



SciFinder[®]

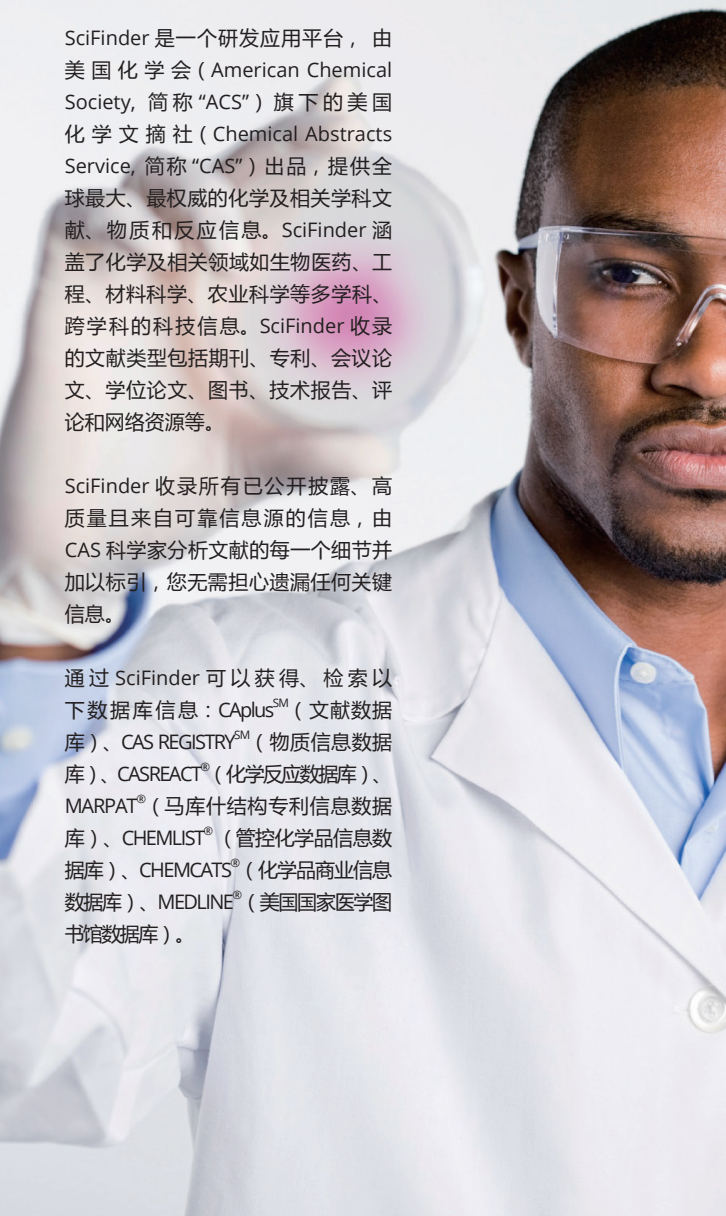
快速入门指南

SciFinder®——最全面的化学及相关学科信息资源， 加速实现科学突破

SciFinder 是一个研发应用平台，由美国化学会（American Chemical Society, 简称“ACS”）旗下的美国化学文摘社（Chemical Abstracts Service, 简称“CAS”）出品，提供全球最大、最权威的化学及相关学科文献、物质和反应信息。SciFinder 涵盖了化学及相关领域如生物医药、工程、材料科学、农业科学等多学科、跨学科的科技信息。SciFinder 收录的文献类型包括期刊、专利、会议论文、学位论文、图书、技术报告、评论和网络资源等。

SciFinder 收录所有已公开披露、高质量且来自可靠信息源的信息，由 CAS 科学家分析文献的每一个细节并加以标引，您无需担心遗漏任何关键信息。

通过 SciFinder 可以获得、检索以下数据库信息：CAplusSM（文献数据库）、CAS REGISTRYSM（物质信息数据库）、CASREACT[®]（化学反应数据库）、MARPAT[®]（马库什结构专利信息数据库）、CHEMLIST[®]（管控化学品信息数据库）、CHEMCATS[®]（化学品商业信息数据库）、MEDLINE[®]（美国国家医学图书馆数据库）。



文献检索

文献记录详情

REFERENCE DETAIL | [Get Substances](#) | [Get Reactions](#) | [Get Related Citations](#) | [Link to Other Sources](#) | **6** | [Send to SciPlanner](#)

[Return](#) | [Previous](#) | [Next](#)

1. Highly transparent and organosoluble polyimides derived from 2,2'-disubstituted-4,4'-oxydianilines **1**

By: Chen, Yi-Chieh; Rajendran, Kuppasath; Chang, Yi-Hsi; Huang, Sheng-Iliu; [Chen, Yao-Chi](#)

To improve the optical transparency and organosolubility of arom. polyimides derived from 4,4'-oxydianiline (4,4'-ODA), two new arom. diamines, 2,2'-di(2,4'-oxydianiline (DI-ODA) and 2,2'-bis(p-trifluoromethyl)phenyl)-4,4'-oxydianiline (BTPF-ODA) were synthesized by using 4,4'-ODA as a starting material. Novel polyimides were prepd. from these two diamines with various com. available arom. diacidhydrides via a one-step high-temp. polycondensation procedure. Most of the polyimides showed enhanced solub. in common org. solvents compared with those corresponding polyimides derived from 4,4'-ODA. Esp., polyimide derived from BTPF-ODA and rigid pyromellitic dianhydride (PMDA) was also sol. in DMF, DMAc, DMSO, NMP, and m-cresol at room temp. These polyimides had inherent viscosities from 0.41 to 1.26 dl/g¹ in NMP or m-cresol at 30°. Transparent, flexible, and tough films can be obtained by casting from their DMAC or m-cresol solns. These films had the UV onset wavelengths in the range of 243-293 nm and the wavelengths at 80% transmission of 445-544 nm, indicating high optical transparency. They also exhibited good thermal stability with glass transition temps. in the range of 260°-327°. The decomp. temps. of these polyimides at 5% wt. loss under nitrogen were >20°-260°. Because of the weak carbon-iodine bonds, polyimides derived from DI-ODA decompd. at lower temps. than polyimides derived from BTPF-ODA. The effects of the substituents at the 2 and 2' positions of 4,4'-ODA on the properties of polyimides are also discussed. High optical transparency and good solub. combined with high thermal stability make these polyimides potential candidates for soft electronics applications. © 2011 Wiley Periodicals, Inc. *J Appl Polym Sci*, 2011.

Indexing
Chemistry of Synthetic High Polymers (Section35-5)

Concepts
Polyimides **3**
polyether-, aromatic-, fluoro-containing; prepn. and properties of highly transparent and organosol. polyimides derived from disubstitutedoxydianilines
Properties; Synthetic preparation; Preparation

Substances
101-63-3P **4**
100125-47-1P **4**
128796-39-4P p-(Trifluoromethyl)pyromellitic acid **4**
Intermediate; prepn. and properties of highly transparent and organosol. polyimides derived from disubstitutedoxydianilines

QUICK LINKS
0 Tags, 0 Comments

SOURCE
Journal of Applied Polymer Science
Volume 120
Issue 4
Pages 3159-31
Journal
2011
CODEN: JAPMAB
ISSN: 0021-8995
DOI: 10.1002/app.33520

COMPANY/ORGANIZATION
Department of Polymer Engineering
National Taiwan University of Science and Technology
Taipei, Taiwan 10607

ACCESSION NUMBER
2011:294432
CASL5410987
CAPLUS

Citations

Widulski, M; *Polym Sci* 2009, 50, 1299 **7**
Zhou, X; *J Appl Polym Sci* 2010, 117, 1144 **7**
Feng, Y; *Macromolecules* 1996, 29, 5037 **7**
Zhang, C; *Polymer* 2008, 49, 2678 **7**
Peters, H; *Prog Polym Sci* 2010, 35, 1022 **7**
Jin-Ho, K; *Macromol Chem* 1973, 145, 189 **7**
Pharmis, M; *Eur Polym J* 2009, 45, 1861 **7**
Peech, H; *Polyimides: Fundamentals and applications* 1996
Sato, T; *High-Performance Polym* 1995, 1, 2 **7**
Iwasawa, M; *Prog Polym Sci* 2001, 26, 259 **7**
Kuan, S; *J Appl Polym Sci* 2009, 113, 3993 **7**
Wang, S; *J Polym Sci Part A: Polym Chem* 1997, 35, 1487 **7**

