

余敏

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- 美国化学文摘社(CAS)内容特色及定制服务
- 为什么需要SciFinderⁿ

美国化学文摘社(CAS)各类科学信息研究工具

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美国化学文摘社(CAS)隶属美国化学会(ACS), 致力于追踪、收录、标引科学信息

- 拥有超过110年的经验; 创立权威化学索引《化学文摘》(CA)
- 密切追踪、标引和提炼着全球化学相关的文献 (包括专利)
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新, 助力于解决科研方面的难题与挑战



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为什么需要美国化学文摘社 (CAS)



CAS拥有互联大数据内容，助力跨学科创新

为什么需要美国化学文摘社 (CAS)

- **生物化学：**
 - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- **有机化学各领域：**
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- **大分子化学各领域：**
 - 纤维素、木质素、造纸;涂料、墨水
 - 染料、有机颜料; 合成橡胶纺织品、纤维
- **应用化学各领域：**
 - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **物理、无机、分析化学各领域：**
 - 表面化学、催化剂、相平衡、核现象、电化学

广泛意义的化学, 不仅包含传统化学, 几乎包含了所有与化学相关的学科。

为什么需要美国化学文摘社 (CAS)

数据量和更新频率全球领先

- 化学物质数量全球领先。目前收录的物质数量已经超过1.67亿个，是进行新化合物确认的唯一可用资源
- 由CAS创建的CAS登记号是化学物质的黄金标准；是对物质进行确认的唯一身份识别号；是在进行化学品进出口交易时，必须向相关国家管控机构提供的身份识别号；是在申报课题项目时，需向评议组提供的身份识别号
- CAS几乎收录了从高分子聚合物到纳米颗粒的所有类别的物质，包括有机物、无机物、聚合物、合金、矿物质、配合物、混合物、生物序列等
- CAS不但收录专利中报道的确定结构的物质，还收录专利中的通式结构（马库什结构），帮助用户在使用CAS的数据后能够最大程度的避免专利法律风险

为什么需要美国化学文摘社 (CAS)

- 化学反应数量全球领先，目前收录的化学反应数量超过1.29亿条，是确认新的化学反应、工艺和方法时必不可缺的资源
- 近千名科学家每天阅读来自全球的科技文献，并根据CAS制定的规则 and 标准、从信息专家和科学家的角度对原文中重要的信息进行改写和标引，从而节省CAS的用户花在阅读、理解、总结科技原文文献所需的时间，将更多的时间投入到其他的工作中

CAS科学家对数据的解读，有助于节省用户检索、分析、
阅读和理解信息所花费的时间

为什么需要美国化学文摘社 (CAS)

1000页! 篇幅太长, 难以短时间内理解其中的信息, 是否太难?

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
15 June 2017 (15.06.2017)

WIPO | PCT

(10) International Publication Number
WO 2017/100668 A1

(51) International Patent Classification:
C07D 495/16 (2006.01) *A61P 35/00* (2006.01)
A61K 31/519 (2006.01)

(21) International Application Number:
PCT/US2016/065964

(22) International Filing Date:
9 December 2016 (09.12.2016)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
62/265,780 10 December 2015 (10.12.2015) US

Row, San Diego, California 92121 (US). **GHOSH, Brahmananda**; 1400 McKean Road, Spring House, Pennsylvania 19477 (US). **HAO, Baoyu**; c/o Hutchinson Medipharma Limited, Building 4, 720 Cailun Road, Zhangjian Hi-Tech Park, Shanghai 201203 (CN). **KREUTTER, Kevin**; c/o Janssen Research & Development LLC, 1400 McKean Road, Spring House, Pennsylvania 19477 (US). **LI, Gang**; c/o Hutchinson Medipharma Limited, Building 4, 720 Cailun Road, Zhangjian Hi-Tech Park, Shanghai 201203 (CN). **TICHENOR, Mark S.**; 3210 Merryfield Row, San Diego, California 92121 (US). **VENABLE, Jennifer D.**; 3210 Merryfield Row, San Diego, California 92121 (US). **WEL, Jianmei**; 3210 Merryfield Row, San Diego, California

为什么需要美国化学文摘社 (CAS)

Table 2

Ex #	Compound Name	BTK_I_binding pIC50
1	N-((3R,5R)-1-Acryloyl-5-fluoropiperidin-3-yl)-5-(2-methyl-4-phenoxyphenyl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	7.7
2	N-((3R,5S)-1-Acryloyl-5-hydroxypiperidin-3-yl)-5-(*S)-(2-methyl-4-phenoxyphenyl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	8.2

近千个化合物，要确定其结构式和CAS号，是否太难？

974	(R)-N-(1-Acryloylpyrrolidin-3-yl)-5-(2-methyl-6-(pyridazin-3-yloxy)pyridin-3-yl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	5.6
975	(R)-N-(1-Acryloylpiperidin-3-yl)-5-(2-methyl-6-(pyridazin-3-yloxy)pyridin-3-yl)-4-oxo-4,5-dihydro-3H-1-thia-3,5,8-triazaacenaphthylene-2-carboxamide;	5.0



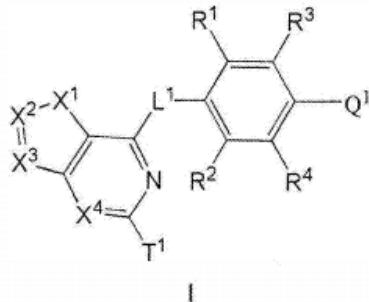
为什么需要美国化学文摘社 (CAS)

CN 106232118 A

权利要求书

1/12 页

1. 式I的化合物或其药学上可接受的盐用于治疗哺乳动物的D1-介导的(或D1-相关)障碍的用途:



结构式复杂, 难以根据定义绘制其结构, 是否太难?

