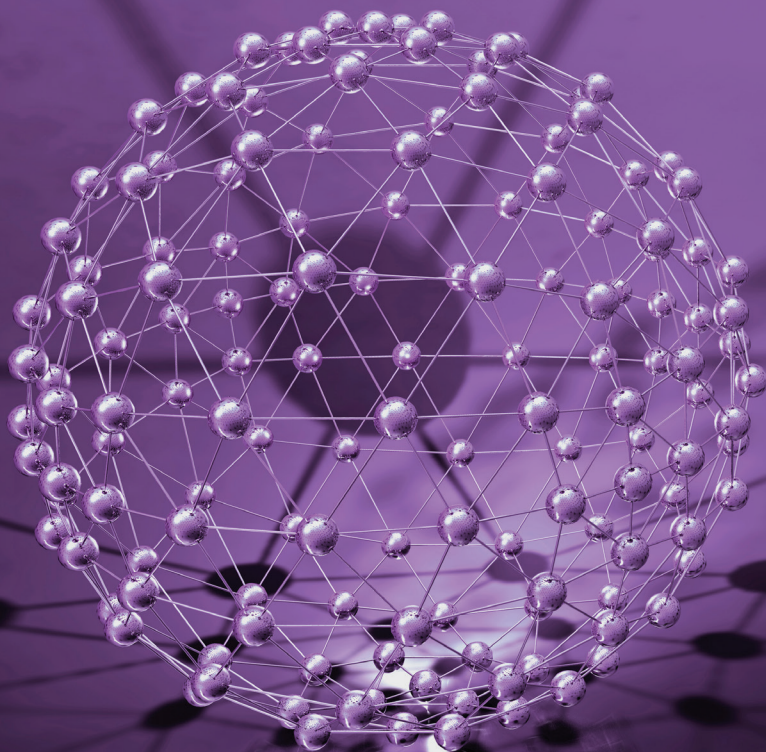




MethodsNow™

合成/分析方法合集



METHODSNow™
A CAS SOLUTION

//CODiE//
2017 SIIA CODiE WINNER

www.cas.org/MethodsNow
www.MethodsNow.com

MethodsNow™简介

MethodsNow是美国化学文摘社（CAS）最新发布的全球最大的合成及分析方法应用，收录高质量标引、增值的分析方法和合成方法，聚焦于：

- 活性药物成分及代谢物分析
- 毒素分析
- 毒品分析
- 阴阳离子
- 生物鉴定
- 天然产物分离/分析
- 有机化合物分析
- 农药残留检测
- 蛋白质分析
- 土壤分析
- 生物合成探针
- 痕量元素分析
- 塑料加工
- 同位素分析
- 手性化合物拆分
- 环境分析
- 大气分析
- 脂肪酸分析
- 石油产品分析
- 食品分析
- 化妆品分析
- 炸药分析
- 除草剂分析
- 有机金属化合物
- 无机化合物
- 生物分子分离
- 法医分析
- 合成方法

★共有近50种方法分类，随着更多科学信息被收录，分类量还将持续增加

通过MethodsNow:

- 轻松获取来自数千种顶级期刊及专利中披露的分析方法和合成方法
- 轻松获取合成方法详情，包括底物、催化剂、溶剂、产物、操作步骤（多步反应的每步操作步骤）、产物谱图数据、产物性状、实验量级
- 轻松获取实验方法详情，包括实验用原料、操作步骤、实验条件、仪器等详细信息
- 快速对比多种分析方法，轻松定位可实施的实验方法
- 无需花费额外费用获取原文，即可轻松获取实验所需的所有信息
- 经过科学家的标引、筛选，可为您节省阅读和理解文献所需时间
- 新的CAS Method Number™有助于快速定位相关文献



界面友好，操作简单（一个产品，两个界面）

通过SciFinder获取MethodsNow合成方法

The screenshot displays the CAS Solutions SciFinder interface. At the top, there's a navigation bar with 'Launch MethodsNow: Analysis' and 'A CAS SOLUTION' logo. Below this, a breadcrumb trail shows 'Substance Identifier "aspirin" > substances (1) > get reactions (190) > keep analysis "MethodsNow" (11)'. The main content area is titled 'REACTIONS' and shows a chemical reaction scheme for the synthesis of aspirin (acetylsalicylic acid) from salicylic acid and acetic anhydride. The reaction is labeled with a yield of 78% and a reference number of ~113. Below the reaction scheme, there are sections for 'Overview', 'Notes', 'References', and 'Experimental Procedure'. The 'Experimental Procedure' section is highlighted with a red box and contains the following text: 'METHODSNow™ Procedure 1. Place iron (III) chloride (0.01 mmol) and acetic anhydride (11 mmol) in a test tube. 2. Keep the test tube at room temperature for 10 min in air. View more... View with MethodsNow'.

