提问互动。



CAS SCIFINDER DISCOVERY PLATFORM

2025 春季专题论坛直播时间表



3月21日 | 零基础入门

演讲人：刘子露 博士



3月28日 | 解锁新功能

演讲人：杜德鑫 博士



4月18日 | 助攻论文写作

演讲人：潘娜 博士



4月25日 | 探索科研成果转化

演讲人：钱欣 博士



5月9日 | 结构绘制面板
及案例详解

演讲人：刘子露 博士



5月23日 | 反应检索策略及典型
案例

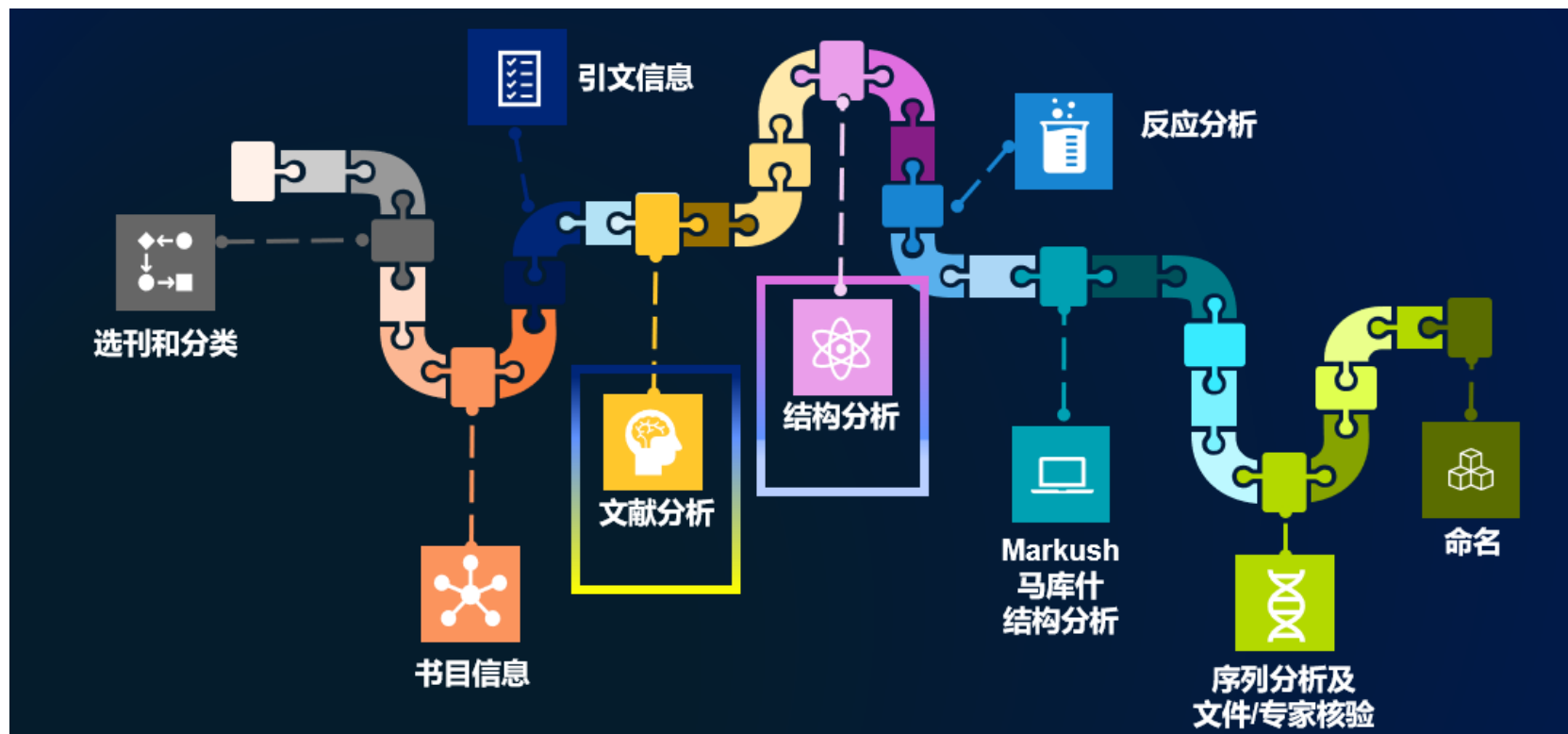
演讲人：陈开乾 博士

“

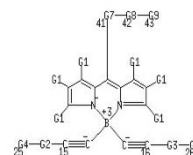
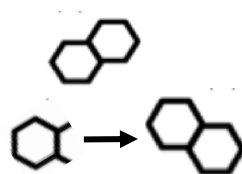
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CAS 科学家的智力标引



1990
Smith, M.
anthracene



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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS独特的内容合集



来源：

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

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

提纲

- 文献检索
- 物质检索
- 反应检索

高度互联的标引信息

☐ 10 Results

Sort: Relevance ▾ View: Partial Abstract ▾

☐ 1

Bimetallic MOF synergy molecularly imprinted ratiometric electrochemical sensor based on MXene decorated with polythionine for ultra-sensitive sensing of catechol 

By: Lu, Zhiwei; Wei, Kai; Ma, Hao; Duan, Rongtao; Sun, Mengmeng; Zou, Ping; Yin, Jiajian; Wang, Xianxiang; Wang, Yanying; Wu, Chun; et al

Analytica Chimica Acta (2023), 1251, 340983 | Language: English, Database: CAPlus and MEDLINE

Dual-signal ratiometric molecularly imprinted polymer (MIP) electrochem. sensors with bimetallic active sites and high-efficiency catalytic activity were fabricated for the sensing of catechol (CC) with high selectivity and sensitivity. The amino-functionalization bimetallic organic framework materials (Fe@Ti-MOF-NH₂), coupled with two-dimensional layered titanium carbide (MXene) co-modified glassy carbon electrode provides an expanded surface while amplifying the output signal through the electropolymerization immobilization of polythionine (pTHi) and MIP. The oxidation of CC and pTHi were pr...

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Full Text ▾

Substances (12)

Reactions (3)

Citing (35)

Citation Map

[CAS Concepts](#)

[MEDLINE® Medical Subject Headings](#)

[Supplementary Concepts](#)

[Substances](#)

[Reactions](#)

[Analytical Methods](#)

[Cited Documents](#)

文献中重要的研究点、物质和反应

CAS Concepts

Binding energy

Crystallinity

Electric current-potential relationship

Electric impedance

Electrochemical polymerization

Electron transfer

Faraday constant

Glassy carbon electrodes

Substances

87257-37-2

$(C_{12}H_{10}N_3S.Cl)_x$
 Phenothiazin-5-ium, 3,7-diamino-, chloride (1:1), homopolymer
 Role: Analytical Reagent Use, Properties, Synthetic Preparation, Technical or Engineered Material Use, Analytical Study, Uses, Preparation

30604-81-0

$(C_4H_5N)_x$
 1H-Pyrrole, homopolymer
 Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

12070-08-5

Image Not Available

CTi
 Titanium carbide (TiC)
 Role: Analytical Reagent Use, Properties, Synthetic Preparation, Analytical Study, Uses, Preparation
 Notes: multilayerd

10312-55-7

$C_8H_7NO_4$
 1,4-Benzenedicarboxylic acid, 2-amino-
 Role: Analytical Reagent Use, Properties, Synthetic Preparation, Analytical Study, Uses, Preparation
 Notes: titanium complexes

