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Overview



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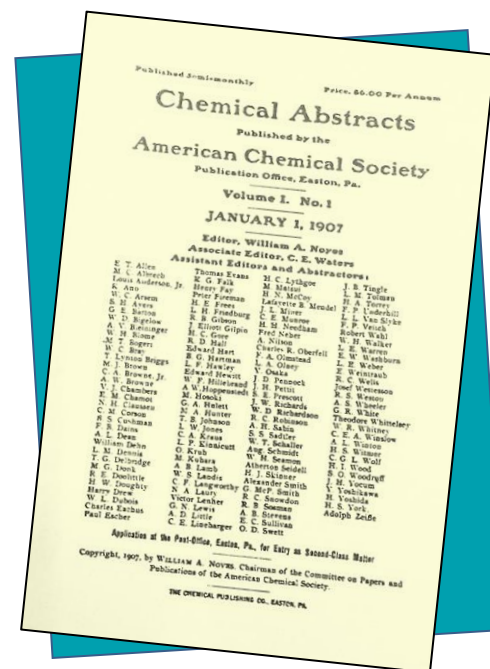


成立於1876年，美國化學學會所出版的專業期刊，廣泛地涵蓋化學相關領域主題－分析化學、食品科學、材料科學、醫藥化學、毒物學、生物化學等，經過同儕評論高品質的文章，累積近130年化學的原始研究，包含三百萬頁超過750,000篇的文章，擁有耀眼的影響指數，被ISI的Journal Citation Report (JCR) 評為:化學領域中，被引用次數最多之化學期刊。



成立於1907年，主要內容有：

1. Chemical Abstracts
2. CAS REGISTRYSM



SciFinder 背景說明

1. 美國化學文摘服務社(Chemical Abstracts Service)以下簡稱CAS，致力於提供最完整化學相關情報予科學家及研究人員，促進科學進步與提升研究水平。旗下產品與服務如SciFinder/STN/NCI Global/ScienceIP等。
2. CAS-SciFinder資料庫特性：
 - a) 研究領域: 適用化學/化工/生醫/生技/製藥/石化/材料/高分子/妝品/光電/農科。
 - b) 版本: SciFinder以雲端連線方式進行，使用者利用個人帳號密於授權IP範圍內，以瀏覽器進行操作，無同時上線人數限制。

SciFinder個人帳號註冊: 簡單4步驟

1. 利用圖書館提供的[特定申請網址\(URL\)](#)進行。
2. [填入](#)申請者相關資訊。*(星號)部分為必填欄位(皆英文填寫)
 - a. email : [使用學校的email domain](#)
 - b. username : [5-15字元](#) , ex: **xyz7890**
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96 hrs!!



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Value & Benefit

SciFinder 獨特性-人工索引價值

- ✓ CAS**超過100年 (1907~)**的資料編撰歷史(CA, Chemical Abstracts) , 由**1,200位**各領域的博士學者或科學家 , 進行文獻資料的分析與整理編寫而成索引。並**非**由機器翻譯與整理 , 每一篇文獻皆會由CAS編輯群審閱分析與整理。讓使用者利用CAS索引進行研究決策時有可靠的依據。



CAS scientists make chemistry discoverable through intellectual indexing

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

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
13 June 2002 (13.06.2002)

(10) International Publication Number
WO 02/46157 A2

(51) International Patent Classification: **C07D 211/00**

(21) International Application Number: PCT/US01/47037

(22) International Filing Date: 4 December 2001 (04.12.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/251,209 4 December 2000 (04.12.2000) US
60/275,600 13 March 2001 (13.03.2001) US

(71) Applicant: SEPRACOR, INC. [US/US]; 111 Locke Avenue, Marlborough, MA 01752 (US).

(72) Inventors: **WU, Xinhai**; One Royal Crest Drive, Marlborough, MA (US). **BANNISTER, Thomas, D.**; 112 Green Street, Marlborough, MA 01532 (US). **CUNY, Gregory, D.**; 100 Tower Street #210, Hudson, MA 01749 (US).

(74) Agents: **GORDON, Dana, M.** et al.; Patent Group, Foley, Hoag & Elliot, LLP; One Post Office Square, Boston, MA 02109 (US).

(81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW.