- 1** 标题
- 2** 摘要
- 3** 文献中标引的技术术语
- 4** 文献中标引的物质
- 5** 书目信息
- 6** 获得文献中的物质、反应、引文等
- 7** 参考文献

文献检索方式及举例

主题检索

SciFinder CAS SOLUTION | Preferences | SciFinder Help | Sign Out

Explore | Saved Searches | SciPlanner

Research Topic: "suzuki"

REFERENCES **1**

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS
Reaction Structure

REFERENCES: RESEARCH TOPIC

suzuki reaction with catalyst **2**

Example:
The effect of antibiotic residues on dairy products.
Photocrosslinking of aromatic compounds

Search **3**

Advanced Search

SAVED ANSWER SETS
Autosaved Reaction Set
Learn how to:
Create Saved Answer Sets
View All | Import

KEEP ME POSTED
You have no profiles.
Learn how to:
Create Keep Me Posted

SciFinder CAS SOLUTION | Preferences | SciFinder Help | Sign Out

Explore | Saved Searches | SciPlanner

Research Topic: "suzuki reaction with catalyst"

REFERENCES

Select All Deselect All **4**

0 of 5 Research Topic Candidates Selected

86 references were found containing "suzuki reaction with catalyst" as entered. **5**

8803 references were found containing the two concepts "suzuki reaction" and "catalyst" closely associated with one another. **6**

10723 references were found where the two concepts "suzuki reaction" and "catalyst" were present anywhere in the reference. **6**

18708 references were found containing the concept "suzuki reaction". **6**

2493732 references were found containing the concept "catalyst". **6**

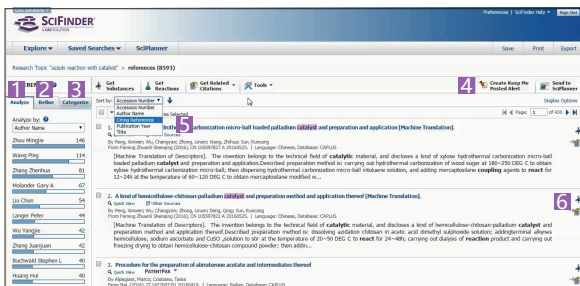
86
8803
10723
18708
2493732

Get References

- 1** 选择Research Topic
- 2** 输入关键词, 用介词 (of , with , to , in) 将关键词连接
- 3** 点击Search

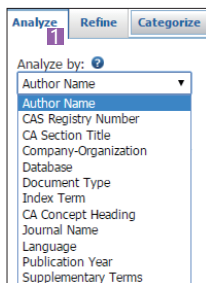
- 4 Concept, 表示SciFinder后台做了同义词、近义词扩展
- 5 Closed associated with one another, 表示两个关键词出现在同一个句子中
- 6 Were present anywhere in the reference, 表示两个关键词出现在同一条记录的任意位置

文献筛选

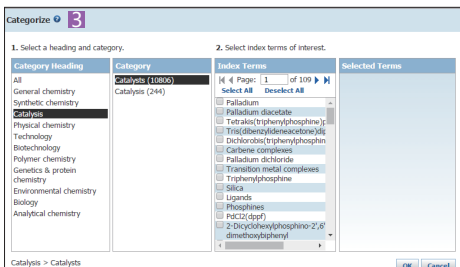
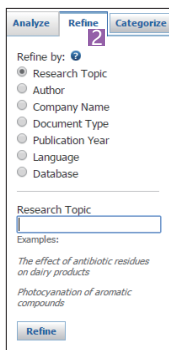


- 1 Analyze 分析工具
- 2 Refine 限定工具
- 3 Categorize 学科分析工具
- 4 Keep Me Posted Alert 定题跟踪服务
- 5 依据被引次数排序
- 6 文献的被引次数

筛选工具



- 1 Analyze 中的12种选项
- 2 Refine 中的7种选项
- 3 Categorize 学科分类工具, 依据学科自动分类



PatentPak™使用*

PatentPak™——专利工作流程解决方案

2. Exploiting the Differential Reactivities of Halogen Atoms: Development of a Scalable Route to IK02 Inhibitor AZD3264

By **Murugan, Anilgoppan**; Sachu, Sneekath; Marjanatha, Sufar G; Ramakrishnan, Ravi; Kadambur, Vasantha Krishna; Reddy, Chandrasekhara; Tollkonda, Venkata Rao; George, Sajay; Ramasubramanian, Srinivasan; Nambiar, Sudhar

From Organic Process Research & Development [2014], 18(5), 646-651. Language: English, Database: CASPLUS

An efficient and scalable synthesis of AZD3264 (1) is described in which the differential reactivities of various halogen atoms have been employed. The process involves five linear chem. steps with three isolated stages starting from com. available fragments.

3. Preparation of 2-(2,4,5-substituted-arylino)pyrimidine derivatives as EGFR modulators useful for treating cancer

By **Richard Andrew, Kadambur, Vasantha Krishna; Chandrasekhara, Reddy C; Murugan, Anilgoppan; Redifman, Heather Marie**

Patent No. WO 2013014448 A1 English

Patent Family

- US 201300857409 A1 English
- US 8940235 B2 English
- JP 2013544273 T Japanese
- JP 5427321 B2 Japanese
- KR 2014030089 A Korean
- KR 1410982 B1 Korean
- CN 103702990 A Chinese
- KR 2014047741 A Korean
- KR 1422619 B1 Korean
- KR 2014052181 A Korean

Abstract: The present invention relates to certain 2-(2,4,5-substituted-arylino)pyrimidine compds. [1: G = 4,5,6,7-tetrahydro[1,5-a]pyridin-1-yl, 1H-indol-3-yl, 1-methyl-1H-indol-3-yl, pyrazolo[1,5-a]pyridin-3-yl; R¹ = H, fluoro, chloro, Me, cyano; R² = methoxy, R³ = (3R)-3-(dimethylamino)pyrrolidin-1-yl, (3S)-3-(dimethylamino)pyrrolidin-1-yl, 3-(dimethylamino)azetidin-1-yl, [2-aminoethyl]methylamino, [2-(methylamino)ethyl]methylamino, 5-methyl-2,5-diazaspiro[3.4]oct-2-yl, (3aR,6aR)-2-oxahydro[3,4-e]pyrrolo[1,2-h]-1,1-methyl-1,2,3,5-tetrahydropyridin-4-yl, 4-...

4. A process for the synthesis of 2-(2,4,5-substituted-arylino)pyrimidine derivatives as EGFR modulators useful for treating cancer

By **Richard Andrew, Kadambur, Vasantha Krishna; Chandrasekhara, Reddy C; Murugan, Anilgoppan; Redifman, Heather Marie**

Abstract: The present invention relates to certain 2-(2,4,5-substituted-arylino)pyrimidine compds. [1: G = 4,5,6,7-tetrahydro[1,5-a]pyridin-1-yl, 1H-indol-3-yl, 1-methyl-1H-indol-3-yl, pyrazolo[1,5-a]pyridin-3-yl; R¹ = H, fluoro, chloro, Me, cyano; R² = methoxy, R³ = (3R)-3-(dimethylamino)pyrrolidin-1-yl, (3S)-3-(dimethylamino)pyrrolidin-1-yl, 3-(dimethylamino)azetidin-1-yl, [2-aminoethyl]methylamino, [2-(methylamino)ethyl]methylamino, 5-methyl-2,5-diazaspiro[3.4]oct-2-yl, (3aR,6aR)-2-oxahydro[3,4-e]pyrrolo[1,2-h]-1,1-methyl-1,2,3,5-tetrahydropyridin-4-yl, 4-...

