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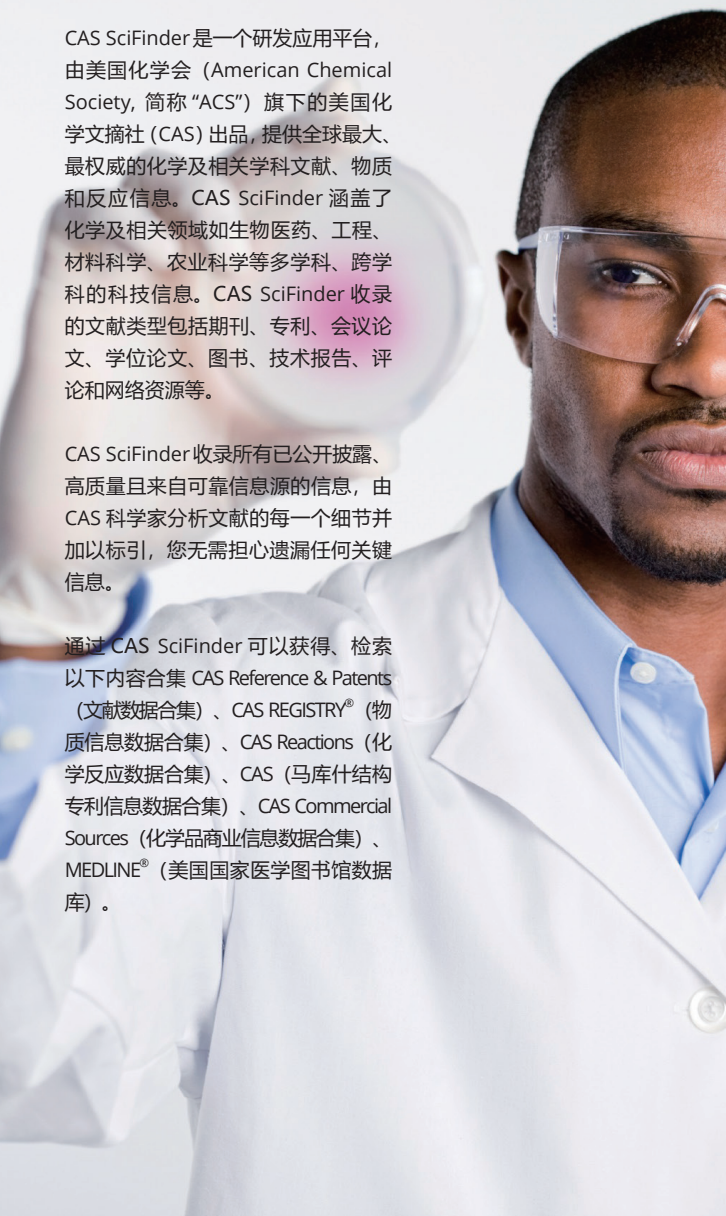
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1. Highly transparent and organosoluble polyimides derived from 2,2'-disubstituted-4,4'-oxydianilines **1**

By: Chen, Yi-Chieh; Rajendran, Kappachari; Chang, Yi-Hsi; Huang, Sheng-Kwei; [Chem. Title](#)

To improve the optical transparency and organosol. of arom. polyimides derived from 4,4'-oxydianiline (4,4'-ODA), two new arom. diamines, 2,2'-di(2o-4,4'-oxydianiline (DI-ODA) and 2,2'-bis(p-trifluoromethylphenyl)-4,4'-oxydianiline (BTFF-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. dianhydrides via a one-step high-temp. polycondensation procedure. The new polyimides showed enhanced sol. in common org. solvents compared with those corresponding polyimides derived from 4,4'-ODA. Esp., polyimide derived from BTFF-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/g) 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 347-391 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 267-327°. The decomp. temps. of these polyimides at 5% wt. loss under nitrogen were 420^o-609^o. Because of the weak carbon-iodine bond, polyimides derived from DI-ODA decreapt. at lower temps. than polyimides derived from BTFF-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 sol. 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

3

Polyimides

polyether-, aromatic, fluorine-containing; prepn. and properties of highly transparent and organosol. polyimides derived from disubstitutedoxydianilines

Properties; Synthetic preparation; Preparation

Substances

4

101-63-3P [Q](#)
100125-47-1P [Q](#)
128796-39-9P p-(Trifluoromethyl)pyromellitic acid [Q](#)

Intermediate; prepn. and properties of highly transparent and organosol. polyimides derived from disubstitutedoxydianilines

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SOURCE
Journal of Applied Polymer Science
Volume120
Issue4
Pages3159-3
Journal
2011
CODEN:JAPNAB
ISSN:1002-8955
DOI:10.1002/app.33520