通过www.MethodsNow.com获取MethodsNow分析方法

The screenshot shows the homepage of the MethodsNow website. At the top, there's a navigation bar with the 'METHODSNow' logo and a 'CAS SOLUTION' tag. To the right of the logo are links for 'Saved' and 'Account'. Below the navigation bar is a large search area with the heading 'Search'. A text input field is labeled 'Enter keyword, matrix, analyte, etc.' and has a magnifying glass icon to its right. Below the search field is a link for 'Advanced Search' and a green box containing the text '输入关键词、物质名称等信息进行检索'. Below the search area is a section titled 'Browse Method Categories' which lists various categories in a grid: 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Fuels / Geology / Biofuels', 'Historical Analysis / Dating', 'Miscellaneous', 'Organic Compound Analysis', 'Organometallics / Inorganics', 'Pharmacology / Toxicology', 'Polymer Analysis', and 'Water Analysis'. At the bottom of the page, there's a 'Recent Searches' section and a green box containing the text '按分析类别，浏览分析方法'.

分析方法详情示例

CAS Solutions

METHODSNow

A GAS SOLUTION

Browse: Active Pharmaceutical Ingredient and Metabolite Analysis

Return to Results

Method Detail (1 of 49320)

PrevNext

Analysis of Diclofenac sodium in Tablets by Liquid chromatographic UV detectors

CAS MN: 1-101-CAS-45187

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: Liquid chromatographic UV detectors; Reversed-phase HPLC

Materials	Role	Image	CAS RN
Diclofenac sodium	analyte	View Structure	15307-79-6
Tablets	matrix		
ODSC ₁₈ (25 cm x 4.6 mm id and 5 µm particle size) column	material		
0.45 µm filter	material		
Methanol	reagent	View Structure	67-56-1

Source

A validated stability-indicating UPLC method for determination of diclofenac sodium in its pure form and matrix formulations

Elzayat, Ehab M.; Ibrahim, Mohamed F.; Abdel-Rahman, Ali A.; Ahmed, Sayed M.; Alanazi, Fars K.; Habib, Walid A.

Arabian Journal of Chemistry, . . Elsevier B.V.

CODEN: AJCRDR | ISSN: 18785352 | DOI: 10.1016/j.arabjc.2013.12.022

Document Sources

Abstract

The aim of this work is to develop a validated stability indicating reverse phase ultra performance liquid chromatog. (UPLC) method for the rapid and accurate determination of diclofenac sodium in its pure form and in matrix formulations. This UPLC method is composed of isocratic mobile phase, 0.05 M ammonium acetate buffer (pH = 2.5) and acetonitrile (50:50), with flow rate 0.5 mL/min, column BEH C18 (2.1 x 50 mm, 1.7 µm). The method is rapid (1.2 min run), selective with well resolved diclofenac peak with retention time 0.94 min and sensitive (LOD = 2 ppm and LLOQ = 6 ppm) with UV detection at 254 nm. The drug was subjected to acidic, alk. media, boiling and oxidizing agent to apply stress conditions. The developed method was able to sep. degradation product generated under forced degradation studies. The developed method was validated as per the FDA guidelines for specificity, linearity, accuracy, precision, LOD, LLOQ and found to be satisfactory. The study suggests that the developed UPLC method can be used for the assessment of drug purity and stability. It can be also used to monitor the drug content and release from different formulations without any interference of excipients and/or degradation products.

Equipment Used

HPLC system

UV - detector

实验设备

Conditions

Chromatographic

Mobile phase - 16% acetonitrile in 0.02M sodium acetate buffer pH (5.5); flow rate - 1 ml/min; column temperature - 30 °C

Instructions

Standards Preparation

1. Prepare Diclofenac sodium (DS) stock solution in 0.2 M phosphate buffer; pH 6.8 to produce final concentration of 2500 µg/ml.
2. Serially dilute standard solutions to eleven working standard solutions covering the range (1 - 2500 µg/ml).

Diclofenac sodium extraction from matrix formulations

1. Dissolve the matrix formulation (HPMC matrix tablets and enteric coated non pareil seeds (40 - 60 mesh size)) in mixture of water and methanol (30:70).
2. Sonicate it for 15 min, and then centrifuge at 5000 rpm for 5 min.
3. Filter the clear supernatant through a 0.45 µm filter.

Reverse phase high performance liquid chromatography (RP - HPLC)

1. Inject 20 µL solution onto ODSC₁₈ (25 cm x 4.6 mm id and 5 µm particle size) column.
2. Maintain the column temperature at 30 °C.
3. Perform the isocratic elution using mobile phase consisting of 16% acetonitrile in 0.02M sodium acetate buffer pH (5.5) at flow rate of 1 ml/min.
4. Set the UV detector at 220 nm.