1 点击PatentPak，获取PatentPak浏览器

Key Substances in Patent

CAS RN 1421373-38-7

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization International Bureau

(10) International Publication Number WO 2013/014448 A1

(43) International Publication Date 31 January 2013 (31.01.2013)

(51) International Patent Classification: C07D 401/02 (2006.01) A61K 31/437 (2006.01) C07D 473/04 (2006.01) A61P 35/00 (2006.01) A61K 31/586 (2006.01)

(21) International Application Number: PCT/GB2012/051783

(22) International Filing Date: 25 July 2012 (25.07.2012)

(25) Filing Language: English

(26) Publication Language: English

(36) Priority Data: 61/512,064 27 July 2011 (27.07.2011) US 61/591,363 27 January 2012 (27.01.2012) US

(74) Agent: ASTRAZENECA INTELLECTUAL PROPERTY; AstraZeneca AB, SE-151 85 Södertälje (SE).

2 PatentPak浏览器

Key Substances in Patent

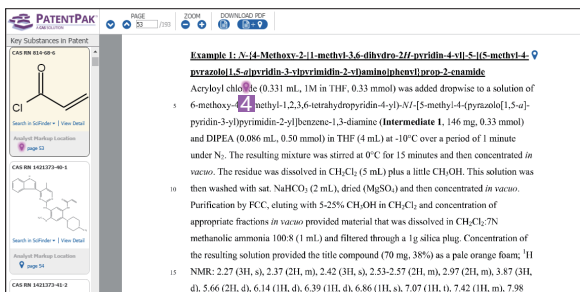
CAS RN 1421373-38-7

Example 1: N-[4-Methoxy-2-[1-methyl-3,6-dihydro-2H-pyridin-4-yl]-5-[5-methyl-4-pyrazolo[1,5-a]pyridin-3-yl]pyrimidin-2-yl]amino]phenyl]prop-2-enamide

Acryloyl chloride (0.331 mL, 1M in THF, 0.33 mmol) was added dropwise to a solution of 6-methoxy-4-(1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-N-[5-methyl-4-pyrazolo[1,5-a]pyridin-3-yl]pyrimidin-2-yl]benzene-1,3-diamine (Intermediate 1, 146 mg, 0.33 mmol) and DIPEA (0.086 mL, 0.50 mmol) in THF (4 mL) at -10°C over a period of 1 minute under N₂. The resulting mixture was stirred at 0°C for 15 minutes and then concentrated *in vacuo*. The residue was dissolved in CH₂Cl₂ (5 mL) plus a little CH₃OH. This solution was then washed with sat. NaHCO₃ (2 mL), dried (MgSO₄) and then concentrated *in vacuo*. Purification by FCC, eluting with 5-25% CH₃OH in CH₂Cl₂ and concentration of appropriate fractions *in vacuo* provided material that was dissolved in CH₂Cl₂:7N methanolic ammonia 100:8 (1 mL) and filtered through a 1g silica plug. Concentration of the resulting solution provided the title compound (70 mg, 38%) as a pale orange foam; ¹H NMR: 2.27 (3H, s), 2.37 (2H, m), 2.42 (3H, s), 2.53-2.57 (2H, m), 2.97 (2H, m), 3.87 (3H,

3 在PatentPak Viewer中点击物质下面的页码，快速定位到专利PDF文件中的物质信息

*PatentPak为新增模块，用户需要与学校图书馆查询是否已获得访问权限



Key Substances in Patent

CAS RN 814-08-0

Search in SciFinder | View Detail

Analyst Markup Location

page 12

CAS RN 1421373-40-1

Search in SciFinder | View Detail

Analyst Markup Location

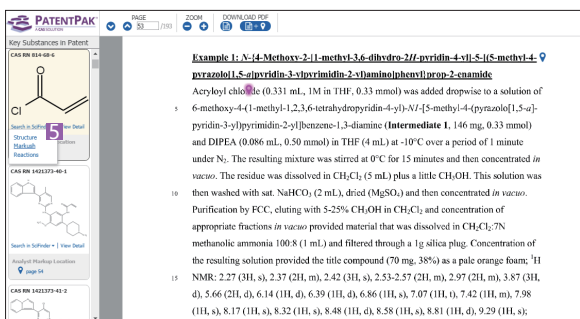
page 54

CAS RN 1421373-41-2

Example 1: [N-\[4-Methoxy-2-\[1-methyl-3,6-dihydro-2H-pyridin-4-yl\]-5-\[5-methyl-4-pyrazolo\[1,5-a\]pyridin-3-yl\]pyrimidin-2-yl\]amino\]phenyl\]prop-2-enamide](#)

Acryloyl chloride (0.331 mL, 1M in THF, 0.33 mmol) was added dropwise to a solution of 6-methoxy-4-(1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-N-[5-methyl-4-(pyrazolo[1,5-a]pyridin-3-yl)pyrimidin-2-yl]benzene-1,3-diamine (**Intermediate 1**, 146 mg, 0.33 mmol) and DIPEA (0.086 mL, 0.50 mmol) in THF (4 mL) at -10°C over a period of 1 minute under N₂. The resulting mixture was stirred at 0°C for 15 minutes and then concentrated *in vacuo*. The residue was dissolved in CH₂Cl₂ (5 mL) plus a little CH₃OH. This solution was then washed with sat. NaHCO₃ (2 mL), dried (MgSO₄) and then concentrated *in vacuo*. Purification by FCC, eluting with 5-25% CH₃OH in CH₂Cl₂ and concentration of appropriate fractions *in vacuo* provided material that was dissolved in CH₂Cl₂:7N methanolic ammonia 100:8 (1 mL) and filtered through a 1g silica plug. Concentration of the resulting solution provided the title compound (70 mg, 38%) as a pale orange foam; ¹H NMR: 2.27 (3H, s), 2.37 (2H, m), 2.42 (3H, s), 2.53-2.57 (2H, m), 2.97 (2H, m), 3.87 (3H, d), 5.66 (2H, d), 6.14 (1H, d), 6.39 (1H, d), 6.86 (1H, s), 7.07 (1H, t), 7.42 (1H, m), 7.98

4 也可以在PDF文件中与PatentPak进行互动



Key Substances in Patent

CAS RN 814-08-0

Search in SciFinder | View Detail

Structure Markups Reactions

page 5

CAS RN 1421373-40-1

Search in SciFinder | View Detail

Analyst Markup Location

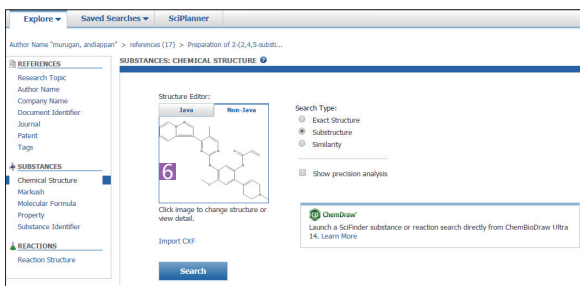
page 54

CAS RN 1421373-41-2

Example 1: [N-\[4-Methoxy-2-\[1-methyl-3,6-dihydro-2H-pyridin-4-yl\]-5-\[5-methyl-4-pyrazolo\[1,5-a\]pyridin-3-yl\]pyrimidin-2-yl\]amino\]phenyl\]prop-2-enamide](#)

Acryloyl chloride (0.331 mL, 1M in THF, 0.33 mmol) was added dropwise to a solution of 6-methoxy-4-(1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-N-[5-methyl-4-(pyrazolo[1,5-a]pyridin-3-yl)pyrimidin-2-yl]benzene-1,3-diamine (**Intermediate 1**, 146 mg, 0.33 mmol) and DIPEA (0.086 mL, 0.50 mmol) in THF (4 mL) at -10°C over a period of 1 minute under N₂. The resulting mixture was stirred at 0°C for 15 minutes and then concentrated *in vacuo*. The residue was dissolved in CH₂Cl₂ (5 mL) plus a little CH₃OH. This solution was then washed with sat. NaHCO₃ (2 mL), dried (MgSO₄) and then concentrated *in vacuo*. Purification by FCC, eluting with 5-25% CH₃OH in CH₂Cl₂ and concentration of appropriate fractions *in vacuo* provided material that was dissolved in CH₂Cl₂:7N methanolic ammonia 100:8 (1 mL) and filtered through a 1g silica plug. Concentration of the resulting solution provided the title compound (70 mg, 38%) as a pale orange foam; ¹H NMR: 2.27 (3H, s), 2.37 (2H, m), 2.42 (3H, s), 2.53-2.57 (2H, m), 2.97 (2H, m), 3.87 (3H, d), 5.66 (2H, d), 6.14 (1H, d), 6.39 (1H, d), 6.86 (1H, s), 7.07 (1H, t), 7.42 (1H, m), 7.98 (1H, s), 8.17 (1H, s), 8.32 (1H, s), 8.48 (1H, d), 8.58 (1H, s), 8.81 (1H, d), 9.29 (1H, s);