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

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CANISH-410987
CAPUS

Citations

Widulski, H.; *Polym Sci* 2009, 58, 1299 [Q](#)
Zhai, X.; *J Appl Polym Sci* 2010, 117, 1144 [Q](#)
Feng, Y.; *Macromolecules* 1996, 31, 5032 [Q](#)
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Kuan, S.; *J Appl Polym Sci* 2009, 113, 3993 [Q](#)
Wang, S.; *J Polym Sci Part A: Polym Chem* 1997, 35, 1487 [Q](#)

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- 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

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8803 references were found containing the two concepts "suzuki reaction" and "catalyst" closely associated with one another. **5**

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**

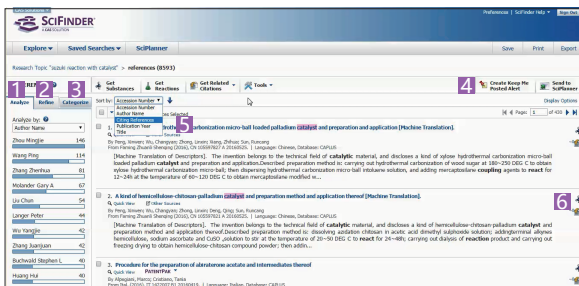
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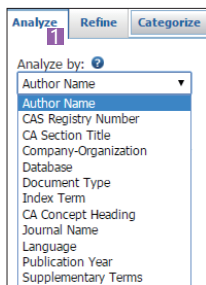
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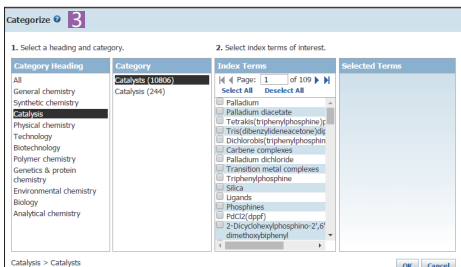
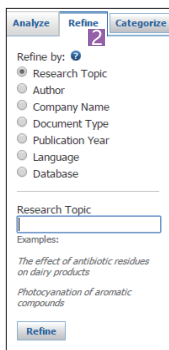


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CAS PatentPak™——专利工作流程解决方案

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

By **Murugan, Andappan**; Sachu, Sreerath; Marjantha, Sufar G.; Ramakrishnan, Ravi; Kadambur, Vasantha Krishna; Reddy, Chandrashekar; Tollkonda, Venkata Rao; George, Sajay; Ramasubramanian, Srinivasan; Nambiar, Sudhar

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

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-aryl)pyrimidine derivatives as EGFR modulators useful for treating cancer

By **Richard Andrew, Kadambur, Vasantha Krishna; Chandrashekar, Reddy C.; Murugan, Andappan; Redfern, Heather Marie**

Patent No. WO 2013014448 A1 English

Patent Family

Patent No.	Kind	Language
US 201300857409	A1	English
US 8940235	B2	English
JP 2013544273	T	Japanese
JP 5427321	B2	Japanese
KR 2014030089	A	Korean
KR 2014010982	B1	Korean
CN 103702990	A	Chinese
KR 2014047741	A	Korean
KR 1422619	B1	Korean
KR 2014062181	A	Korean

Abstract: ...carboxylate azaspiroindocanymethylphenylethylaminohydroxyethylhydroxybenzothiazole

By **Stuart P.; Meadows, Rebecca Elizabeth; Harfield, Eric; Mitchell, Christopher William; Murugan, Andappan; O'Keefe, Philip; Patel, Zakariya**

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Key Substances in Patent

CAS RN 1421373-38-7

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(19) World Intellectual Property Organization International Bureau

(10) International Publication Number WO 2013/014448 A1

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

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

(25) Filing Language: English

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

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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-ynamide**

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,

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Key Substances in Patent

CAS RN 014-08-G

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Analyt. Markup Location

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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

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Key Substances in Patent

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Structure Markups Reactions

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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);

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物质检索

物质记录详情

1 63968-64-9

2 ~4297

3

4 ~122

Absolute stereochemistry.