L¹为O、S、NR^N、C(=O)、CH(OH)或CH(OCH₃);
Q¹为含N的5元至10元杂芳基、含N的4元至12元杂环烷基或苯基, 它们各自任选地被一个R⁹取代且进一步任选地被1、2、3或4个R¹⁰取代;

X¹为O、S、NH、N(C₁₋₄烷基)、N(环丙基)或N(-CH₂-环丙基);

X²为N或C-T²;

X³为N或C-T³;

前提条件是当X¹为O或S时, 则X²和X³中的至少一个不为N;

X⁴为N或C-T⁴;

T¹为H、-OH、卤素、-CN或任选被取代的C₁₋₂烷基;

T²、T³和T⁴各自独立地选自由下列选项组成的组: H、-OH、卤素、-CN、任选被取代的C₁₋₄烷基、任选被取代的C₃₋₄环烷基、任选被取代的环丙基甲基以及任选被取代的C₁₋₄烷氧基;

R^N为H、C₁₋₄烷基、C₃₋₄环烷基或-C₁₋₂烷基-C₃₋₄环烷基;

R¹和R²各自独立地选自由下列选项组成的组: H、卤素、-CN、C₁₋₆烷基、C₁₋₆卤代烷基、C₁₋₆烷氧基、C₁₋₆卤代烷氧基以及C₃₋₆环烷基, 其中所述的C₁₋₆烷基和C₃₋₆环烷基各自任选地被各自独立地选自下列选项的1、2、3、4或5个取代基取代: 卤代、-OH、-CN、C₁₋₄烷基、C₁₋₄卤代烷基、C₁₋₄烷氧基以及C₁₋₄卤代烷氧基;

R³和R⁴各自独立地选自由下列选项组成的组: H、卤素、-OH、-NH₂、-NH(CH₃)、-N(CH₃)₂、-NO₂、-CN、-SF₅、C₁₋₆烷基、C₁₋₆卤代烷基、C₁₋₆卤代烷氧基、C₂₋₆烯基、C₂₋₆炔基、C₃₋₇环烷基、4元至10元杂环烷基、-N(R⁵)(R⁶)、-N(R⁷)(C(=O)R⁸)、-C(=O)-N(R⁵)(R⁶)、-C(=O)-R⁸、-C(=O)-OR⁸、-N(R⁷)(S(=O)₂R⁸)、-S(=O)₂-N(R⁵)(R⁶)、-SR⁸以及-OR⁸, 其中所述的C₁₋₆烷基、C₃₋₇环烷基及杂环烷基各自任选地被各自独立地选自由下列选项组成的组的1、2或3个取代基取代: 卤素、-CN、-OH、C₁₋₄烷基、C₁₋₄烷氧基、C₁₋₄卤代烷基、C₁₋₄卤代烷氧基、C₃₋₆环烷基、-N(R⁵)(R⁶)、-N(R⁷)(C(=O)R⁸)、-C(=O)-OR⁸、-C(=O)H、-C(=O)R⁸、-C(=O)N(R⁵)(R⁶)、-N(R⁷)(S



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为什么需要美国化学文摘社 (CAS)

WO 2006/016684

PCT/JP2005/014867

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DESCRIPTION

PDF原文中的标题和摘要

METHOD FOR SYNTHESIS OF AROMATIC AMINE

(57) Abstract: One embodiment of the present invention provides a method for synthesis of substituted secondary amine by the reaction of aniline with aryl halide by using a Pd catalyst including (t-Bu)₃P as a ligand.

Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)₃P as a ligand as an electroluminescence source for display devices

By: Nakashima, Harue; Kawakami, Sachiko

Assignee: Semiconductor Energy Laboratory Co., Ltd., Japan

CAS科学家改写的标题和摘要

A process for the synthesis of secondary amines is presented via condensation of aniline with an aryl halide using palladium as a catalyst and (t-Bu)₃P as a ligand in the key step. Thus, N-(4-diphenylamino)phenylaniline is synthesized in 42% yield by condensation of N,N-diphenyl-N-(4-bromophenyl)amine with aniline. The process avoids protecting groups though the use of a palladium catalyst and (t-Bu)₃P as a ligand. N-(4-diphenylamino)phenylaniline can be used as an electroluminescence source for display devices including a light-emitting diodes, flat panel displays, liq. crystal display devices (no data).

CAS的科学家对专利进行必要改写，使其更容易被理解和获取



为什么需要美国化学文摘社 (CAS)

Indexing

Heterocyclic Compounds (More Than One Hetero Atom) (Section28-16)

Section cross-reference(s): 1, 63

Concepts

Antirheumatic agents
Homo sapiens
Pharmaceutical excipients

Antitumor agents
Human

prepn. of oxodihydrothiazacacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

CAS科学家标引的信息揭示了本专利的发明主题

Neoplasm
Rheumatoid arthritis
nematosis

treatment of; prepn. of oxodihydrothiazacacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

2101210-72-2P
2101210-73-3P
2101210-82-4P
2101211-31-6P
2101211-41-8P
2101211-62-3P
2101212-16-0P
2101212-26-2P
2101212-84-2P
2101214-41-7P
2101216-00-4P
2101216-02-6P
2101216-63-9P
2101216-66-2P
2101216-70-8P
2101216-72-0P
2101216-74-2P

CAS科学家标引的物质信息。此两组物质都为被制备的物质，有何异同？

Page 211 in PATENTPAK
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Page 710 in PATENTPAK
Page 714 in PATENTPAK
Page 716 in PATENTPAK

prepn. of oxodihydrothiazacacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

Pharmacological activity; Physical, engineering or chemical process; Synthetic preparation; Therapeutic use; Biological study; Preparation; Process; Uses

2101212-82-0P
2101212-92-2P
2101215-45-4P

Page 364 in PATENTPAK
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Page 598 in PATENTPAK

prepn. of oxodihydrothiazacacenaphthylenecarboxamides as inhibitors of Bruton's tyrosine kinase

Pharmacological activity; Physical, engineering or chemical process; Reactant; Synthetic preparation; Therapeutic use; Biological study; Preparation; Process; Uses; Reactant or reagent



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The screenshot displays a patent document on the PatentPak platform. On the left, a sidebar lists 'Key Substances in Patent' with two entries: 'CAS RN 54878-25-0' and 'CAS RN 7758-19-2'. The first entry includes a chemical structure of a spiro compound and a 'page 21' marker. The main text of the patent is visible, containing several paragraphs and examples. Annotations from CAS are shown as blue location pins on the text. A yellow callout box points to the 'page 21' marker in the sidebar, containing the text: 'CAS科学家标引专利中以名称表示的物质，并提供物质的结构式、CAS号及在专利中的位置信息'.

medium was prepared by inoculating 50 mL of SDE-ura medium with CALI-5 or ALX7-95 containing YEp-HPS-ura. This culture was grown until early stationary phase (24-48 hr). One mL of this culture was inoculated into 500 mL of SDE-ura medium and grown for 24 hr. A 400-mL aliquot (5% inoculum) was used to inoculate the 8 L of medium.

[0188] The fermentor was maintained at 26° C. The air flow was 4.5 L/min and the dO₂ was maintained above 30% by adjusting the rpm. Furthermore, the pH was maintained at 4.5 using acetic acid and NaOH.