[Continued on next page]

(54) Title: METHODS FOR THE STEREOSSELECTIVE SYNTHESIS OF SUBSTITUTED PIPERIDINES

Examples of Substituted Piperidines Accessible Via the Methods of the Present Invention

Structure A: C1CCN(C1)C2=CC=CC=C2

Structure B: C1CCN(C1)C2=CC=CC=C2C

Structure C: C1CCN(C1)C2=CC=CC=C2C

Structure D: C1CCN(C1)C2=CC=CC=C2C

For Structures A, B, C, and D:
n = 0, 1, or 2
R₁ = H, alkyl, aryl, heteroaryl, aralkyl, -CO₂R₄, or -C(O)NHR₄
R₂ = alkyl
X = O, N(O)R₄, or N(O)R₄, NH, NR₄, S, or S(O)
R₃ = alkyl, aralkyl, aryl, or heteroaryl
R₄ = alkyl, aryl, heteroaryl, or aralkyl



23 novel substances

153 reactions schemes

3 Markush structures

27 single step reactions

42 known substances with new info

6 new novel subjects/concepts

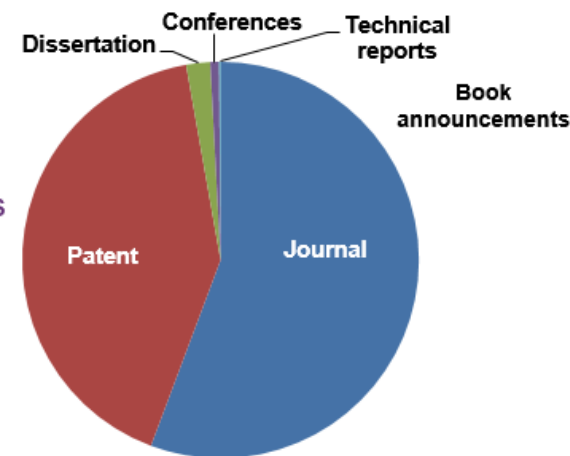


為 CAS 於1994年發展出之線上資訊檢索系統

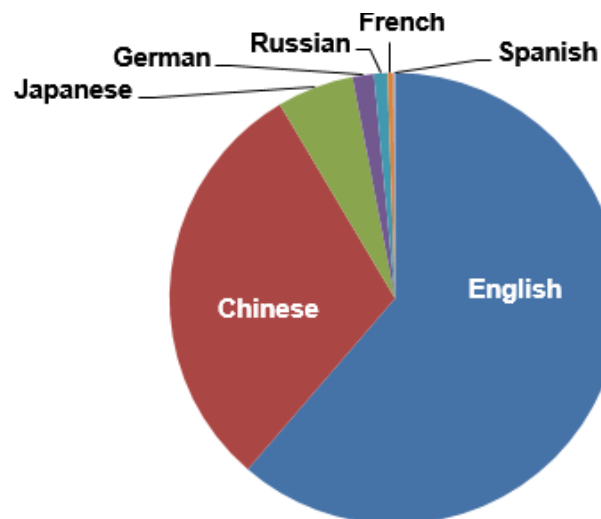
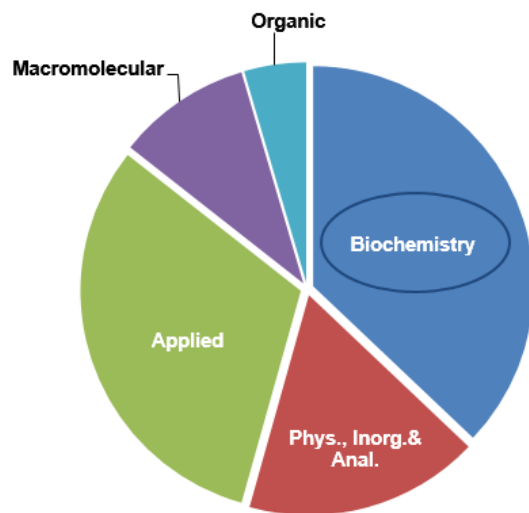
涵蓋量

1. 1907年至現今 (Early 1800's)
2. 專利 & 專利家族 – 全球 63國專利局的專利文獻。
3. 化學摘要 – 50,000知名科學期刊，以及當地國家語言寫的期刊。
4. 文獻型態 – 期刊、專利、技術報告、書本、論文、會議紀錄與摘要、評論與回顧。
5. 更新速度 – Daily (每日更新)。

Disclosure types – 44%
not published in journals



Discipline areas – 54%
not in traditional chemistry



Original publication languages –
40% not published in English

SciFinder 資料涵蓋量

子資料庫

- CAplus (包含下頁文獻型態:專利、期刊...等等)
- Medline (<http://www.cas.org/products/scifinder/content>)
- CAS Registry (化學結構資料)
- CASReact (反應資料)
- Chemlist (物質管制清單)
- Chemcats (化學品供應商)
- Marpat (Markush 專利結構)

