



**SciFinder**<sup>®</sup>  
**Part of the process.**<sup>™</sup>

# CAS / SciFinder Web Basic Training

2009.10



*A division of the American Chemical Society*  
[www.cas.org](http://www.cas.org)

# 內容綱要

- SciFinder Web新介面介紹
- 文獻檢索(Explore Reference)
- 物質檢索(Explore Substance)
- 反應檢索(Explore Reaction)

# SciFinder Web網址 <https://scifinder.cas.org>

-https 連線透過 “[port 443](#)”; IP: [134.243.5.42](#)

-Windows / Mac : [IE, FireFox, Safari, Chrome](#)

-Java Runtime Environment ([JRE 6.x](#)) ; Java Plug-In



<https://scifinder.cas.org/>

## Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

## What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

## Welcome to SciFinder

**NEW!** The new web version of SciFinder makes access to SciFinder even more essential to your scientists research process. Some of the **new features** include:

- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Visit [www.cas.org](http://www.cas.org) for more information about the latest release.

## CAS - Science Connections

The CAS - Science Connections series showcases the value of CAS databases in light of important general-interest, science, and technology news and highlights CAS database enhancements and editorial milestones.

From CAS - Science Connections articles, you can link directly to Substance Details and Reference Details in the web version of SciFinder.

To read the latest article on *Charles Darwin and radiometric*

請尊重智財權及著作權，  
勿違法使用及大量下載~



Welcome Coach Hsu | Sign Out

## License Agreement

As a SciFinder Authorized User, I acknowledge the following:

I have been assigned a unique loginid/password and will not share my loginid/password with any other person.

I will search only for myself and not for others or other organizations.


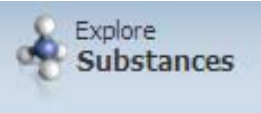

I will not use any automated program or script for extracting and downloading CAS data, or any other systematic retrieval of data.

I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.

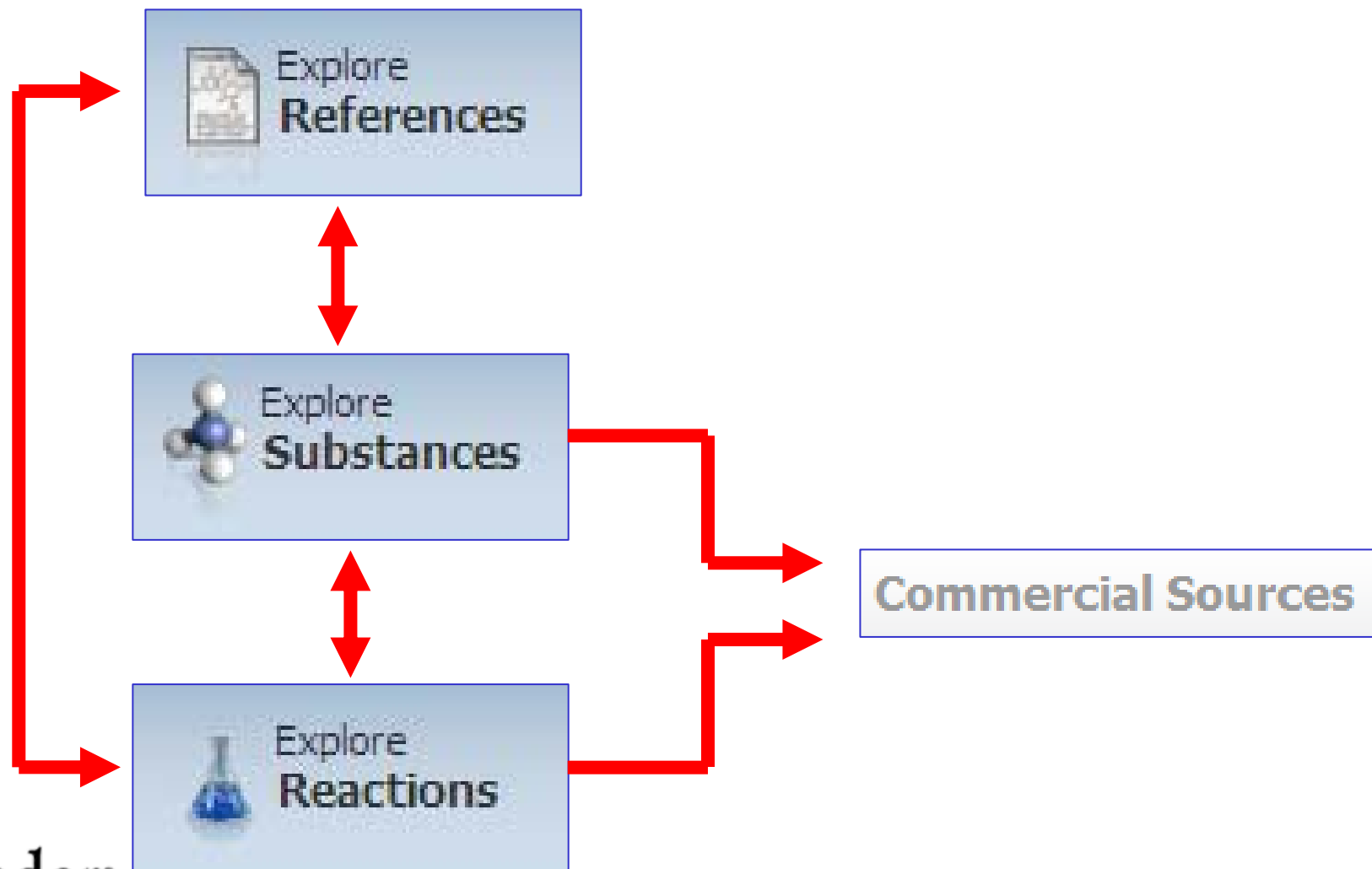
My company's SciFinder License and the [CAS Information Use Policies](#) apply to my use of SciFinder.

I will contact my SciFinder Key Contact if I have any questions.