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

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

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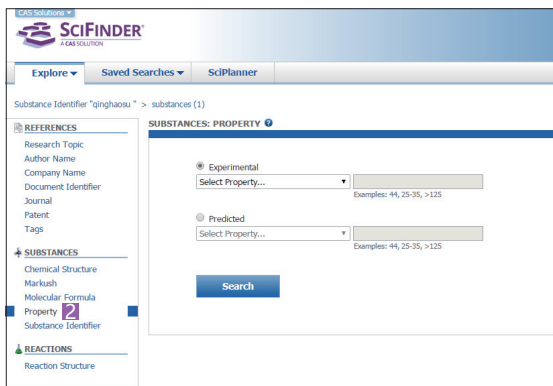
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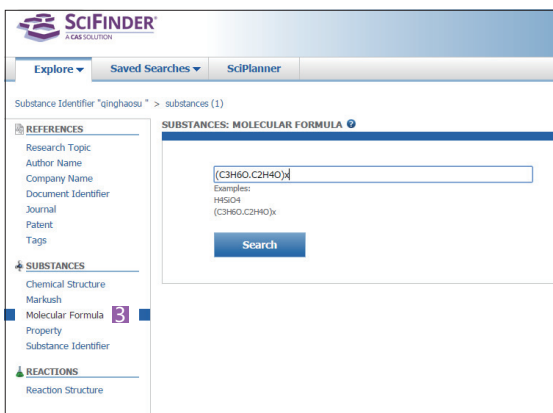
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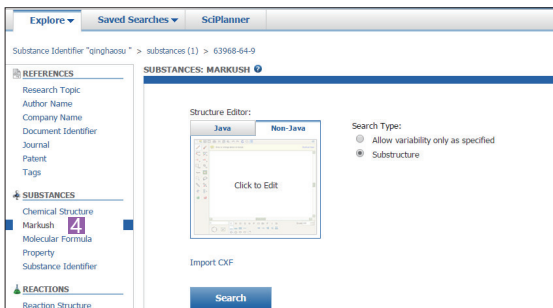
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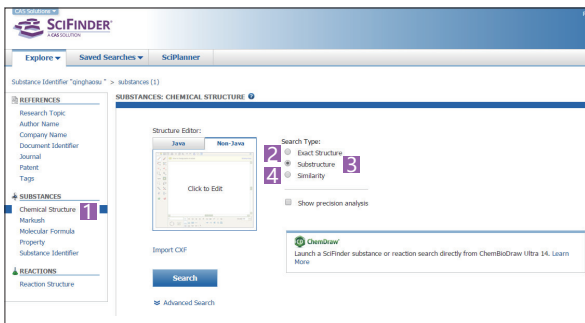


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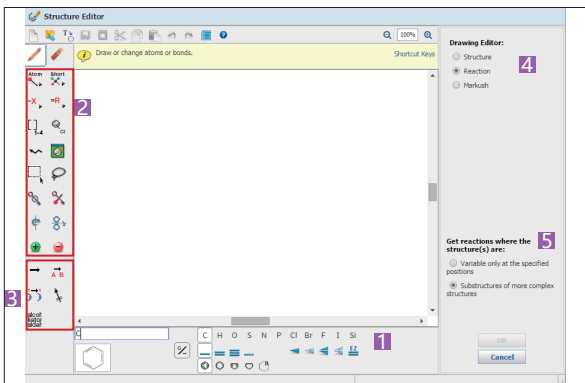
物质检索举例



- 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

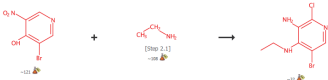
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1. View Reaction Detail Link 1

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



Overview Steps/Stages 2

1.1 R:POCl₂, R':RNEt₂, cooled; (PC) (PC) (PC) (PC) → rt; 2 h, reflux
 2.1 S:H₂O, S:THF, 3 h, rt
 3.1 R:HC, R':SnCl₄, S:H₂O, RPC: 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. Quis *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, 13ml). 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-ethylpyridine-3,4-diamine (V). 3-bromo-4-chloro-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

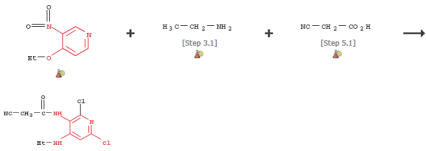
重排反应式

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 Full Text
 4 Reactions 2

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

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:

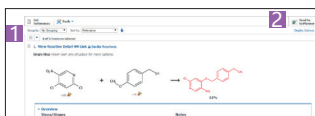
- All reactions
- Current answer set

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

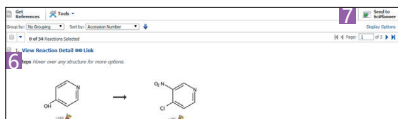
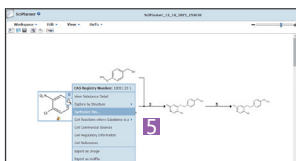
SciPlanner™使用



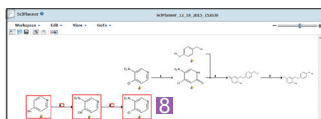
- 1 勾选想要的反应
- 2 点击Send to SciPlanner



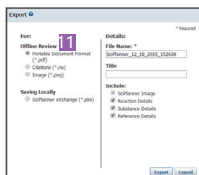
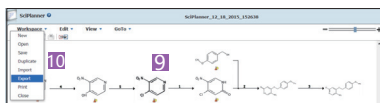
- 3 workspace 下新建一个文件
- 4 进入SciPlanner, 将刚推送过来的反应拖动到屏幕中间