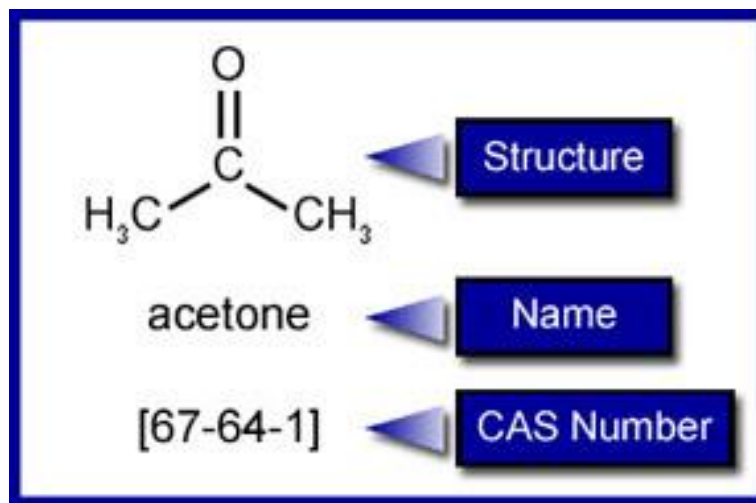
特點

- 人工索引(人工閱讀，摘錄重點)
- 文獻、物質(化學結構)與反應資訊
- 涵蓋化學以及科學領域

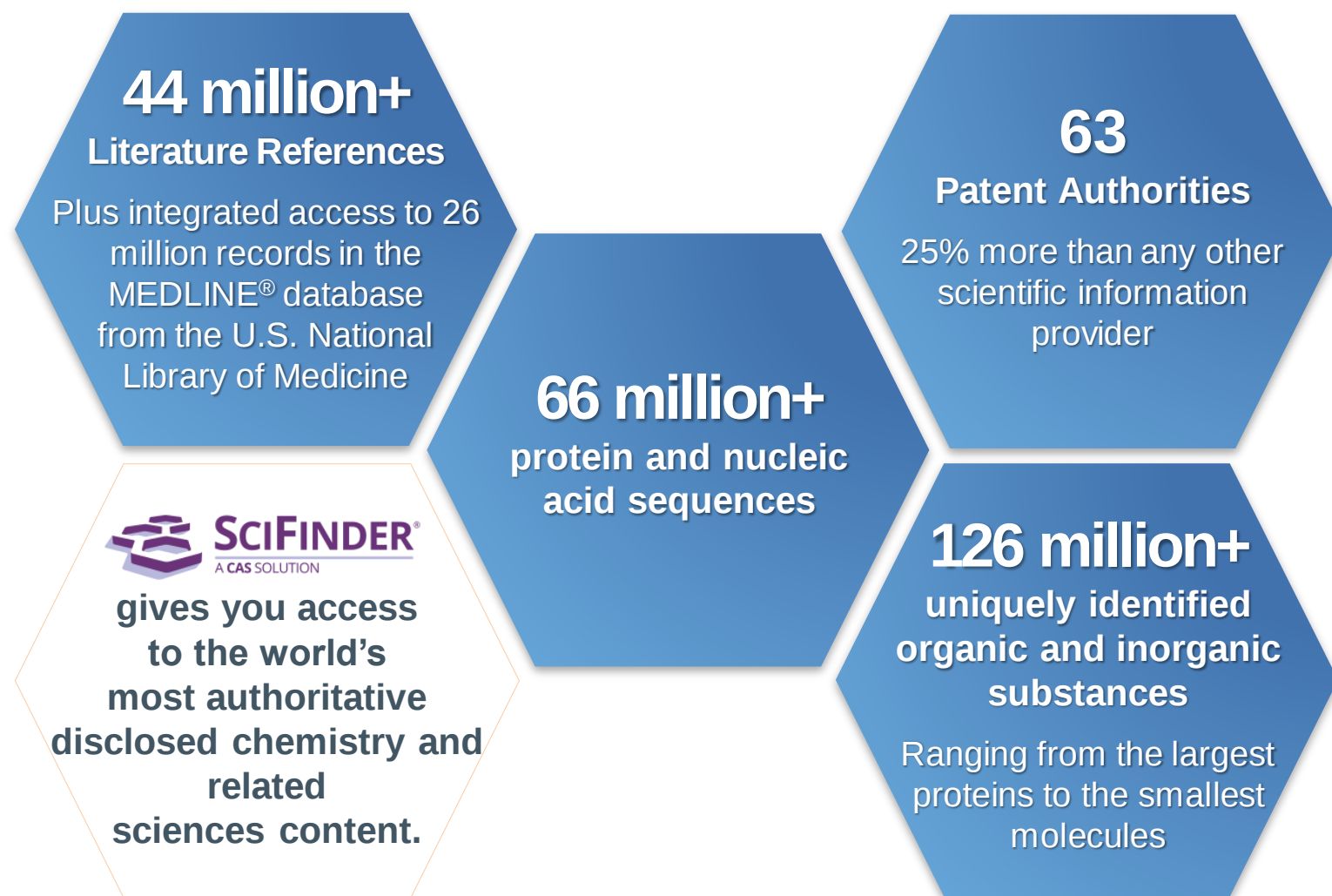
文獻量	>4千3百萬筆資料；50,000 期刊
文獻 - 專利	全球63個(國家)專利局: EP/DPMA/JPO/USPTO/UK-IPO/WIPO/CIPO.....等等
文獻型態	-專利 -期刊 -會議記錄與摘要 -技術報告 -書本 -Reviews -學位論文 -網頁預印本
文獻涵蓋年份	1800年~至今
涵蓋學科	- 化學/化工/ 物理/無機/化妝品 - 生物/畜產 (生命科學) - 光電/電化學 - 環境工程 - 食品/農業/藥學
更新頻率	Daily

