

# CAS – SciFinder Training

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# 簡介



Chemical Abstracts

- 人工建置索引

CAS REGISTRY<sup>SM</sup>

- CAS Number 核發與完整物質資訊

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CAS REGISTRY<sup>SM</sup> 申請

2

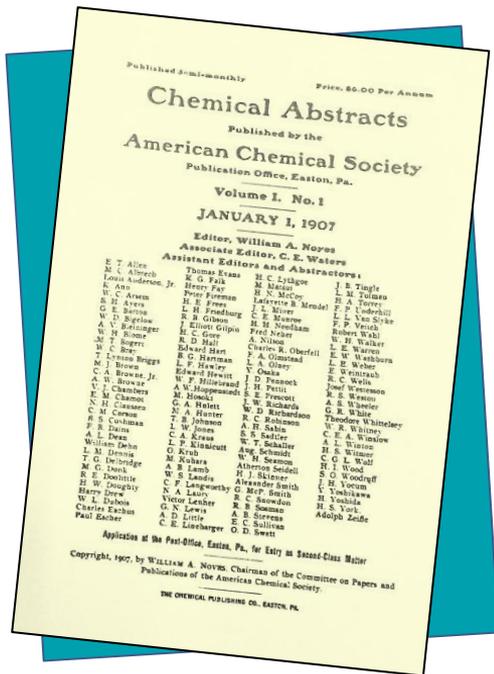
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3



# CAS 建立於兩個原則

- 全世界科學家發表的研究成果可互相交換訊息。
- 科學家沒有多餘時間閱讀完相關研究訊息。



REFERENCE DETAIL

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### 4. Mass and velocity of the $\alpha$ -particles expelled from radium and actinium

By: [Rutherford, Ernest](#)

The author has previously found the values  $e/m = 6 \times 10^3$ , and the highest velocity of the  $\alpha$ -particle =  $2.5 \times 10^9$  cm./sec. Des Coudres found  $e/m = 6.3 \times 10^3$ , and the average velocity  $1.65 \times 10^9$  cm./sec., whilst Mackenzie obtained the values  $4.6 \times 10^3$  and  $1.37 \times 10^9$ . The question is made complex by the fact that the  $\alpha$ -particles come from four different  $\alpha$ -ray products with different ionisation ranges and different projection velocities. In the present investigation homogeneous  $\alpha$ -rays were employed by means of a small wire made active by exposure to radium emanation, which, after fifteen minutes, emits only radium C  $\alpha$ -particles. The method and theory of the experiments are explained and the results and calculations recorded. The values finally obtained are  $e/m = 5.07 \times 10^3$  and  $v = 2.06 \times 10^9$ , these results being considered accurate to about 2 p. the value of  $e/m$  varies with the passage of the  $\alpha$ -particle through matter. It is equivalent to 3.5 cm. and 6.5 cm. of air were  $5.07 \times 10^3$  and  $4.8 \times 10^3$  respectively. The  $\alpha$ -particles from radium A were obtained by the use of a number of act after its exposure to the emanation. The values obtained were  $5.6 \times 10^3$  and in the previous case) tend to give too high a value for  $e/m$ , and the author has radium C have the same mass and differ only in initial velocity. The radium F  $\alpha$ -particle was obtained by the use of a bismuth rod coated with radiotellurium, and values  $e/m = 5.3 \times 10^3$  and  $v = 1.73 \times 10^9$  were obtained; for actinium,  $e/m = 4.7 \times 10^3$  and  $v = 1.21 \times 10^9$ . These results indicate that the  $\alpha$ -particles expelled from the different radio-elements have the same mass in all cases, and that uranium, radium, actinium, and thorium (see succeeding abstract) have a common product of transformation. The value obtained for  $e/m$  is about one-half of that of the hydrogen atom. This may be explained on the assumption that the  $\alpha$ -particle is (1) a molecule of hydrogen carrying the ionic charge, (2) a helium atom carrying twice the ionic charge, or (3) one-half of the helium atom carrying the ionic charge. Of these, (1) is evidently improbable, and the other two hypotheses are briefly discussed. From the quantity of contained helium the age of two radioactive minerals is calculated, being in each case about 400 million years. The energy and heating effects of the  $\alpha$ -particles are calculated, the results being in good accord with observed values.

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SOURCE  
Philosophical Magazine (1798-1977)  
Volume 12  
Issue vi  
Pages 348-71

1906  
CODE: PHMMA4

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126744  
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CAPLUS

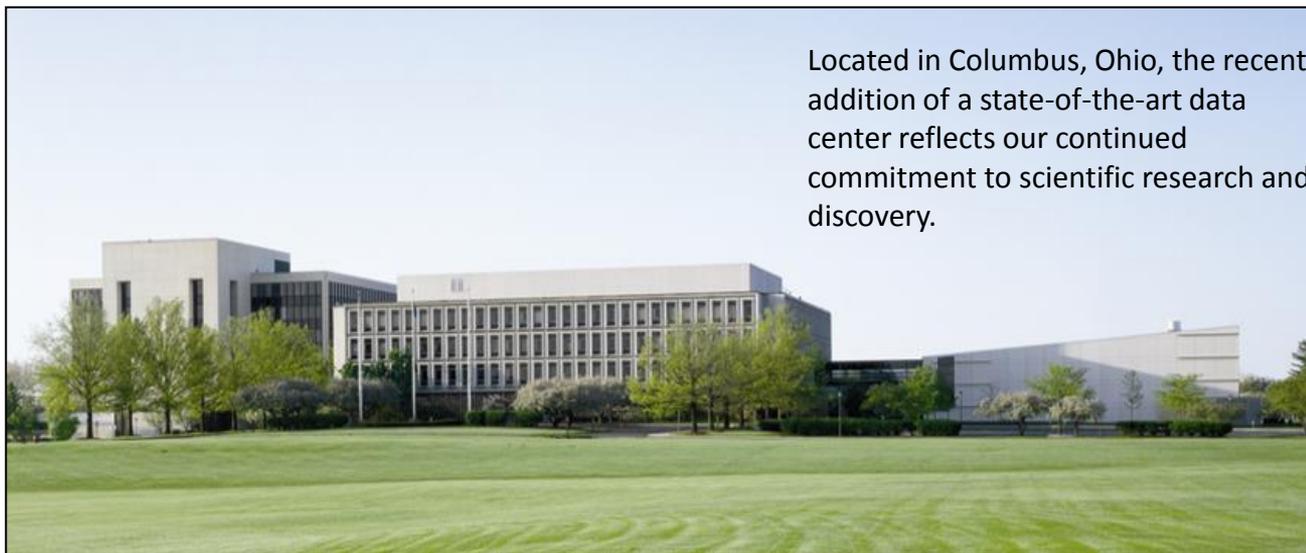
PUBLISHER  
From: J. Chem. Soc., Abstr. 90, II, 719 1906

LANGUAGE  
Unavailable

Indexing  
General and Physical Chemistry (Section2)