# 輕鬆選擇從何種角度出發進行檢索

Type of information	Content and coverage	Starting points for locating chemical synthesis information
	<ul style="list-style-type: none"> <li>• &gt;31 million references from <b>59 patent authorities</b> worldwide and <b>&gt;10,000</b> major scientific journals</li> <li>• &gt;18 million references from MEDLINE®</li> <li>• <b>1907</b> to present, plus selected pre-1907 articles and patents</li> </ul>	<ul style="list-style-type: none"> <li>• Research topic</li> </ul>
	<ul style="list-style-type: none"> <li>• &gt;50 million organic and inorganic substances</li> <li>• &gt;61 million sequences</li> <li>• <b>&gt;1.9 billion</b> predicted and experimental properties, spectra, and data tags, plus</li> <li>• <b>&gt;23.8 million proton NMR spectra</b> 1957 to present, plus selected substances back to the early 1900s</li> <li>• Commercial source information <b>from &gt;900 suppliers</b> for &gt;26 million substances</li> <li>• Regulatory information for more than 245,000 substances</li> </ul>	<ul style="list-style-type: none"> <li>• Chemical name or CAS Registry Number®</li> <li>• Molecular formula</li> <li>• Chemical structure drawing</li> </ul>
	<ul style="list-style-type: none"> <li>• <b>&gt;29 million</b> preparations, including</li> <li>• <b>&gt;18 million</b> single- and multi-step reactions</li> <li>• <b>1840 to present</b></li> </ul>	<ul style="list-style-type: none"> <li>• Reaction structure drawing</li> <li>• Functional group transformation</li> </ul>

自由地想像，在不同類型資料中恣意轉換與串連，獲得最精準與最廣泛的訊息！！



# 透過SciFinder可以在6個資料庫進行整合查詢，其中包含CAS 最重要的5個化學資料庫!!

CAplus <sup>SM</sup>	CAS REGISTRY <sup>SM</sup>	CASREACT <sup>®</sup>	CHEMCATS <sup>®</sup>	CHEMLIST <sup>®</sup>
<ul style="list-style-type: none"> <li>• &gt;31M bibliographic records</li> <li>• &gt;10K journals covered</li> <li>• Patents from 59 patent offices</li> <li>• Updated daily (~3K daily)</li> <li>• Links to almost 400 publishers and 5 patent offices</li> <li>• Literature back to early 1800s</li> <li>• Cited articles from 1997 onward</li> </ul>	<ul style="list-style-type: none"> <li>• &gt;50M small molecules</li> <li>• &gt;61M sequences</li> <li>• Updated daily (&gt;12K daily)</li> <li>• Substances reported comprehensively in literature back to 1957</li> <li>• Includes nomenclature, spectra, and properties (experimental and predicted)</li> </ul>	<ul style="list-style-type: none"> <li>• &gt;18M single and multi-step reactions</li> <li>• Extracted from patents and journal articles</li> <li>• Updated weekly (~30K weekly)</li> <li>• Reactions back to 1840</li> <li>• Reaction conditions starting in 2003</li> </ul>	<ul style="list-style-type: none"> <li>• &gt;24M commercially available compounds</li> <li>• &gt;900 suppliers</li> <li>• &gt;1000 chemical catalogs</li> <li>• Updated when new or revised catalogs are available</li> <li>• Contact/ordering information including quantity and pricing (when available)</li> </ul>	<ul style="list-style-type: none"> <li>• &gt;248K inventoried / regulated substances</li> <li>• &gt;100 inventories &amp; regulated lists from 1979 to present</li> <li>• Updated weekly (~50 additions)</li> <li>• Contains regulatory requirements for substances</li> </ul>

以及NLM製作的MEDLINE<sup>®</sup>資料庫，可  
檢索生物醫學相關領域的文獻！

### MEDLINE<sup>®</sup>

- >18M bibliographic records
- 4,800 biomedical journals
- Updated 5 times per week
- 1950 -1966 from OLDMEDLINE database

更多資訊，請  
上網..

<http://www.cas.org/expertise/cascontent/caplus/patcoverage/worldcov.html>  
<http://www.cas.org/expertise/cascontent/caplus/corejournals.html>  
<http://www.cas.org/expertise/cascontent/ataglance/index.html>  
<http://www.cas.org/cgi-bin/cas/regreport.pl>



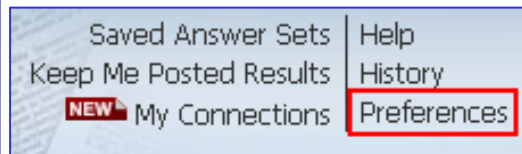
# SciFinder Web新介面介紹:

全新介面，加強個人化功能(KMP)與直覺式檢索頁面.....

The screenshot shows the SciFinder Web interface with several key features highlighted:

- Top Navigation:** "Explore References", "Explore Substances", and "Explore Reactions" buttons are highlighted in a red box.
- User Profile:** "Coach Hsu" and "Sign Out" links are highlighted in a red box. A yellow callout box below them says "註冊名字/登出鍵".
- Search Area:** A search bar with a "Search" button is highlighted in a red box. A yellow callout box below it says "檢索資料型態選擇區，可選擇找文獻、物質、反應".
- Saved Answer Sets:** A sidebar on the right shows a list of saved sets (e.g., nctu160, 1007, 1007-2) and an "Import" button, both highlighted in red boxes. A yellow callout box points to this area, stating "基本設定與存檔管理區，可對儲存之Answer Sets或KMP進行管理。另有Help、檢索歷史查詢".
- Filtering Options:** The "Publication Year(s)", "Document Type(s)", and "Language(s)" sections are highlighted in red boxes. A yellow callout box points to the "Import" button, stating "Answer Sets,紀錄最新10筆存檔紀錄。" and "Import,可自電腦輸入'.akx'檔案。".
- Personalized Features:** The "Keep Me Posted Results" and "My Connections" sections are highlighted in red boxes. A yellow callout box points to these sections, stating "KMP,呈現有無更新文章的狀況。" and "My Connection,呈現社群connection的狀況。".

Preferences: 可設定常用的檢索方式為歡迎頁面，以及KMP的通知功能~



## Preferences

### Starting Page

Select the default starting page

- Explore References
- Explore Substances
- Explore Reactions

可依自己最常使用的檢索方式(文獻、物質或反應)設定為登入歡迎頁面!

### Keep Me Posted Notification

- Receive e-mail notification of Keep Me Posted results

KMP通知功能，預設值為勾選。

The e-mail address can be specified or changed using myCAS.