[0189] Once the glucose concentration was below 1 g/L, a feeding regimen was initiated such that the glucose in the fermentor was kept between 0 and 1 g/L. The glucose feed was made by mixing 1400 mL of 60% glucose and 328 mL of 12.5% yeast extract.

[0190] After 5 days, the air and agitation were turned off, and the oil was allowed to rise to the top of the tank and decanted.

Example 3
Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]dec-6-en-8-one (the "(–)-solavetivone") (5)

[0191] 3,5-Dimethylpyrazole (47 g, 0.49 mol) was dissolved in a mixture of CH₂Cl₂ (650 mL) and t-butyl alcohol (31 mL). The solution was then cooled to ±78° C. Chromyl chloride (CrO₂Cl₂) (13.3 mL) was added over 15 min and stirred for another 15 min before it was allowed to warm to room temperature. Premnaspirodiene (6.69 g, 32.7 mmol) was dissolved in CH₂Cl₂ (650 mL) and added rapidly to the reaction. The dark red solution was stirred for 48 hours. The

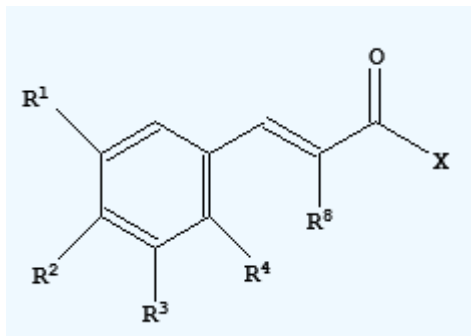
Example 5
Preparation of 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-2,6-dien-8-one (3) & 2-Isopropyl-6,10-dimethyl-spiro[4.5]deca-1,6-dien-8-one (4).

[0193] To a solution of (–)-solavetivone (5) (100 mg, 0.46 mmol) dissolved in ethanol (2 mL) was added Amberlyst® IR-15 (150 mg). The suspension was then heated at 105° C. in a sealed reaction flask for 96 hours. The suspension was then filtered through Celite and evaporated under vacuum. The residue was purified on a silica gel column (hexane:ether, 85:15) to afford the mixture as a colorless oil (67 mg, 67%). ESIMS m/z 219 (M+H), 78.7% at 14.71 min; 219 (M+H), 17.1% at 14.89 min.

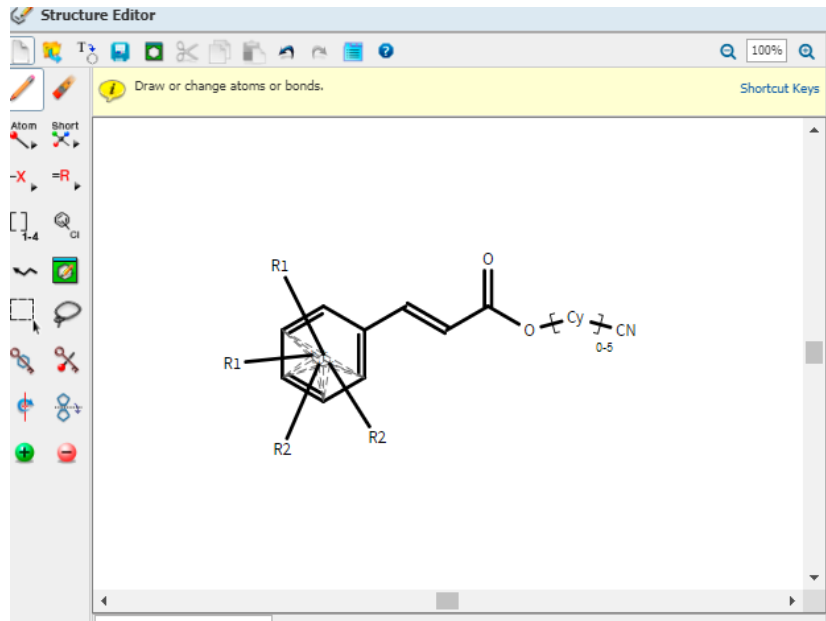
Example 6
Oxidation of (+)-Valencene to (+)-Nootkatone

[0194] In order to test various reaction conditions for the oxidation of premnaspirodiene to solavetivone, reactions were carried out on commercially available valencene, a compound that is chemically similar to premnaspirodiene and would be expected to oxidized under similar reaction conditions. Reactions were carried out using 250 mg of starting material in a single reaction, using combinations of sodium chlorite and either t-butylhydroperoxide (t-BuOOH) or N-hydroxyphthalimide (NHPI) as described (S. M. Silvestre & I.

为什么需要美国化学文摘社(CAS)



R¹-R⁴相同或不同，分别为H、F、Cl、Br
R¹-R⁴至少有两个不能同为氢
X=O-[Ar]₀₋₅-CN
R⁸为任意原子



CAS的解决方案具有强大的结构绘制功能，能够绘制较复杂的结构

LIMITLESS POSSIBILITIES 无限可能

定制服务应对挑战



CONTENT SERVICES

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Data structure
- 数据平台
Data platforms



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- 技术评估
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科研分析



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美国化学文摘社(CAS)为抗击新冠病毒发布的分析报告



COVID-19治疗药物及疫苗研发数据分析报告
ACS Cent. Sci. 2020, 6, 3, 315–331

发布日期: March 12, 2020

<https://doi.org/10.1021/acscentsci.0c00272>

Table 2. Key Proteins and Their Roles during the Viral Infection Process

target candidate	full name	role during viral infection	drug candidate
3CLpro	coronavirus main protease 3CLpro	a protease for the proteolysis of viral polyprotein into functional units	lopinavir ^{19,30}
PLpro	papain-like protease PLpro	a protease for the proteolysis of viral polyprotein into functional units	lopinavir ^{19,30}
RdRp	RNA-dependent RNA polymerase	an RNA-dependent RNA polymerase for replicating viral genome	remdesivir, ^{19,26,32} ribavirin ^{16,29,31}
S protein	viral spike glycoprotein	a viral surface protein for binding to host cell receptor ACE2	Arbidol ^{20,22,33a}
TMPRSS2	transmembrane protease, serine 2	a host cell-produced protease that primes S protein to facilitate its binding to ACE2	camostat mesylate ¹¹
ACE2	angiotensin-converting enzyme 2	a viral receptor protein on the host cells which binds to viral S protein	Arbidol ^{20,22,33a}
AT2	angiotensin AT2 receptor	an important effector involved in the regulation of blood pressure and volume of the cardiovascular system	L-163491 ²⁸

^aAn inhibitor of viral entry to host cells. Its direct action on S protein and ACE2 is yet to be confirmed.