Reactions

31-614-CAS-35837877

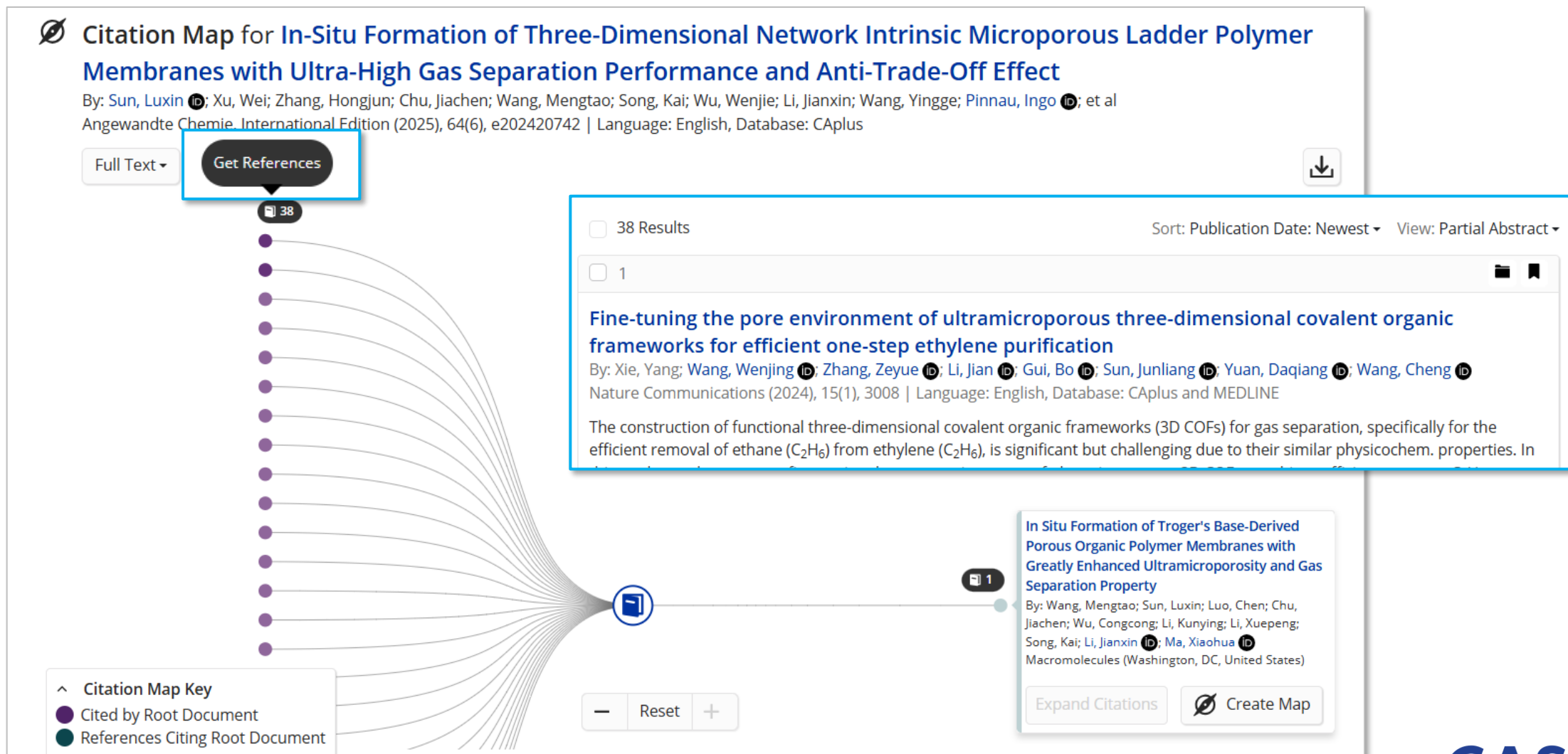
View Experimental Protocols
 Steps: 1
 1.1 Reagents: [Titanium tetrabutoxide](#)
 Solvents: [Methanol](#), [Dimethylformamide](#); 48 h, 150 °C

8

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引文地图



CAS标引的分析方法详情

■ Analysis of Catechol in Urine by Square wave voltammetry

CAS Method Number
1-143-CAS-551503

Method Category
Water / Wastewater / Sludge Analysis

Technique

Square wave voltammetry

Analyte

Catechol

Matrix

Urine
Drinking waters

Material

Glassy carbon electrodes
Titanium aluminum
carbide 200 mesh (Ti_2AlC)

Reagent

Methanol
Sodium hydroxide
Chitosan

Instructions

Preparation of urine samples

1. Collect human urine samples for analysis.
2. Centrifuge the samples to remove solid impurities and store in re
3. Dilute the samples 100 times with phosphate buffered saline (PBS) to a blank urine sample for quantitative analysis.

Preparation of water samples

1. Collect tap water samples for analysis.
2. Filter the samples using a cellulose filter membrane (pore size of 0.45 µm) for further use.

Preparation of amino-functionalized bimetallic organic framework (MOF)-NH₂)

1. Dissolve 0.675 g of ferric chloride hexahydrate, 0.44 g of 2-aminotriethylborane (TEBA) in a mixture solution of 36 mL of N,N-dimethylformamide (DMF) and 4 mL of acetic acid to form an orange-red homogeneous solution.
2. Place the above solution in a Teflon-lined stainless steel autoclave.
3. Cool to room temperature and wash the solid product continuously with distilled water.
4. Place under a vacuum drying oven at 60 °C to dry overnight to obtain the final product.

Preparation of two-dimensional layered titanium carbide (MXene)

1. Add 1 g Ti_3AlC_2 to 20 mL of hydrofluoric acid solution (40%) and stir at a frequency of 15 Hz.
2. Filter the obtained black Ti_3C_2 precipitate and disperse in 1 M sodium hydroxide for 60 min of ultrasound.
3. Wash the dispersion with ultrapure water several times.
4. Dry the filtered material under a vacuum oven at 80 °C overnight to obtain black MXene material.

Validation

Linearity Range 1.0 - 4000 μ M

Limit of $0.54 \mu\text{M}$

Recovery

100.85, 98.86, 96.45, 101.30 and 97.58% in 100, 200, 300, 400 and 500 μM spiked concentrations, respectively (Tap water)
98.37, 101.54, 98.38, 99.64 and 99.25% in 100, 200, 300, 400 and 500 μM spiked concentrations, respectively (Urine)

Precision

1.95% (RSD, reproducibility) at 100 μ M concentration

- ### Preparation of pol

- | | | |
|---|------------------|---|
| 1. Disperse 4 mg of MXene/Fe@Ti-MOF-NH ₂ /GCE respectively. | Recovery | 100.85, 98.86, 96.45, 101.30 and 97.58% in 100, 200, 300, 400 and 500 µg/L respectively (Tap water) |
| 2. Drop 10 µL of Fe solution (1:1), etc. | | 98.37, 101.54, 98.38, 99.64 and 99.25% in 100, 200, 300, 400 and 500 µg/L respectively (Urine) |
| 3. Drop 10 µL of pH 7.0 buffer solution | | |
| 4. Prepare 0.1 M phosphate buffer solution (pH 7.0) | Precision | 1.95% (RSD, reproducibility) at 100 µM concentration |
| 5. Immerse the prepared electrode (MXene/Fe@Ti-MOF-NH ₂ /GCE) in 10 mL of the above solution. | | |
| 6. Perform the cyclic voltammetry (CV) method from -0.4 V to 0.4 V for 20 cycles at a scan rate of 40 mV/s to obtain the electrochemical response of the electrode. | | |

Preparation of molecularly imprinted polymer (MIP)/pTHi/MXene/Fe@Ti-MOF-NH₂/GCE

1. Prepare MIP/pTHi/MXene/Fe@Ti-MOF-NH₂/GCE composite via electrochemical polymerization.
2. Immerse the electrode in 0.1 M PBS (pH 7.0) solution that contains 2 mM catechol (CC) and 2 mM pyrrole.
3. Incubate in dark for 15 min and then carry out CV method from -0.2 V to 0.8 V with 5 cycles at scan rate of 50 mV/s to obtain the pyrrole polymer membrane embedded with thionin and CC molecules.
4. Immerse the electrode in 0.5 M hydrochloric acid solution after electrochemical polymerization and stir slowly for 3 min.
5. Immerse in PBS solution (pH 7.0) with slow stirring for 2 h to completely remove CC and THi from the MIP membrane to form imprinted holes with specific recognition ability.
6. Prepare nonimprinted polymer (NIP) through the same method as MIP but without CC and THi in the electrolyte.

Square wave voltammetry (SWV) detection of catechol

1. Perform SWV analysis using a CHI660E electrochemical workstation (purchased from Chen Hua, Shanghai, China).
2. Use MIP/pThi/MXene/Fe@Ti-MOF-NH₂/GCE as working electrode, Ag/AgCl electrode as reference electrode and platinum wire electrode as counter electrode.
3. Carry out SWV analysis in 0.1 M PBS (pH 7.0) with successive addition of different concentration of catechol (urine or tap water samples) at an applied potential from -0.5 V to 0.8 V with an amplitude of 25 mV, a potential increment of 4 mV and a frequency of 15 Hz.

- 所用材料
- 仪器
- 实验条件
- 操作步骤
- 数据有效性

CAS标引的配方工艺与实验数据

Paclitaxel-Piperine Pharmaceutical Nanoparticles: Drug Delivery Systems or Antitumor Agents

 Save

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents, Drug delivery systems	paclitaxel, Homo sapiens, Mammary gland neoplasm, Ovary neoplasm, lungs cancer	Oral drug delivery systems	Particles	View

U.S. Pharmacopeia

Formulation Ingredients

Expand All Groups | Collapse All Groups

Component	Function	Amount Reported	Optionality
Group: paclitaxel nanoparticles	-	-	Mandatory
Paclitaxel	Antitumor agents	0.5 mg	Mandatory
Acrylic polymers	-	0.1 g	Mandatory
Water	Solvents	90 mL	Mandatory
Poly(vinyl alcohol)	Surfactants		
Piperine	bioenancers		

More Formulations like this...

Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
 Purpose: improving oral bioavailability...
 Target: Homo sapiens, paclitaxel
 Delivery Route: Oral drug delivery syst...
 Physical Form: Powders, nanosuspensi...

Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
 Purpose: improving oral bioavailability...
 Target: Homo sapiens, paclitaxel
 Delivery Route: Oral drug delivery syst...
 Physical Form: Powders, nanosuspensi...

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 Purpose: improving oral bioavailability...
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Oral Paclitaxel Nanosuspensions: Improving Oral Bioavailability or Inhibiting Intestinal P-GP Efflux
 Purpose: improving oral bioavailability...
 Target: Homo sapiens, paclitaxel
 Delivery Route: Oral drug delivery syst...
 Physical Form: Powders, nanosuspensi...

Process

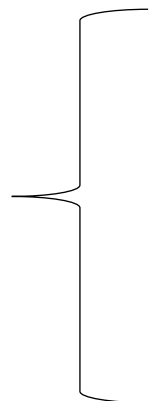
the paclitaxel-piperine pharmaceutical nanoparticles is prepared by: adding the Eudragit and drug which contain paclitaxel is dissolved in acetone to obtain the organic phase; pouring it into the aqueous phase having surfactant which is composed of polyvinyl alcohol and distilled water to produce the oil in water type emulsion; crushing it into the nanoparticles using sonicator-driven external energy; the organic solvent is evaporated during magnetic stirrer for 2 hours at 300 rpm under the atmospheric conditions to the obtain paclitaxel nanoparticles is prepared; the obtained paclitaxel nanoparticles are combined with piperine.

Experimental Activity

Descriptor	Notes	Details
area under curve(0-infinite)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-infinite).	12315.2 ± 916.3
area under curve(0-t)	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of area under curve(0-t).	10335.3 ng. h/mL ± 983.2 ng. h/mL
clearance rate of drug	the plasma concentration of paclitaxel after oral administration of nanoparticle to 10 rats, was evaluated in terms of clearance rate of drug (CL).	6.9 L/h ± 1.8 L/h
cytotoxicity test	the cytotoxic action of cell lines was determined by high throughput MTT assay and the cell growth was measured by calorimetric assay.	cell apoptosis and better anticancer activity.
drug diffusion	the drug diffusion of the composition was evaluated at 0.5 hours.	9.15 %
drug diffusion	the drug diffusion of the composition was evaluated at 1 hours.	9.55 %

提纲

- 文献检索
- 物质检索
- 反应检索

- 
- ✓ 获取关键词
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 - ✓ 高效筛选和追踪文献

关键词从哪里来？

1. **初步确定的关键词**：根据课题的研究方向和学科知识，提炼基本关键词进行初步检索
2. **积累文献中的关键词**：在初步检索的文献中积累相关的关键词

例如：来自标题、摘要、Keywords、Concept、物质标引信息、全文

3. **CAS Lexicon**：浏览CAS科学家标引的不同层级概念词和物质，拓展检索词
4. **精炼或扩展关键词**：基于初步检索到的文献，结合自己对课题本身的理解，锁定多个关键词，
进行组合检索

例如：专业术语、同义词/近义词、上下位概念词

一篇文献中的关键词

Highly Selective Inhibition of Tyrosine Kinase 2 (TYK2) for the Treatment of Autoimmune Diseases: Discovery of the Allosteric Inhibitor BMS-986165

97

234

230



Citation Map



In this Reference

Concepts ^

[CAS Concepts](#)

[MEDLINE MeSH](#)

[Supplementary Concepts](#)

[Substances](#)

[Reactions](#)

[Life Science Data](#) v

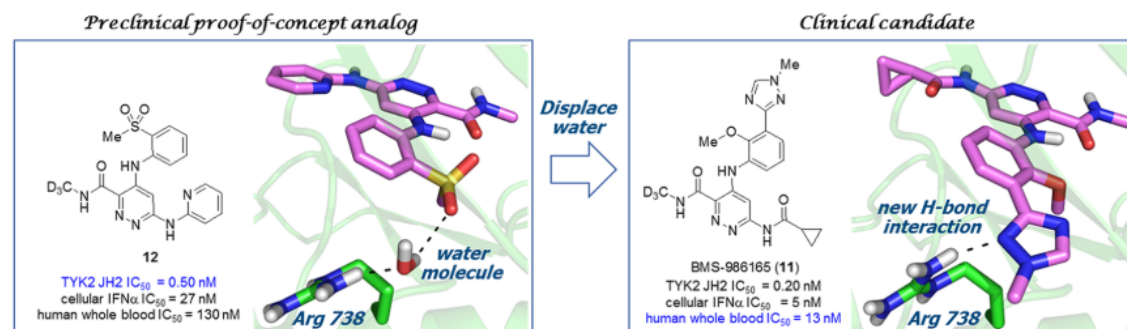
[Cited Documents](#)

By: Wroblewski, Stephen T. ; Moslin, Ryan ; Lin, Shuqun; Zhang, Yanlei; Spergel, Steven ; Kempson, James ; Tokarski, John S.; Strnad, Joann; Zupa-Fernandez, Adriana; Cheng, Lihong; et al

[View All](#) v

DOI: 10.1021/acs.jmedchem.9b00444

Small mol. JAK inhibitors have emerged as a major therapeutic advancement in treating autoimmune diseases. The discovery of isoform selective JAK inhibitors that traditionally target the catalytically active site of this kinase family has been a formidable challenge. Our strategy to achieve high selectivity for TYK2 relies on targeting the TYK2 pseudokinase (JH2) domain. Herein we report the late stage optimization efforts including a structure-guided design and water displacement strategy that led to the discovery of BMS-986165 (11, I) as a high affinity JH2 ligand and potent allosteric inhibitor of TYK2. In addition to unprecedented JAK isoform and kinome selectivity, I shows excellent pharmacokinetic properties with minimal profiling liabilities and is efficacious in several murine models of autoimmune disease. On the basis of these findings, I appears differentiated from all other reported JAK inhibitors and has been advanced as the first pseudokinase-directed therapeutic in clin. development as an oral treatment for autoimmune diseases.



- 标题
- 摘要
- Keywords
- Concepts

从文献结果集中获得概念词

Filter Behavior

Filter by Exclude

Search Within Results

Concept

CAS Content

CA Section

Publication Year

Language

Publication Name

Organization

Document Type

Author

Database

Formulation Purpose

Life Science Data

Concept

Top Count Alphanumeric Search

6 Selected

☐ Autoimmune disease (1,443)	☐ Pancreatic neoplasm (316)	☐ Kidney neoplasm (232)
☐ Homo sapiens (1,389)	☐ Lung neoplasm (314)	☐ Interleukin 6 (231)
☐ Human (1,389)	☐ Antibodies and Immunoglobulins (313)	☐ Antiviral agents (229)
☐ Antitumor agents (1,084)	☒ Tyrosine kinase inhibitors (312)	☐ Myasthenia gravis (228)
☐ Neoplasm (995)	☐ Transplant rejection (305)	☒ Alzheimer disease (224)
☐ Inflammation (918)	☐ Proliferative disorders (303)	☐ Antiangiogenic agents (224)
☐ Anti-inflammatory agents (864)	☒ Diabetes mellitus (291)	☒ Chronic obstructive pulmonary disease (224)
☐ Rheumatoid arthritis (783)	☒ Tyrosine kinase receptor FLT3 (289)	☐ Atherosclerosis (223)
☐ Immunomodulators (603)		☐ B cell (220)

利用CAS Lexicon拓展检索词

References Suppliers

Patent Number, PubMed ID, AN, CAN, and/or

e, first name middle name.