- 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™

快速获取更加详细的合成方法

1 Analyze for: 1,2-diol

2 Sort by: 1. Most Reactions Selected

3 View with MethodsNow

Overview

Steps/Stages

- 1.1 R.NaH, S.THF, 0°C, 70 min, rt, 10 min, 0°C
- 1.2 2 min, 0°C, 10 h, rt
- 2.1 R.Hg(OAc)₂, S.EtOAc, 2.5 h, rt; 20 h, reflux; reflux - 0°C
- 2.2 R.sodium carbonate, S.H₂O, 0°C
- 3.1 S.PfCl₅, overnight, 120°C
- 4.1 R.H₂, C.CS₂/50-5, S.MgCl₂, 5 min, rt; 15 min, rt; 5 min, rt
- 4.2 reflux
- 5.1 R.NaH, 40', S.THF, 30 min, rt
- 6.1 R.NaH, 4(AcO)₂H, S.MgCl₂, S.AcOEt, overnight, reflux
- 7.1 Cs₂CO₃, S.C₆H₆, overnight, rt
- 8.1 R.Py, S.C₆H₆, 1 h, rt
- 8.2 R.Et₃O, S.HCO₂Et, S.Py, 4 h, rt
- 9.1 R.Me₂CH₂Me, S.THF, 12 h, rt

Notes

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

References

Synthesis of D- and L-Carboxylic Nucleosides via Rhodium-Catalyzed Asymmetric Hydroxylation as the Key Step
 B. Quirk, S. J. O'Brien
 In: Stereo. Methods at 2008
 From Organic Letters, 19(21), 4155-4156, 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, ELEM. ANAL. 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 Hydroxylation as the Key Step
 By Marco, Fabrizio, Diaz, Yolanda, Maffeo, M. Isabella, Castillon, Sergio
 From Organic Letters, 19(21), 4155-4156, 2008
 Published by American Chemical Society

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

4 **5**

6

7

8 Print/Export Close

Products

2-Propan-1-ol, 2-[[[(1,1-dimethyl-2-phenylethyl)phenyl]oxy]methyl]-, 98%, CAS RN: 17769-51-6

Reactants

1,3-Propanediol, 2-methylene-, CAS RN: 3513-61-3
 1,1'-[Chloro(1,1-dimethyl-2-phenylethyl)oxy]bis(benzene), CAS RN: 58479-61-1

Reagents

Sodium hydride, CAS RN: 7549-69-7

Solvents

Tetrahydrofuran, CAS RN: 109-69-9

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 100PCC (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 × 30 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, 136.0, 127.9 (Ar), 111.3 (C-3), 67.8 (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


*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

CAS Analytical Methods快速获取详细的分析方法

CAS Analytical Methods (methods.cas.org)

- 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...



CAS
Analytical
Methods

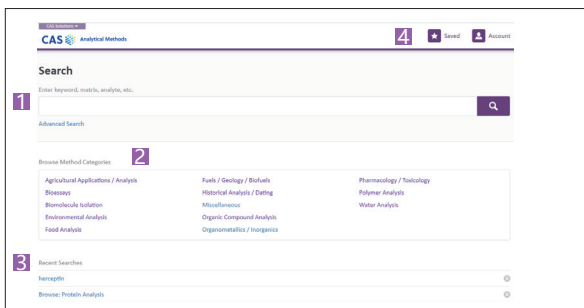
Log In to Analytical Methods

1

Username or Email Address

1 登录methods.cas.org网址，输入用户名和密码

*此为新增模块，用户需要与学校图书馆确认是否已获得访问权限

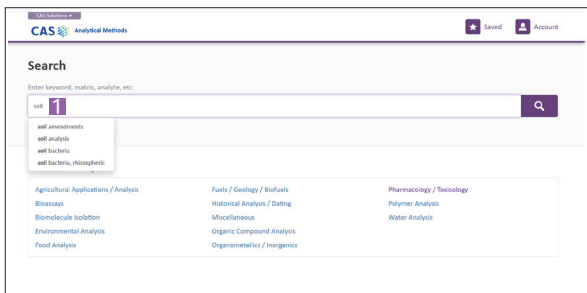


- 1 可以在检索框输入关键词或者分析物等进行检索
- 2 也可以通过浏览方法分类，点击一个浏览类别查看相关方法
- 3 点击历史检索重新运行检索，点击X删除检索历史
- 4 保存结果集