5 在PatentPak浏览器中直接进行SciFinder结构、马库什和反应检索



Explore | Saved Searches | SciPlanner

Author Name "munagan, andhapan" > references (17) > Preparation of 2-(2,4,5-substituted...)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Search Type:

Exact Structure

Substructure

Similarity

Show precision analysis

ChemDraw®

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More

Import CXF

Search

6 从PatentPak浏览器直接跳转到结构检索界面，同时无需绘制，系统会自动将相应的结构直接导入到绘图面板，点击Search即开始SciFinder检索，拓展新的研究方向

物质检索

物质记录详情

1 63968-64-9

2 ~4297

3

~122

4

Absolute stereochemistry.

C₁₅ H₂₂ O₅
 3,12-Epoxy-12H-pyrano[4,3-f]-1,2-benzodioxepin-10(3H)-one, octahydro-3,6,9-trimethyl-, (3R,5aS,6R,8aS,9R,12S,12aR)-

► **Key Physical Properties**
 Regulatory Information 5
 6 Spectra
 Experimental Properties 7

1 物质详情链接

5 物质管制信息链接

2 物质文献链接

6 物质谱图链接

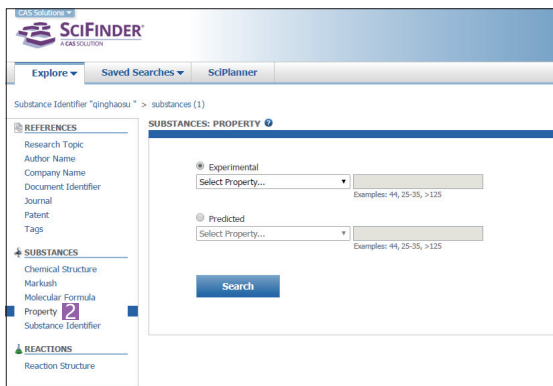
3 物质反应链接

7 物质实验性质链接

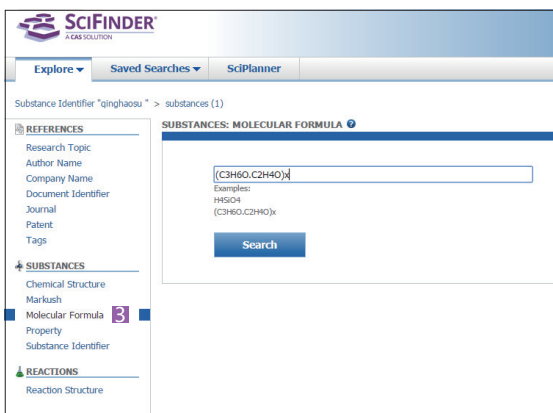
4 物质供应商链接

物质检索举例

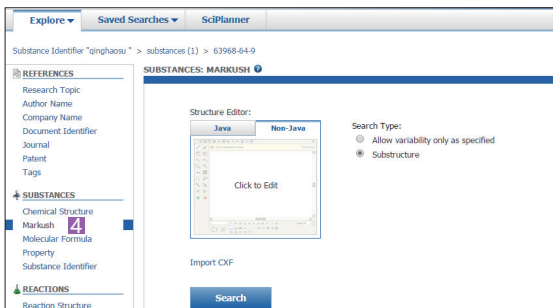
1 物质标识符 (CAS RN[®]、化学名、商品名、俗名等)



2 理化性质数据（实验数据、预测数据）

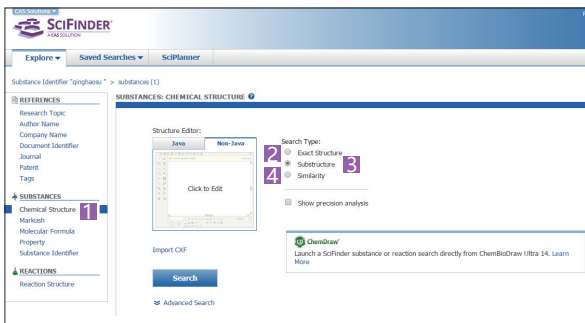


3 分子式（分子式输入需要遵守Hill排序规则：不含碳化合物，分子式按元素符号的字母顺序排列；含碳化合物，则“C”在前；如有氢则紧随其后，其它元素符号则按字母顺序排在氢的后面）



4 马库什检索，获取专利权利要求（说明书）中的Markush结构，用于确认化合物结构保护范围及获取最新化合物信息

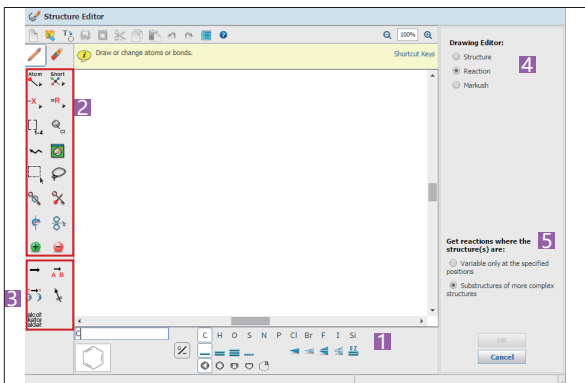
物质检索举例



- 1 结构检索
- 2 精确结构检索：获得被检索结构的盐、混合物、配合物、聚合物等，被检结构不能被取代
- 3 亚结构检索：包括精确结构检索结果，及被检索结构的修饰结构
- 4 相似结构检索：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

反应检索

结构绘制面板



- 1 常用原子、环、化学键
- 2 结构绘制工具组
- 3 反应定义工具组
- 4 结构检索、反应检索、马库什检索选项
- 5 当前检索模式下的功能选择

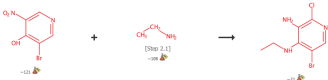
反应记录详情

REACTIONS 6 Send to SciPlanner

Analyze Refine 7 Group by: No Groups 4 Sort by: Relevance 5 0 of 3 Reactions Selected Display Options

1. **View Reaction Detail** 1 Link

3 Steps *Hover over any structure for more options.*



Overview Steps/Stages 2

1.1 R:POCl₂, R':RNEt₂, cooled; (PC) (PC) (PC) → rt; 2 h, reflux
 2.1 S:H₂O, S:THF, 3 h, rt
 3.1 R:HC, R':SnCl₄, S:H₂O, RDC: 1 h, reflux

Notes

3) regioselective, Reactants: 2, Reagents: 4, Solvents: 2, Steps: 3, Stages: 3, Most stages in any one step: 1

References

Preparation of affinity matrix for the identification of poly(ADP-ribose) polymerase (PARP) interacting molecules and for purification of PARP proteins
 G. Quik *et al.* **PatentPak**™
 In: *Drugs, Genes and Health: Volume*
 From PCT Int. Appl., 2009136229, 19 Nov 2009

Experimental Procedure

Step 1

Synthesis of 3-bromo-4-chloro-5-nitropyridine (III). To phosphorus oxychloride (50ml) cooled in ice was slowly added 3-bromo-5-nitropyridin-4-ol (6.57g, 30mmol). The resulting suspension was stirred at 0°C and N,N-diethylamine(4.17ml, 30mmol) was added drop wise. The resulting mixture was warmed at room temperature, then refluxed for 2 hours. The resulting black solution was concentrated under vacuum and the residue poured onto ice. The mixture was extracted with ether (200ml). The organic layer was washed with water, brine, and dried on MgSO₄. After filtration the solvent was removed to yield the desired compound as a brown oil which solidified upon further drying (5.46g, 85%). LCMS Rt=3.18min, no significant MS trace.