## 超過100年的時間，CAS支持與輔助科學家

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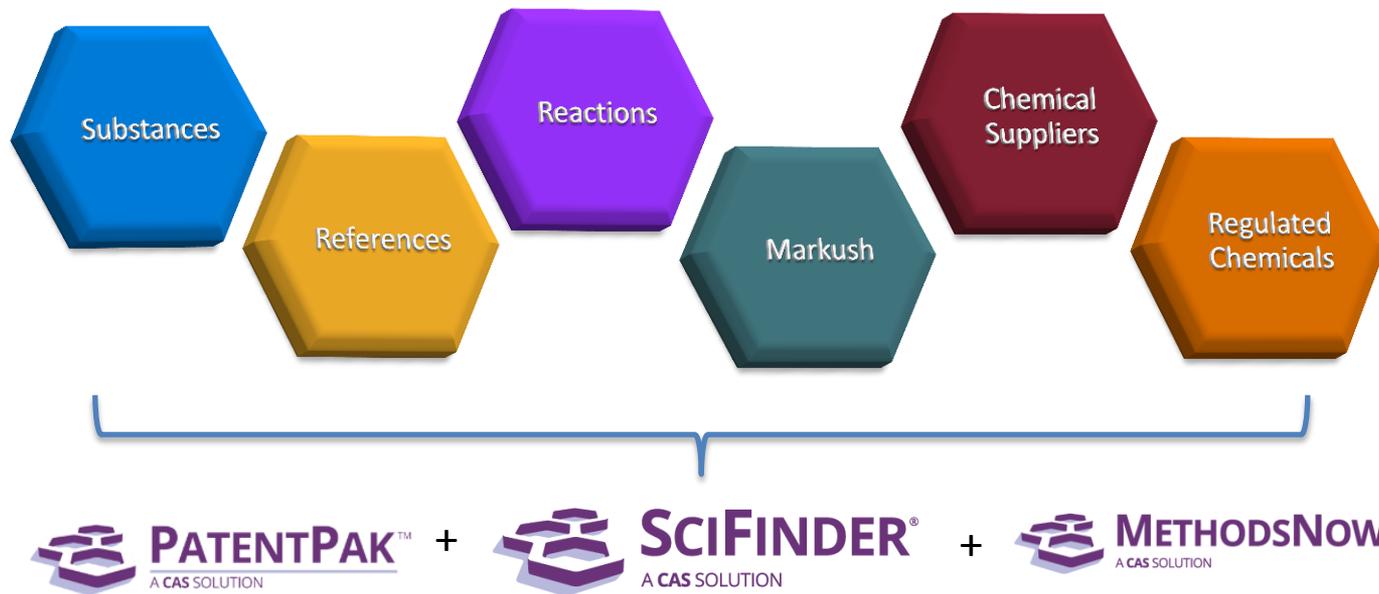
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## CAS 提供的訊息與平台幫助科學家查詢專利與期刊工作流程