SciFinder 獨特性- 完整物質資料

- ✓ CAS為全球權威性-CAS Number 物質登入碼的核發單位，使用SciFinder即擁有**最完整**的物質(化學結構/生醫基因)資料。



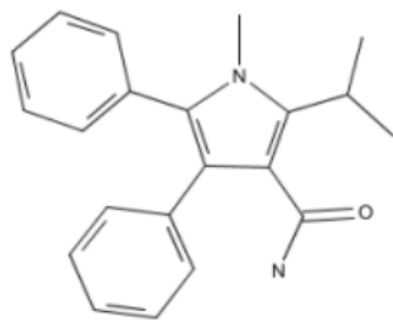
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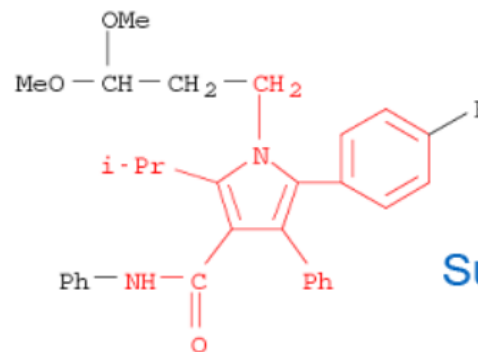
Data as of January 2017

SciFinder 獨特的專利與文獻檢索

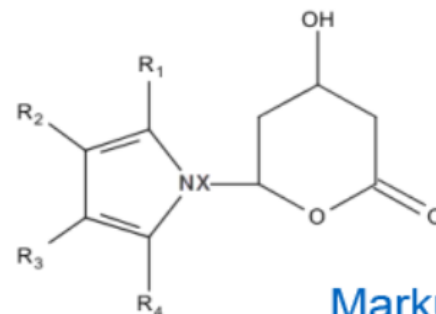
- ✓ SciFinder檢索區分為一般檢索與高級檢索(SSM)，一般檢索如關鍵字查詢、簡易結構式查詢、反應查詢、專利期刊文獻查詢等；高級檢索(SSM)如衍伸結構查詢(substructure)、Markush結構查詢等，對於進行化學物質/藥物/高分子開發非常需要，可大幅提升查找資料效能，進而加速研發腳步與開發。



Structure query



Substructure match



Markush match





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Patent "US20080078739" > references (3)

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0 of 3 References Selected

Analyze by: ?
Author Name ▾

Author	Count
Booth Jean Paul	1
Fujita Minoru	1
Hattori Kazuhiro	1
Hibi Mikiharu	1
Kajii Yoshio	1

1. **Capacitively-coupled electrostatic (CCE) probe arrangement for detecting strike step in a plasma processing chamber**

By Booth, Jean-Paul
From PCT Int. App. No. PCT/US2009/049757

Patent No.	Kind	Language
WO 201005930	A2	English
CN 102084473	A	Chinese
JP 2011527521	T	Japanese
JP 5427888	B2	Japanese
CN 104320899	A	Chinese

Patent Family

Language: English, Database: CAPLUS

processing chamber of a plasma processing system in a processing chamber to generate a plasma. The strike step is formed in the processing chamber and maintaining a low radio frequency plasma in the processing chamber. A probe head is positioned in the processing chamber, wherein the surface is within close proximity to the strike step. The probe head is used for collecting a set of characteristic parameter measurements from the surface of the processing chamber, wherein the surface is within close proximity to the strike step. The set of characteristic parameter measurements is compared against a pre-defined range. If the set of characteristic parameter measurements is within the pre-defined range, the stabilized plasma exists.