Step 2

Synthesis of 3-bromo-N-ethyl-5-nitropyridin-4-amine (IV). To a solution of 3-bromo-4-chloro-5-nitropyridine (6.45g, 25.4mmol) in THF (194ml) was added slowly a solution of ethyl amine in water (70% solution, 1012mmol, 24ml). The solution was stirred at room temperature for 3 hours then poured into water. The resulting solution was extracted twice with ethyl acetate. The organic layer was washed with brine, then dried over MgSO₄. The solvent was removed. The crude product was purified by flash chromatography (ethyl acetate:hexane 1:9 to 3:7) to yield the desired compound as a brown oil (5.45g, 92%). LCMS Rt=2.62min [M+H]⁺=246.248.

Step 3

Synthesis of 5-bromo-2-chloro-N-ethyl-4-aminopyridin-3,4-diamine (V). 3-bromo-4-ethyl-5-nitropyridin-4-amine (4.66g, 19mmol) was dissolved in concentrated hydrochloric acid (47ml) and heated at 85°C. Tin Chloride (50.8g, 57mmol) was added in portions. The reaction was heated at reflux for 1 hour then allowed to cool to room temperature overnight. The off white solid was filtered off then suspended in icy water (50ml). The pH was adjusted to 12 by addition of 12% sodium hydroxide. The resulting solution was extracted with ethyl acetate (2x100ml). The organic layer was washed with brine, and dried over MgSO₄. The solvent was removed to yield the desired compound as a yellow oil (3.96g, 83%). LCMS Rt=3.07min[M+H]⁺=246.9-251.9.

- 1 反应详情链接
- 2 反应总览
- 3 反应实验过程
- 4 反应分组
- 5 反应排序
- 6 将反应推送到SciPlanner
- 7 反应分析与限定

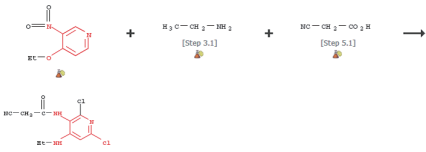
重排反应式

Group by: Document 1 Sort by: Number of Steps Answers per Page [20] Display: []

0 of 75 Reactions Selected Page: 1 of 2

1. **Imidazopyridinyl compounds as inhibitors of AKT activity and their preparation, pharmaceutical compositions and use in the treatment of cancer and arthritis** 4 Reactions 2 Full Text

5 Steps *Hover over any structure for more options.*



Overview

Experimental Procedure

- 1 选择Group by Document
- 2 所有来自同一篇文章的反应全部合并到一条记录中

Group by: Transformation **1** | Frequency | Display Options

0 of 3038 Reactions Selected | Page: 1 of 3

1. Aryl-Alkyne Coupling/ Stephens-Castro Coupling/ Sonogashira Coupling
173 Reactions

$$\text{Ar-X} + \text{HC}\equiv\text{CR} \xrightarrow{\text{cat.}} \text{Ar-C}\equiv\text{CR}$$

2

2. Hydrolysis or Hydrogenolysis of Amides/ Imides/ Carbamates
110 Reactions

$$\text{R-NH-CO-R}^1 \xrightarrow{\text{H}_2\text{O}} \text{R}^1\text{-COOH} + \text{R-NH}_2$$

$$\text{R-NH-CO-R}^1 \xrightarrow{\text{H}_2} \text{R-NH}_2$$

3. Reduction of Nitriles to Amines
20 Reactions

$$\text{R-C}\equiv\text{N} \longrightarrow \text{R-CH}_2\text{-NH}_2$$

4. Coupling of Aryl Compounds with Arylboronic Acid Derivatives/ Suzuki Coupling
15 Reactions

$$\text{Ar-Y} + \text{Ar}^1\text{-B}(\text{OR})_2 \xrightarrow{\text{cat.}} \text{Ar-Ar}^1$$

Y = OCOR', OSO₂R', Halogen

1 选择Group By Transformation

2 总结归纳反应类型

反应检索举例

REACTIONS: REACTION STRUCTURE

Structure Editor:

Java | Non-Java **1**

Search Type:

- Allow variability only as specified
- Substructure

Click image to change structure or view detail.

Import CXF (File uploaded)

2 Search

Advanced Search | Always Show

ChemDraw
Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More

1. View Reaction Detail | Link | Similar Reactions

Single Step | Hover over any structure for more options. **3**

100%

1 待检索的反应式

2 点击，执行反应检索

3 获取相似反应

4 选择不同的相似级别，获得相似反应

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity: **4**

- Broad - Reaction centers only (117483)
- Medium - Reaction centers plus adjacent atoms and bonds (112098)
- Narrow - Reaction centers plus extended atoms and bonds (107216)

Get Reactions | Cancel

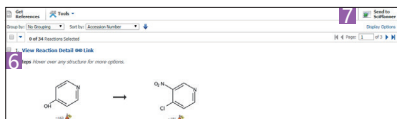
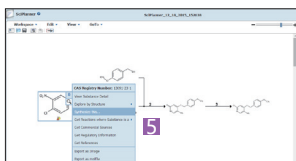
SciPlanner™使用



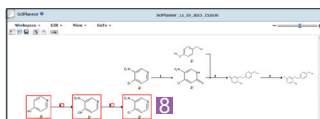
- 1 勾选想要的反应
- 2 点击Send to SciPlanner



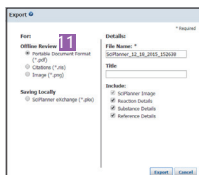
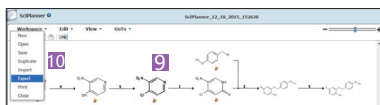
- 3 workspace 下新建一个文件
- 4 进入SciPlanner，将刚推送过来的反应拖动到屏幕中间



- 5 点击反应中的一个物质，单击上面的双箭头，选择Synthesis this
- 6 在检索到的反应中，选择感兴趣的一条反应
- 7 将该条反应继续推送到SciPlanner中



- 8 将推送过来的反应拖动到屏幕中间，可以看到两条反应中存在同样的结构



- 9 用鼠标将两个同样的结构拖动至重叠状态，两条反应合并
- 10 点击 Workspace，选择其中的 Export 输出结果
- 11 选择适当的输出格式，输出结果

MethodsNow™使用*

MethodsNow™快速获取更加详细的合成方法

1 Analyze for: **MethodsNow**

2 **MethodsNow**

3 View with MethodsNow

Overview

Steps/Stages

- 1.1 R₂NH, S₂THF, 0°C, 70 min, rt, 0°C
- 1.2 2 min, 0°C, 16 h, rt
- 2.1 R₂NH(O₂C₂), S₂EtO(CH₂)₂, 2.5 h, rt; 20 h, reflux; reflux → 0°C
- 2.2 R₂NH(O₂C₂), S₂EtO(CH₂)₂, 2.5 h, rt; 20 h, reflux; reflux → 0°C
- 3.1 S₂THF, overnight, 120°C
- 4.1 R₂NH, C₂H₅CO₂Et, S₂THF, 5 min, rt; 15 min, rt; 5 min, rt
- 4.2 reflux
- 5.1 R₂NH, 4⁺, S₂THF, 30 min, rt
- 6.1 R₂NH, 4⁺(AcO)₂H, S₂THF, S₂AcOEt, overnight, reflux
- 7.1 Cs₂CO₃, S₂THF, overnight, rt
- 8.1 R₂NH, S₂THF, 1 h, rt
- 8.2 R₂NH, S₂THF, 1 h, rt
- 9.1 R₂NH, S₂THF, 12 h, rt

Notes

4) stereoselective, 6) stereoselective, 8) stereoselective, Reactants: 5, Reagents: 5, Catalysts: 2, Solvents: 10, Steps: 9, Stages: 13, Most steps in any one step: 2

References

Synthesis of D- and L-Carboxylic Nucleosides via Rhodium-Catalyzed Asymmetric Hydroacylation as the Key Step
 B. Zhou, P. Zhou, et al.
 From Organic Letters, 33(21), 4755-4758, 2008

Experimental Procedure

METHODSNOW™

Procedure

1. Add by cannula a solution of 2-methylene-1,3-propanediol (57.1 mmol) in dry THF (44 mL) slowly to NaH (2.38 g, 57.1 mmol, 60% dispersion in mineral oil) at 0°C.
2. Stir the reaction mixture for 70 minutes at room temperature under nitrogen.