Table 8. Target Analysis of Patents on Developing Therapeutic Antibodies for SARS

patent number	antigen of SARS antibody	patent title	organization	priority date
EP2112164	lipid attachment signals or GPI	Antiviral peptides linked to a lipid attachment signals or GPI against enveloped virus such as HIV, avian flu, SARS or Ebola virus	Institute Pasteur of Shanghai	20080229
WO2009128963	spike protein	Cross-neutralizing human monoclonal antibodies to SARS-CoV and methods of use thereof	Institute for Research In Biomedicine	20080117
WO2009128963	spike protein	Cross-neutralizing human monoclonal antibodies to spike protein of SARS coronavirus and methods of use thereof	Humab, LLC	20080117
WO2008035894	viral infection	Preparation of antiviral antibody 3D8 fragments and their use in treatment of viral infection	Sung Kyun Kwan University; Ajou University; Invitroplant Co., Ltd.	20060919
WO2008060331	spike protein	Antibodies to SARS coronavirus	Angen Inc.	20060519
WO2007044695	spike protein	Neutralizing monoclonal anti-spike protein antibodies for diagnosis and treatment of SARS-coronavirus-associated disease and screening of vaccine or anti-SARS agent	Dana-Farber Cancer Institute	20051007
CN1911963	RBD of S protein	Method for preparing neutralizing monoclonal antibody against severe acute respiratory syndrome coronavirus and its application	Chinese Academy of Sciences	20050810
CN1903878	S2 protein	Fab fragment of human antibody IgG against SARS coronavirus	Fudan University	20050726
WO2006095180	spike protein	Human monoclonal antibodies against SARS-associated coronavirus and treatment of patients with SARS	Ultra Biotech Ltd.; University of California	20050310
WO2006086561	spike protein	Neutralizing monoclonal antibodies against severe acute respiratory syndrome-associated coronavirus	New York Blood Center, Inc.	20050208



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美国化学文摘社(CAS)为抗击新冠病毒发布的分析报告



COVID-19诊断检测方法与技术开发

ACS Cent. Sci. 2020, 6, 5, 591-605

发布日期: April 30, 2020

<https://doi.org/10.1021/acscentsci.0c00501>

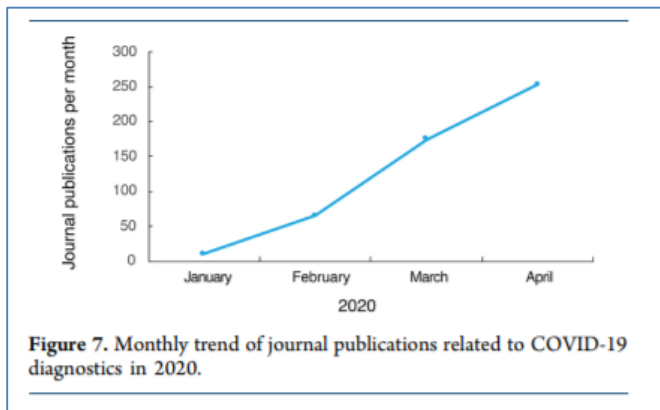


Table 4. Journal Articles with SARS-CoV-2-Related Sequences for Potential Applications in Diagnostics

publication date	title	journal	nucleic acids	proteins
2020	Nanopore Target Sequencing for Accurate and Comprehensive Detection of SARS-CoV-2 and Other Respiratory Viruses	<i>medRxiv</i>	40 primers	
2020	A Single and Two-Stage, Closed-Tube, Molecular Test for the 2019 Novel Coronavirus (COVID-19) at Home, Clinic, and Points of Entry	<i>ChemRxiv</i>	6 COVID-19 LAMP primers	
2020	Transmission and Clinical Characteristics of Coronavirus Disease 2019 in 104-Outside-Wuhan Patients, China	<i>medRxiv</i>	6 primers and probes	
2020	A Pneumonia Outbreak Associated with a New Coronavirus of Probable Bat Origin	<i>Nature</i>	4	50
2020	A New Coronavirus Associated with Human Respiratory Disease in China	<i>Nature</i>	1	10
2020	A Sequence Homology and Bioinformatic Approach Can Predict Candidate Targets for Immune Responses to SARS-CoV-2	<i>Cell Host & Microbe</i>		51
2020	Comparative Analysis of Primer-Probe Sets for the Laboratory Confirmation of SARS-CoV-2	<i>bioRxiv</i>	20 primers, 10 probes	
2020	Spike Protein Binding Prediction with Neutralizing Antibodies of SARS-CoV-2	<i>bioRxiv</i>		3
2020	SARS-CoV-2 Proteome Microarray for Mapping COVID-19 Antibody Interactions at Amino Acid Resolution	<i>bioRxiv</i>		11
2020	Evaluation of Recombinant Nucleocapsid and Spike Proteins for Serological Diagnosis of Novel Coronavirus Disease 2019 (COVID-19)	<i>medRxiv</i>	12 primers	
2020	RBD Mutations from Circulating SARS-CoV-2 Strains Enhance the Structure Stability and Infectivity of the Spike Protein	<i>bioRxiv</i>		8
2020	Teicoplanin Potently Blocks the Cell Entry of 2019-nCoV	<i>bioRxiv</i>	14	134
2020	Differential Antibody Recognition by SARS-CoV-2 and SARS-CoV Spike Protein Receptor Binding Domains: Mechanistic Insights and Implications for the Design of Diagnostics and Therapeutics	<i>bioRxiv</i>		7
2020	A Proposal of an Alternative Primer for the ARTIC Network's Multiplex PCR to Improve Coverage of SARS-CoV-2 Genome Sequencing	<i>bioRxiv</i>	2	
2020	First 12 Patients with Coronavirus Disease 2019 (COVID-19) in the United States	<i>medRxiv</i>	12	109

美国化学文摘社(CAS) 为抗击新冠病毒提供数据集

OPEN ACCESS:
CAS COVID-19 ANTIVIRAL CANDIDATE
COMPOUNDS DATASET

CAS 抗新冠病毒数据集

50,000 候选化合物

包括已知或潜在的抗病毒活性物质以及相关的数据，以支持研究，数据挖掘和分析应用

下载网址：<https://www.cas.org/covid-19-antiviral-compounds-dataset>

L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester
C27H35N6O8P
1809249-37-3 Copyright (C) 2020 ACS
42 45 0 0 1 0 0 0 0 0 0999 V2000
24113.740225083.5116 0.0000 C 0
24738.466831027.3695 0.0000 N 0
14556.860113339.0458 0.0000 O 0
35135.6204 8964.8958 0.0000 C 0
41864.271512849.6839 0.0000 O 0
48592.9226 8964.8958 0.0000 P 0 0 1 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48592.922616734.4721 0.0000 O 0
53768.806911953.1943 0.0000 N 0
48592.9226 2988.2986 0.0000 O 0
58944.6882 8964.8958 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