OK

Cancel

Help: 可幫助您更容易了解SF Web的使用方式，任何時間點選  亦可連結至說明頁面~

Saved Answer Sets	<b>Help</b>
Keep Me Posted Results	History
<b>NEW</b> My Connections	Preferences



Contents | Index | Search

- SciFinder Overview
- INTRODUCTION
- EXPLORE TASKS
- USING ANSWER SETS
- COLLABORATION
- KEEP ME POSTED
- LINK RESOURCES
- HISTORY
- OBTAINING DOCUMENTS
- PREFERENCES
- MISCELLANEOUS



## SciFinder Overview

### What's New

The latest browser-based SciFinder® provides many new capabilities.

### Reactions

- [Solvent limiter](#) for a reaction search
- Search for [similar reactions](#)
- Reaction search results [sorted](#) by product yield, number of steps, or publication date

### Substances

- Refine a substance result answer set by [property values](#)
- [Export](#) substance property values to data table
- ACD predicted [carbon-13 Nuclear Magnetic Resonance \(NMR\)](#) spectra data

### Collaboration

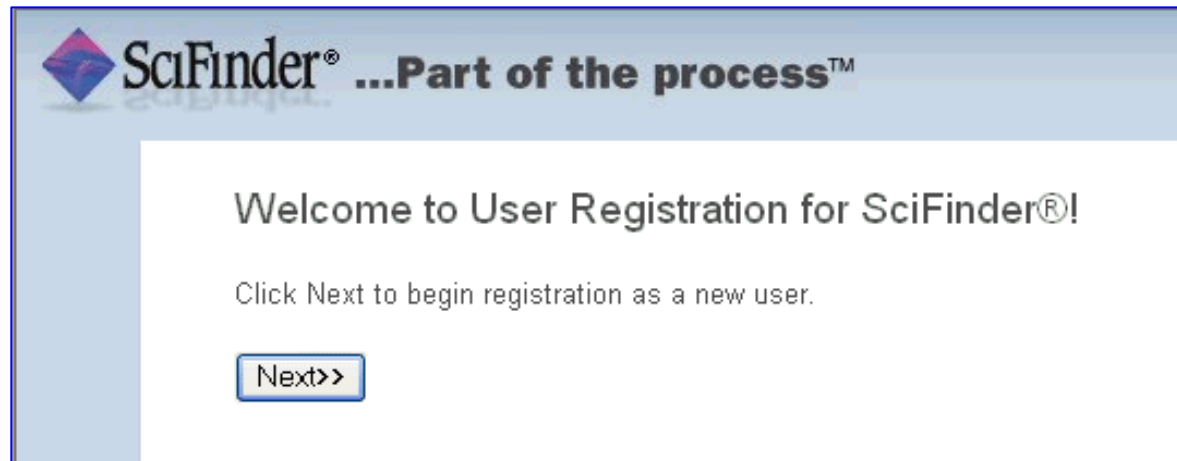
- [Collaborate](#) with colleagues at your research site using My Connections
- [Tags](#) for grouping references and sharing them with colleagues at your research site
- [Commenting](#) for references and for sharing with colleagues at your research site

### Usability Enhancements

- Specify a search type for [reaction](#) and [substance](#) explore pages
- [Search short cut](#) from substance and reaction search results
- One step [transfer of queries](#) between structure and reaction explores
- [Linked CPlus roles](#) to explore references from substances
- CAS Structure Drawing window [resize](#)
- [Page view preferences](#)
- Reference results [viewing options](#)
- Substance results [columns per page options](#)
- Reaction results [viewing options](#)
- Links from [ACS](#) articles to SciFinder substances and reactions search
- Combine [Keep Me Posted](#) results
- [Task Billing](#)

# 立即申請 !!

- 請向學校圖書館洽詢SciFinder Web 註冊URL，點選後進入註冊畫面..



# 忘記密碼時...



## Sign In

Username

Password

Remember my username

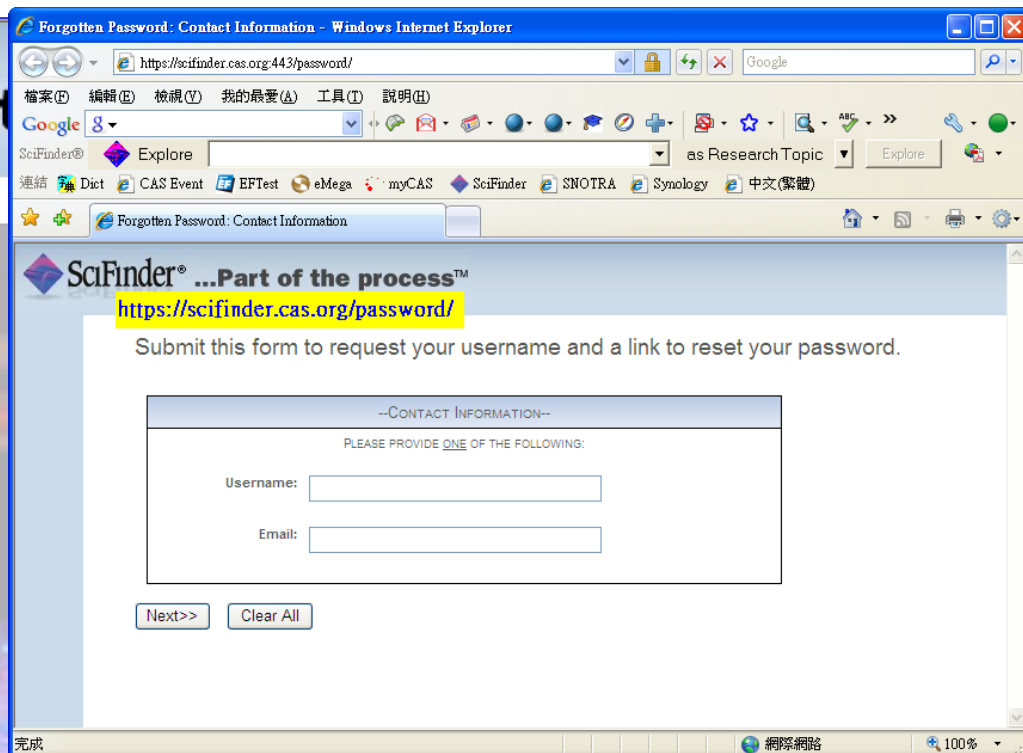
**Forgot Username or Password?**

**Sign In**

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

## What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!



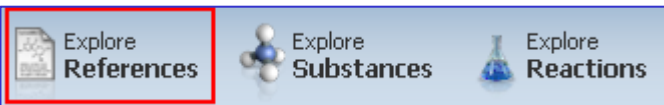
and technology news and highlights CAS database enhancements and editorial milestones.