Available Experimental Data

¹H NMR, ¹³C NMR, IR, DLS, UV, Elemental Analysis, State

View with MethodsNow **3**

- 1 在SciFinder反应结果集的分析选项中，获取有MethodsNow的反应结果
- 2 也可以在反应结果集的排序选项中获取
- 3 点击View with MethodsNow，获取合成方法详情

MethodsNow

Synthesis of D- and L-Carboxylic Nucleosides via Rhodium-Catalyzed Asymmetric Hydroacylation as the Key Step

By Marco, Fabrizio, Diaz, Yolanda, Maffeo, M. Isabella, Castillon, Sergio
 From Organic Letters, 33(21), 4755-4758, 2008
 Published by American Chemical Society

Reaction Steps **1** **2** **3** **4** **5** **6** **7** **8** **9** **10** **11**

4 **5**

Products

2-Propanoic acid, 2-[[[(1,1-dimethylethyl)phenyl]imino]methyl]-, 98%, CAS RN: 17769-51-6

Reactants

1,3-Propanediol, 2-methylene-, CAS RN: 3513-61-3
 1,1'-[Chloro(1,1-dimethylethyl)phosphono]benzene], CAS RN: 58479-61-1

Reagents

Sodium hydride, CAS RN: 7599-97-7

Solvents

Tetrahydrofuran, CAS RN: 109-99-9

Procedure

1. Add by cannula a solution of 2-methylene-1,3-propanediol (57.1 mmol) in dry THF (44 mL) slowly to NaH (2.38 g, 57.1 mmol, 60% dispersion in mineral oil) at 0°C.
2. Stir the reaction mixture for 70 minutes at room temperature under nitrogen.
3. Cool the solution to 0°C.
4. Add 100%PCP (14.9 g, 14.1 mL, 54.2 mmol) to the reaction mixture over 2 minutes, turning the solution cloudy.
5. Stir the reaction mixture for 16 hours at room temperature.
6. Evaporate the solvent.
7. Dissolve the white residue in a mixture of H₂O (20 mL) and Et₂O (20 mL).
8. Extract the aqueous layer with Et₂O (3 × 50 mL).
9. Dry the combined organic layer with MgSO₄.
10. Concentrate the combined organic layer under reduced pressure.
11. Purify the residue by flash chromatography (hexane/EtOAc 5:1).

Scale

milligram

¹H NMR

CDCl₃, 400 MHz δ in ppm: 7.26-7.7 (m, 4H, Ar), 7.47-7.61 (m, 8H, Ar), 5.18 (s, 1H, H-3a), 5.13 (s, 1H, H-3b), 4.28 (s, 2H, H-4), 4.18 (s, 2H, H-1), 1.97 (br, 1H, OH), 1.08 (s, 9H, t-Bu).

¹³C NMR

CDCl₃, 100.6 MHz δ in ppm: 147.3 (C-1), 133.4, 135.7, 130.0, 127.9 (Ar), 111.3 (C-3), 67.6 (CH₂OH), 99.8 (C-1), 27.8 (CH₃, t-Bu), 19.4 (C, t-Bu).

State

colorless oil.

CAS Method Number

3-008-CAS-1096210

8 Print/Export Close


*MethodsNow为新增模块，用户需要与学校图书馆查询是否已获得访问权限

- 4 书目信息
- 5 点击反应步数即可获得该步反应的详细操作信息
- 6 反应中涉及的物质：产物、反应物、催化剂、溶剂和相关物质的CAS登记号等，点击CAS登记号即可转到SciFinder物质检索界面，查看物质信息详情。
- 7 可以获得分步列出的反应过程，反应量级，图谱数据，元素分析和其他可获得的性质数据。
- 8 可以打印或者保存到本地电脑

MethodsNow快速获取详细的分析方法

MethodsNow Analysis (www.methodsnow.com)

- Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析...
- Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析
- Pharmacology / Toxicology: 成瘾药物检测，有毒物检测...
- Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定...
- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析...
- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析...
- Agricultural Applications / Analysis: 除草剂分析...
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析...
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工...
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析...



Your single source to search and compare the latest published scientific methods.
Log in with your CAS Username
[Learn more](#)

Username

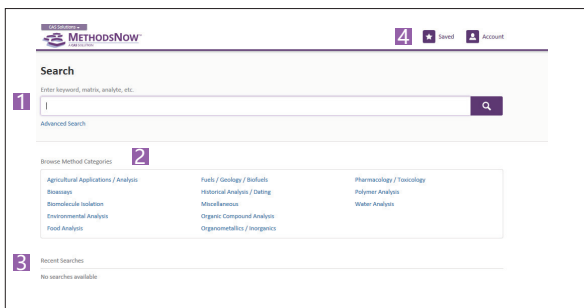
1 Password

[Log In](#)

Forgot Username or Password?

Use of this product means that you agree to the [Terms & Conditions](#).

- 1 登录www.methodsnow.com网址，输入用户名和密码

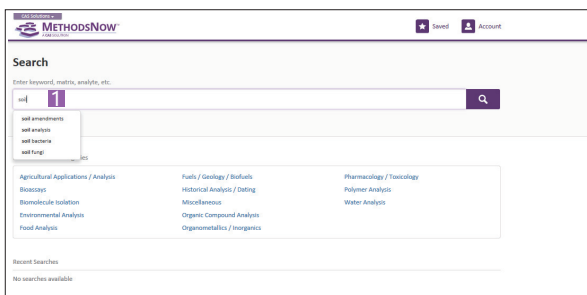


- 1 可以在检索框输入关键词或者分析物等进行检索
- 2 也可以通过浏览方法分类，点击一个浏览类别查看相关方法
- 3 点击历史检索重新运行检索，点击X删除检索历史
- 4 保存结果集

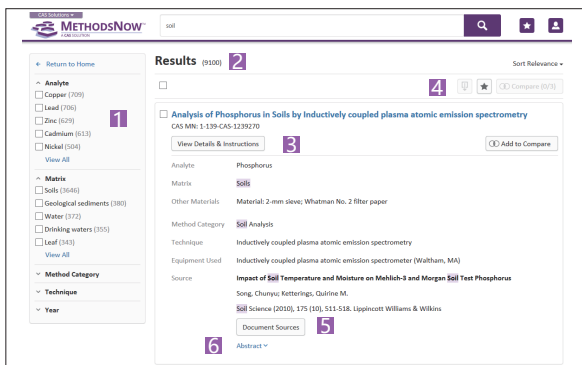


- 1 逻辑运算符：and, or, not
- 2 检索条件包括：关键词，分析物，基质，方法分类，技术手段，CAS方法号，出版物名称
- 3 增加检索条件
- 4 删除检索条件

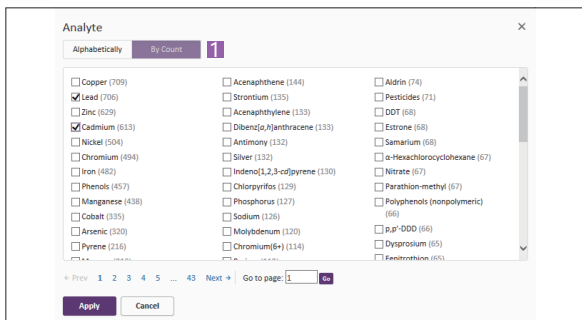
案例：在土壤中检测重金属的方法



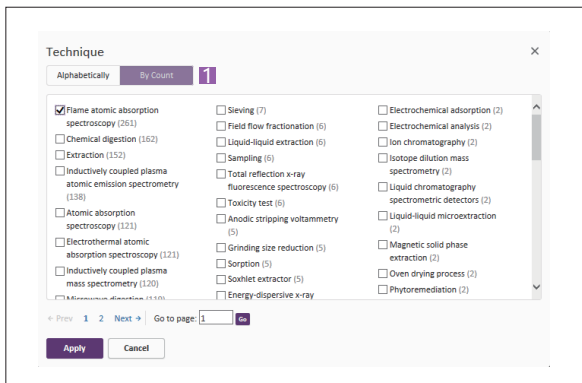
- 1 此处只需要输入物质的一个名称即可，MethodsNow会自动进行同义词的查找