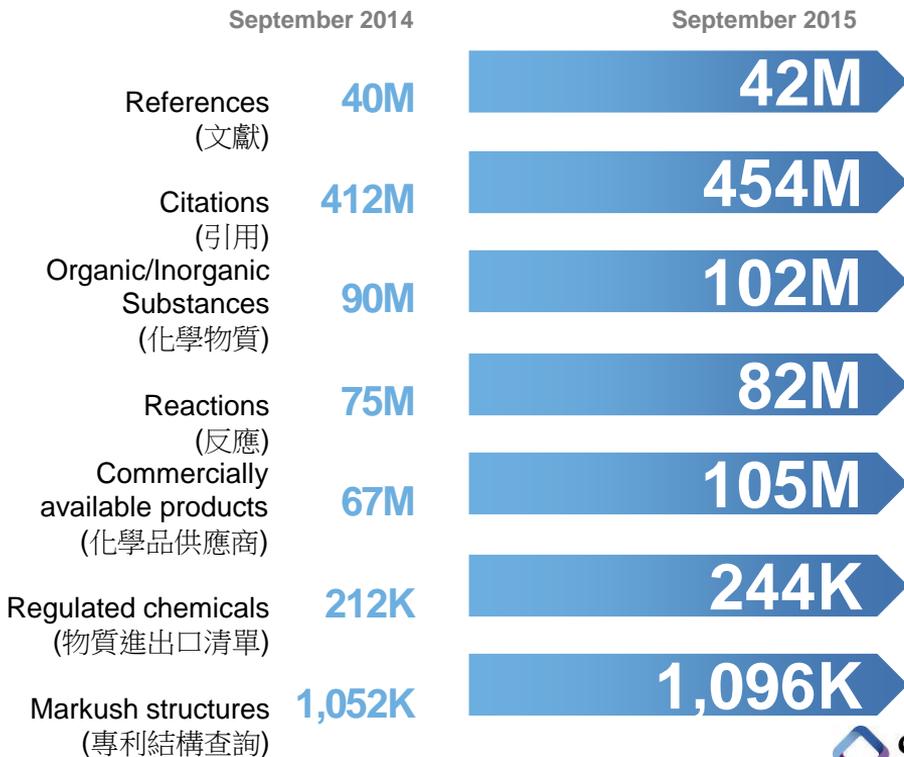


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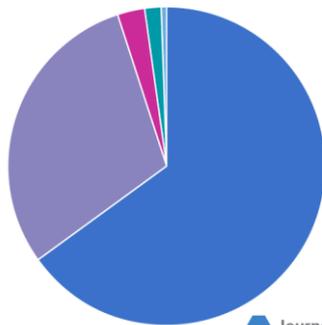
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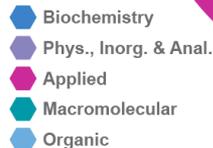
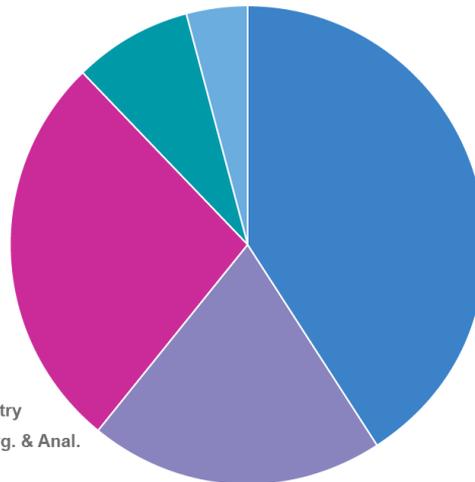
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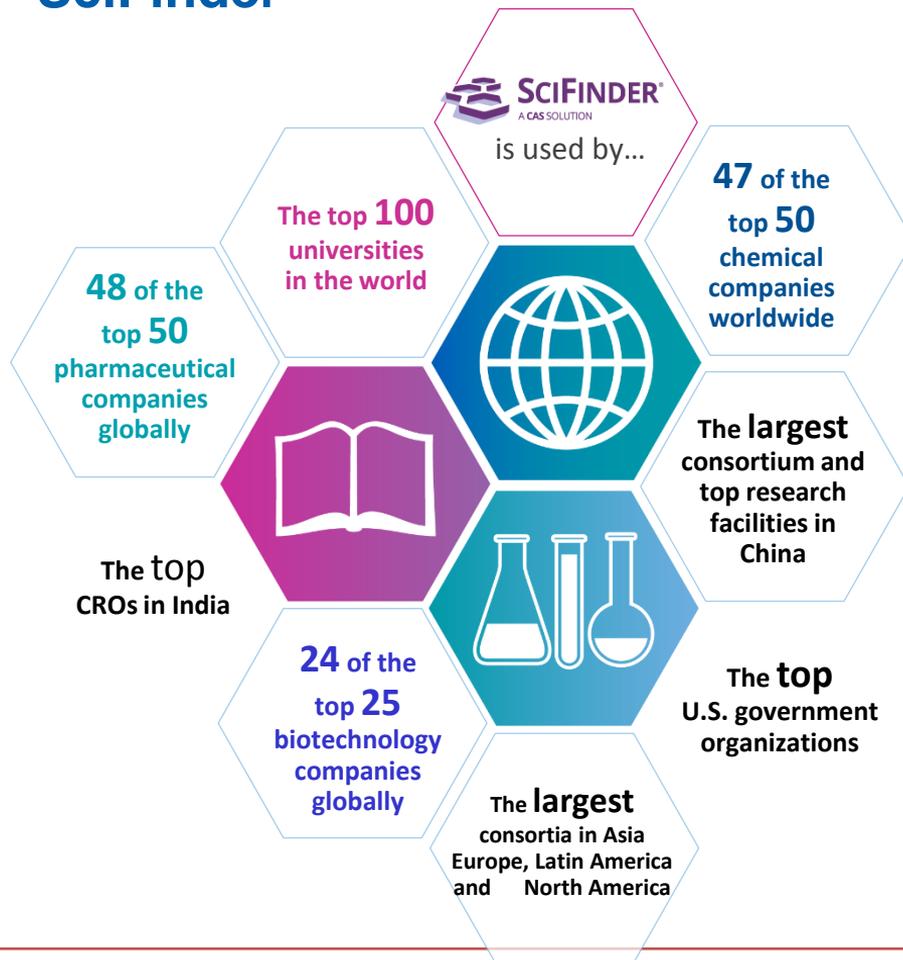
Disclosure types not published in journals **35%**



Discipline areas not in traditional chemistry **61%**



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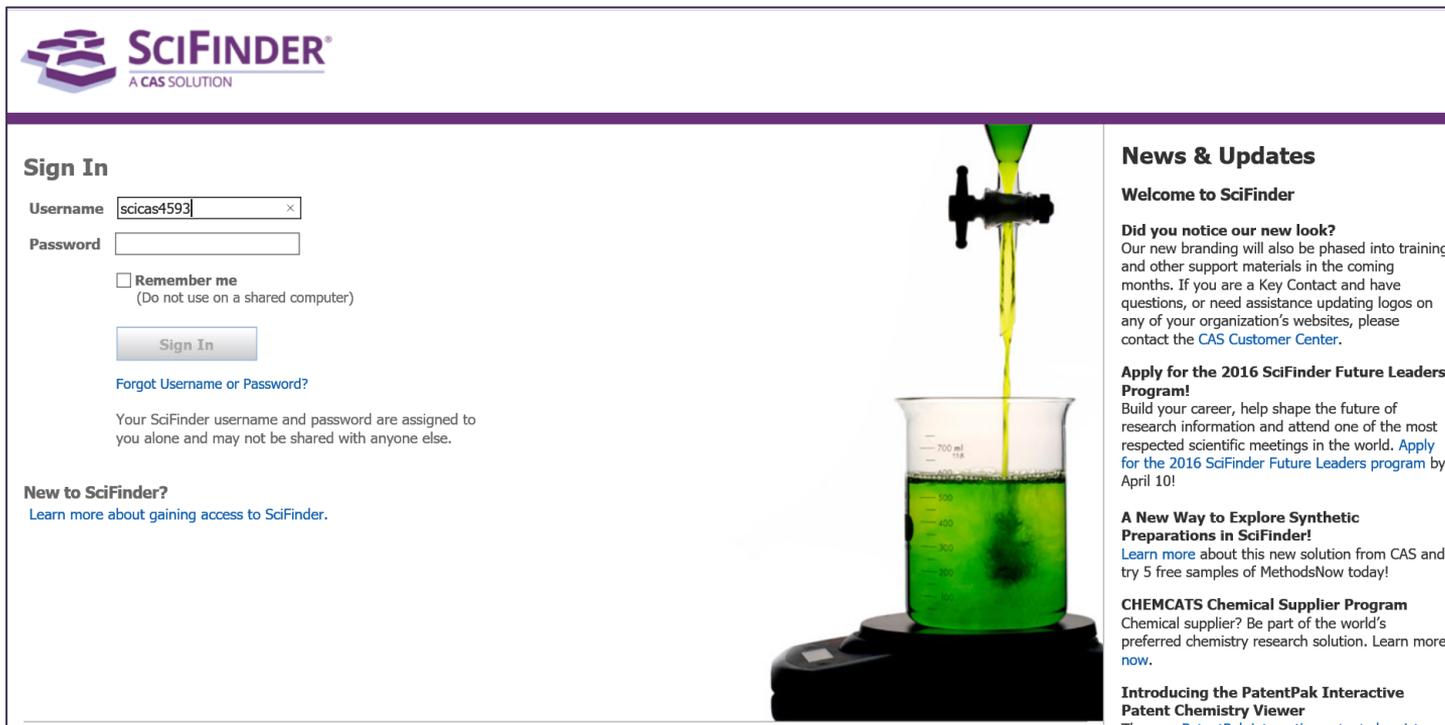


**Sources:**

- *The Academic Ranking of World Universities*
- *Chemical & Engineering News*
- *Genetic Engineering & Biotechnology News*
- *PharmaExec.com*

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3. 申請完成會提醒您CAS寄發確認信至填寫的email信箱中。
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# 如何使用 SciFinder?

- Search for **References, Substances and Reactions**

The screenshot displays the SciFinder web interface. The top navigation bar includes 'CAS Solutions', 'SCIFINDER A CAS SOLUTION', 'Preferences | SciFinder Help', and 'Sign Out'. The left sidebar contains a navigation menu with categories like 'REFE', 'SUBS', and 'REACT'. The main content area shows a search for 'reactions (112)'. Below the search bar, there are tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The 'REACTIONS' section is active, showing a list of reagents and their counts:

Reagent	Count
HCl	30
NaH	20
H <sub>2</sub> SO <sub>4</sub>	17
KOH	15
HNO <sub>3</sub>	13
NaOH	9
H <sub>2</sub> O	8
HCO <sub>2</sub> H	7
NaHCO <sub>3</sub>	7
Zn	7

The reaction scheme shows the synthesis of caffeine from 1,3,7-trimethylxanthine and dimethyl carbonate. The reaction is labeled 'Single Step' and has a yield of 98%.