From CAS - Science Connections articles, you can link directly to Substance Details and Reference Details in the web version of SciFinder.

To read the latest article on [cherry blossoms](#), visit [CAS](#)

# 文獻檢索:

有多種方式查詢文獻，如主題、作者名、公司名...等!!下方並有限制條件區可供設定。



Explore References

Research Topic  Search

Examples:  
*The effect of antibiotic residues on dairy products*  
*Photocyanation of aromatic compounds*

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags **NEW**

Publication Year(s)   
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Language(s)

<input type="checkbox"/> Chinese	<input type="checkbox"/> German	<input type="checkbox"/> Polish
<input type="checkbox"/> English	<input type="checkbox"/> Italian	<input type="checkbox"/> Russian

有多種檢索方式查詢文獻，如主題、作者名、單位名...在上方輸入檢索提問，下方有限制條件區可供選擇。

文獻檢索結果在上方有快速反查區，以及單筆文獻的相關聯結，並可調整結果呈現方式。右方則是自動分析作者名稱與篩選功能。

### Research Topic Candidates

### References

- 223 references were found containing "nano technology" as entered. 223
- 711654 references were found containing the concept "nano technology". ← 選擇包含"觀念"的結果，可完整撈取相關文獻。 711654

Get References



Create Keep Me Posted | Research Topic **nano technology** > references (711654)

References **Get Substances** **Get Reactions** **Get Cited** **Get Citing**

711654 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | **Add Tags**

上方：快速文獻反查區，可反查相關物質、反應、引用及被引用情形。並可設定標籤(Tags)重新定義。  
下方：單筆文獻相關聯結，如反查物質、反應、被引用、全文、評語及標籤等。

自動完成分析(預設值為Author Name)，並有其他11項分析功能與篩選(Refine)功能。

Answers per Page [20] | 1 2 3 4 5 6 ... 35583 | Save | Print | Export | View: [List Icon]

檢索結果呈現方式，可選擇每頁筆數以及是否要完整呈現摘要。另有儲存、列印、輸出等選項。

From Chemistry & Industry (London, United Kingdom) (2009), (18), 9. Language: English, Database: CAPLUS

**+**Substances **▲**Reactions **📄**Citing **📄**Full Text **🔗**Link **💬**0 Comments **🏷️**0 Tags

2. **Interaction between water-soluble hydroxylated single-wall carbon nanotubes and human serum albumin**  
By Liu, Shu-Fang; Yin, Jun-Fa; Song, Mao-Yong; Wang, Hai-Lin  
From Gaodeng Xuexiao Huaxue Xuebao (2009), 30(9), 1733-1738. Language: Chinese, Database: CAPLUS

The interaction between water-sol. hydroxylated single-wall carbon **nanotube** and human serum albumin and other related effects were investigated using fluorescence spectroscopy, absorption spectroscopy, synchronous fluorescence spectroscopy and transmission electron microscopy (TEM) methods. Fluorescence quenching of human serum albumin by a hydroxylated single-wall carbon **nanotube** was obsd., indicating the interaction between them occurs. TEM images show the hydroxylated carbon **nanotubes** system can be stabilized and dispersed by the absorption of human serum albumin on the surface of the hyd...

**+**Substances **▲**Reactions **📄**Citing **📄**Full Text **🔗**Link **💬**0 Comments **🏷️**0 Tags

**Analysis** | Refine

Sample Analysis

Author Name

Biswas Pratim

Iijima Sumio

Laudon Matthew

Yudasaka Masako

Ajayan Pulickel M

Bando Yoshio

Chen George Z

感興趣(或最終篩選得到)的文章，可透過"Link"功能快速複製一串URL(物質/反應檢索亦同)，此URL可分享給他人。只要登入SF Web並貼上此URL即可快速獲得此篇文獻，減少重複查詢的工作。

Select All Deselect All | Sort by: Accession Number | Answers per Page

1. **Energy flow, thermoelectricity and Fourier's law at the nanoscale**  
By Dubi, Yonatan; Di Ventra, Massimiliano  
From arXiv.org, e-Print Archive, Condensed Matter (2009), 1-29, arXiv:0910.0425v1 [cond-mat.mes-hall]. Language: English, Database: CAPLUS  
Advances in the fabrication and characterization of **nanoscale** systems now allow for a deeper understanding of one of the most technol.: the flow of energy at the microscopic level. This knowledge is also likely to impact our ability to build more efficient de storage and conversion. In this Colloquium we survey recent advances and present understanding of phys. mechanis **nanostructures**. We examine basic issues such as thermoelectricity, local temp. and heating, and the relation between energy c.d

+Substances ▲Reactions 📄Citing 📄Full Text **🔗Link** 💬0 Comments 🏷️0 Tags

2. **Damping of a nanomechanical oscillator str**  
By Bennett, Steven D.; Cockins, Lynda; Miyahara, Yoichi; Gr  
From arXiv.org, e-Print Archive, Condensed Matter (2009), 1  
We present theor. and exptl. results on the mec  
the cantilever oscillation amplitude is large, its n  
of the cantilever. We observe highly asym. lineshapes or Coulomb blockade peaks in the damping that reflect the degeneracy of  
excellent agreement with our strong coupling theory. Furthermore, we predict that excited state spectroscopy is possible by s...

Copy and paste link for quick access to this reference.  
[https://scifinder.cas.org/scifinder/view/link\\_v1/reference.jsf?l=Br](https://scifinder.cas.org/scifinder/view/link_v1/reference.jsf?l=Br)  
Create a bookmark, save in a document, or e-mail to a colleague.