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

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
14 January 2010 (14.01.2010)

(10) International Publication Number
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(51) International Patent Classification:
H01L 21/66 (2006.01) H01L 21/205 (2006.01)
H01L 21/3065 (2006.01)

(21) International Application Number:
PCT/US2009/049757

(22) International Filing Date:
7 July 2009 (07.07.2009)

(25) Filing Language:
English

(26) Publication Language:
English

(30) Priority Data:
61/078,739 7 July 2008 (07.07.2008) US

(71) Applicant (for all designated States except US): LAM RESEARCH CORPORATION [US/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US).

(72) Inventors and Applicants (for US only): BOOTH, Jean-paul [FR/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US); KEHL, Douglas, L. [US/US]; 4650 Cushing Parkway, Fremont, CA 94538 (US).

(74) Agent: NGUYEN, Joseph, A.; P.O. Box 700640, San Jose, CA 95170 (US).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published: without international search report and to be republished upon receipt of that report (Rule 48.2(g)).

- 31國專利PDF全文直接下載。
- 專利家族全文亦可直接下載，可選擇較熟悉語言。
- 全文為可檢索PDF，非一般影像檔。
- CA科學家進行索引/摘錄的化學物質，可直接透過互動方式定位在專利全文中。(Patent Viewer)

Patent Viewer

每篇專利中的索引物質 (key substances) 將會有專利全文頁碼的連結，**不需要花費時間**慢慢在專利全文尋找結構。

The screenshot displays the Patent Viewer interface. On the left, a list of key substances is shown, with the entry **1636182-63-2P** highlighted in a red box. This entry is linked to **Page 127 in PATENTPAK**. The main view on the right shows the patent document for **WO 2014/179562** (PCT/US2014/036355). The document includes a chemical reaction scheme (Scheme 1) and a list of compounds (1-5) with their respective NMR and HRMS data. The entry for **Compound 1-4** is highlighted in a red box, showing its ¹H NMR and HRMS data. The interface also includes a search bar, a list of key substances, and a detailed view of the selected patent document.

Key Substances in Patent

- CAS RN 1626333-91-2**
Search in SciFinder | View Detail
Analyst Markup Location
page 127
- CAS RN 1636182-65-4**
Search in SciFinder | View Detail
Analyst Markup Location
page 127
- CAS RN 24511-62-9**
Search in SciFinder | View Detail
Analyst Markup Location
page 127
- CAS RN 35161-70-7**

WO 2014/179562 (PCT/US2014/036355)

Scheme 1 Exemplary synthesis of certain compounds of Formula (I), wherein R^A and R^B are as described herein.

[00269] In one set of experiments, a mixture of compounds 1 and 4 in EtOH was irradiated in the microwave oven at 150 °C for 5 h. The reaction mixture was purified by flash column chromatography to yield a compound of Formula (I). Compound

[00270] **Compound 1-1:** ¹H NMR (500 MHz, CDCl₃) δ 4.08-4.13 (m, 3H), 3.99-4.01 (m, 3H), 3.84-3.88 (m, 3H), 2.30-2.48 (m, 12H), 2.24 (s, 9H), 1.27-1.44 (m, 24H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C₃₀H₄₂N₆O₆ [M+H]⁺ 613.5122, found 613.5203.

[00271] **Compound 1-2:** ¹H NMR (500 MHz, CDCl₃) δ 4.08-4.13 (m, 3H), 3.98-4.00 (m, 3H), 3.83-3.85 (m, 3H), 2.33-2.47 (m, 12H), 2.24 (s, 9H), 1.26-1.46 (m, 36H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C₃₀H₄₂N₆O₆ [M+H]⁺ 727.6056, found 727.6116.

[00272] **Compound 1-3:** ¹H NMR (500 MHz, CDCl₃) δ 4.08-4.13 (m, 3H), 3.99-4.00 (m, 3H), 3.84-3.87 (m, 3H), 2.30-2.47 (m, 12H), 2.24 (s, 9H), 1.26-1.44 (m, 60H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C₃₁H₄₄N₆O₆ [M+H]⁺ 895.7934, found 895.7937.