- 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，CAS Analytical Methods会自动进行同义词的查找

Results (30932) **2** Sort Relevance

1 Analyte

- Copper (2914)
- Zinc (2805)
- Lead (2706)
- Cadmium (2652)
- Chromium (2019)

2 Matrix

- Soils (11655)
- Leaf (2135)
- Geological sediments (1339)
- Root (1192)
- Water (749)

3 Method Category

- Solvent extraction (8582)
- Extraction (4246)
- Spectrophotometry (3834)
- Solid phase extraction (3528)
- HPLC (2483)

4 Analysis of 1,6-Dinitropyrene by Solvent extraction
CAS Mn: 2-107-CAS-129012

5 View Details & Instructions

6 Full Text

Abstract

- 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

Analyte

Alphabetically **By Count** **1**

- Copper (2914)
- Zinc (2805)
- Lead (2706)
- Cadmium (2652)
- Chromium (2019)
- Nickel (1941)
- Iron (1923)
- Manganese (1752)
- Arsenic (1644)
- Phenols (1433)
- Cobalt (1151)
- Flavonoids (866)
- Pyrene (835)
- Calcium (829)
- Phenanthrene (825)
- Mercury (800)
- Anthracene (749)
- Benzo[ghi]perylene (504)
- Sodium (502)
- DNA (487)
- Dibenz[ah]anthracene (477)
- Barium (467)
- Indeno[1,2,3-cd]pyrene (452)
- Polycyclic aromatic hydrocarbons (442)
- Heavy metals (440)
- Antimony (414)
- Atrazine (412)
- Strontium (404)
- Silver (393)
- Molybdenum (389)
- Thorium (364)
- Lead 83, Lithium 17 (atomic) (354)
- Samarium (220)
- Cu²⁺ (218)
- p,p'-DDE (216)
- Cr³⁺ (213)
- Simazine (213)
- DDT (206)
- Nitrogen (204)
- Gallic acid (202)
- Ferulic acid (198)
- Polyphenols (nonpolymeric) (198)
- Europium (189)
- Scandium (189)
- Lead(2+) (188)
- Rutin (188)
- Saponins (186)
- p,p'-DDD (185)

- 1 点击分析物列表，选择目标分析物

Technique

Alphabetically **By Count** **1**

- Acid digestion (993)
- Inductively coupled plasma atomic emission spectrometry (774)
- Inductively coupled plasma mass spectrometry (666)
- Flame atomic absorption spectroscopy (659)
- Extraction (592)
- Atomic absorption spectroscopy (588)
- Microwave digestion (546)
- Electrothermal atomic absorption spectroscopy (435)
- Solvent extraction (364)
- Chemical digestion (315)
- Solid phase extraction (177)
- Preconcentration (80)
- Leaching (75)
- Ultrasonic extraction (65)
- Differential pulse anodic stripping voltammetry (16)
- Slotted-tube atom traps (16)
- Ashing (15)
- Dry ashing (15)
- Total reflection x-ray fluorescence spectroscopy (14)
- PIXE (13)
- Reflux separation (13)
- Coprecipitation (12)
- High-resolution continuum source graphite furnace atomic absorption spectroscopy (12)
- Microbial cell culture (12)
- Soxhlet extractor (12)
- Acids (10)
- Anodic stripping voltammetry (10)
- Atomic fluorescence spectroscopy (10)
- Gamma ray (7)
- Liquid-liquid extraction (7)
- Sampling (7)
- Sequential injection analysis (7)
- Sieving (7)
- Square wave voltammetry (7)
- Vision (7)
- Chronopotentiometry (6)
- Fluorescence spectroscopy (6)
- Grinding size reduction (6)
- Immobilization, cellular, microbial cell (6)
- Ion chromatography (6)
- Liquid-liquid microextraction (6)
- Size exclusion chromatography (6)
- Ultrasound-assisted chemical digestion (6)
- Calcination (5)

Apply Cancel

- 1 点击技术手段列表，选择技术手段

Analysis of Cadmium in Soils by Electrothermal atomic absorption spectroscopy

CAS MN: 1338-0838RS

Method Category: Soil Analysis, Trace Element Analysis
Technique: Flow Injection Analysis, Electrothermal atomic absorption spectroscopy, Microwave digestion, Solid phase extraction