感興趣(或最終篩選得到)的文章，可增加 **Comments** 以及 **Tags**，可分享給 **"My Connection"** 設定的朋友。

- 1. **Energy flow, thermoelectricity and Fourier's law at the nanoscale**  
By Dubi, Yonatan; Di Ventra, Massimiliano  
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Advances in the fabrication and characterization of **nanoscale** systems now allow for a deeper understanding of the flow of energy at the microscopic level. This knowledge is also likely to impact our technology: the flow of energy at the microscopic level. This knowledge is also likely to impact our storage and conversion. In this Colloquium we survey recent advances and present understanding of **nanoscale** systems. We examine basic issues such as thermoelectricity, local temperature, and heating, and  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)
- 2. **Damping of a nanomechanical oscillator strongly coupled to a quantum dot**  
By Bennett, Steven D.; Cockins, Lynda; Miyahara, Yoichi; Grutter, Peter; Clerk, Aashish A.  
From arXiv.org, e-Print Archive, Condensed Matter (2009), 1-5, arXiv:0910.0308v1 [cond-mat.mes-hall]. Language: English  
We present theoretical and experimental results on the mechanical damping of an atomic force microscope cantilever system. When the cantilever oscillation amplitude is large, its motion dominates the charge dynamics of the dot with

**Comments** **BETA**

Energy flow, thermoelectricity and Fourier's law at the nanoscale

**0 Comments** Sort by: Newer First | Older First

No comments

**Add Comment:** Maximum of 1024 characters per comment; 50 comments per user.  
Reminder: Your comments and tags can be viewed by your connected colleagues.

this is a good reference !!

**Save**

**Edit Tags** **BETA**

Energy flow, thermoelectricity and Fourier's law at the nanoscale

**All Tags:** Click tag to add it to "My Tags"  
No tags available.

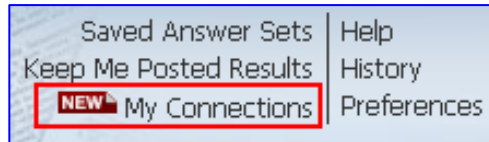
**My Tags:** Click 'x' to remove tag from "My Tags".  
You have not added any tags for this reference.

**Add Tags:** Separate multiple tags with semicolons, max. of 100 characters per tag, 50 tags max. per user.  
Reminder: Any colleague you connect with will be able to view your comments and tags.

for Nano Tech. Project

**Save** **Cancel**

My Connections:於同一訂購單位(學校)中，可設定多組社群連結，  
設為連結的人員可互相查看”Comments”以及”Tags”資料。



My Connections **BETA** **+ Invite Colleagues To Connect**

**Connections** | **Invitations**

2 Connections | 0 Selected | Remove

My Connections allows you to share comments and tags with these colleagues

**Connected Colleagues**

- Chang, Joey
- Hsu, Coach

**Invite Colleagues To Connect**

Enter the full or partial name of a colleague **within your organization** \* Required

Last Name: \*  First Name:

1 Colleagues | 0 Selected

Colleagues	E-mail	Profile
<input type="checkbox"/> Chang, Joey	joey.chang@igrouptaiwan.com	Taiwan Online Plus Inc <b>Connected</b>

Tags:於文獻檢索區中可點選Tags查看自己與連結人員所設定的資料，以加速文獻分享與團隊合作研究。

Explore References

Research Topic  
Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
**Tags** NEW

Tags are shared between you and your connected colleagues. Click a tag to retrieve references associated with that tag. **BETA**

0 - 9 (and Special Characters)

- 123

A

- a plan

C

- cyut1013

F

- for tmu
- friends

H

- h1n1 of vaccine in mr. k

I

- ipamacase\_cyyc substance get related references on...

N

- nctu160

S

- sweet potato



文獻結果可進行”Save”(Answer Set)、“Print”、“Export”等動作。Export可輸出成多種格式，如akx, pdf, rtf, txt等。”Save”與”Export”皆有最大存檔/輸出筆數限制。

The screenshot displays the SciFinder interface. At the top, there are navigation buttons: "Get Reactions", "Get Cited", and "Get Citing". Below these are action buttons: "Keep Selected", "Remove Selected", "Remove Duplicates", and "Add Tags". On the right side of the top bar, there are buttons for "Save", "Print", and "Export", which are highlighted with a red box. A red arrow points from this box to the "Export" button in the dialog box below.

The "Export" dialog box is open, showing a warning message: "Only 20,000 answers from a single answer set can be exported in .akx file format. The most recent 20,000 answers will be exported." Below the warning, there are radio buttons for "All answers" (selected) and "Only selected answers". There is a "File Name:" field and a "File Type:" dropdown menu. The dropdown menu is open, showing several options: "Answer Key eXchange (\*.akx)", "Portable Document Format (\*.pdf)", "Rich Text Format (\*.rtf)", "Answer Keys (\*.txt)", "Quoted Format (\*.txt)", and "Tagged Format (\*.txt)". The "Answer Key eXchange (\*.akx)" option is highlighted with a blue bar and a red box. At the bottom of the dialog box, there are "Export" and "Cancel" buttons.

The background shows the main results page with a table of results. The table has columns for "Answers per Page [50]" and "1 2 3 4 5 6 ... 14259". The first row of the table contains text: "6%-20%, potassium dihydrogen phosphate 15%- 25%, conditioning agent can rapidly supplement Ca and Mg lost". The second row contains text: "arid red soil". The third row contains text: "carbonate 20-30, potassium dihydrogen phosphate 10- oil microorganism amt. and enzymic activity, improving".

文獻結果可以不同形式排序，  
如登錄號、作者名、發表年  
份、標題等

References Get Substances Get Reactions Get Cited Get Citing

12943 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [50] 1 2 3 4 5 6 ... 259 View:

1. **Optimal degradation of *rhodamine B* by ultrasound/Fenton method in the presence of nanoscale iron**  
By Hsieh, Ling-Ling; Kang, Hui-De; Chen, Chen-Yu  
From Water Science and Technology (2009), 60(5), 1295-1301. Language: English, Database: CAPLUS

An advanced ultrasound/Fenton/nanoscale iron oxidn. process was applied for treatment of dye wastewater. In this study, the Taguchi statistical method was used to design expts. for the optimization of the ultrasound/Fenton/nanoscale iron process. The exptl. design consisted of testing five factors (dosage of H2O2, concn. of Fe2+, amt. of nanoscale iron added, treatment time, and initial pH), with four levels of each factor tested. COD (COD) measurements were conducted to det. the efficiency of the water samples. An anal. of the mean sign-to-noise (S/N) ratio indicated that the optimum comb...

Substances Reactions Citing Full Text Link 0 Comments 0 Tags

2. **Zinc-doping in TiO2 films to enhance electron transport in dye-sensitized solar cells under low-intensity illumination**  
By Wang, Kai-Ping; Teng, Hshiheng  
From Physical Chemistry Chemical Physics (2009), 11(41), 9489-9496. Language: English, Database: CAPLUS

A nanocryst. TiO2 film with highly dispersed Zn-doping shows its capability for efficient electron transport in dye-sensitized solar cells (DSSCs). The Zn-doping is conducted via Zn2+ introduction into a layered titanate followed by hydrothermal treatment and calcination. The Zn-doped films exhibit an elevated electron Fermi level, which may enhance band bending to lower the d. of empty trap states. Because of this Zn-doping, the consequent DSSCs can alleviate the decay of light-to-elec. energy conversion efficiency due to light intensity redn. Intensity-modulated spectroscopic anal. revea...