Options for viewing the reaction details include:

- 1. View Reaction Detail [Link](#) [Similar Reactions](#)

The interface also includes a 'Get References' button, a 'Tools' dropdown, and a 'Send to SciPlanner' button. The bottom of the page shows a navigation bar with 'Overview', 'Steps/Stages', and 'Notes'.

## 如何使用 SciFinder?

- 創新介面：**analyze** and **refine** answer sets; **save** and **export** results; **navigate** from reference to substance to reaction search **seamlessly**

Stay current in your field and keep track of competition

Quickly find and analyze information (research topic, structure, reaction)

Share ideas with colleagues and collaborators

The screenshot displays the SciFinder interface with the following elements:

- Header:** SciFinder logo, navigation tabs (Explore, Saved Searches, SciPlanner), and utility buttons (Save, Print, Export).
- Search Bar:** A search query "Keep Me Posted 'carbon nanotubes'[Jun 27, 2015] (288)" is entered and highlighted with a red box.
- Navigation:** Buttons for "Get Substances", "Get Reactions", "Get Related Citations", and "Tools". A "Send to SciPlanner" button is highlighted with a red box.
- Analysis Panel:** A dropdown menu for "Analyze by:" is open, showing "Company-Organization" selected and highlighted with a red box. Below it, a list of organizations is shown with bar charts: ULVAC Inc, Japan (7); Chongqing University, Peop Rep China (4); Fuzhou University, Peop Rep China (3); and another entry (3).
- Results:** A list of 288 references is shown, sorted by "Access Number". The first result is highlighted: "1. Fabrication and dielectric properties of poly(ether ether ketone)/polyimide blends with selectively distributed multi-walled carbon nanotubes".



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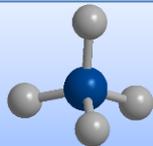
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MethodsNow : Analysis



## MethodsNow : Synthesis



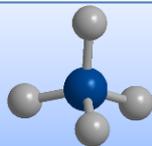
## 優點介紹

詳細的合成資訊完整的實驗步驟，以及化合物完整光譜資訊，一併條列式的呈現。  
\*有機合成研究人員最適合的功能~

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# MethodsNow : Synthesis



如何使用?

反應查詢結果頁面

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0 of 36 Reactions Selected

1. View Reaction Detail [Link](#)

4 Steps Hover over any structure for more options.

[Step 2.1] ~59

[Step 4.1] ~145

Overview

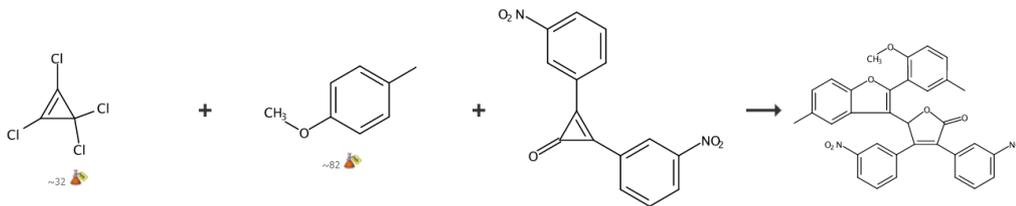
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Procedure

1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.001 mol)

15. [View Reaction Detail](#) [Link](#)

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



[Step 2.1]

Overview

Steps/Stages

- 1.1 R: AlCl<sub>3</sub>, S: CH<sub>2</sub>Cl<sub>2</sub>, 5 min, -20°C; 10 min, -20°C
- 1.2 5 min, -20°C; -20°C → rt; 45 min, rt
- 1.3 R: NH<sub>4</sub>Cl, S: H<sub>2</sub>O
- 2.1 C: CuBr, S: ClCH<sub>2</sub>CH<sub>2</sub>Cl, 12 h, 75°C
- 3.1 R: BBr<sub>3</sub>, S: CH<sub>2</sub>Cl<sub>2</sub>, 20 min, 0°C; 3 h, rt
- 3.2 R: H<sub>2</sub>O

Notes

Reactants: 3, Reagents: 4, Catalysts: 1, Solvents: 3, Steps: 3, Stages: 6, Most stages in any one step: 3

References

Synthesis of benzofuran-containing spiro lactones from diarylcyclopropanes

[Quick View](#) [Other Sources](#)

By Syu, Jia-Ru et al  
From *Tetrahedron Letters*, 55(6), 1207-1211, 2014

METHODSNow™

Procedure

1. Charge a flame dried, argon-fed three neck flask fitted with a reflux condenser with AlCl<sub>3</sub> (1024 mg, 7.8 mmol) and dry methylene chloride (50 mL).
2. Cool the flask to -20 °C.

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Available Experimental Data

<sup>1</sup>H NMR, <sup>13</sup>C NMR, IR, HRMS, MP, R<sub>f</sub>, State

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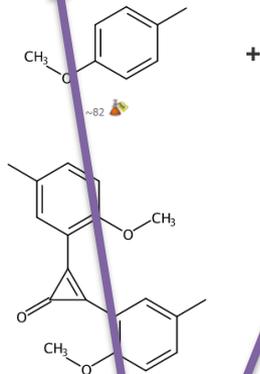
# MethodsNow 畫面

## MethodsNow

### Synthesis of benzofuran-containing spirolactones from diaryl

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-Cyclopropenone, 2,3-bis(2-methoxyphenyl)cyclopropenone

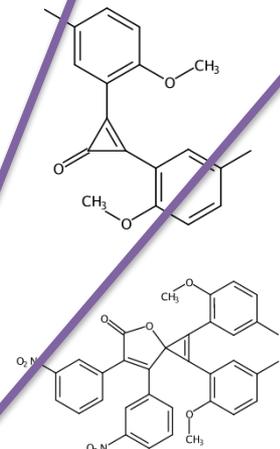
**Reactants** 4-Methylanisole, CAS RN: 104-90-5  
Cyclopropenone, 1,2,3-trichloro-

## MethodsNow

### Synthesis of benzofuran-containing spirolactones from diaryl

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



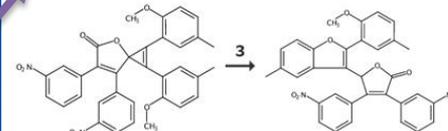
**Products** 4-Oxaspiro[2.4]hepta-1,6-dien-5-one  
RN: 1547074-36-1