 **Search CAS Lexicon**
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Search CAS Lexicon [Learn more about CAS Lexicon searching.](#)

Neoplasm

^ Preferred Concept

☒ Neoplasm

This will search synonyms: Animal tumors; MeSH ID: D009370; Neoplasia; **Neoplasm** by histologic type; **Neoplasm** by site; Neoplastic disease; Neoplastic disorder; Neoplastic disorders; Oncological disease; Oncological diseases; Oncological disorder; Oncologic disorder; Organ, **neoplasm**; Organ tumors; Tumor cell; Tumor cells; Tumor disease; Tumors (animal); Tumour; Tumours
[View fewer synonyms](#)

^ Broader Concepts (1) [Select All](#)

☐ Proliferative disorders

^ Narrower Concepts (76) [Select All](#)

☐ Abdominal neoplasm

☐ Acanthoma

☐ Adenolymphoma

☐ Ascitic neoplasm

☐ Benign neoplasm

Personalized medicine - Preferred Concept

AND [Remove All](#)

Neoplasm - Preferred Concept

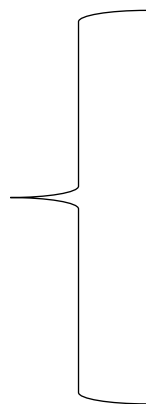
添加主题词

一键获取关联文献

AND OR NOT

提纲

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灵活缩放检索式——逻辑算符和通配符的使用

示例:

“tyrosine kinase 2” OR “TYK2” AND inhibitors AND autoimmun* (524)

“tyrosine kinase 2” OR “TYK2” AND inhibitors AND biomarker (118)

References search for "tyrosine kinase 2" OR "TYK2" AND inhibitors AND autoimmun*

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results. [Learn about result relevance.](#)

[Load All Results](#)

524 Results Sort: Relevance View: Partial Abstract

1

Discovery of Tyrosine Kinase 2 (TYK2) Inhibitor (PF-06826647) for the Treatment of Autoimmune Diseases

By: Gerstenberger, Brian S.; Ambler, David; Alpay, Dowty, Martin E.; Fensome, Andrew; Vincent, Michael; et al

Journal of Medicinal Chemistry (2020), 63(1), 1-12

Heterocycle core electrostatic potential map

Engineered polar C-H hydrogen bond to Val 981

PF-06826647 / TYK2

was accomplished through computational chemistry

[View More](#)

[Full Text](#)

References search for "tyrosine kinase 2" OR "TYK2" AND inhibitors AND biomarker

Substances Reactions Citing Knowledge Graph

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118 Results Sort: Relevance View: Partial Abstract

1

The Safety, Tolerability, Pharmacokinetics, and Pharmacodynamics of a TYK2/JAK1 Inhibitor (PF-06700841) in Healthy Subjects and Patients With Plaque Psoriasis

By: Banfield, Christopher; Scaramozza, Matthew; Zhang, Weidong; Kieras, Elizabeth; Page, Karen M.; Fensome, Andrew; Vincent, Michael; Dowty, Martin E.; Goteti, Kosalaram; Winkle, Peter J.; et al

Journal of Clinical Pharmacology (2018), 58(4), 434-447 | Language: English, Database: CAlplus and MEDLINE

The safety, tolerability, pharmacokinetics, and pharmacodynamics of PF-06700841 were assessed in a randomized, double-blind, placebo-controlled, single- and multiple-dose escalation, parallel-group study in healthy subjects and patients with plaque psoriasis. The single ascending dose (1, 3, 10, 30, 100, or 200 mg) and multiple ascending dose (MAD; PF-06700841; up to 175 mg once daily or 50 mg twice daily for 10 days) periods included 54 healthy participants. In addition, 30 patients with psoriasis received PF-06700841 30 or 100 mg or placebo once daily for 28 days. Single PF-06700841 doses were well tolerated. The pharmacokinetics of PF-06700841 were consistent across the dose range. The pharmacodynamics of PF-06700841 were consistent across the dose range. The safety, tolerability, pharmacokinetics, and pharmacodynamics of PF-06700841 were assessed in a randomized, double-blind, placebo-controlled, single- and multiple-dose escalation, parallel-group study in healthy subjects and patients with plaque psoriasis. The single ascending dose (1, 3, 10, 30, 100, or 200 mg) and multiple ascending dose (MAD; PF-06700841; up to 175 mg once daily or 50 mg twice daily for 10 days) periods included 54 healthy participants. In addition, 30 patients with psoriasis received PF-06700841 30 or 100 mg or placebo once daily for 28 days. Single PF-06700841 doses were well tolerated. The pharmacokinetics of PF-06700841 were consistent across the dose range. The pharmacodynamics of PF-06700841 were consistent across the dose range.

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Substances (5) Reactions (0) Citing (72) Citation Map

锁定研究了目标结构的文献

同时识别关键词与结构式

CAS SciFinder

References Organic photovoltaic cell

References search for "Organic photovoltaic cell" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match

As Drawn (0)

Substructure (1,877)

Filter Behavior

Filter by Exclude

Search Within Results

Publication Year

Language

Publication Name

1,877 Results

1

Fused-Ring Acceptors with Asymmetric Side Chains for High-Performance Solar Cells

By: Feng, Shiyu; Zhang, Cai-e; Liu, Yahui; Bi, Zhaozhao; Zhang, Zhe; Xu, Xinjun; Advanced Materials (Weinheim, Germany) (2017), 29(42), n/a | Language: English

A kind of new fused-ring electron acceptor, IDT-OB, bearing asym. side chains, is introduced. The introduction of asym. side chains can increase the solubility of acceptors, and devices exhibit high and balanced hole and electron mobility and give a high power conversion efficiency. Importantly, the IDT-OB-based devices are not very sensitive to the film thickness.

View More

Full Text

Substances (17)

2213434-11-6

C76H86N4O2S2

Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

Notes: electron acceptor with asym. fused ring side chain

2213434-10-5

C84H86N4O2S2

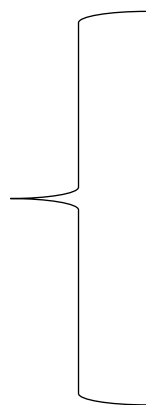
Propanedinitrile, 2,2'-[[4,9-bis(4-hexylphenyl)-4,9-dihydro-4,9-dioctyl-s-indace...

Role: Properties, Synthetic Preparation, Technical or Engineered Material Use, Preparation, Uses

Notes: electron acceptor with asym. fused ring side chain

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丰富的筛选工具

文献类型、语言、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、下载数据分析报告...

Filter Behavior

Filter by Exclude

^ Search Within Results

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

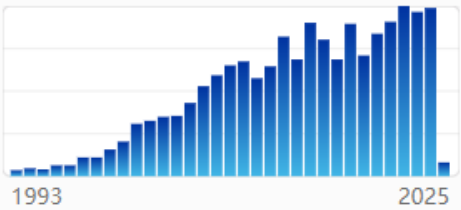
Enter a query...

Search

Searching for... [Clear All](#)

Signal transduction ×

^ Publication Year



1993 2025

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^ Language

^ Publication Name

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☐ Pharmacology (1,541)

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☒ Immunochemistry (112)

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☒ Formulations (83)

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In-Situ Formation of Three-Dimensional Network Intrinsic Microporous Ladder Polymer Membranes with Ultra-High Gas Separation Performance and Anti-Trade-Off Effect

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Publication Year

Language

Publication Name

Filtering: Publication Year: 2020 to No Ma

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The e13a3 (b2a3) and e14a3 (b3a3)

By: Leske, Inga B. ; Hantschel, Oliver

Leukemia (2024), 38(9), 2041-2045 | Language

Asciminib is a first-in-class allosteric **BCR::AB**

(Ph) chromosome-pos. chronic myeloid leuke

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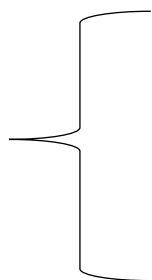
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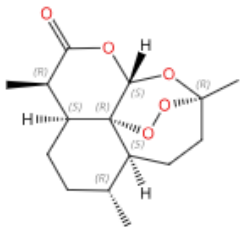
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✓ 生物学数据

谱图信息

☐ 1

63968-64-9



Absolute stereochemistry shown

$C_{15}H_{22}O_5$

3,12-Epoxy-12H-pyrano[4,3-j]-1,
2-benzodioxepin-10(3H)-one,
octahydro-3,6,9-trime...

 9,268
References

 3,039
Reactions

 101
Suppliers

Expand All | Collapse All

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Other Names and Identifiers

Experimental Properties

Experimental Spectra

Pharmacological Data

ADME

Toxicity

Predicted Properties

Predicted Spectra

Bioactivity Indicators

Target Indicators

Regulatory Information

GHS Hazard Statements

Additional Details

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谱图信息

核磁、红外、质谱、拉曼、红外、UV-vis、X-Ray等

Experimental Spectra

1H NMR

13C NMR

Hetero NMR

IR

Mass

Raman

UV and Visible

Additional Spectra

View Carbon-13 NMR Spectrum (Image Available)

View Carbon-13 NMR Spectrum (Image Available)

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

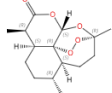
View Carbon-13 NMR Spectrum

View Carbon-13 NMR Spectrum

Carbon-13 NMR Spectrum - 8 Sources

Sources

63968-64-9



Absolute stereochemistry shown

C₁₅H₂₂O₅

CAS Name

3,12-Epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

Conditions

Solvent

Chloroform-d (865-49-6)

Spectrum Summary

Spectrum ID

12NTPR01_75.C

Peak Data

171.9, 105.2, 93.6, 79.4, 49.9, 44.8, 37.4, 35.8, 33.5, 32.8, 25.1, 24.8, 23.3, 19.7, 12.5 ppm