- 1 按照分析物、基质、方法分类、技术手段、公开年份等条件筛选结果
- 2 方法结果数量
- 3 查看方法信息详情
- 4 导出或者保存方法
- 5 获得全文链接
- 6 展示摘要



- 1 点击分析物列表，选择目标分析物



- 1 点击技术手段列表，选择技术手段

Analysis of Cadmium in Soils by Flame atomic absorption spectroscopy

CAS MN: 1-139-CAS-93451

Method Category: **Soil** Analysis; Trace Element Analysis
 Technique: Electrothermal atomic absorption spectroscopy; Flame atomic absorption spectroscopy

1

Materials	Role	Image	CAS RN
Cadmium	analyte	View Structure	7440-43-9
Soils	matrix		
Cd hollow cathode lamp	material		
Hydrochloric acid	reagent	View Structure	7647-01-0
Perchloric acid	reagent	View Structure	7601-00-3
Nitric acid	reagent	View Structure	7697-37-2
Hydrofluoric acid	reagent	View Structure	7664-39-0

2

Source
Atomic absorption spectrometric determination of cadmium and lead in **soil after total digestion**
 Naeem, Kashif, Yawar, Wasim, Akhter, Perveen, Rehana, Ishrat
 Asia-Pacific Journal of Chemical Engineering (2012), 7 (2), 295-301. John Wiley & Sons Ltd.
 CODEN: AJCEBK | ISSN: 19922135 | DOI: 10.1002/apj.535

3

[Document Sources](#)

4

Abstract
 To establish the baseline levels of Cd and Pb in Pakistani **soil**, samples were collected from various eco. areas of the country. A total digestion procedure using an acid mixture of HF-HClO₄ was investigated for heavy metal anal. of **soil** samples. Concentrations of these elements were measured using flame and graphite furnace at. absorption spectrometry. Measured contents of Cd and Pb varied from 0.41-1.18 and 22.47-85.75 µg/g with geometric mean 0.73 and 47.39 and geometric standard deviation concentrations of 1.16 and 1.65 µg/g, resp. Two certified reference materials (JAEA-**soil** 7 and IAEA-405 (soil/trace element)) were introduced for the validation of anal. data. The estimated values were compared with other regions of the world and found lower than the world average values, Cd 27% and Pb 13%, and therefore considered comparatively safe and may not be a cause of concern for environmental pollution.

5

Equipment Used
 Flame and graphite furnace atomic absorption spectrophotometer, 2-8000, Hitachi, Ltd., Tokyo, Japan

6

Conditions
 Instrument
 lamp current: 7.5 mA, wavelength: 228.8 nm, slit: 1.3 mm, burner height: 7.5 mm, acetylene flow rate: 2.2 L/min, air flow rate: 9.4 L/min, argon flow rate: 100 mL/min, injection volume: 10 µL.

7

Instructions
Preparation of **soil sample**
 1. Collect 5 kg of **soil** from suburb area in a clean plastic bags and mark.
 2. Air dry the sample.
 3. Grind in an agate mill and pass through 100 µm sieve.
 4. Dry the sample in an oven at 110 °C.
 5. Weigh 0.5 g **soil** and place in a Teflon beaker.
 6. Add 10 drops of distilled water, 5 mL HClO₄ and 5 mL HF in a beaker.
 7. Allow to stand for 16 h.
 8. Dry on sand bath at 50-60 °C.
 9. Add 5 mL HF and 5 mL HClO₄ to dry sample.
 10. Add 2.5 mL HClO₄ and dry to eliminate HF.
 11. Add residue to 10 mL water and 2.5 mL HCl.
 12. Heat on sand bath to dissolve the residue completely.
 13. Make the volume up to 25 mL.

Flame and graphite furnace atomic absorption spectrophotometer method
 1. Analyze the sample using flame atomic absorption spectrophotometer (FAAS) and graphite atomic absorption spectrophotometer (GFAAS) (Hitachi, Ltd., Tokyo, Japan).
 2. Set the instrument condition as follows: Cd lamp current: 7.5 mA, wavelength: 228.8 nm, slit: 1.3 mm, burner height: 7.5 mm, acetylene flow rate: 2.2 L/min, air flow rate: 9.4 L/min, argon flow rate: 100 mL/min.
 3. Inject 10 µL sample to instrument.

8

Validation
 Recovery: 112.2%

1 分析方法所用材料

2 书目信息

3 原文链接

4 摘要

5 使用仪器

6 实验条件

7 分析方法操作步骤

8 方法有效性

Results (261)

Sort Relevance ▾



[Compare \(0/3\)](#)

Analysis of Cadmium in Soils by Flame atomic absorption spectroscopy

CAS MN: 1-139-CAS-93451

[View Details & Instructions](#)

1

[Add to Compare](#)

Analyte: **Cadmium**

Matrix: **Soils**

Other Materials: **Reagent:** Hydrochloric acid; Perchloric acid; Nitric acid; Hydrofluoric acid
Material: Cd hollow cathode lamp

Method Category: **Soil** Analysis; Trace Element Analysis

Technique: **Electrothermal atomic absorption spectroscopy; Flame atomic absorption spectroscopy**

Equipment Used: **Flame and graphite furnace atomic absorption spectrophotometer**

Source: **Atomic absorption spectrometric determination of cadmium and lead in **soil** after total digestion**
 Naeem, Kashif, Yawar, Wasim, Akhter, Perveen, Rehana, Ishrat
 Asia-Pacific Journal of Chemical Engineering (2012), 7 (2), 295-301. John Wiley & Sons Ltd.

[Document Sources](#)

[Abstract ▾](#)

METHODSNOW
FOR SOLUTION

Compare Methods **2**

Expand All Collapse All **3**

	1	2	3
Title	Analysis of Cadmium in Soils by Flame atomic absorption spectroscopy	Analysis of Cadmium in Soils by Flame atomic absorption spectroscopy	Analysis of Lead in Soils by Flame atomic absorption spectroscopy
CAS Method Number	1-139-CAS-93451	1-139-CAS-93840	1-139-CAS-103728
Method Category	Soils Analysis; Trace Element Analysis	Soils Analysis; Element Detection	Soils Analysis; Trace Element Analysis
Technique	Electrothermal atomic absorption spectroscopy; Flame atomic absorption spectroscopy	Oven drying process; Flame atomic absorption spectroscopy	Electrothermal atomic absorption spectroscopy; Flame atomic absorption spectroscopy
Analyte	Cadmium	Cadmium	Lead
Matrix	Soils	Soils	Soils
Other Materials	Hydrochloric acid, Perchloric acid, Nitric acid, Hydrofluoric acid, Cd hollow cathode lamp	2-Heptanone; Potassium iodide; Tricrythylammonium chloride; Nitric acid; Whatman #42 filter paper	Hydrofluoric acid, Perchloric acid, Hydrochloric acid, Nitric acid, Pb hollow cathode lamp
Equipment Used	Flame and graphite furnace atomic absorption spectrophotometer; Z-6000, Hitachi, Ltd., Tokyo, Japan	Spectrometer	Flame and graphite furnace atomic absorption spectrophotometer; Z-6000, Hitachi, Ltd., Tokyo, Japan
Conditions	Instrument: lamp current: 7.5 mA, wavelength: 228.8 nm, slit: 1.3 nm; burner height: 7.5 mm; acetylene flow rate: 2.3 View All	Instrument: Detection at: 228.8 nm.	Instrument: lamp current: 7.5 mA, wavelength 283.3 nm; slit: 1.3 nm; burner height: 7.5 mm; acetylene flow rate: 2.3 View All
Source	Atomic absorption spectrometric determination of cadmium and lead in soils after total digestion View All	A comparison of reliability of soils cadmium determination by standard spectrometric methods View All	Atomic absorption spectrometric determination of cadmium and lead in soils after total digestion View All
Preparation	Preparation of soils sample 1. Collect 5 kg of soils from suburb area View All		Preparation of soils sample 1. Collect 5 kg of soils from suburb area View All
Method	Flame and graphite furnace atomic absorption spectrophotometer method 1. Analyze the sample using flame View All	Extraction of the soils samples and flame atomic absorption (FAA) detection of cadmium 1. Prepare a set of 50 soils associated to View All	Flame and graphite furnace atomic absorption spectrophotometer method 1. Analyze the sample using flame View All
Recovery	112.3%	73% (SRM-2702); 55% (SRM-2709)	108.3%
Concentration		0.108 - 3.90 mg/kg	