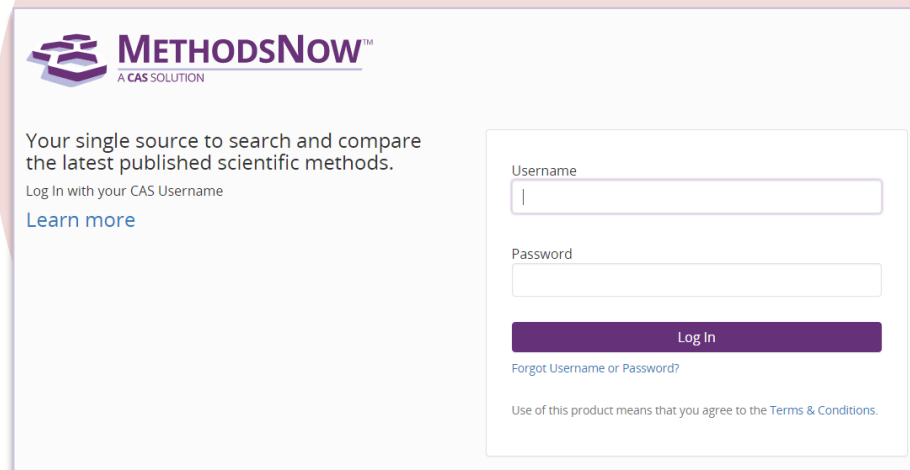
[00273] **Compound 1-4:** ¹H NMR (500 MHz, CDCl₃) δ 4.08-4.11 (m, 3H), 3.98-3.99 (m, 3H), 3.84-3.87 (m, 3H), 2.33-2.45 (m, 12H), 2.24 (s, 9H), 1.25-1.44 (m, 96H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C₃₀H₄₂N₆O₆ [M+H]⁺ 1148.0751, found 1148.0615.

[00274] **Compound 1-5:** ¹H NMR (500 MHz, CDCl₃) δ 4.08-4.13 (m, 3H), 3.93-3.95 (m, 3H), 3.82-3.84 (m, 3H), 1.34-1.42 (m, 12H), 1.26-1.33 (m, 12H), 1.39-1.41 (m, 12H), 1.27-1.30 (m, 12H), 0.89 (t, J = 7.0 Hz, 18H). HRMS (ESI) calcd for C₃₀H₄₂N₆O₆ [M+H]⁺ 685.5592, found 685.5597.



Analysis

分析方法



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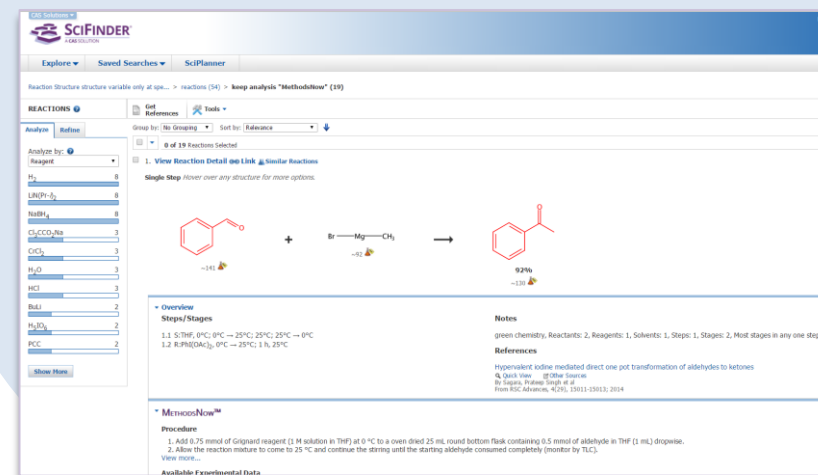
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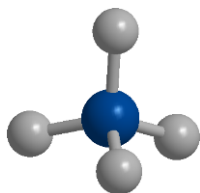
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Synthesis

合成步驟



Synthesis



MethodsNow

Synthesis of benzofuran-containing spirolactones from diarylcyclopropanones

By Syu, Jia-Ru; Lin, Chi-Hui; Kuo, Chiao-Wen; Yang, Ding-Yah
From Tetrahedron Letters, 55(6), 1207-1211; 2014
Published by Elsevier Ltd.