Parameter	Unit	Range	CAS RN
Cadmium	analyte	View Structure	7540-49-9
Soils	matrix		
0.8 mm i.d. polytetrafluoroethylene (PTFE) tubing	material		
Multisulfated carbon nanotubes (diameter 60-120 nm, length 5-15 nm, purity 95%, ash 0.2 wt%, surface area 40-500 m ² /g, amorphous carbon <1%)	material		
22 mm length of PTFE tubing (2.0 mm i.d., 1.2 mm o.d.)	material		
Metal column	material		
Mercuric nitrate	reagent	View Structure	12842-48-4
Van (oxide) (P ₂ O ₅)	reagent	View Structure	7705-08-0
Thiothiourea/dithionite/hydrochloric acid	reagent	View Structure	1385-03-1
Nitric acid	reagent	View Structure	7667-07-2
Hydrofluoric acid	reagent	View Structure	7664-09-3
Hydrochloric acid	reagent	View Structure	7647-01-9
Ethanol	reagent	View Structure	64-17-5
Sodium hydroxide	reagent	View Structure	1310-73-2
Magnesium phosphate	reagent	View Structure	7558-80-7

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Source
Requirement on the selectivity and sensitivity of cadmium by low-baked carbon nanotubes with detection by electrothermal atomic absorption spectroscopy
Zheng, Xiaohong, Zhang, Lian, Yang, Ting, Shen, Liming, Chen, Ming, Zhang, Junhua
Journal of Analytical Atomic Spectrometry (2012), 27 (15), 1860-1867. Royal Society of Chemistry

CODEN: JAAPEX ISSN: 0263-7077 DOI: 10.1039/C2JA30006K

Full Text >

Abstract >
Multisulfated carbon nanotubes (MWCNTs) were functionalized by incubating in H₂O₂ solution for the purpose of improving its selectivity and sensitive capacity to cadmium. High resolution transmission electron microscopy, Raman spectroscopy, x-ray diffraction, and surface charge area demonstrated that the MWCNTs were decorated by a layer of iron nanoparticles. In a relative medium pH (6), the non-phosphate carbon nanotubes (CNFs) offer a much improved sorption capacity of 22.84 mg/g for cadmium over a 12 mg/g by the same carbon nanotubes (CN) solution. The low-baked carbon nanotubes generally exhibit specific adsorption for various species, when the MWCNTs composite powder and high sensitivity to cadmium agent complex sample matrix components, i.e., the standard limit for correcting species were 9-220 fold improved. The MWCNTs composite were tested with a microcolumn for some selected preconcentration of cadmium with detection by electrothermal atomic absorption spectroscopy. A 100% enrichment with enrichment of pH 6, and 50% of aqueous mixture of 0.002 mol L⁻¹ H₂PO₄⁻ and 0.2 mol L⁻¹ H₂PO₄⁻ was fitted to a recovery of 17%, with a sample volume of 100 μL, an enrichment factor of 22.2 is obtained, along with a detection limit of 2.2 μg L⁻¹ (20 nL × 11) and a LOD of 2.26 μg L⁻¹ (n = 11) within a linear calibration range of 0.020-0.2 μg L⁻¹. The procedure is validated by determining cadmium in two certified reference materials (GBW08308 and GBW08310) and environmental water samples.

Equipment Used
Atomic absorption spectrophotometer: WFX-LSDA, Beijing瑞利 Analytical Instrumental Co., Ltd, China
Cadmium hollow cathode lamp, Beijing瑞利 Photoelectricity Factory, China
pH meter, OHA-80A, Thermofisher
Sequential injection system, FIAS4000, FIAS instruments, Bellefonte, PA, USA

Conditions
Inactivated
Drying temperature: 120 °C (pump time: 10 s), holding time: 20 s (pulsation temperature: 325 °C (pump time: 20 s), holding time: 20 s (atomization temperature: 1800 °C) (pulsing time: 3 s), cleaning temperature: 2000 °C (pulsing time: 2 s), injection volume: 20 μL
Wavelength: 228.8 nm; Current: 5.0 mA; Spectral bandpass: 0.4 nm

Instructions
Preparation of stock solution
1. Prepare the stock solution of iron (1000 mg/L) by dissolving 0.8637 g of Fe(NO₃)₃·9H₂O in 50 mL distilled water.
2. Prepare working standards of different concentrations by stepwise dilution of the stock solution.
Preparation of standard solution
1. Prepare stock solution of cadmium (1000 mg/L) by dissolving 0.1004 g of CdCl₂·2 H₂O in nitric acid (0.1 mol/L).
2. Dilute to 50 mL.
3. Prepare working standards of different concentrations by stepwise dilution of the stock solution.
Preparation of MWCNTs
1. To remove carbonaceous and catalyst impurities on their surface, preheat the multisulfated carbon nanotubes (MWCNTs) by heating 0.5 g of the commercial MWCNTs in 50 mL nitric acid (20% v/v).
2. Sonicate the mixture for 16 h, 60 min to wipe off the carbonaceous impurities.
3. Centrifuge the mixture by centrifugation.
4. Rinse with distilled water.
5. Dispense the MWCNTs into 50 mL of HCl solution (2% v/v).
6. Stir for 16 h to remove the residual metallic catalyst.
7. Wash the collected MWCNTs with distilled water until the pH of the wash-out solution is the same as distilled water.
8. Dry the collected MWCNTs at 100 °C in vacuum.
Validation of MWCNTs
1. Take 0.5 g of the purified MWCNTs in a 500 mL flask.
2. Mix with 200 mL of H₂SO₄/HNO₃ (3:1 v/v).
3. Sonicate for 2 h.
4. Dilute the mixture and wash thoroughly with distilled water.
5. Centrifuge by centrifugation.
6. Dry at 100 °C.