Solvent

Chloroform-d

Source

(1) ACD



生物学数据信息

Structure Activity Relationships

CAS LIFE SCIENCES

Clear All Filters Knowledge Graph

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Multidrug 1		IC50			HOMO SAPIENS	View Detail	(1) CAS

Filter Target

- ☒ Multidrug resistance protein 1 (265)
- ☐ Fibroblast growth factor receptor 1 (155)
- ☐ P-glycoprotein (45)
- ☐ ATP-dependent translocase ABCB1 (40)

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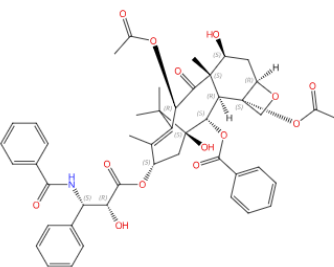
Filter Parameter

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- ☐ RATIO (65)
- ☐ Change (7)
- ☐ GI50 (6)
- ☐ RELATIVE RESISTANCE (6)

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Assay Data

Ligand 33069-62-4



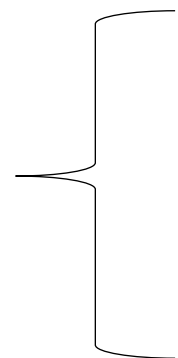
C₄₇H₅₁NO₁₄
Benzenepropanoic acid, β-(benzoylamino)-α-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS,12cS,12dS,12eS,12fS,12gS,12hS,12iS,12jS,12kS,12lS,12mS,12nS,12oS,12pS,12qS,12rS,12sS,12tS,12uS,12vS,12wS,12xS,12yS,12zS,12a1S,12b1S,12c1S,12d1S,12e1S,12f1S,12g1S,12h1S,12i1S,12j1S,12k1S,12l1S,12m1S,12n1S,12o1S,12p1S,12q1S,12r1S,12s1S,12t1S,12u1S,12v1S,12w1S,12x1S,12y1S,12z1S,12a2S,12b2S,12c2S,12d2S,12e2S,12f2S,12g2S,12h2S,12i2S,12j2S,12k2S,12l2S,12m2S,12n2S,12o2S,12p2S,12q2S,12r2S,12s2S,12t2S,12u2S,12v2S,12w2S,12x2S,12y2S,12z2S,12a3S,12b3S,12c3S,12d3S,12e3S,12f3S,12g3S,12h3S,12i3S,12j3S,12k3S,12l3S,12m3S,12n3S,12o3S,12p3S,12q3S,12r3S,12s3S,12t3S,12u3S,12v3S,12w3S,12x3S,12y3S,12z3S,12a4S,12b4S,12c4S,12d4S,12e4S,12f4S,12g4S,12h4S,12i4S,12j4S,12k4S,12l4S,12m4S,12n4S,12o4S,12p4S,12q4S,12r4S,12s4S,12t4S,12u4S,12v4S,12w4S,12x4S,12y4S,12z4S,12a5S,12b5S,12c5S,12d5S,12e5S,12f5S,12g5S,12h5S,12i5S,12j5S,12k5S,12l5S,12m5S,12n5S,12o5S,12p5S,12q5S,12r5S,12s5S,12t5S,12u5S,12v5S,12w5S,12x5S,12y5S,12z5S,12a6S,12b6S,12c6S,12d6S,12e6S,12f6S,12g6S,12h6S,12i6S,12j6S,12k6S,12l6S,12m6S,12n6S,12o6S,12p6S,12q6S,12r6S,12s6S,12t6S,12u6S,12v6S,12w6S,12x6S,12y6S,12z6S,12a7S,12b7S,12c7S,12d7S,12e7S,12f7S,12g7S,12h7S,12i7S,12j7S,12k7S,12l7S,12m7S,12n7S,12o7S,12p7S,12q7S,12r7S,12s7S,12t7S,12u7S,12v7S,12w7S,12x7S,12y7S,12z7S,12a8S,12b8S,12c8S,12d8S,12e8S,12f8S,12g8S,12h8S,12i8S,12j8S,12k8S,12l8S,12m8S,12n8S,12o8S,12p8S,12q8S,12r8S,12s8S,12t8S,12u8S,12v8S,12w8S,12x8S,12y8S,12z8S,12a9S,12b9S,12c9S,12d9S,12e9S,12f9S,12g9S,12h9S,12i9S,12j9S,12k9S,12l9S,12m9S,12n9S,12o9S,12p9S,12q9S,12r9S,12s9S,12t9S,12u9S,12v9S,12w9S,12x9S,12y9S,12z9S,12a10S,12b10S,12c10S,12d10S,12e10S,12f10S,12g10S,12h10S,12i10S,12j10S,12k10S,12l10S,12m10S,12n10S,12o10S,12p10S,12q10S,12r10S,12s10S,12t10S,12u10S,12v10S,12w10S,12x10S,12y10S,12z10S,12a11S,12b11S,12c11S,12d11S,12e11S,12f11S,12g11S,12h11S,12i11S,12j11S,12k11S,12l11S,12m11S,12n11S,12o11S,12p11S,12q11S,12r11S,12s11S,12t11S,12u11S,12v11S,12w11S,12x11S,12y11S,12z11S,12a12S,12b12S,12c12S,12d12S,12e12S,12f12S,12g12S,12h12S,12i12S,12j12S,12k12S,12l12S,12m12S,12n12S,12o12S,12p12S,12q12S,12r12S,12s12S,12t12S,12u12S,12v12S,12w12S,12x12S,12y12S,12z12S,12a13S,12b13S,12c13S,12d13S,12e13S,12f13S,12g13S,12h13S,12i13S,12j13S,12k13S,12l13S,12m13S,12n13S,12o13S,12p13S,12q13S,12r13S,12s13S,12t13S,12u13S,12v13S,12w13S,12x13S,12y13S,12z13S,12a14S,12b14S,12c14S,12d14S,12e14S,12f14S,12g14S,12h14S,12i14S,12j14S,12k14S,12l14S,12m14S,12n14S,12o14S,12p14S,12q14S,12r14S,12s14S,12t14S,12u14S,12v14S,12w14S,12x14S,12y14S,12z14S,12a15S,12b15S,12c15S,12d15S,12e15S,12f15S,12g15S,12h15S,12i15S,12j15S,12k15S,12l15S,12m15S,12n15S,12o15S,12p15S,12q15S,12r15S,12s15S,12t15S,12u15S,12v15S,12w15S,12x15S,12y15S,12z15S,12a16S,12b16S,12c16S,12d16S,12e16S,12f16S,12g16S,12h16S,12i16S,12j16S,12k16S,12l16S,12m16S,12n16S,12o16S,12p16S,12q16S,12r16S,12s16S,12t16S,12u16S,12v16S,12w16S,12x16S,12y16S,12z16S,12a17S,12b17S,12c17S,12d17S,12e17S,12f17S,12g17S,12h17S,12i17S,12j17S,12k17S,12l17S,12m17S,12n17S,12o17S,12p17S,12q17S,12r17S,12s17S,12t17S,12u17S,12v17S,12w17S,12x17S,12y17S,12z17S,12a18S,12b18S,12c18S,12d18S,12e18S,12f18S,12g18S,12h18S,12i18S,12j18S,12k18S,12l18S,12m18S,12n18S,12o18S,12p18S,12q18S,12r18S,12s18S,12t18S,12u18S,12v18S,12w18S,12x18S,12y18S,12z18S,12a19S,12b19S,12c19S,12d19S,12e19S,12f19S,12g19S,12h19S,12i19S,12j19S,12k19S,12l19S,12m19S,12n19S,12o19S,12p19S,12q19S,12r19S,12s19S,12t19S,12u19S,12v19S,12w19S,12x19S,12y19S,12z19S,12a20S,12b20S,12c20S,12d20S,12e20S,12f20S,12g20S,12h20S,12i20S,12j20S,12k20S,12l20S,12m20S,12n20S,12o20S,12p20S,12q20S,12r20S,12s20S,12t20S,12u20S,12v20S,12w20S,12x20S,12y20S,12z20S,12a21S,12b21S,12c21S,12d21S,12e21S,12f21S,12g21S,12h21S,12i21S,12j21S,12k21S,12l21S,12m21S,12n21S,12o21S,12p21S,12q21S,12r21S,12s21S,12t21S,12u21S,12v21S,12w21S,12x21S,12y21S,12z21S,12a22S,12b22S,12c22S,12d22S,12e22S,12f22S,12g22S,12h22S,12i22S,12j22S,12k22S,12l22S,12m22S,12n22S,12o22S,12p22S,12q22S,12r22S,12s22S,12t22S,12u22S,12v22S,12w22S,12x22S,12y22S,12z22S,12a23S,12b23S,12c23S,12d23S,12e23S,12f23S,12g23S,12h23S,12i23S,12j23S,12k23S,12l23S,12m23S,12n23S,12o23S,12p23S,12q23S,12r23S,12s23S,12t23S,12u23S,12v23S,12w23S,12x23S,12y23S,12z23S,12a24S,12b24S,12c24S,12d24S,12e24S,12f24S,12g24S,12h24S,12i24S,12j24S,12k24S,12l24S,12m24S,12n24S,12o24S,12p24S,12q24S,12r24S,12s24S,12t24S,12u24S,12v24S,12w24S,12x24S,12y24S,12z24S,12a25S,12b25S,12c25S,12d25S,12e25S,12f25S,12g25S,12h25S,12i25S,12j25S,12k25S,12l25S,12m25S,12n25S,12o25S,12p25S,12q25S,12r25S,12s25S,12t25S,12u25S,12v25S,12w25S,12x25S,12y25S,12z25S,12a26S,12b26S,12c26S,12d26S,12e26S,12f26S,12g26S,12h26S,12i26S,12j26S,12k26S,12l26S,12m26S,12n26S,12o26S,12p26S,12q26S,12r26S,12s26S,12t26S,12u26S,12v26S,12w26S,12x26S,12y26S,12z26S,12a27S,12b27S,12c27S,12d27S,12e27S,12f27S,12g27S,12h27S,12i27S,12j27S,12k27S,12l27S,12m27S,12n27S,12o27S,12p27S,12q27S,12r27S,12s27S,12t27S,12u27S,12v27S,12w27S,12x27S,12y27S,12z27S,12a28S,12b28S,12c28S,12d28S,12e28S,12f28S,12g28S,12h28S,12i28S,12j28S,12k28S,12l28S,12m28S,12n28S,12o28S,12p28S,12q28S,12r28S,12s28S,12t28S,12u28S,12v28S,12w28S,12x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提纲