Reaction Steps **1** **2** **3**

Products 2-(5*H*-Furanone, 5-[2-(2-methoxy-5-methylphenyl)-5-methyl-3-benzofuranyl]-3,4-bis(3-nitrophenyl)-, 64%, CAS RN: 1547074-39-4

Reactants 4-Oxaspiro[2.4]hepta-1,6-dien-5-one, 1,2-bis(2-methoxy-5-methylphenyl)-6,7-bis(3-nitrophenyl)-, CAS RN: 1547074-36-1

Reagents Water, CAS RN: 7732-18-5
Boron tribromide, CAS RN: 10294-33-4

Solvents Dichloromethane, CAS RN: 75-09-2

Procedure

1. Add BBr₃ (120 mg, 0.48 mmol, 1.0 M in methylene chloride) dropwise to a solution of the reactant (0.40 mmol) in methylene chloride (20 mL) over the course of 20 minutes at 0 °C.
2. Stir the resulting mixture at 0 °C for 3 hours.
3. After completion, quench the reaction with water.
4. Extract with methylene chloride twice (60 mL each).
5. Dry the combined organic extracts over MgSO₄.
6. Filter and concentrate in a vacuum.
7. Purify the resulting crude product by column chromatography.

Scale milligram

¹H NMR (CDCl₃, 300 MHz) δ 8.28-8.25 (m, 3H), 8.12-8.08 (m, 1H), 7.80-7.77 (m, 2H), 7.61 (dd, *J* = 8.7, 7.8 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.27-7.20 (m, 1H), 7.14-7.10 (m, 2H), 6.91 (d, *J* = 2.7 Hz, 1H), 6.74 (s, 1H), 3.72 (s, 3H), 2.42 (s, 3H), 2.30 (s, 3H)

¹³C NMR (CDCl₃, 75 MHz) δ 170.9, 157.6, 154.9, 153.9, 153.1, 148.5, 148.1, 135.0, 133.7, 133.1, 132.4, 131.9, 131.6, 130.9, 130.5, 130.1, 129.9, 127.3, 126.5, 126.3, 124.9, 124.2, 124.15, 122.9, 118.8, 117.8, 111.7, 111.3, 109.6, 76.6, 55.9, 21.6, 20.3

IR (KBr) 2924, 1756, 1523, 1346, 1006, 806 cm⁻¹

HRMS (EI) calcd for C₃₃H₂₄N₂O₈ [M⁺] 576.1533 found 576.1523

MP 94-95 °C

R_f 0.6 (30% EtOAc/hexanes)