Parameter	Value
Linearity Range	0.020-0.2 μg/L
Limit of Detection	2.7 ng/L
Precision	2.2% (RSD) at 0.1 μg/L
Concentration	0.03 ± 0.08 mg/kg (GBW07504), 0.28 ± 0.08 mg/kg (certified value)

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

Analysis of Cadmium in Soils by Flame atomic absorption spectroscopy
CAS MN: 1-139-CAS-236465

[View Details & Instructions](#) **1** [Add to Compare](#)

Analyte: Lead; Cadmium

Matrix: **Soils**

Other Materials: Reagent: Tungsten carbide; Nitric acid; Perchloric acid; Hydrofluoric acid
Material: Plastic spatula; Sieve (2 mm); Polyethylene bags; Swing mill; Teflon vessels; Hot plate

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

Technique: Flame atomic absorption spectroscopy; Microwave digestion

Equipment Used: Flame atomic absorption spectrophotometer

Source: **Cadmium and Lead Distribution in Marine Soil Sediments, Terrestrial Soil, Terrestrial Rock, and Atmospheric Particulate Matter around Split, Croatia**
Buljac, Masa; Bogner, Danijela; Bralic, Marija; Peris, Nenad; Buzuk, Marijo; Brinic, Slobodan; Vladislavic, Nives
Analytical Letters (2014), 47 (11), 1952-1964. Taylor & Francis, Inc.