物质

-物质详情

-检索方法

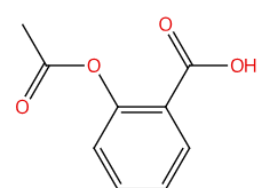
- 
- ✓ 标识符、分子式
 - ✓ 属性值、谱图数值
 - ✓ 结构检索
 - ✓ 序列检索

物质的检索策略

Search interface showing results for **Aspirin** (50-78-2).

Navigation: All | Substances | Reactions | References | Suppliers

50-78-2



C9H8O4
Aspirin

92K | 2,311 | 110 | View Spectra

Key Physical Properties

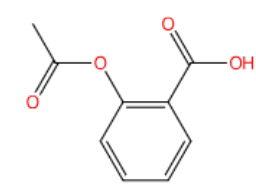
Molecular Weight 180.16	Melting Point 135 °C	Boiling Point 145-150 °C Press: 3 Torr	Density 1.40 g/cm³
-----------------------------------	--------------------------------	---	---

pKa (Predicted)
3.482±0.10
Most Acidic Temp: 25 °C

Search interface showing results for **50-78-2**.

Navigation: All | Substances

50-78-2



C9H8O4
Benzoic acid, 2-(acetyloxy)-

92K | 2,311 | 110

References | Reactions | Suppliers

Search interface showing results for **Al.Ca.Na.O**.

Navigation: All | Substances | Reactions

Al.Ca.Na.O

AND | Molecular Formula

44 Results

12004-54-5

Component	Ratio
O	9
Ca	4
Al	3
Na	1

Al.Ca.Na.O
Components: 4
Aluminum calcium sodium oxide (Al3Ca4NaO9)

54 | 0 | 0

References | Reactions | Suppliers

64764-01-8

Component	Ratio
O	x
Ca	x
Na	x
Al	x

Al.Ca.Na.O
Components: 4
Aluminum calcium sodium oxide

28 | 0 | 0

References | Reactions | Suppliers

利用属性值、谱图数值检索物质

Navigation: All Substances Reactions References Suppliers

Search by Substance Name, CAS RN, Patent Number, Pub

Filters:

- Molecular Weight: 220 to 280 (Predicted values only.)
- AND pKa: 1.3 to 1.8 (Predicted values only.)
- AND Carbon-13 NMR: 114 to 171, 96, 11.5 (Allowance of ± 2 ppm.)

Filter Behavior

Filter by Exclude

Search Within Results

Reference Role

Substance Class

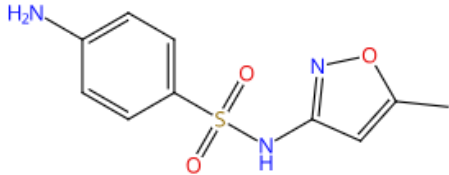
Aromatic Rings

- ☐ No aromaticity (5)
- ☐ 1 (38)
- ☐ 2 (31)
- ☐ 3 (12)

86 Results Sort: Number of Ref

1

723-46-6



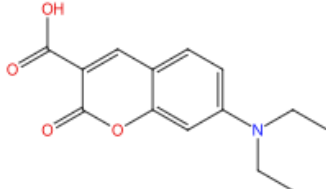
Cc1cc2nc(NC(=O)c3ccc(N)cc3)oc2

$C_{10}H_{11}N_3O_3S$
Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)-

30K References 1,046 Reactions 112 Suppliers

2

50995-74-9



CCN(CC)c1ccc2c(c1)oc(=O)c(=O)c2C(=O)O

$C_{14}H_{15}NO_4$
2*H*-1-Benzopyran-3-carboxylic acid, 7-(diethylamino)-2-oxo-

744 References 985 Reactions 84 Suppliers

结构检索

R1 Co, Ni, Cu, Pd, Rh, Fe

Filter Behavior

Filter by Exclude

Search Within Results

Substance Class

☒ Coordination Compound (32)

☐ Salt and Compound With (1)

Reference Role

Reaction Role

☐ Product (60)

☐ Reactant (32)

☐ Reagent (11)

☒ Catalyst (32)

☐ Solvent (1)

Aromatic Rings

Functional Group

Element

4

33991-60-5

$C_{36}H_{30}NiP_2$
Bis(triphenylphosphine)nickel

47 References 24 Reactions 0 Suppliers

5

33775-59-6

$C_{36}H_{30}NiP_2$
Bis(triphenylphosphine)nickel(2+)

3 References 1 Reaction 0 Suppliers

7

24355-89-3

$C_{36}H_{30}CuP_2$

8

69878-70-2

$C_{36}H_{30}P_2Pd_2$

Markush检索

CAS SciFinder[®]

← Return to Home

Substances search for

References Reactions

Structure Match

As Drawn (0)

Substructure (0)

Similarity (127K)

CAS SciFinder[®]

Substances Enter a query...

Edit

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (1)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

CA Section

Filter Content Report

1 Result

1

WO2018062978

Preparation of heteroaryl compounds as antiviral agents

By: Min, Ji Young; Chang, So Young; Lee, Ji Hye; Kang, Sun Hee; Kong, Sun Ju; Jo, Su Yeon; Park, Kaapjoo; Kim, Young Mi; Choi, Junghwan

World Intellectual Property Organization, WO2018062978 A1 2018-04-05 | Language: Korean, Database: CAplus

Assignee: Institut Pasteur Korea

Patent claim 1

PatentPak Full Text

substd. by G16

Search Patent Markush

Chemical structure diagram of a heteroaryl compound, showing a pyridine ring connected to a benzene ring, which is further connected to a pyrazole ring, and finally to a phenyl ring.

Patent	Language	Kind Code	PatentPak Options
WO2018062978	Korean	A1	PDF PDF+ Viewer
KR2018036415	Korean	A	PDF PDF+ Viewer
US20200031816	English	A1	PDF
US11149033	English	B2	PDF

序列检索

Search CAS Sequences

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BLAST

CDR

Motif

Clear Search

ucacuuucauaaugcugg

例：寡核苷酸 ucacuuucauaaugcugg

Advanced Sequence Search

Upload Sequence (.fasta or .txt)

Sequence Type:

Nucleotide

Protein

Search Within:

Nucleotides

Proteins

Include NCBI Sequences

Search Sequences

Substance Detail

Reference (1)

Reactions (0)

Suppliers (0)

CAS Registry Number
2307521-26-0

Unspecified

Not Yet Assigned

Nucleic Acid Sequence
Sequence Length: 18
4 a, 4 c, 3 g, 7 u
modified

Related Sequences (118)

Sequence Modifications					
Type	修饰类型	Location	修饰位点	修饰详情	Description
	modified base		uridine-1		m5u
	modified base		uridine-1		2'-moe
	modified base		cytidine-2		m5c
	modified base		cytidine-2		2'-moe
	modified base		adenosine-3		2'-moe

提纲

反应

- 检索方法
- 逆合成设计

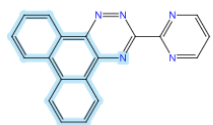
合成反应操作详情

CAS Reaction Number: 31-289-CAS-15718311

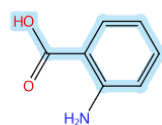
Get Similar Reactions



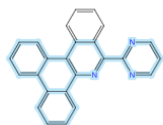
Save



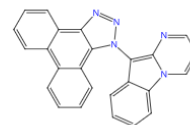
+



→



+



Suppliers (46)

Experimental Protocols



Synthetic Methods (7)

Procedure

1. Suspend 3-(pyrimidine-2-yl)phenanthro[9,10-e]-1,2,4-triazole
2. Add isoamyl nitrite (0.47 ml, 3.5 mmol) to the mixture.
3. Stir the resulting mixture under reflux.
4. Add a solution of corresponding anthranilic acid (3.5 mmol) dropping funnel for 30 minutes.
5. Heat the reaction mixture under reflux for 1 hour.
6. Cool the reaction mixture to room temperature.
7. Wash the reaction mixture with potassium hydroxide solution.
8. Dry the reaction mixture with anhydrous sodium sulfate.
9. Concentrate the crude product under reduced pressure.
10. Dry the crude product under vacuum.
11. Separate the crude product by column chromatography (Si (1:2) as eluent).