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分析欄位增加“**CA Concept Heading**”，可更清楚了解文獻檢索結果中包含的“**重要觀念**”。點選“**Full Analysis**”可秀出每個分析選項的筆數，也可點選“**more**”做完整的分析查看。

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Sample Analysis ⓘ

- CA Concept Heading
- Author Name
- CAS Registry Number
- CA Section Title
- Company/Organization
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- Document Type
- Index Term
- CA Concept Heading
- Journal Name
- Language
- Publication Year
- Supplementary Terms

Nanostructures

Electroluminescent devices

Films

Catalysts

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CA Concept Heading

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Nanoparticles	472
Nanotubes	372
Metals	137
Coating process	135
Vapor deposition process	123
Semiconductor device fabrication	111
Coating materials	107
Nanostructures	106
Electroluminescent devices	105
Field emission displays	98

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<input type="checkbox"/> Nanotubes	372
<input type="checkbox"/> Metals	137
<input type="checkbox"/> Coating process	135
<input type="checkbox"/> Vapor deposition process	123
<input type="checkbox"/> Semiconductor device fabrication	111
<input type="checkbox"/> Coating materials	107
<input type="checkbox"/> Nanostructures	106
<input type="checkbox"/> Electroluminescent devices	105
<input type="checkbox"/> Field emission displays	98

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點選感興趣的分析項目(ex. Nanocomposites)，結果會先以黃色區塊表示，並在其他分析項目中以黃色表示重複文章所佔比例。若此分析結果為所需，則點選”keep analysis”!!

References

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12943 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

904 references with CA Concept Heading **Nanocomposites** are displayed Keep Analysis Clear Analysis

Select All Deselect All Sort by: Accession Number Answers per Page [50] 1 2 3 4 5 6 ... 19 View: [icon]

88. **Biomimetic Synthesis of Nacrelike Faceted Mesocrystals of ZnO-Gelatin Composite**  
By Tseng, Yao-Hung; Lin, Hsia-Yu; Liu, Ming-Han; Chen, Yang-Fang; Mou, Chung-Yuan  
From Journal of Physical Chemistry C (2009), 113(42), 18053-18061. Language: English, Database: CAPLUS  
A fabrication of ZnO hierarchical mesocrystal was achieved by a biomimetic method using gelatin as structure-directing agent. It was found that the ZnO-gelatin microcrystal with well-defined hexagonal twin plate shape is built by the stacking of **nanoplates**. The irregularly edged **nanoplates** can adjust themselves to each other throughout the microcrystal, resulting in a roughly hexagonal edge. Selected area electron diffraction (SAED) anal. of the ZnO-gelatin microcrystal demonstrates that all the stacked **nanoplates** are aligned and oriented to form a single-crystal structure with hexagonal sy...  
Substances Reactions Citing Full Text Link 0 Comments 1 Tag

159. **Modulation and Improvement on Separation of Photoinduced Charge Carriers in CdS-Metal Nanoheterostructures**  
By Cheng, Wei-Yun; Chen, Wei-Ta; Hsu, Yung-Jung; Lu, Shih-Yuan  
From Journal of Physical Chemistry C (2009), 113(40), 17342-17346. Language: English, Database: CAPLUS  
We demonstrate the feasibility of modulating and improving the sepr. of photoinduced charge carriers of CdS-M **nanoheterostructures** through partial replacement of S with two group 16 elements of larger at. size, Se and Te. With the incorporation of Se or Te into the CdS **nanowires** (NWs), the defect states of the CdS NWs were effectively passivated, enabling a fuller extent of participation of the photoinduced electrons in the charge sepr. process, thus resulting in a more pronounced photoluminescence quenching and photocurrent depression for the CdS<sub>1-x</sub>Sex and CdS<sub>1-x</sub>Tex NWs. The present study p...  
Substances Reactions Citing Full Text Link 0 Comments 0 Tags

293. **Dynamic mechanical study of clay dispersion in maleated polypropylene/organoclay nanocomposites**  
By Wang, Yeh; Huang, Syh-W.; Guo, Jiang-Y.  
From Polymer Composites (2009), 30(9), 1218-1225. Language: English, Database: CAPLUS  
Morphol. characteristics and the dynamic mech. properties of maleic anhydride grafted polypropylene (PPGMA) and its clay-filled **nanocomposites** with different degrees of clay exfoliation have been investigated. Fully and partially exfoliated samples were prepd. through powered sonication and melt blending, resp. Our results indicated that both mech.  $\alpha$  and  $\beta$  relaxations can be identified. The glass ( $\beta$ ) transition of the **nanocomposites** shifted to slightly lower temps. for nearly all formulations because of reduced chain cooperative motion. However, the broad  $\alpha$  transition became more distinct ...

Analysis Refine

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Nanoparticles	2443
Nanotubes	1471
Nanostructures	1067
<b>Nanocomposites</b>	<b>904</b>
Microstructure	886
Surface structure	739
Particle size	686
Vapor deposition process	667
Luminescence	605
Nanowires	605

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Select All Deselect All | Sort by: Accession Number | Answers per Page [50] 1 2 3 4 5 6 ... 19 | View: [icon]

1. **Biomimetic Synthesis of Nacrelike Faceted Mesocrystals of ZnO-Gelatin Composite**  
By Tseng, Yao-Hung; Lin, Hsia-Yu; Liu, Ming-Han; Chen, Yang-Fang; Mou, Chung-Yuan  
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2. **Modulation and Improvement on Separation of Photoinduced Charge Carriers in CdS-Metal Nanoheterostructures**  
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 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

3. **Dynamic mechanical study of clay dispersion in maleated polypropylene/organoclay nanocomposites**  
By Wang, Yeh; Huang, Syh-W.; Guo, Jiang-Y.  
From Polymer Composites (2009), 30(9), 1218-1225. Language: English, Database: CAPLUS

**Analysis** Refine

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Nanocomposites	904
Polymer morphology	249
Nanoparticles	167
Thermal stability	165
Glass transition temperature	129
Microstructure	114
Nanotubes	103



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Select All Deselect All Sort by: Accession Number Answers per Page [50] 1 2 3 4 5 6 ... 19 View: [icon]

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- 2. Modulation and Improvement on Separation of Photoinduced Charge Carriers in CdS-Metal Nanoheterostructures**  
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Nanocomposites	904
Polymer morphology	249
Nanoparticles	167
Thermal stability	165
Glass transition temperature	129
Microstructure	114
Nanotubes	103
Tensile strength	97
Young's modulus	93

分類(Categorize)，位於分析欄位下方，點選後會出現大型對話框，選擇每一階層感興趣的欄位，點選"Refine"即可進行分類!!