Full Text >

Abstract >

Compare Methods 2

3

	1	2	3
Title	Analysis of Lead in Soils by Microwave Digestion	Analysis of Copper in Soils by Chemical Digestion	Analysis of Cadmium in Soils by Flame Atomic Absorption Spectrometry
CAS Method Number	1-239-045-0030A	1-239-045-0030B	1-239-045-0030C
Method Category	SEM Analysis, Element Detection	SEM Analysis, Trace Element Analysis	SEM Analysis, Element Detection
Technique	Flame atomic absorption spectrometry; Microwave digestion	Flame atomic absorption spectrometry; Chemical digestion	Flame atomic absorption spectrometry; Microwave digestion
Analyte	Cadmium, Zinc, Lead, Iron	Iron, Lead, Copper, Manganese, Zinc, Cadmium	Cadmium, Lead
Matrix	Soil	Soil	Soil
Other Materials	Acid reagent; Cadmium chloride; Silver (99.99% purity); Whatman no. 4 filter paper	Fluoroboric acid; Hydrofluoric acid; Nitric acid	Fluoroboric acid; Nitric acid; Hydrofluoric acid; Fungicide carbendazim; Plastic spoons; Low pH zinc; Methionine; Tap; Strong acid; View All
Equipment Used	Microwave oven, 1000-2000, 1500 Flame atomic absorption spectrophotometer (FAAS), AAS200, Varian	Reaction, 2000, PH202; Flame atomic absorption spectrophotometer (FAAS), Model 200, Analytik Jena	Flame atomic absorption spectrophotometer, 2000, PerkinElmer
Conditions	Unknown; Soils; analyzer		
Source	Electrochemical EDPA reagent after SEM washing of Pb, Zn and Cd contaminated soil: measuring trace function, dispersion, cadmium. View All	Improving the relationship between SEM characteristics and metal bioavailability by using tracers: function of SEM parameters. View All	Cadmium and Lead Distribution in Marine Sediments, Terrestrial Soil, Sewerage Sludge, and Bioremediation-Perforated Sludge. View All
Preparation	Collection and processing of SEM samples 1. Collect the SEM samples which have been exposed to tracers above three. View All	Collection of SEM samples 1. Place 200 mg of 1, 1 kg of unspiked and spiked cadmium SEM sediments in containers. View All	Collection of SEM samples 1. Collect SEM from 5 - 15 cm depth under a small plastic inside after. View All
Method	Microwave digestion followed by flame atomic absorption spectrophotometry (FAAS) analysis 1. Serial dilution of SEM samples (2 g) in acid. View All	Wet digestion and detection of Cu, Ni, Cd, Co, Pb and Zn by flame atomic absorption spectrophotometry (FAAS) method. View All	Flame atomic absorption spectrophotometry (FAAS) 1. The flame atomic absorption. View All
Limit of Quantitation	0.2 mg/L, Lead, 0.20 mg/L, Zinc, 0.02 mg/L, Cadmium, 0.20 mg/L, Iron	0.2 mg/L, Copper, 0.1 mg/L, Lead, 0.2 mg/L, Zinc, 0.2 mg/L, Cadmium, 0.1 mg/L, Iron, 0.2 mg/L, Manganese	
Units of Detection		0.2 mg/L, Cadmium	
Contributions			0.4 mg/L SEM collected in spring, sample 4000; Cadmium, 0.7 mg/L SEM collected in 04; sample 4000; Cadmium, 0.11 mg/L SEM . View All
Source	Electrochemical EDPA reagent after SEM washing of Pb, Zn and Cd contaminated soil: measuring trace function, dispersion, cadmium. View All	Improving the relationship between SEM characteristics and metal bioavailability by using tracers: function of SEM parameters. View All	Cadmium and Lead Distribution in Marine Sediments, Terrestrial Soil, Sewerage Sludge, and Bioremediation-Perforated Sludge. View All
Preparation	Collection and processing of SEM samples 1. Collect the SEM samples which have been exposed to tracers above three. View All	Collection of SEM samples 1. Place 200 mg of 1, 1 kg of unspiked and spiked cadmium SEM sediments in containers. View All	Collection of SEM samples 1. Collect SEM from 5 - 15 cm depth under a small plastic inside after. View All
Method	Microwave digestion followed by flame atomic absorption spectrophotometry (FAAS) analysis 1. Serial dilution of SEM samples (2 g) in acid. View All	Wet digestion and detection of Cu, Ni, Cd, Co, Pb and Zn by flame atomic absorption spectrophotometry (FAAS) method. View All	Flame atomic absorption spectrophotometry (FAAS) 1. The flame atomic absorption. View All
Limit of Quantitation	0.2 mg/L, Lead, 0.20 mg/L, Zinc, 0.02 mg/L, Cadmium, 0.20 mg/L, Iron	0.2 mg/L, Copper, 0.1 mg/L, Lead, 0.2 mg/L, Zinc, 0.2 mg/L, Cadmium, 0.1 mg/L, Iron, 0.2 mg/L, Manganese	
Units of Detection		0.2 mg/L, Cadmium	
Contributions			0.4 mg/L SEM collected in spring, sample 4000; Cadmium, 0.7 mg/L SEM collected in 04; sample 4000; Cadmium, 0.11 mg/L SEM . View All

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

Search

Enter keyword, matrix, analyte, etc.

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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	Organic Compound Analysis 2
Chiral Separation		

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)
- 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

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Analysis of Tannins in Coriandrum sativum by Extraction
CAS MN: 1-131-CAS-43974

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](#)
Smith, Jazia; Bettaleb, Ines; Bachrouh, Olla; 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 (28 of 276)

Prev Next

Analysis of Tannins in Coriandrum sativum by Extraction

CAS MN: 1-131-CAS-102587

Method Category: [Natural Product Isolation Analysis](#)

Technique: Spectrophotometry; Extraction

1 **Materials**

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
Smith, Jazia; Bettaleb, Ines; Bachrouh, Olla; Talou, Thierry; Marzouk, Brahim
Arabian Journal of Chemistry (2019), 12 (7), 1763–1773. Elsevier B.V.
CODEN: AJCRRD ISSN: 18785352 DOI: 10.1016/j.ajoc.2014.11.043

[Full Text](#)

3 **Abstract**

This study was designed to examine the effect of operating conditions on essential oil composition and antioxidant activity of coriander cakes. Twenty-nine components were determined in essential oils, which were mostly alc. monoterpenes. The highest essential oil yields (0.11%) were obtained by the nozzle diameter of 5 mm. The main components of cake essential oil linolol, γ -terpinene, geranyl acetate, linally 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 9.11 mg GA/g. The screening of antioxidant activity of the different coriander cakes using the di(phenyl)(2,4,6-trinitrophenyl) iminoazanium 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 $\mu\text{g/ml}$, as compared with bigger diameter ($IC_{50} = 88 \mu\text{g/ml}$). 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 ($EC_{50} = 700 \mu\text{g/ml}$) compared to ascorbic acid ($EC_{50} = 40 \mu\text{g/ml}$).

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 (Model OMEGA 20, France) with a motor (0.75 kW, 230 V of maximal tension, 5.1 A of maximal intensity), 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-placed 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 (2–6 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-carbide 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 1.5 ml of concentrated H_2SO_4 to 50 μl 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 **Validation**

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

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