## MethodsNow

### Synthesis of benzofuran-containing spirolactones from diarylcyclopropenones

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



<b>Products</b>	2-(5-Furanone)-5-[2-(2-methoxy-5-methylphenyl)-5-methyl-3-benzofuryl]-3,4-bis(3-nitrophenyl)-, 64%, CAS RN: 1547074-39-4
<b>Reactants</b>	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
<b>Reagents</b>	Water, CAS RN: 7732-18-5 Boron tribromide, CAS RN: 10294-33-4
<b>Solvents</b>	Dichloromethane, CAS RN: 75-09-2
<b>Procedure</b>	1. Add BBr <sub>3</sub> (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 (50 mL each). 5. Dry the combined organic extracts over MgSO <sub>4</sub> . 6. Filter and concentrate in a vacuum. 7. Purify the resulting crude product by column chromatography.
<b>Scale</b>	milligram
<b><sup>1</sup>H NMR</b>	(CDCl <sub>3</sub> , 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)
<b><sup>13</sup>C NMR</b>	(CDCl <sub>3</sub> , 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
<b>IR</b>	(KBr) 2924, 1756, 1523, 1346, 1006, 806 cm <sup>-1</sup>
<b>HRMS</b>	(EI) calcd for C <sub>33</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> [M <sup>+</sup> ] 576.1533 found 576.1523
<b>MP</b>	94-95 °C
<b>R<sub>f</sub></b>	0.6 (30% EtOAc/hexanes)
<b>State</b>	White solid
<b>CAS Method Number</b>	3-614-CAS-581989

Print/Export

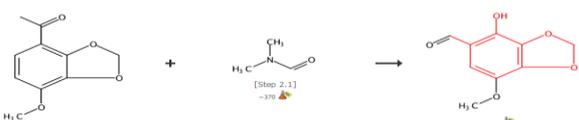
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## ■ 詳細三步驟反應過程

## ■ 匯出功能

# Experimental procedures VS MethodsNow

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



**Overview**

**Steps/Stages**

- 1.1 R:Na<sub>2</sub>HPO<sub>4</sub>, R:mCPBA, Si:CH<sub>2</sub>Cl<sub>2</sub>, cooled; 1 h; rt
- 1.2 R:KOH, S:MeOH, 2 h; rt
- 1.3 R:KHSO<sub>5</sub>, S:H<sub>2</sub>O, acidic
- 2.1 R:POCl<sub>3</sub>, S:DMF, 15 min, 5°C → rt; 20 min; rt
- 2.2 R: rt → 75°C; 2 h, 75°C; 75°C → 0°C
- 2.3 R:H<sub>2</sub>O, 5°C

**Notes**

1) Baeyer-Villiger oxidation (stage 1), 2) regioselective, Vilsmeier reaction, Reagents: 2, Reagents: 6, Solvents: 6, Steps: 2, Stages: 6, Most stages in any one step: 3

**References**

Total Synthesis of Bulbophyol-B  
 By Liu, Zhilun et al  
 From Journal of Natural Products, 71(11), 1938-1941; 2008

**Experimental Procedure**

**Step 1**

**4-Methoxy-2,3-methylenedioxyphenyl Acetate (8).** To a suspension of **7** (5.0 g, 25.5 mmol) and anhydrous Na<sub>2</sub>HPO<sub>4</sub> (4.7 g, 32.2 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL) was added *m*-CPBA (85%, 23.4 g, 127.5 mmol), in portions and in an ice-water bath, and the mixture was stirred at room temperature for 1 h. The resulting mixture was refluxed overnight, then cooled and filtered. The filter cake was washed with CH<sub>2</sub>Cl<sub>2</sub> (3 × 30 mL). Evaporation of the solvent *in vacuo* gave a residue, which was directly used in the next reaction. **4-Methoxy-2,3-methylenedioxyphenol (9).** KOH (1.4 g, 25 mmol) in H<sub>2</sub>O (10 mL) was added to the crude **8** (5.5 g, 25.8 mmol) in MeOH (20 mL), and the mixture was stirred for 2 h at room temperature. The mixture was concentrated to 10 mL and acidified with 2 M HCl (5 mL). The aqueous layer was extracted with CHCl<sub>3</sub> (3 × 20 mL), washed with H<sub>2</sub>O (2 × 20 mL) and brine (20 mL), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and concentrated. The residue was purified by column chromatography (CC) (n-hexane/EtOAc, 3:1) to give **9** (4.38 g, two steps total yield 78%) as a white solid. **4-Methoxy-2,3-methylenedioxyphenol (9).** yield 4.38 g, 78% mp 103-105 °C (lit.<sup>11</sup> mp 100-101 °C); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 6.43 (1H, s, H-6), 6.42 (1H, s, H-5), 5.99 (2H, s, OCH<sub>3</sub>), 4.48 (1H, s, OH), 3.85 (1H, s, OCH<sub>2</sub>).

**Step 2**

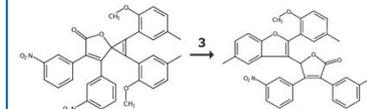
**2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10).** POCl<sub>3</sub> (5.5 mL, 59.5 mmol) was added dropwise to DMF (10 mL, 129.4 mmol) over 15 min at 5 °C, then stirred at room temperature for 20 min followed by addition of **9** (2.5 g, 14.9 mmol) in portions. The mixture was slowly heated to 75 °C and then stirred at this temperature for 2 h. The resulting mixture was cooled to 5 °C and poured into H<sub>2</sub>O (50 mL), after filtration, the filter cake was purified by CC (n-hexane/CHCl<sub>3</sub>, 1:1) to give **10** (2.3 g, 79%) as a white solid; **2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10).** yield 2.3 g, 79% mp 181-182 °C (lit.<sup>11</sup> mp 179-180 °C); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 10.83 (1H, s, CHO), 9.73 (1H, s, OH), 6.75 (1H, s, Ar-H), 6.18 (2H, s, OCH<sub>2</sub>O), 3.93 (3H, s, OCH<sub>3</sub>).

## MethodsNow

Synthesis of benzofuran-containing spinolactones from diarylylcyclopropanes

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

Reaction Steps 1 2 3



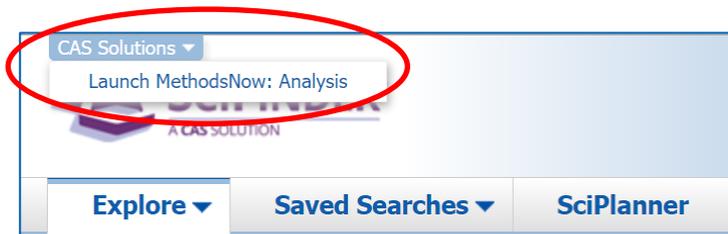
<b>Products</b>	2-(5H-Furanone, 5-[2-(2-methoxy-5-methylphenyl)-5-methyl-3-benzofuranyl]-3,4-bis(3-nitrophenyl), 64%, CAS RN: 1547074-39-4
<b>Reactants</b>	4-Oxaspiro[2.4]hepta-1,6-dien-5-one, 1,2-bis(2-methoxy-5-methylphenyl)-6,7-bis(3-nitrophenyl), CAS RN: 1547074-36-1
<b>Reagents</b>	Water, CAS RN: 7732-18-5 Boron tribromide, CAS RN: 10294-33-4
<b>Solvents</b>	Dichloromethane, CAS RN: 75-09-2
<b>Procedure</b>	1. Add 98g (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 (50 mL each). 5. Dry the combined organic extracts over MgSO <sub>4</sub> . 6. Filter and concentrate in a vacuum. 7. Purify the resulting crude product by column chromatography.
<b>Scale</b>	milligram
<b><sup>1</sup>H NMR</b>	(CDCl <sub>3</sub> , 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, 2H), 2.42 (s, 2H), 2.30 (s, 2H)
<b><sup>13</sup>C NMR</b>	(CDCl <sub>3</sub> , 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, 130.3, 130.5, 130.1, 129.9, 127.3, 126.5, 126.3, 124.9, 124.2, 124.15, 122.9, 118.8, 117.8, 117.7, 111.3, 109.6, 76.6, 55.9, 21.6, 20.3
<b>IR</b>	(KBr) 2924, 1756, 1523, 1346, 1006, 806 cm <sup>-1</sup>
<b>HRMS</b>	(EI) calcd for C <sub>31</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub> [M] <sup>+</sup> 576.1533 found 576.1523
<b>MP</b>	94-95 °C
<b>R<sub>f</sub></b>	0.6 (30% EtOAc/hexanes)
<b>State</b>	White solid
<b>CAS Method Number</b>	3-614-CAS-581989