Characterization Data

1H-Phenanthro[9,10-d]-1,2,3-triazole, 1-pyrimido[1,2-a]indol-10-yl-

Proton NMR Spectrum

δ , ppm (CDCl₃): 6.70 (dd, 1H, J 7.1, 3.7 Hz, H-3 (pyrimidoindole)), 7.19 (m, 1H), 7.42-7.61 (m, 5H), 7.72 (m, 1H), 7.80 (m, 1H), 8.04 (m, 1H), 8.35 (dd, 1H, J 3.7, 2.0 Hz, H-4 (pyrimidoindole)), 8.67 (m, 1H), 8.71 (m, 1H), 8.79 (dd, 1H, J 7.1, 2.0 Hz, H-2 (pyrimidoindole)), 8.97 (dd, 1H, J 8.1, 0.9 Hz).

Carbon-13 NMR

δ , ppm (CDCl₃): 101.9, 105.6, 110.9, 118.4, 120.8, 122.5, 122.7, 123.1, 123.4, 124.0, 125.0, 125.4, 125.7, 125.9, 126.9, 127.0, 127.6, 128.1, 129.1, 130.5, 131.2, 131.9, 138.1, 141.4, 151.8.

Elemental Analysis

Calcd for C₂₅H₁₅N₅: C 77.91; H 3.92; N 18.17. Found: C 77.80; H 3.81; N 17.98.

Mass Spectrum

ESI-MS, m/z : found 386.14, calculate 386.14 (M+H)⁺.

Melting Point

181-183°C.

R_f

0.8.

反应检索方法

Navigation: All Substances **Reactions** References Suppliers For You NEW

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

Draw

Reactions search for "29022-11-5"

References

Filter Behavior: Filter by Exclude

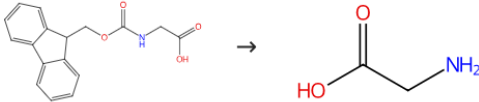
Search Within Results: Yield

- 90-100% (2,064)
- 80-89% (1,119)
- 70-79% (1,098)

93,626 Results

Group: By Scheme Sort: Publication Date: Oldest View: Expanded

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



Reactions search for "10.1002/adfm.201200729"

References

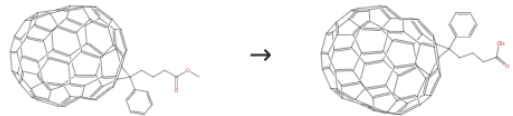
Filter Behavior: Filter by Exclude

Search Within Results: Yield Reaction Scale Number of Steps

3 Results

Group: By Scheme Sort: Publication Date: Oldest View: Expanded

Scheme 1 (1 Reaction) Steps: 1 Yield: 63%



Suppliers (60)

1

910463-68-2

Image Not Available

Unspecified Semaglutide

Protein/Peptide Sequence
Sequence Length: 34

1,527 References 259 Reactions 32 Suppliers

利用自然语言便捷检索反应

Reactions search for "synthesis of paclitaxel from acetic anhydride"

References

醋酸酐合成紫杉醇

258 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (10 Reactions) Steps: 1 Yield: 85-96%

Absolute stereochemistry shown

Suppliers (65)

31-355-CAS-20587342

1.1 Reagents: [Hexamethyldisilane](#)
Catalysts: [4-\(Dimethylamino\)pyridine](#)
Solvents: [Acetonitrile](#); rt

1.2 Reagents: [Hydrochloric acid](#)
Solvents: [Water](#); rt

Filter Behavior

Filter by Exclude

Search Within Results

Non-Participating Functional Groups

Experimental Protocols

Catalyst

Number of Steps

Reaction Type

Yield

90-100% (2)

80-89% (3)

Reactions search for "suzuki coupling reaction"

References

Suzuki偶联反应

1,391,065 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (20 Reactions) Steps: 1 Yield: 98-100%

Suppliers (119)

Suppliers (68)

Suppliers (41)

31-179-CAS-12086025 Steps: 1 Yield: 100%

1.1 Reagents: [Potassium carbonate](#)
Catalysts: [\(SP-4-1\)-Bis\(acetato-κO\)bis\(N"-butyl-N,N,N',N'-tetramethylguanidine-κN"\)palladium\(II\) chloride](#)
Solvents: [Ethanol](#), [Water](#); 20 h, 80 °C

Experimental Protocols

Full Text

Guanidine/Pd(OAc)₂-Catalyzed Room Temperature Suzuki Cross-Coupling Reaction in Aqueous Media under Aerobic Conditions

By: Li, Shenghai; et al

Journal of Organic Chemistry (2007), 72(11), 4067-4072

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Reaction Scale

Milligram (117K)

Gram (31K)

Kilogram (89)

No Scale Provided (1.2M)

Reaction Notes

Microwave Irradiation (155K)

Thermal (59K)

Chemoselective (56K)

结构式检索

Reactions search for drawn structure

References ▾

Structure Match

As Drawn (0)

Substructure (472)

Similarity (0)

Filter Behavior

Filter by Exclude

- Search Within Results
- Yield
- Reaction Scale
- Reaction Notes
- Number of Steps
- Catalyst

472 Results

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

Scheme 1 (1 Reaction) Steps: 1 Yield: 91% ●●●

31-087-CAS-17090818 Steps: 1 Yield: 91% ●●●

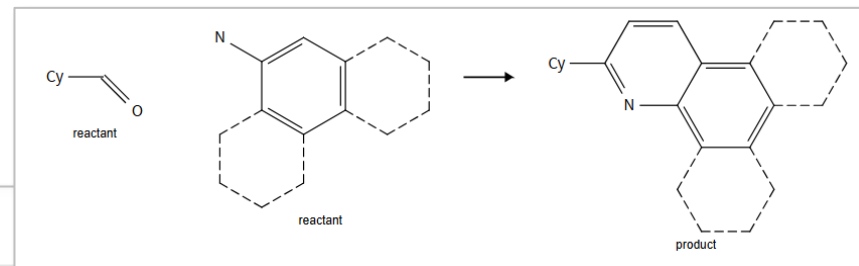
1.1 Reagents: [Phosphorus oxychloride](#)
Solvents: [Nitrobenzene](#); 4 h, reflux

Preparation benzothiophene-fused heterocyclic compound for organic light emitting device
Assignees: Heesung Material Ltd.; LT Materials Co., Ltd.
Korea, Republic of, KR2016051212 A 2016-05-11

PatentPak ▾ Full Text ▾

Collapse Scheme ^

Scheme 2 (1 Reaction) Steps: 1 Yield: 91% ●●●



高效筛选目标反应

反应筛选类别：产率、规模、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

Filter Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Reaction Notes

Number of Steps

Catalyst

Reagent

Solvent

Experimental Protocols

Non-Participating Functional Groups

Reaction Mapping

Reaction Type

Commercial Availability

Source Reference

Document Type

Language

Publication Year

Organization

Publication Name

CA Section

Filter Content Report

Download filter data from this result set.