> <cas.index.name>

L-Alanine, N-[(S)-hydroxyphenoxyphosphinyl]-, 2-ethylbutyl ester, 6-ester with 2-C-(4-aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-2,5-anhydro-D-altrnonitrile

> <molecular.formula>

C27H35N6O8P

> <molecular.weight>

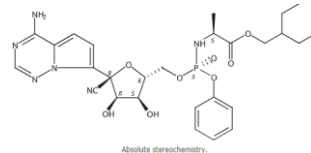
602.58

> <density.predicted>

1.47Å±0.1 g/cm3 Temp: 20 Å°C; Press: 760 Torr

> <pka.predicted>

12.00Å±0.70 Most Acidic Temp: 25 Å°C



CAS
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美国化学文摘社(CAS) 为抗击新冠病毒提供数据集

COVID-19 Protein Target Thesaurus

CAS 抗新冠病毒候选靶向蛋白数据集

包括SARS-CoV-2 病毒蛋白，病毒入侵所依赖的宿主蛋白，宿主免疫反应相关蛋白等，下载网址：

<https://www.cas.org/covid-19-protein-target-thesaurus>

63个靶向蛋白以及它们的常用名

5	328404-18-8	Angiotensin-converting enzyme 2	Carboxypeptidase, angiotensin-converting enzyme-related Angiotensin-converting enzyme-related carboxypeptidase Carboxypeptidase ACE2 ACE2 APN 01 Angiotensin I converting enzyme II Angiotensin I converting enzyme 2 Angiotensin 1 converting enzyme 2 Angiotensin 1 converting enzyme II E.C. 3.4.17.23 EC 3.4.17.23 ACE-II ACE-2 Angiotensin-converting enzyme II ACEII
---	-------------	---------------------------------	--



CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

大纲

- 美国化学文摘社(CAS)内容特色及定制服务
- 为什么需要SciFinderⁿ

为什么需要SciFinderⁿ

- SciFinderⁿ完全涵盖SciFinder中的内容
- SciFinderⁿ整合了专利流程解决方案PatentPak，利于快速定位专利中的关键信息及节省阅读、理解专利原文所花费的时间
- SciFinderⁿ整合了方法学解决方案MethodsNow-Synthesis，无需获取全文即可获得合成方法所需的详细信息
- 采用先进的技术和算法，可按相关性排列检索结果，提高获取信息的效率
- 多样化的聚类选项，细化研究，拓展思路
- 利用CAS的大数据及新技术，提供逆合成设计工具Retrosynthesis，触发创新灵感

为什么需要SciFinderⁿ

The screenshot displays the SciFinderⁿ interface. At the top, there is a navigation bar with the SciFinderⁿ logo, a 'Saved' button, a 'History' button, and an 'Account' button. Below this is a purple banner with text about COVID-19 research. The main content area is divided into two columns. The left column, titled 'Searching for...', contains a vertical menu with options: 'All', 'Substances', 'Reactions', 'References' (highlighted in purple), and 'Suppliers'. The right column, titled 'References', shows a search bar with the text 'lead free' and a search button. Below the search bar is a list of search results, with 'Petrol, lead-free' highlighted in purple. At the bottom of the interface, there is a 'Recent Search History' section showing a search for 'COVID-19 (83K)' on 'September 28, 2020' at '4:28 PM'. There are 'Rerun Search' and 'Edit Search' buttons next to the history entry.

无需逐步在不同信息中检索，提高检索效率

利用CAS科学家编制的叙词表，创建高质量的检索式。

为什么需要SciFinder[®]

按相关性排序，无需花费更多时间查找相关信息

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

Return to Home

References (25,403) **Sort: Relevance** View: No Abstract

Substances Reactions Cited By

1

The effects of ethanol-unleaded gasoline blends on engine performance and exhaust emissions in a spark-ignition engine
By: Koc, Mustafa; Sekmen, Yakup; Topgul, Tolga; Yucesu, Huseyin Serdar
Renewable Energy (2009), 34(10), 2101-2106 | Language: English, Database: CPlus
View Abstract

Full Text Substances (3) Reactions (0) Cited By (148) **Citation Map**

2

The effect of compression ratio on the performance, emissions and combustion of an SI (spark ignition) engine fueled with pure ethanol, methanol and unleaded gasoline
By: Balki, Mustafa Kemal; Sayin, Cenk
Energy (Oxford, United Kingdom) (2014), 71, 194-201 | Language: English, Database: CPlus
View Abstract

Full Text Substance (1) Reactions (0) Cited By (78) Citation Map

3

A chronic inhalation study with unleaded gasoline vapor
By: MacFarland, H. N.; Ulrich, C. E.; Holdsworth, C. E.; Kitchen, D. N.; Halliwell, W. H.; Blum, S. C.

Filter by

- Document Type
 - Journal (162)
 - Review (22)
 - Conference (2)
- Author
 - Masjuki, H. H. (13)
 - Kalam, M. A. (7)
 - Masum, B. M. (7)
 - Palash, S. M. (5)
 - Venu, Harish (5)
- Concept
 - Gasoline (100)
 - Hydrocarbons (76)
 - Exhaust gases (engine) (74)
 - Combustion (65)
 - Spark-ignition engines (59)

References This Document Cites

- Ethanol-diesel fuel blends - a review
Bioresource Technology (2004)
Cited By 525
- Engine performance and pollutant emission of an SI engine using ethanol-gasoline blended fuels
Atmospheric Environment (2002)
Cited By 266
- Ethanol in gasoline: environmental impacts and sustainability. Review article
Renewable & Sustainable Energy Reviews (2005)
Cited By 190
- The use of ethanol-gasoline blend as a fuel in an SI engine
Renewable Energy (2004)
Cited By 160
- Experimental study of some performance parameters of a constant speed stationary diesel engine using ethanol-diesel blends as fuel
Biomass and Bioenergy (1999)
Cited By 134
- Experimental and theoretical investigation of using gasoline-ethanol blends in spark-ignition engines
Renewable Energy (2005)
Cited By 129
- A study on emission characteristics of an FI engine with ethanol blended gasoline fuels
Atmospheric Environment (2003)