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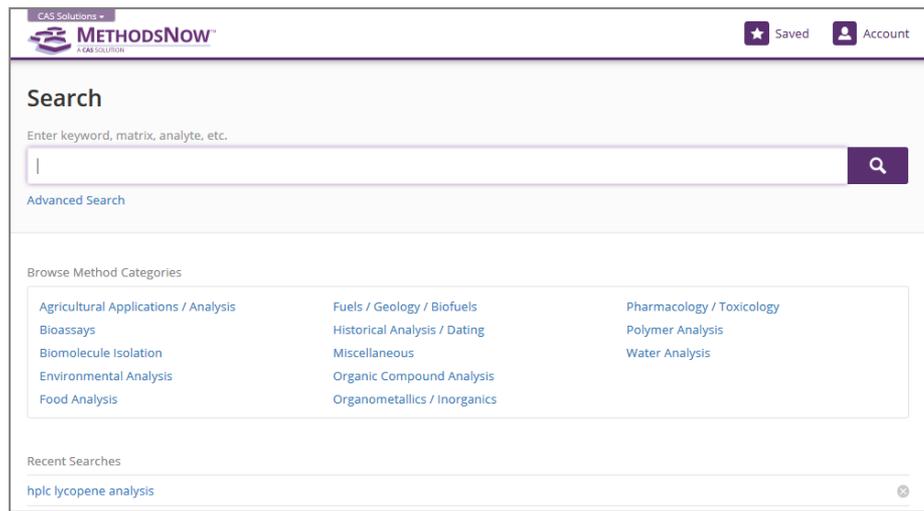
# MethodsNow : Analysis



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- wastewater treatment anaerobic sludge
- wastewater treatment plants
- wastewater treatment sludge**

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The screenshot displays the SciFinder METHODSNow interface. At the top, the search bar contains the text 'wastewater sludge'. The left sidebar features a filter menu with categories: Analyte (listing Copper, Lead, Cadmium, Nickel, Mercury), Matrix (listing Drinking waters, River waters, Water, Wastewater, Seawater), Method Category, Technique, and Year. The main content area shows a search result for 'Analysis of Phosphorus in Wastewater treatment sludge by Dehydration process' with CAS MN: 1-143-CAS-4734. A table below the title lists key details:

Analyte	Phosphorus
Matrix	Municipal wastewater; Wastewater treatment sludge
Other Materials	Reagent: Perchloric acid; Molybdic acid; L-Ascorbic acid; Sulfuric acid Material: Oven
Method Category	Water / Wastewater / Sludge Analysis
Technique	Dehydration process; UV-visible spectroscopy
Equipment Used	UV-VIS spectrometer
Source	Method validation and uncertainty estimation for total phosphorus determination in wastewater sludge samples

## 查看所有分析物

### Analyte

Alphabetically **By Count**

<input type="checkbox"/> Copper (627)	<input type="checkbox"/> Indeno[1,2,3- <i>cd</i> ]pyrene (119)	<input type="checkbox"/> Polycyclic aromatic hydrocarbons (79)
<input type="checkbox"/> Lead (573)	<input type="checkbox"/> Ciprofloxacin (116)	<input type="checkbox"/> Terbutylazine (79)
<input type="checkbox"/> Cadmium (495)	<input type="checkbox"/> Ethinylestradiol (115)	<input type="checkbox"/> Trimethoprim (79)
<input type="checkbox"/> Nickel (339)	<input type="checkbox"/> Vanadium (115)	<input type="checkbox"/> Dimethyl phthalate (78)
<input type="checkbox"/> Mercury (333)	<input type="checkbox"/> Dibenz[ <i>a,h</i> ]anthracene (112)	<input type="checkbox"/> Selenium (78)
<input type="checkbox"/> Zinc (275)	<input type="checkbox"/> Naproxen (111)	<input type="checkbox"/> Diethyl phthalate (75)
<input type="checkbox"/> Cobalt (254)	<input type="checkbox"/> Enrofloxacin (110)	<input type="checkbox"/> $\alpha$ -Endosulfan (74)
<input type="checkbox"/> Chromium (253)	<input type="checkbox"/> Chromium(6+) (107)	<input type="checkbox"/> p,p'-DDD (74)
<input type="checkbox"/> Iron (242)	<input type="checkbox"/> Uranium (107)	<input type="checkbox"/> Carbofuran (73)
<input type="checkbox"/> Arsenic (209)	<input type="checkbox"/> Chlorpyrifos (105)	<input type="checkbox"/> Sulfadiazine (73)
<input type="checkbox"/> 2,2'-Bis(4-hydroxyphenyl)propane (199)	<input type="checkbox"/> Lead(2+) (104)	<input type="checkbox"/> 2,4,6-Trichlorophenol (72)

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### Technique

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<input type="checkbox"/> Adsorptive stripping voltammetry (1)	<input type="checkbox"/> Electrochemical adsorption (1)	<input type="checkbox"/> HPLC (24)
<input type="checkbox"/> Affinity (1)	<input type="checkbox"/> Electrochemical analysis (29)	<input type="checkbox"/> HPLC stationary phases (2)
<input type="checkbox"/> Amperometric biosensors (2)	<input type="checkbox"/> Electrochemical catalysis (1)	<input type="checkbox"/> HPLC-tandem mass spectrometry (6)
<input type="checkbox"/> Amperometric sensors (1)	<input type="checkbox"/> Electrochemical immunoassay (3)	<input type="checkbox"/> Hemagglutination test (1)
<input type="checkbox"/> Amperometry (32)	<input type="checkbox"/> Electrochemical oxidation (2)	<input type="checkbox"/> High-performance liquid chromatography-mass spectrometry (2)
<input type="checkbox"/> Analysis (1)	<input type="checkbox"/> Electrochemical reaction kinetics (1)	<input type="checkbox"/> High-performance size exclusion chromatography (1)
<input type="checkbox"/> Anion exchange (1)	<input type="checkbox"/> Electrochemical sensors (1)	<input type="checkbox"/> High-performance thin layer chromatography (2)
<input type="checkbox"/> Anion exchange HPLC (1)	<input type="checkbox"/> Electrochemiluminescence (7)	<input type="checkbox"/> High-resolution NMR spectroscopy (1)
<input type="checkbox"/> Anodic stripping voltammetry (4)	<input type="checkbox"/> Electrochemiluminescence spectroscopy (1)	<input type="checkbox"/> Hydrolysis (2)
<input type="checkbox"/> Anodization (1)	<input type="checkbox"/> Electrodeposition (2)	<input type="checkbox"/> Hydrolytic polymer degradation (2)
<input type="checkbox"/> Atmospheric precipitation (3)		
<input type="checkbox"/> Atomic absorption spectroscopy (1)		