Nanocomposites	904
Polymer morphology	249
Nanoparticles	167
Thermal stability	165
Glass transition temperature	129
Microstructure	114
Nanotubes	103
Tensile strength	97
Young's modulus	93
Storage modulus	83

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1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Proteins & peptides (45)	<b>Select All</b> <b>Deselect All</b>	Click 'X' to remove the term or entire category from 'Selected Terms'
Technology	Miscellaneous substances (45)	<input checked="" type="checkbox"/> Transformation, genetic 2	<input checked="" type="checkbox"/> <b>Technology &gt; Ceramics(3)</b>
Physical chemistry	Nucleic acids (7)	<input checked="" type="checkbox"/> Chromosome 1	<input checked="" type="checkbox"/> Hybrid organic-inorganic materials
General chemistry	Genetics (4)	<input type="checkbox"/> PCR (polymerase chain reaction) 1	<input checked="" type="checkbox"/> Annealing
Polymer chemistry	Protein & peptide topics (2)	<input type="checkbox"/> Plasmids 1	<input checked="" type="checkbox"/> Sintering
Synthetic chemistry			<input checked="" type="checkbox"/> <b>Catalysis &gt; Catalysis(2)</b>
Environmental chemistry			<input checked="" type="checkbox"/> Catalysts
Catalysis			<input checked="" type="checkbox"/> Photolysis catalysts
Genetics & protein chemistry			<input checked="" type="checkbox"/> <b>Genetics &amp; protein chemistry &gt; Genetics(2)</b>
Analytical chemistry			<input checked="" type="checkbox"/> Transformation, genetic
Biotechnology			<input checked="" type="checkbox"/> Chromosome
Biology			

Genetics & protein chemistry > Genetics > 2 Index Term(s) Selected

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## 2. Modulation and Improvement on Separation of Photoinduced Charge Carriers in CdS-Metal Nanoheterostructures

By: Cheng, Wei-Yun; Chen, Wei-Ta; Hsu, Yung-Jung; Lu, Shih-Yuan

We demonstrate the feasibility of modulating and improving the sepn. of photoinduced charge carriers of CdS-M nanoheterostructures through partial replacement of S with two group 16 elements of larger at. size, Se and Te. With the incorporation of Se or Te into the CdS nanowires (NWs), the defect states of the CdS NWs were effectively passivated, enabling a fuller extent of participation of the photoinduced electrons in the charge sepn. process, thus resulting in a more pronounced photoluminescence quenching and photocurrent depression for the CdS<sub>1-x</sub>Sex and CdS<sub>1-x</sub>Tex NWs. The present study provides a facile way of improving the photocatalytic efficiency of CdS through the improvement in retarding the recombination of photoinduced charge carriers.

### Indexing

Optical, Electron, and Mass Spectroscopy and Other Related Properties (Section 73-5)

Section cross-reference(s): 76, 74

### Concepts

Charge separation	Electric current-potential relationship
Exciton luminescence	Luminescence quenching
Nanocomposites	Nanoparticles
Nanowires	Passivation
Photocurrent	Photoelectrons
Photolysis catalysts	Suspensions

### Substances

1306-23-6P Cadmium sulfide (CdS)  
 107103-13-9P Cadmium selenide sulfide (CdSe<sub>0.1</sub>SO.<sub>9</sub>)  
 149293-62-9P Cadmium sulfide telluride (CdS<sub>0.95</sub>Te<sub>0.05</sub>)

modulation and sepn. of photoinduced charge carriers in CdS-metal nanoheterostructures

Catalyst use; Properties; Synthetic preparation; Technical or engineered

### Quick Links

0 Tags, 0 Comments

### Source

*Journal of Physical Chemistry C*  
 Volume 113  
 Issue 40  
 Pages 17342-17346  
 Journal  
 2009  
 CODEN: JPCCCK  
 ISSN: 1932-7447

### Company/Organization

Department of Chemical Engineering  
 National Tsing Hua University  
 Hsinchu, Taiwan 30013

### Accession Number

2009:1119730  
 CAPLUS

### Publisher

American Chemical Society

### Language

Concepts 區塊 提供超連結點選，方便研究人員 快速轉換 至相關主題!!

**Indexing**

Optical, Electron, and Mass Spectroscopy and Other Related Properties (Section 73-5) ⓘ


Section cross-reference(s): 76, 74

**Concepts** ⓘ

Charge separation	Electric current-potential relationship
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Nanowires	Passivation
Photocurrent	Photoelectrons
Photolysis catalysts	Suspensions

modulation and seprn. of photoinduced charge carriers in CdS-metal nanoheterostructures

Substances 區塊提供本文章中相關物質超連結點選，方便研究人員快速查看相關物質資訊，下方並有此物質在本文章中扮演的角色說明!!