- 1 选择感兴趣的方法进行对比
- 2 一次最多可以比较三种不同方法，所有方法信息详情的内容都可以进行对比
- 3 可以将方法比较结果下载成pdf或者excel格式文件到本地电脑

天然产物分离

METHODSNOW
FOR SOLUTION

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

Agricultural Applications / Analysis	Fuels / Geology / Biofuels	Pharmacology / Toxicology
Bioassays	Historical Analysis / Dating	Polymer Analysis
Biomolecule Isolation	Miscellaneous	Water Analysis
Environmental Analysis	Organic Compound Analysis 1	
Food Analysis	Organometallics / Inorganics	

Browse Method Categories > Organic Compound Analysis

Active Pharmaceutical Ingredient and Metabolite Analysis	Natural Product Isolation Analysis	2
Chiral Separation	Organic Compound Analysis	

- 1 浏览方法分类，选择有机化合物分析
- 2 获得全部关于天然产物分离/分析的文獻

[Return to Home](#)

Analyte

- Phenols (11417) **1**
- Flavonoids (7834)
- Polyphenols (nonpolymeric) (2571)
- Tannins (2288)
- Quercetin (2134)
- [View All](#)

Matrix

- Leaf (8807)
- Root (2522)
- Stem (2361)
- Seed (2039)
- Flower (1597)
- [View All](#)

Method Category

Technique

Year

Results (41895)

Sort Relevance ▾

🔍 ★ 🔍 Compare (0/3)

Analysis of Tannins in Coriandrum sativum by Extraction

CAS MN: 1-131-CAS-43974

[View Details & Instructions](#) [Add to Compare](#)

Analyte	Tannins
Matrix	Coriandrum sativum
Other Materials	Reagent: Methanol; Sulfuric acid
	Material: Whatman No. 4 filter paper
Method Category	Natural Product Isolation Analysis
Technique	Spectrophotometry; Extraction
Equipment Used	Spectrophotometer
Source	Chemical composition and antioxidant activity of the coriander cake obtained by extrusion Srih, Jazia; Bettaleb, Iness; Bachrouch, Ofra; Talou, Thierry; Marzouk, Brahim Arabian Journal of Chemistry, - Elsevier B.V.

[Document Sources](#)

1 根据需要，对相应的分离物、基质进行筛选

[Return to Results](#)

Method Detail (1 of 1)

◀ Prev Next ▶

🔍 ★

Analysis of Tannins in Coriandrum sativum by Extraction

CAS MN: 1-131-CAS-43974

Method Category: **Natural Product Isolation Analysis**

Technique: Spectrophotometry; Extraction

1

Materials	Role	Image	CAS RN
Tannins	analyte		
Coriandrum sativum	matrix		
Whatman No. 4 filter paper	material		
Methanol	reagent	View Structure	67-56-1
Sulfuric acid	reagent	View Structure	7664-93-9

2

Source

Chemical composition and antioxidant activity of the coriander cake obtained by extrusion
Srih, Jazia; Bettaleb, Iness; Bachrouch, Ofra; Talou, Thierry; Marzouk, Brahim
Arabian Journal of Chemistry, - Elsevier B.V.
CODEN: AJCRRD | ISSN: 18785352 | DOI: 10.1016/j.ajoc.2014.11.043

[Document Sources](#)

3

Abstract

This study was designed to examine the effect of operating conditions on essential oil composition and antioxidant activity of coriander cakes. Twenty-one components were determined in essential oils, which were mostly α -monoterpenes. The highest essential oil yields (0.12%) were obtained by the nozzle diameter of 3 mm. The main components of cake essential oil (linalool, γ -terpinene, geranyl acetate, linalyl acetate and camphor) showed significant variations with different nozzle diameter. The total phenol contents and condensed flavonoid contents varied between different nozzle diameters; the highest values obtained of small diameters (5 and 6 mm). Significant differences were also found in total tannin contents among different nozzle diameters. The total phenol contents decreased significantly ($p < 0.05$) when increased the nozzle diameter to 9 mm and reached 8.11 mg GAE/g. The screening of antioxidant activity of the different coriander cakes using the diphenyl-(2,4,6-trinitrophenyl)aminoazanium radical (DPPH) assay showed an appreciable reduction of the stable radical DPPH, although small nozzle diameter was the most efficient method with an IC_{50} reached of 55 μ g/ml, as compared with bigger diameter ($IC_{50} = 88 \mu$ g/ml). All the extracts had lower β -carotene bleaching activity than that of synthetic antioxidant BHA and BHT. Coriander cake extracts presented a very low reducing power ability ($EC_{50} = 700 \mu$ g/ml) compared to ascorbic acid ($EC_{50} = 40 \mu$ g/ml).

4

Equipment Used

Spectrophotometer

5

Conditions

Instrument

Wavelength: 500 nm

6

Instructions

Extraction

1. Extract the fruits from coriander with single screw press extruder, and collect the cake samples immediately for further analysis.
2. Perform extrusion using a single-screw (Mitsui OMRGA 20, France) with a motor (0.75 kW, 230 V of maximal tension), a screw length of 18 cm, a pitch screw of 1.8 cm, with an internal diameter of 1.4 cm, a channel depth of 0.5 cm and a sleeve of 2.5 cm of internal diameter equipped with a filter-perforated outlet for liquid at the end of the screw and at the surface of the nozzles.
3. Use the filter section of 2 mm in diameter to separate extracted oil.
4. Maintain the feed rate and the screw rotation speed at 15 g/min (0.9 kg/h) and 40 rpm, respectively.
5. Use the nozzles of different diameters (9-6 mm) in the pressing of the coriander seed and the nozzle/screw distance of 3 cm.
6. First run the screw press for 15 min without seed material but with heating via an electrical resistance-heating ring attached around the press barrel, to raise the screw press barrel temperature to the desired value.
7. Adjust the running temperature with a thermocouple.

Extraction

1. Finely grind the air-dried coriander cake with a blade/corbis grinding.
2. Extract separately the triplicate subsamples of 2.5 g of each ground sample by stirring with 10 ml of pure methanol for 30 min.
3. Place the extracts for 24 h at 4 °C and filter through a Whatman No. 4 filter paper.
4. Evaporate under vacuum to dryness and store at 4 °C until the analysis.

Determination of total condensed tannin content

1. Add a total of 3 ml of 4% methanol vanillin solution and 2.5 ml of concentrated H_2SO_4 to 50 μ l of suitably diluted sample.
2. Incubate the mixture for 15 min.
3. Measure the absorbance at 500 nm against methanol as a blank.
4. Express the amount of total condensed tannins as milligrams of (+)-catechin equivalent per gram of dry weight (mg of CE/g of DW) through the calibration curve with catechin.

7

Validation

Concentration	3.00 mg CE/g DW
---------------	-----------------

8

1 实验所用材料

2 书目信息

3 摘要

4 使用的仪器

5 实验条件

6 提取、分离步骤详情

7 产物的表征

8 方法有效性

美国化学文摘社 (Chemical Abstracts Service, 简称“CAS”) 是美国化学会 (American Chemical Society, 简称“ACS”) 旗下的分支机构, 是全球提供化学及相关信息解决方案的权威机构。秉承美国化学会“通过化学的力量改善人们的生活”的愿景, 美国化学文摘社专业的科学家团队致力于发现、收集及管理所有公开的化学物质信息, 创建了世界上对于创新至关重要的、最有价值的内容集合。全球的科研人员及从事专利的专业人士依靠美国化学文摘社提供的研究解决方案实现其科研发现并完成工作流程。

Connect with SciFinder:



美国艾赛思国际有限公司北京代表处
Tel: 010-62508026/7
Email: china@acs-i.org



scifinder.cas.org