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- Copper (627)
- Lead (573)
- Cadmium (495)
- Nickel (339)
- Carbamazepine (96)

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Matrix

Method Category

Technique

Year

Analysis of Carbamazepine in Wastewater by Atmospheric pressure chemical ionization mass spectrometry  
CAS MN: 1-101-CAS-27867

View Details & Instructions

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Analyte Carbamazepine

Matrix Wastewater treatment sludge; Wastewater

Other Materials Material: Environmental analytical cartridges; Glass-fiber (0.45mm); Stainless steel vessel (34 mL); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).  
View All

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis; Water / Wastewater / Sludge Analysis

Technique Atmospheric pressure chemical ionization mass spectrometry

Equipment Used Milli-Q/Milli-RO system; ASE extractor; Vacuum pump; LDTD-APCI ionization source; Mass Spectrometer

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wastewater sludge

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## Compare Methods

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	1	2
Title	Analysis of Carbamazepine in <b>Wastewater</b> by Atmospheric pressure chemical ionization mass spectrometry	Analysis of Carbamazepine in <b>Wastewater</b> by Atmospheric pressure chemical ionization mass spectrometry
CAS Method Number	1-101-CAS-27867	1-101-CAS-29149
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis; Water / <b>Wastewater</b> / <b>Sludge</b> Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis; Water / <b>Wastewater</b> / <b>Sludge</b> Analysis
Technique	Atmospheric pressure chemical ionization mass spectrometry	Atmospheric pressure chemical ionization mass spectrometry
Analyte	Carbamazepine	Carbamazepine
Matrix	Wastewater treatment sludge; <b>Wastewater</b>	Wastewater treatment sludge; <b>Wastewater</b>
Other Materials	Environmental cartridges; Glass-fiber (0.45mm); Stainless steel vessel (34 mL); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W)	Environmental cartridges; Glass-fiber (0.45mm); LazWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).

# 查詢結果詳細資訊

CAS Solutions  
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# 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	<a href="#">View Structure</a>	2224-88-6
<b>Aspirin</b>	analyte	<a href="#">View Structure</a>	50-78-2
Benzoic acid, 2-(acetyloxy)-, methyl ester	analyte	<a href="#">View Structure</a>	580-02-9
Benzoic acid, 2-(acetyloxy)-, butyl ester	analyte	<a href="#">View Structure</a>	52602-16-1
Benzoic acid, 2-(acetyloxy)-, ethyl ester	analyte	<a href="#">View Structure</a>	529-68-0
Benzoic acid, 2-(acetyloxy)-, 3-hydroxyphenyl ester	analyte	<a href="#">View Structure</a>	1429226-88-9
Benzoic acid, 2-(acetyloxy)-, phenylmethyl ester	analyte	<a href="#">View Structure</a>	52602-17-2
Kromasil C18 (180 × 4.6 mm, 5 μm) column	material		

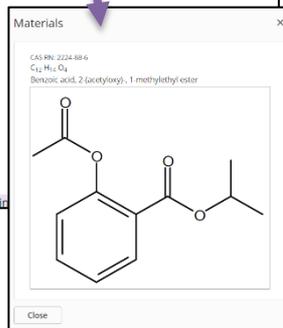
**Source**

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: IJRPGF ISSN: 22312781

Document Sources

Abstract ^  
A simple, rapid, precise, and accurate HPLC method for differentiating **aspirin** from the derivatives of **Aspirin**



### Abstract ^

A simple, rapid, precise, and accurate HPLC method for differentiating **aspirin** from the derivatives of **Aspirin** synthesized. The instrument used for carrying out HPLC was Shimadzu LCVP2010C integrated system equipped with quaternary gradient pump. Column utilized Kromasil C<sub>18</sub> (180 × 4.6 mm), 5μm and the detection made possible using UV-Vis detector at a wavelength of 277 nm and the mobile phase employed was acetonitrile:MeOH 60:40(volume/volume). The R<sub>t</sub>(Retention time) of **aspirin** was found to be 4.303 and that of derivatives as SR01-2.543, SR02-3.797, SR03-4.133, SR05-2.553, SR06-3.277, SR07-2.903. Proving the fact that the **aspirin** and its derivatives synthesized are pure.

### Equipment Used

HPLC system, LCVP2010C, Shimadzu  
Pump, Shimadzu  
UV-Vis detector

### Conditions

Instrument  
Mobile phase-acetonitrile:methanol (60:40, v/v)  
Wavelength-277 nm

### Instructions

#### High performance liquid chromatography (HPLC)

1. Perform analysis using Shimadzu LCVP2010C integrated system equipped with quaternary gradient pump.
2. Use Kromasil C18 (180 × 4.6 mm, 5 μm) column.
3. Use mobile phase consisting of acetonitrile:methanol (60:40, v/v).
4. Perform detection using UV-Vis detector at 277 nm.

### Validation

Retention Time	
4.303 min,	<b>Aspirin</b>
2.543 min,	Benzoic acid, 2-(acetyloxy)-, butyl ester
3.797 min,	Benzyl-2-acetoxy benzoate
4.133 min,	3-Hydroxy phenyl-2-acetoxy benzoate

# PatentPak™

一個強大的工具解決專利閱讀的工作流程，使科學家使用一半時間快速定位並追蹤專利中的化學物質。

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- ✓ 全新**專利閱讀導航**-Patent Viewer，點選物質對應頁碼立即開啟Patent Viewer 瀏覽，專利訊息**解讀更容易**，並可連結SciFinder進行物質進階查詢，讓**流程更加簡化**。

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直接點選Patent No. 即可下載全文。

The screenshot displays the SciFinder interface. The main search results show a patent entry for "US20080078739" with 3 references. A table of patent families is highlighted with a red box:

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

An inset window shows the full patent document for WO 2010/005930 A2, including the title, international classification, filing date, and applicant information.



# Patent Viewer

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The screenshot displays the Patent Viewer interface. On the left, a list of patents is shown, with the entry "1636182-69-8P" highlighted in red. A blue arrow points from this entry to the detailed view of the patent on the right. In the detailed view, the "Key Substances in Patent" section is visible, with the entry "CAS RN 1626333-91-2" highlighted in red. A blue arrow points from this entry to the list on the left. The detailed view also shows a chemical structure and associated text, with a red box highlighting the entry "[00273] Compound 1-4" in the text.