References Citing This Document

- Effect of ethanol-gasoline blend on NOx emission in SI engine
Renewable & Sustainable Energy Reviews (2013)
Citing 136
- Effect of spark timing and load on a DISI engine fuelled with 2,5-dimethylfuran
Fuel (2010)
Citing 104
- The effect of different alcohol fuels on the performance, emission and combustion characteristics of a gasoline engine
Fuel (2011)
Citing 99
- Influence of diethyl ether (DEE) addition in ethanol-biodiesel-diesel (EBD) and methanol biodiesel-diesel (MBD) blends in a diesel engine
Fuel (2017)
Citing 83
- The effect of compression ratio on the performance, emissions and combustion of an SI (spark ignition) engine fuelled with pure ethanol, methanol and unleaded gasoline
Energy (Oxford, United Kingdom) (2014)
Citing 78
- Potential emissions reduction in road transport sector using biofuel in developing countries
Atmospheric Environment (2010)
Citing 76
- Impact of alcohol-gasoline fuel blends on the exhaust emission of an SI

在一个页面获取完整的前向、后向引文，并有多多个聚类选项对引文进行筛选

为什么需要SciFinderⁿ

依据CAS科学家利用人类智慧标引的信息，精准定位文献

The screenshot displays the SciFinder search results page. On the left, a 'Filter by' sidebar includes sections for Document Type (Journal: 2, Patent: 46), Substance Role (Biological Study: 48, Preparation: 38, Process: 3, Prophetic In Patents: 2, Reactant or Reagent: 16, Uses: 48), Language (English: 39, Chinese: 9), and Publication Year (2010 to 2020). A bar chart shows an increasing trend in publications from 2010 to 2020. The main area is titled 'References (48)' and shows three results. Each result includes a title, author information, and a 'View Abstract' link. Below each title are buttons for 'PATENTPAK', 'Full Text', and counts for 'Substances', 'Reactions', and 'Cited By'. A 'Citation Map' button is also present for each entry.

Filter by

- Document Type
 - Journal (2)
 - Patent (46)
- Substance Role
 - Biological Study (48)
 - Preparation (38)
 - Process (3)
 - Prophetic In Patents (2)
 - Reactant or Reagent (16)
 - Uses (48)
- Language
 - English (39)
 - Chinese (9)
- Publication Year
 - 2010 to 2020
 - Apply
 - View Larger

References (48) Sort: Relevance View: No Abstract

Substances Reactions Cited By Save

1

Heterocyclic compound capable of serving as SHP2 inhibitor
By: Ma, Cunbo; Gao, Panliang; Hu, Shaojing; Xu, Zilong; Han, Huifeng; Wu, Xinpeng; Kang, Di; Long, Wei
China, CN110143949 A 2019-08-20 | Language: Chinese, Database: CAplus
View Abstract

PATENTPAK Full Text Substances (548) Reactions (1,257) Cited By (2) Citation Map

2

Preparation of novel heterocyclic derivatives useful as SHP2 inhibitors
By: Ma, Cunbo; Gao, Panliang; Hu, Shaojing; Xu, Zilong; Han, Huifeng; Wu, Xinpeng; Kang, Di; Long, Wei
World Intellectual Property Organization, WO2018172984 A1 2018-09-27 | Language: English, Database: CAplus
View Abstract

PATENTPAK Full Text Substances (531) Reactions (2,055) Cited By (6) Citation Map

3

SHP2 inhibitors and methods of use thereof for treatment of diseases
By: Yu, Hongtao; Choi, Eunhee
United States, US20190231805 A1 2019-08-01 | Language: English, Database: CAplus
View Abstract

为什么需要SciFinderⁿ

← Return to Home

Filter by

- Document Type
- Substance Role
- Language
 - English (39)
 - Chinese (9)
- Publication Year
- Author
- Organization
- Publication Name
- Concept**
 - Antitumor agents (44)
 - Homo sapiens (27)
 - Human (27)
 - Lung neoplasm (27)
 - Mammary gland neoplasm (27)
 - [View All](#)
- CAS Solutions
- Formulation Purpose

Concept

Top Count **Alphanumeric** Search

A B C D E F G H I J K L M N O P Q R S

1 Selected

- Schwannoma (1)
- Short hairpin RNA (1)
- Signal transduction (1)
- siRNA (2)
- Skin neoplasm (1)
- Small-cell lung carcinoma (1)
- Small intestine neoplasm (1)
- Sodium-dependent glucose transporter SGLT2 inhibitors (1)
- Sodium-dependent phosphate transport protein 2B (1)
- Spinal cord (1)
- Spinal cord neoplasm (1)
- Spiro compounds (1)
- Squamous cell carcinoma (2)
- Stomach carcinoma (11)
- Str (2)**

2 Selected

- Pancreatic neoplasm (12)
- Pharmaceutical carriers (21)
- Pharmaceutical diluents (2)
- Pharmaceutical dosage forms (1)
- Pharmaceutical excipients (6)**
- Pharmaceutical formulations (2)
- Pharmaceutical intravenous injections (1)
- Pharmaceutical liposomes (1)
- Pharmaceutical nanoparticles (1)
- Polycythemia vera (1)
- Primary myelofibrosis (1)
- Prodrugs (3)**
- Prognosis (1)
- Programmed cell death (1)
- Programmed cell death protein 1 (1)
- Programmed cell death protein 1 inhibitors (3)
- Programmed death-ligand 1 (1)
- Proliferation inhibition (1)
- Proliferative disorders (2)
- Protein Binding (1)
- Protein phosphorylation (3)
- Proteins (1)
- Protein Tyrosine Phosphatase, Non-Receptor Type 11 (2)
- Protein tyrosine phosphatase PTP1B inhibitors (1)
- Psoriasis (1)
- Pyrazoles (1)
- Pyridines (1)
- Pyrimidines (1)
- Pyrimidinones (2)

Apply Cancel

Apply Cancel

依据CAS科学家利用人类智慧标引的信息细化研究点

为什么需要SciFinderⁿ

化合物新颖性的依据

为化合物设计提供新的想法

Structure Match

- As Drawn (10)
- Substructure (14)
- Similarity (802)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Regulatory Information
- Bioactivity Indicator
- Target Indicator

Substances (9)

Sort: Relevance View: Partial

References Reactions Suppliers

1 1801765-04-7

Absolute stereochemistry shown

C18H24ClN7OS
(3S,4S)-8-[6-Amino-5-[(2-amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-...

11 References 109 Reactions 6 Suppliers

2 2414487-37-7

Absolute stereochemistry shown

C18H24ClN7OS.xClH
Components: 2
Component RN: 1801765-04-7
2-Oxa-8-azaspiro[4.5]decan-4-amine, 8-[6-amino-5-[(2-amino-3-chloro-4-pyridinyl)...