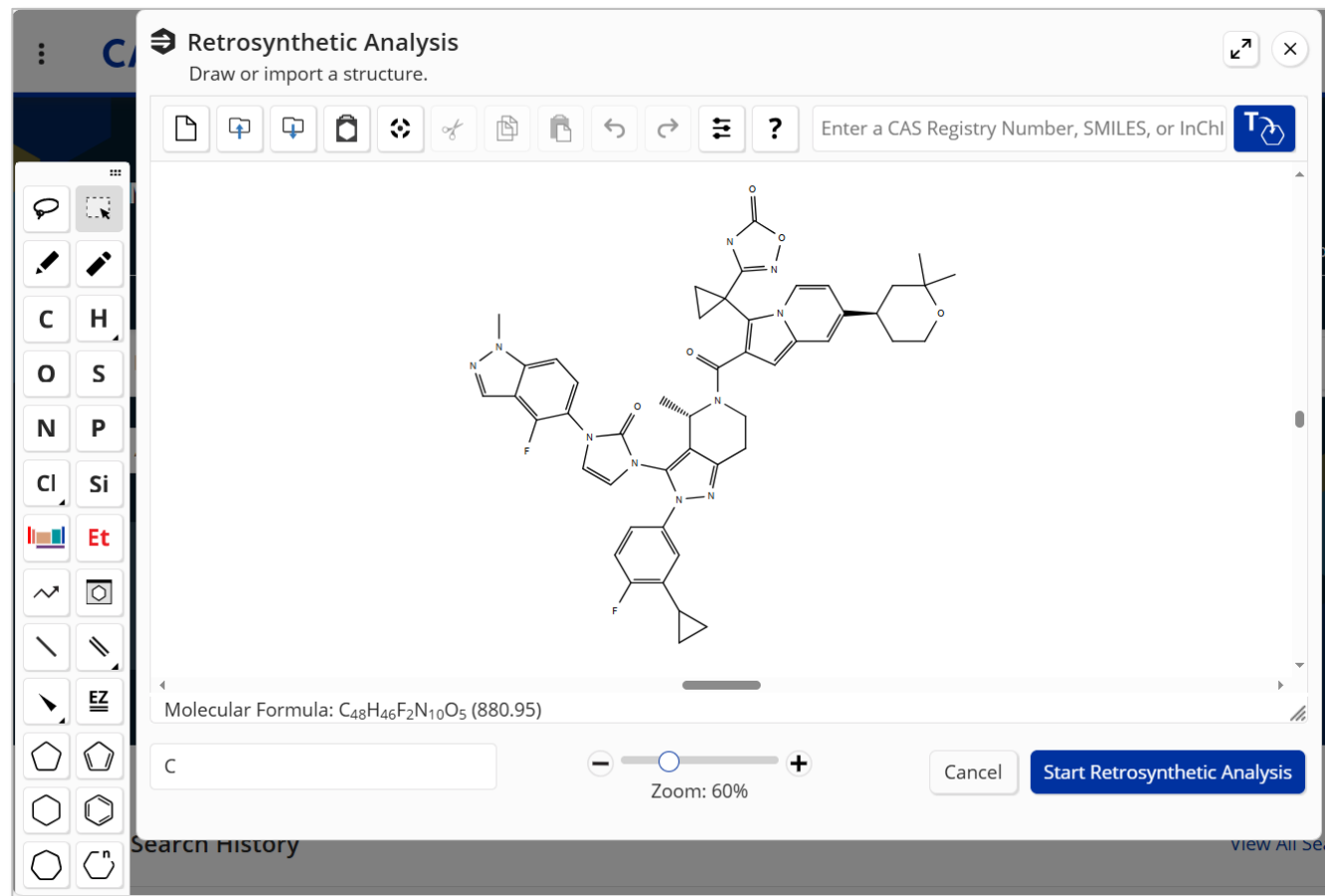
提纲

反应

- 检索方法
- 逆合成设计

启发逆合成路线的设计

可用于未知化合物或已知化合物和的逆合成路线设计



Retrosynthetic Analysis

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

预设合成参数

Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions

[Learn more](#)

☒ Common **反应规则常见性**

☐ Uncommon (includes common rules)

☐ Rare (includes common and uncommon rules)

Set Starting Materials Cost Limit

[Learn more](#)

Set Starting Materials Cost Limit

100 USD/mol

起始原料费用

☒ Email me when my plan is complete

[Continue to Retrosynthesis Plan](#)

Break and Protect Bonds (Optional)

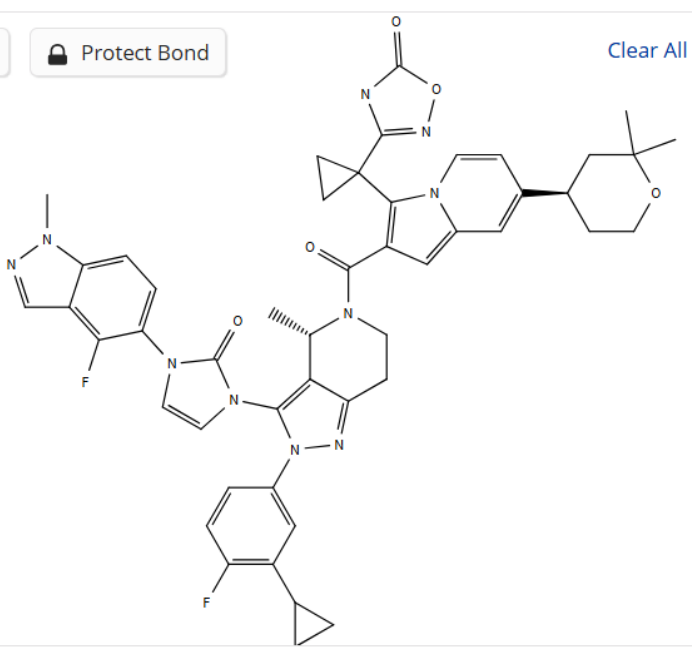
断裂键或保护键

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

☐ Break Bond

☐ Protect Bond

[Clear All Bond Selections](#)



获得逆合成反应路线

Retrosynthesis Plan for drawn structure Powered by ChemPlanner®

Key Experimental Steps Predicted Steps [Edit Plan Options](#) [View Excluded Options](#) [Save](#)

实验报道路线

预测型反应路线

View all alternatives (9)
View evidence
Exclude this step

Step Evidence

A ⇒ B + C + D

Average Yield: 60%
Evidence
Alternative steps (9)

1.1 Reagents: Diisopropylethylamine, O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluoro phosphate
Solvents: Dimethylformamide; 1 h, 25 °C
[View All](#)

查看文献支持与替换路线

Reactions from Retrosynthesis Plan Evidence

References ▾

Filter Behavior

Filter by Exclude

Search Within Results

Yield

☐ 50-69% (2)

☐ No Yield Available (116)

Reaction Scale

☐ Gram (2)

☐ No Scale Provided (116)

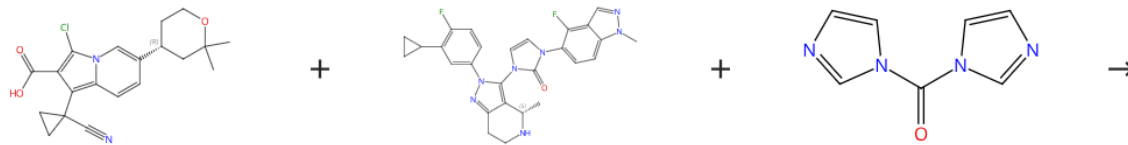
Number of Steps

☐ 1 (118)

118 Results

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

Scheme 1 (2 Reactions) Steps: 1 ⋮



Absolute stereochemistry shown

A ⇒ B + C + D Alternative Steps (9)

Filter by

Alternative Step Type

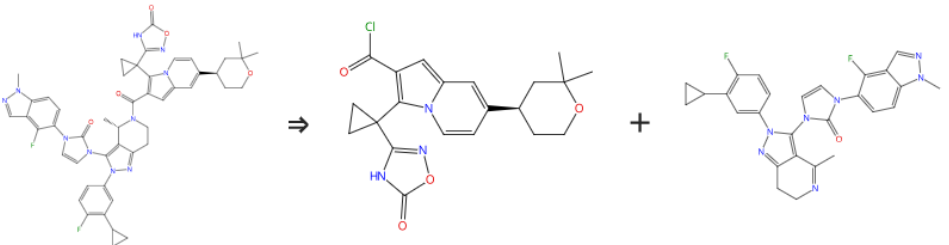
☐ Predicted (9)

Predicted Stereochemistry

☐ Non-Selective (8)

☐ Exact (1)

1 of 4 Stereoselective



Select View 5 similar Alternatives View evidence Average yield: 87%

总结

文献检索

- 基于数据关联，高效查看文献中的核心研究点、物质、反应、分析方法及配方信息
- 利用**Concept**、**Lexicon**辅助关键词的积累，灵活构建检索式，利用丰富的筛选工具高效筛选

物质检索

- 基于数据关联，高效获取物质的属性、谱学、生物学数据、**GHS**危险说明等信息
- 利用物质/文献标识符、分子式、属性值/谱图数值、结构检索物质

反应检索

- 利用物质或文献标识符、自然语言或结构式灵活检索，高效筛选目标反应，利用**Synthetic Methods**高效查看合成反应详情
- **Retrosynthetic Analysis**获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

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

谢谢!

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