1636182-64-3P Page 127 in PatentPak<sup>™</sup>

prepn. of triazinane trione derivs. and comps. thereof useful for treatment of diseases

Biological use, unclassified; Cosmetic use; Food or feed use; Other use, unclassified; Pharmacokinetics; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses

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1636182-62-1P Page 127 in PatentPak<sup>™</sup>

1636182-63-2P Page 127 in PatentPak<sup>™</sup>

1636182-65-4P Page 127 in PatentPak<sup>™</sup>

1636182-66-5P Page 128 in PatentPak<sup>™</sup>

1636182-67-6P Page 128 in PatentPak<sup>™</sup>

1636182-68-7P Page 128 in PatentPak<sup>™</sup>

1636182-69-8P Page 128 in PatentPak<sup>™</sup>

prepn. of triazinane trione derivs. and comps. thereof useful for treatment of diseases

Biological use, unclassified; Cosmetic use; Food or feed use; Other use, unclassified; Synthetic preparation; Therapeutic use; Biological study; Preparation; Uses

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Key Substances in Patent

CAS RN 1626333-91-2

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CAS RN 1636182-69-8P

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Analyst Markup Location

page 127

CAS RN 2451-62-9

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Analyst Markup Location

page 127

WO 2014/17962 PCES20140635

Scheme 1. Exemplary synthesis of certain compounds of Formula (I), wherein R<sup>1</sup> and R<sup>2</sup> 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: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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 C<sub>27</sub>H<sub>36</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 643.5122, found 643.5203.

[00271] Compound 1-2: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08-4.13 (m, 3H), 3.98-4.00 (m, 3H), 3.83-3.86 (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 C<sub>30</sub>H<sub>40</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 727.6056, found 727.6116.

[00272] Compound 1-3: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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 C<sub>31</sub>H<sub>40</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 805.7934, found 805.7937.

[00273] Compound 1-4: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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, 90H), 0.88 (t, J = 7.0 Hz, 9H). HRMS (ESI) calcd for C<sub>30</sub>H<sub>36</sub>N<sub>6</sub>O<sub>6</sub> [M+H]<sup>+</sup> 643.5122, found 643.5122.

**PatentPak™**  
Key Substances in Patent

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Analyst Markup Location  
page 127

**CAS RN 1626333-91-2**  
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Analyst Markup Location  
page 127

**CAS RN 1636182-65-4**  
Search in SciFinder | View Detail  
Analyst Markup Location  
page 127

**CAS RN 2451-62-9**

Chemical structure: CC1(C)N(C)C(=O)N(C)C(=O)N1C

**專利全文**

**標示物質在專利全文中出現的頁碼與句子或反應式中。**

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*Scheme 1. Exemplary synthesis of certain compounds of Formula (I), wherein R<sup>A</sup> and R<sup>B</sup> 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: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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 C<sub>27</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub> [M+H]<sup>+</sup> 643.5122, found 643.5203.

**[00271]** Compound 1-2: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.98–4.00 (m, 3H), 3.83–3.86 (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 C<sub>30</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub> [M+H]<sup>+</sup> 727.6056, found 727.6116.

**[00272]** Compound 1-3: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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 C<sub>31</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub> [M+H]<sup>+</sup> 895.7934, found 895.7937.

**[00273]** Compound 1-4: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 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 C<sub>30</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub> [M+H]<sup>+</sup> 1148.0751, found 1148.0615.

MHz, CDCl<sub>3</sub>) δ 4.08–4.13 (m, 3H), 3.93–3.95 (m, 3H), 3.84–3.87 (m, 3H), 2.33–2.45 (m, 12H), 2.24 (s, 9H), 1.26–1.33 (m, 12H), 1.39–1.41 (m, 12H). HRMS (ESI) calcd for C<sub>30</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub> [M+H]<sup>+</sup>

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# 讓結構繪圖更省時



# 如何加速SciFinder 查詢流程

ChemBioDraw Ultra 14 提供了一個SciFinder按鈕，讓使用者要查詢SciFinder變的更加快速方便。

The screenshot shows the ChemBioDraw Ultra 14 interface. A chemical structure of a substituted indole is highlighted with a blue box and labeled '1 選定結構' (Select structure). A red arrow points to the SciFinder button in the top toolbar, labeled '2'. Below the main window, the 'Search SciFinder' dialog box is open, showing search options for 'Substance Search' (Substructure, Exact Structure) and 'Reaction Search (Substructure)' (Selected Structure(s) are Products, Selected Structure(s) are Reactants). The 'Selected Structure(s) are Reactants' option is selected and circled in red, labeled '3'. The dialog box also includes a 'Proxy Settings...' button and 'OK' and 'Cancel' buttons.

The screenshot shows the SciFinder REACTIONS search results page. The 'Analyze' tab is active, displaying a list of reagents and their counts: BuLi (1379), K<sub>2</sub>CO<sub>3</sub> (1192), PPh<sub>3</sub> (1189), H<sub>2</sub>O (1184), P(OEt)<sub>3</sub> (1130), NaOBr-t (822), H<sub>2</sub>SO<sub>4</sub> (735), I<sub>2</sub> (676), Me<sub>2</sub>SiC (648), and S64483-19-B (642). The 'Refine' tab is also visible. The main content area shows a reaction scheme with a yield of 65% and a reference: '1.1 R:P(OEt)<sub>3</sub>, overnight, reflux'. The 'Notes' section contains: 'Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1'. The 'References' section lists: 'Metal complexes, methods, and uses thereof', 'Quick View PatentPak™', 'By Li, Jian and Turner, Eric', and 'From PCT Int. Appl., 2014109814, 17 Jul 2014'.

直接導向SciFinder檢索頁面

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The screenshot shows the iGroup website homepage. At the top left is the iGroup logo with the text 'iGroup 智泉國際事業'. To the right of the logo is a navigation bar with links: '研究員入口', '電子報', '客服中心', '網站地圖', 'iGroup TW 粉絲團', and 'CAS 粉絲團'. The 'CAS 粉絲團' link is circled in red. Below the navigation bar is a search bar with the text '在此搜尋 ...'. A secondary navigation bar contains links: '首頁', '關於我們', '服務對象', '產品', '資料下載', '常見問題', and '新聞中心'. Below this is a row of links: 'CAS 專頁', 'Submit 專頁', 'iG Publishing 專頁', and '\*TAEBDC 推薦專區'. The 'CAS 專頁' link is circled in red. The main content area features a section titled '匯聚全球資訊' with a circular graphic divided into four segments: '多元服務', '豐富資源', '專業分析', and '全方位主題'. Below this graphic is a blue button labeled '開始了解'. To the right is a large red banner for the Chinese New Year (Year of the Monkey) with the text 'iGroup Wishing You 2016 元宵快樂 猴賽雷' and the iGroup Taiwan logo.

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