1 Reference 1 Reaction 0 Suppliers

3 2414487-38-8

Absolute stereochemistry shown

C18H24ClN7OS.CH4O3S
Components: 2

1 Reference 1 Reaction 0 Suppliers

4 2414487-43-5

5 2414487-41-3

6 2414487-42-4

为什么需要SciFinderⁿ

聚类筛选项节省时间，一目了然。无需逐步二次检索和限定，直接勾选即可定位所需信息

The screenshot displays the SciFinder search results interface. On the left is a sidebar with various filters, and the main area shows a grid of search results for chemical compounds.

Filters:

- Reactant (2)
- Reference Role**
 - Biological Study (29)
 - Preparation (27)
 - Prophetic in Patents (5)
 - Reactant or Reagent (1)
 - Uses (29)
- Stereochemistry**
- Number of Components**
- Substance Class**
- Isotopes**
- Metals**
- Molecular Weight**
- Regulatory Information**
- Bioactivity Indicator**
 - Antitumor agents (28)
 - Enzyme inhibitors (17)
 - Antidiabetic agents (12)
 - Membrane transport modulators (12)
 - Receptor agonists (12)
- [View All](#)
- Target Indicator**

Search Results:

Reference ID	Chemical Name	References	Reactions	Suppliers
2235394-86-0	C ₁₈ H ₂₃ ClN ₆ O ₅ (3S,4S)-8-[5-[(2-Amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-2-oxa-8-...	2	15	0
1801765-38-7	C ₁₈ H ₂₃ ClN ₆ O ₅ (3R,4R)-8-[5-[(2-Amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-2-oxa-8-...	1	5	0
1801764-84-0	C ₁₈ H ₂₃ ClN ₆ O ₅ (3R,4S)-8-[5-[(2-Amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-2-oxa-8-...	1	14	0
22235394-86-0	C ₁₉ H ₂₆ ClN ₇ O ₅ (3S,4S)-8-[6-Amino-5-[(2-amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-ethyl-2-...	1	0	0
1801765-38-7	C ₁₈ H ₂₄ ClN ₇ O ₅ (4S)-4-Amino-8-[6-amino-5-[(2-amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-2-oxa-8-...	2	0	0
1801764-85-1	C ₁₇ H ₂₂ ClN ₇ O ₅ (4S)-8-[6-Amino-5-[(2-amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-2-oxa-8-azas...	3	1	0
2172650-69-8	C ₁₈ H ₂₃ ClN ₆ O ₅ (3R,4R)-8-[5-[(2-Amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-2-oxa-8-...	1	5	0
1801765-26-3	C ₁₈ H ₂₃ ClN ₆ O ₅ (3R,4S)-8-[5-[(2-Amino-3-chloro-4-pyridinyl)thio]-2-pyrazinyl]-3-methyl-2-oxa-8-...	1	14	0

为什么需要SciFinderⁿ

Patent Markush Match

As Drawn (2)

Substructure (4)

Filter by

Patent Office

World Intellectual Property Organization (4)

Patent Markush (4)

Sort: Patent Number: Ascending ▾

References ▾

Download Email Save

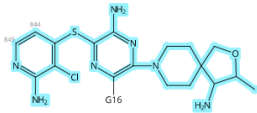
1

WO2015107495

Patent claim 1

PATENTPAK ▾ Full Text ▾

844,845: opt. substd. by G35



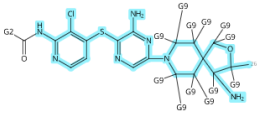
2

WO2017216706

Patent claim 1

PATENTPAK ▾ Full Text ▾

262: opt. substd. by 1 or more F



已公开的专利影响被设计结构的新颖性/创造性?

为什么需要SciFinderⁿ

The screenshot displays the PATENTPAK interface. On the left, there is a sidebar with three patent entries, each showing a CAS RN, a chemical structure, and analyst markup locations. The main content area shows a patent document with a red arrow pointing from a text box to a specific paragraph. The text in the document is as follows:

azaspiro[4.5]decan-4-amine, succinate (1:1) hemihydrate, modification (form) HA, Variant a)

[00327] 50 ml ethanol and 2.5 ml water were added to a 100ml flask containing 3.0 g of free base of 3S,4S)-8-(6-amino-5-((2-amino-3-chloropyridin-4-yl)thio)pyrazin-2-yl)-3-methyl-2-oxa-8-azaspiro[4.5]decan-4-amine (obtained as A18 for example as described in Example 1) and 848.0 mg of succinic acid. The mixture was heated to 50°C to generate a clear solution. The temperature was lowered to 15°C during a period of 3 hours. The solution was kept stirring at 15°C overnight. Precipitated solid was separated via suction filtration and 50 ml of acetone was added to produce a suspension. The suspension was stirred at 50°C for 3 hours. The solid was separated with suction filtration and dried at room temperature under vacuum for 3 hours. Yield was about 60%.

72

WO 2020/065453 PCT/IB2019/057864

利用CAS科学家人类智慧标引的信息，快速定位专利中的目标结构

为什么需要SciFinderⁿ

筛选合成方法的多个聚类选项

Filter by

- Substance Role
- Yield
- Number of Steps
- Non-Participating Functional Groups
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results

Source Reference

- Document Type
- Language
- Publication Year
- Publication Name

Reactions (162)

Group: By Document View: Expanded

References

1

Process of manufacture of a compound for inhibiting the activity of S

By: Fei, Zhongbo; Lu, Gang; Wan, Yinbo; Wang, Jianhua; Wu, Quanbing; et al
World Intellectual Property Organization, WO2020065453 A1 2020-04-02 | Language: English

PATENTPAK Full Text View 100 Related Reactions

Absolute stereochemistry shown

Suppliers (6)

Suppliers (125)

Absolute stereochemistry shown

Reaction Summary

Steps: 1 Yield: 88%

被设计结构（及其相似结构）已有哪些合成方法？如何突破现有的方法？

为什么需要SciFinderⁿ

Reaction Detail (Scheme 1, Reaction 1 of 1)

← Prev Next →
📄 📧 ★ Save

Steps: 1
Yield: 64%

Relative stereochemistry shown
Relative stereochemistry shown
64%

🛒 Suppliers (53)

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrogen peroxide	Iodine	Acetonitrile Water	5 h, 23 °C