Validation

Linearity Range0.01 – 0.06 mg/ml

Limit of Detection3.4 µg/ml

实验有效性

快速对比多种方法，轻松定位可实施的实验方法

- 标题
- CAS方法号
- 方法类别
- 技术
- 分析物
- 基质
- 其他材料
- 所用仪器
- 条件
- 方法来源
- 样品制备详情
- 分析/检测操作详情
- 线性范围
- 检测限制
- 回收
- 浓度

METHODS NOW			
Compare Methods			
方法1方法2方法3			
Expand All Collapse All			
Title	Analysis of Biotin in Milk by HPLC	Analysis of Mitochondrial DNA in Horse meat by Multiplex polymerase chain reaction	Analysis of Anthocyanins in Brassica oleracea capitata rubra by Boiling (cooking)
CAS Method Number	1-124-CAS-2325056	1-124-CAS-2308548	1-124-CAS-1237864
Method Category	Food Analysis	Food Analysis	Food Analysis
Technique	UV-visible spectroscopy; HPLC	Spectrophotometry; Multiplex polymerase chain reaction; DNA extraction; Gel electrophoresis	Liquid chromatography spectrometric detectors; Boiling (cooking); HPLC; Extraction
Analyte	Biotin	12S rRNA; 18S rRNA; Mitochondrial DNA; Animal gene	Anthocyanins
Matrix	Milk; Skim milk	Beef; Glycine max; Pork; Poultry meat; Horse meat; Lamb meat	Brassica oleracea capitata rubra
Other Materials	Ethanol; Acetic acid; Ethylene glycol dimethacrylate; Tetraethoxysilane; 3-Phenylmethoxycarbonyl-methacrylate; View All	Ethylendiaminetetraacetic acid sodium salt; Boric acid (H ₃ BO ₃); Agarose; Tris(hydroxymethyl)aminomethane; View All	Formic acid; Methanol; Hydrochloric acid; C ₁₈ column; Injection valve
Equipment Used	Liquid chromatograph, 20A, Shimadzu; UV-Vis detector, SPD-20A, Shimadzu; Autosampler, 20i-20A, Shimadzu; Detector, View All	UV-Vis spectrophotometer, NanoDrop2000, USA; Thermo cycler, Techne	High performance liquid chromatography system, Shimadzu, Kyoto, Japan; Diode array detector, SPD-M20DA, Shimadzu
Conditions	Instrument: mobile phase: NaH ₂ PO ₄ 25 mmol/L, methanol in the volume ratio of 80:20; Flow rate: 1.0 mL/min; Injection View All		Instrument: Column, C ₁₈ Detection wavelength, 278 - 538 nm
Source	Magnetically separable polymer (Mag-MIP) for selective analysis of biotin in food samples View All	The development of a hexaplex-conventional PCR for identification of six animal and plant species in foodstuffs View All	Cooking techniques improve the levels of bioactive compounds and antioxidant activity in kale and red cabbage View All
Preparation	Preparation of samples 1. Obtain the samples of raw milk; View All		Sample Preparation 1. Collect vegetable samples (red View All
Method	HPLC analysis 1. Perform the analysis using a Shimadzu View All	DNA extraction 1. Collect commercial foodstuffs such as View All	Cooking of the samples by boiling 1. Add red cabbage to boiling tap water View All
Linearity Range	5.0 - 100 mg/L		
Limit of Detection	0.96 mg/L	0.01%	
Recovery	77 ± 14% in 5.0 mg/g of spiked sample (Milk powder), 83 ± 4% in 5.0 mg/g of spiked sample (Horse meat) mRM: 102 ± 3% in 5.0 View All		
Concentration			2.27 ± 0.88 mg C ₃₀ /100 g, Cy 3-dehydroside-5-hexoside, 10.44 ± 4.63 mg C ₃₀ /100 g, Cy 3-dehydroside-4-hexoside, 5-hexoside, 1-16 ± View All

合成方法详情示例

产物	Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
底物	Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
溶剂	Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
操作过程	Procedure	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzylloxy)phenyl)ethylamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H ₂ O. 4. Basify with potassium carbonate and extract with CH ₂ Cl ₂ . 5. Wash the combined organic layers with brine. 6. Dry over MgSO ₄ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzylloxy)-3,4-dihydroisoquinoline.
实验量级	Scale	gram
谱图数据	¹ H NMR	(CDCl ₃ , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, J = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
谱图数据	¹³ C NMR	(CDCl ₃ , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
谱图数据	IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹
谱图数据	HRMS	(FAB+) calcd for C ₂₂ H ₂₂ NO ₂ (M+H ⁺) 344.1651; found 344.1658
谱图数据	Mass Spec	(FAB+) m/z 344 (M+H ⁺)
产物性状	State	yellow solid
MethodsNow方法号	CAS Method Number	3-614-CAS-200055
Print/Export Close		



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及相关信息，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。

MethodsNow™

全球最大的合成/分析方法合集

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