State White solid

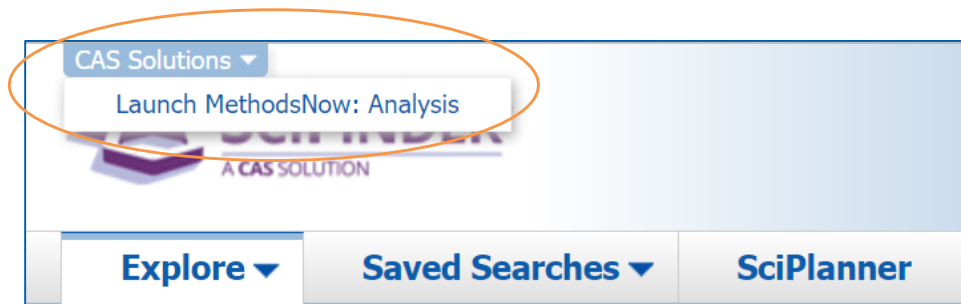
CAS Method Number 3-614-CAS-581989

Print/Export **Close**

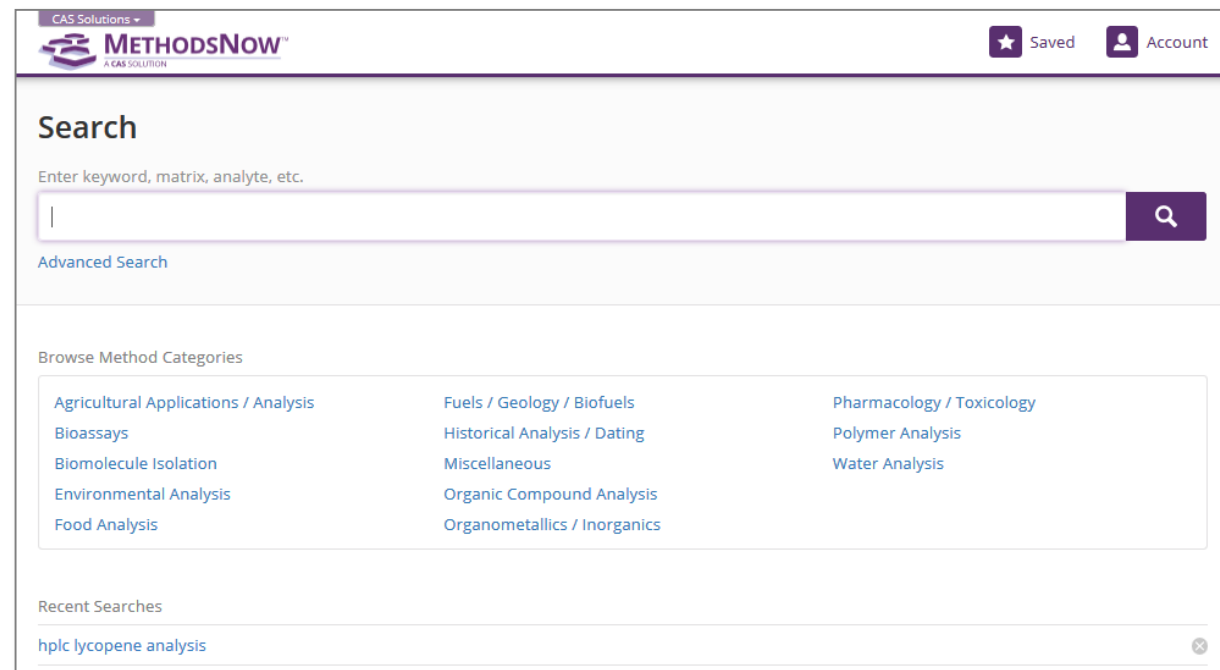
- 不需調閱期刊全文即可看到完整實驗步驟。
- 表格呈現使閱讀容易。
- 可匯出PDF或XLS檔案，方便印出觀看或保存。

匯出功能

Analysis



SciFinder 平台切換 MethodsNow 分析平台



改寫過標題

CAS分析法編號
與
技術方法

物質資訊

原始期刊
(標題、作者、摘要、
出版社連結)

CAS Solutions
METHODSNow™
A CAS SOLUTION

aspirin

Analysis of Aspirin by HPLC

CAS MN: 1-101-CAS-124015

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis
Technique: UV-visible spectroscopy; HPLC

Materials	Role	Image	CAS RN
Benzoic acid, 2-(acetyloxy)-, 1-methylethyl ester	analyte	View Structure	2224-88-6
Aspirin	analyte	View Structure	50-78-2
Benzoic acid, 2-(acetyloxy)-, methyl ester	analyte	View Structure	580-02-9
Benzoic acid, 2-(acetyloxy)-, butyl ester	analyte	View Structure	52602-16-1
Benzoic acid, 2-(acetyloxy)-, ethyl ester	analyte	View Structure	529-68-0
Benzoic acid, 2-(acetyloxy)-, 3-hydroxyphenyl ester	analyte	View Structure	1429226-88-9
Benzoic acid, 2-(acetyloxy)-, phenylmethyl ester	analyte	View Structure	52602-17-2
Kromasil C18 (180 × 4.6 mm, 5 µm) column	material		

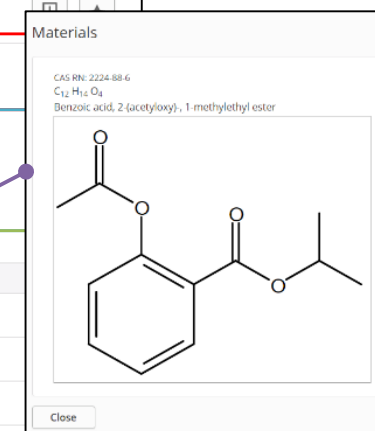
Source

HPLC study of aspirin and aspirin derivatives

Ramjith, U. S.; Sunith, D. K.; Radhakrishnan, Smrithi; Sameer, P. A.
International Journal of Research in Pharmacy and Chemistry (2013), 3 (1), 1 - 5. Catchway Technologies
CODEN: IJRPFQ | ISSN: 22312781

[Document Sources](#)

[Abstract ^](#)
A simple, rapid, precise, and accurate HPLC method for differentiating aspirin from the derivatives of Aspirin synthesized. The instrument used for



總結

- ✓ 進入大數據時代，研究人員必握有強大工具，尚可於新型態資料戰中取得先機。資料庫內容的**涵蓋性為首要**，提供強大的**進階工具(分析/篩選)為必要**。
- ✓ SciFinder兼具以上**二大優勢**，協助研究人員**更有效率**於茫茫資料海中**精準撈取**所需資料，毋須多花時間進行後段篩選與解讀。
- ✓ 創新研究必仰賴於既有的研究基礎進行發想與堆疊，SciFinder提供強大功能，協助研究人員**更有系統與效率**進行研究創新。

iGroup Taiwan 智泉國際事業有限公司

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