CAS Reaction Number: 31-207-CAS-18256071

Notes
safety

Experimental Protocols

MethodsNow™

Products 1803406-76-9
, Yield: 64%

Reactants cis-Tetrahydro-2,5(1H,3H)-pentalenedione

Reagents Hydrogen peroxide

Catalysts Iodine

Reference
Less sensitive oxygen-rich organic peroxides containing geminal hydroperoxy groups
[View Reference Detail](#)
By: Gamage, Nipuni-Dhanesha H.; et al
[View All](#) v
Chemical Communications (Cambridge, United Kingdom) (2015), 51(68), 13298-13300
[Full Text](#) v

Company/Organization
Department of Chemistry
Wayne State University
Detroit, Michigan 48202
United States

提供反应安全信息，提高实验安全性

Solvents Acetonitrile
Water

Procedure

1. Charge a 50 ml round bottomed flask with a magnetic stir bar, I₂ (0.010 g, 0.040 mmol) in CH₃CN (1 mL).
2. Add a 50 wt.% aqueous solution of H₂O₂ (0.10 mL, 1.7 mmol) to the reaction mixture.
3. Add cis-1,5-dimethylbicyclo[3.3.0]octane-3,7-dione (0.20 mmol) to the solution.
4. Stir the reaction mixture at room temperature (23 °C) for 5 hours.
5. At this point, concentrate the reaction mixture under reduced pressure.
6. Dissolve the reaction mixture in 1 mL of DCM: CH₃OH (20:1).
7. Purify the product by silica gel column chromatography with 4:1 CH₂Cl₂ : EtOAc.

Safety Information Caution: the H₂O₂ solutions are strong oxidizers that may cause explosions. All organic peroxides are potentially explosive and require handling with extreme care. Reactions and manipulations should be run in fume hoods behind blast shields. Personal safety gear should include a face shield, leather gloves, a leather apron and hearing protection. Peroxide compound should not come into contact with strong acid, metal salts, or easily oxidized species. All reaction should be run at or below room temperature and performed on small scales. Specifically, 3 exploded upon concentrating a solution containing approximately 30 mg of crystals on the walls of the flask and shattered the flask and damaged the stir bar and but an explosion occurred upon solvent removal under reduced pressure, the flask shattered and even the stir bar was damaged.
[View Less](#) v

Transformation Formation of Hydroperoxides/ Autoxidation

Scale milligram

Characterization Data

1803406-76-9

Proton NMR Spectrum (400 MHz, CD₃OD, 23 °C, δ) OOH resonances not observed due to exchange with CD₃OD, 2.722.56 (m, 2H, CH), 2.18 (d of d, 4H, J= 14.4, 8.8 Hz), 1.86 (d of d, 4H, J= 14.4, 5.6 Hz).

Carbon-13 NMR (101 MHz, CD₃OD, 23 °C, ppm) 122.10 (peroxy C), 40.54 (CH), 39.03 (CH₂).

Elemental Analysis C₈H₁₄O₈ : C, 40.34; H, 5.92. Found: C, 39.98; H, 5.77.

State white solid.

CAS Method Number 3-614-CAS-2972525

实验详情，无需获取或阅读全文即可获得实验所需的信息



为什么需要SciFinderⁿ

Structure Match

As Drawn (9)

Substructure (13K)

Similarity (1,893)

Filter by

Yield

No Yield Available (9)

Number of Steps

1 (9)

Non-Participating Functional Groups

Alcohol (4)

Cyclic alcohol (4)

Halide (2)

Phenyl halide (2)

Alkene (1)

View All

Reaction Mapping

Mapping Data Available (9)

Reaction Type

Full (13K)

Failed (9)

Reactions (9)

Group: By Scheme View: Expanded

References

Scheme 1 (1 Reaction) Steps: 1

c1ccccc1S + c1ccccc1Br * c1ccc(cc1)Sc2ccccc2

Suppliers (48) Suppliers (78) Suppliers (74)

Reaction Summary Steps: 1 Failed

1.1 Reagents: Potassium carbonate
Catalysts: 1,2,3,4-Tetrahydro-8-quinolinol, Copper bromide
Solvents: Dimethyl sulfoxide; 24 h, 80 °C; 80 °C → rt

A highly efficient and widely functional-group-tolerant catalyst system for copper(I)-catalyzed S-arylation of thiols with aryl halides

By: Feng, Yang; et al
Tetrahedron (2009), 65(47), 9737-9741

View Reaction Detail Full Text

Collapse Scheme

Scheme 2 (2 Reactions) Steps: 1

c1ccccc1Br + c1ccc(cc1)CCBr * c1ccc(cc1)Sc2ccccc2

Suppliers (78) Suppliers (72) Suppliers (77)

失败反应提醒,
避免走弯路

为什么需要SciFinderⁿ

利用逆合成工具，突破现有合成方法，寻找最优的合成路线

Chemical structure: C1=CC=C2C(=C1)C(=O)C=C2

Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

Retrosynthesis

Overview Steps Scoring

Powered by ChemPlanner[®]

Complexity Reduction

Convergence

Evidence

Yield

Atom Efficiency

自定义逆合成设计参数

Reaction network showing steps A through K with associated suppliers and maximum yields.

- A: Suppliers (6), Max. Yield: 87%
- B: Suppliers (32), Max. Yield: 100%
- C: Suppliers (16)
- D: Suppliers (13), Max. Yield: 72%
- E: Suppliers (16), Max. Yield: -
- F: Suppliers (15), Max. Yield: 87%
- G: Suppliers (22)
- H: Suppliers (109)
- I: Suppliers (88)
- J: Suppliers (5), Max. Yield: 68%
- K: Suppliers (82)

Reset +

为什么需要SciFinderⁿ

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Substructure (4)

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Patent Markush (2)

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1

WO2020065453

Patent claim 1

PATENTPAK

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2

WO2015107495

Patent claim 1

PATENTPAK Full Text ▾

844,845: opt. subst. by G35

G1

G16

Save Search

Name

No Alerts As Available Weekly Monthly

Tags (optional)

combine

New Tag (optional)

Save Cancel

实时紧跟最新报道

为什么需要SciFinderⁿ

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- Retrosynthesis (39)

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便捷地管理检索历史，随时运行、编辑之前的检索式

为什么需要SciFinderⁿ

- CAS**科学家解读**的科技信息，有助于提高获取信息的效率
- **多种聚类筛选项**，一目了然，节省逐步筛选/二次检索的时间
- 数据的**全面性和及时性**，有助于确定研究的新颖性，避免潜在的专利风险
- 利用CAS大数据和先进技术的**逆合成设计工具**有助于突破现有合成方法，为获得最优方法提供见解和思路
- CAS科学家利用**人类智慧标引**的信息，有助于细化研究点
- 便捷地**管理检索历史**

SciFinderⁿ ——最先进的化学信息检索工具

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