**Substances** 

<a href="#">1306-23-6P</a> Cadmium sulfide (CdS) <a href="#">107103-13-9P</a> Cadmium selenide sulfide (CdSe <sub>0.15</sub> S <sub>0.9</sub> ) <a href="#">149293-62-9P</a> Cadmium sulfide telluride (CdS <sub>0.95</sub> Te <sub>0.05</sub> )
modulation and seprn. of photoinduced charge carriers in CdS-metal nanoheterostructures  Catalyst use; Properties; Synthetic preparation; Technical or engineered material use; Preparation; <b>Uses</b>
<a href="#">7440-22-4P</a> Silver <a href="#">7440-50-8P</a> Copper
modulation and seprn. of photoinduced charge carriers in CdS-metal nanoheterostructures  Physical, engineering or chemical process; Properties; Synthetic preparation; Technical or engineered material use; Preparation; Process; <b>Uses</b>
<a href="#">7447-39-4</a> Copper chloride (CuCl <sub>2</sub> ) <a href="#">7704-34-9</a> Sulfur <a href="#">7761-88-8</a> Silver nitrate <a href="#">7782-49-2</a> Selenium <a href="#">10325-94-7</a> <a href="#">13494-80-9</a> Tellurium
modulation and seprn. of photoinduced charge carriers in CdS-metal nanoheterostructures  Reactant; Reactant or reagent

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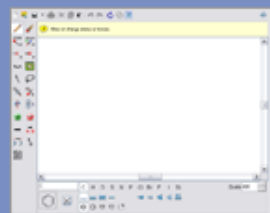
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Characteristic(s) ⓘ

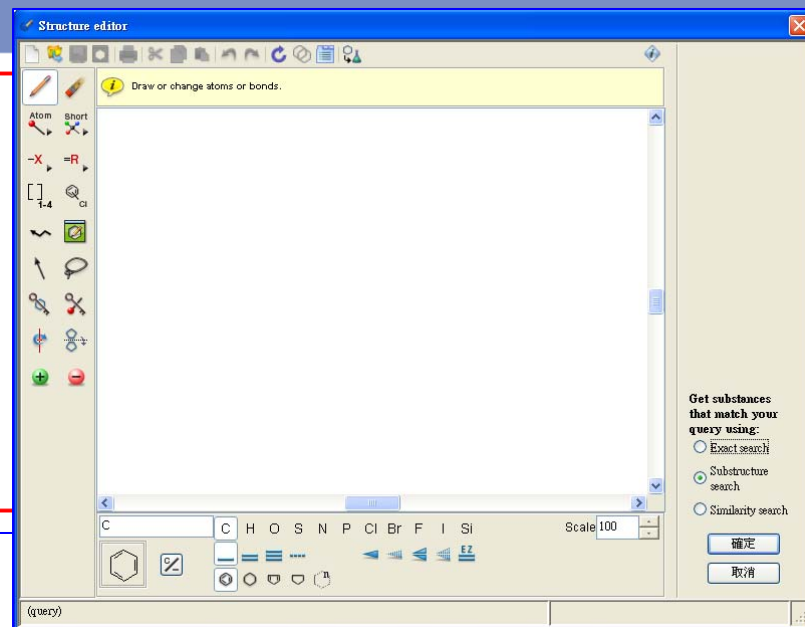
- Single component
- Commercially available
- Included in reference(s)

Class(es) ⓘ

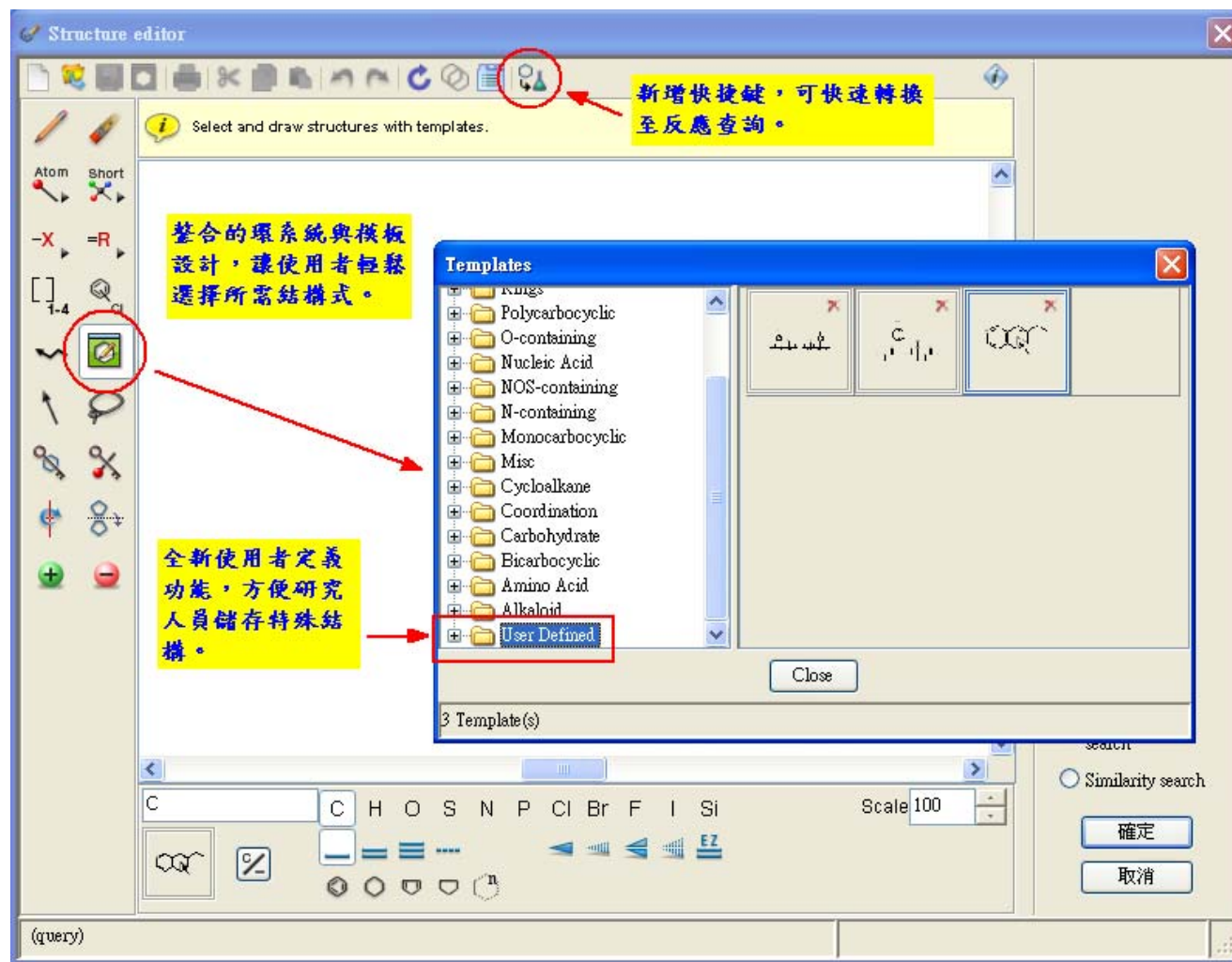
- Alloys
- Coordination compounds
- Incompletely defined

Studies ⓘ

- Analytical
- Biological



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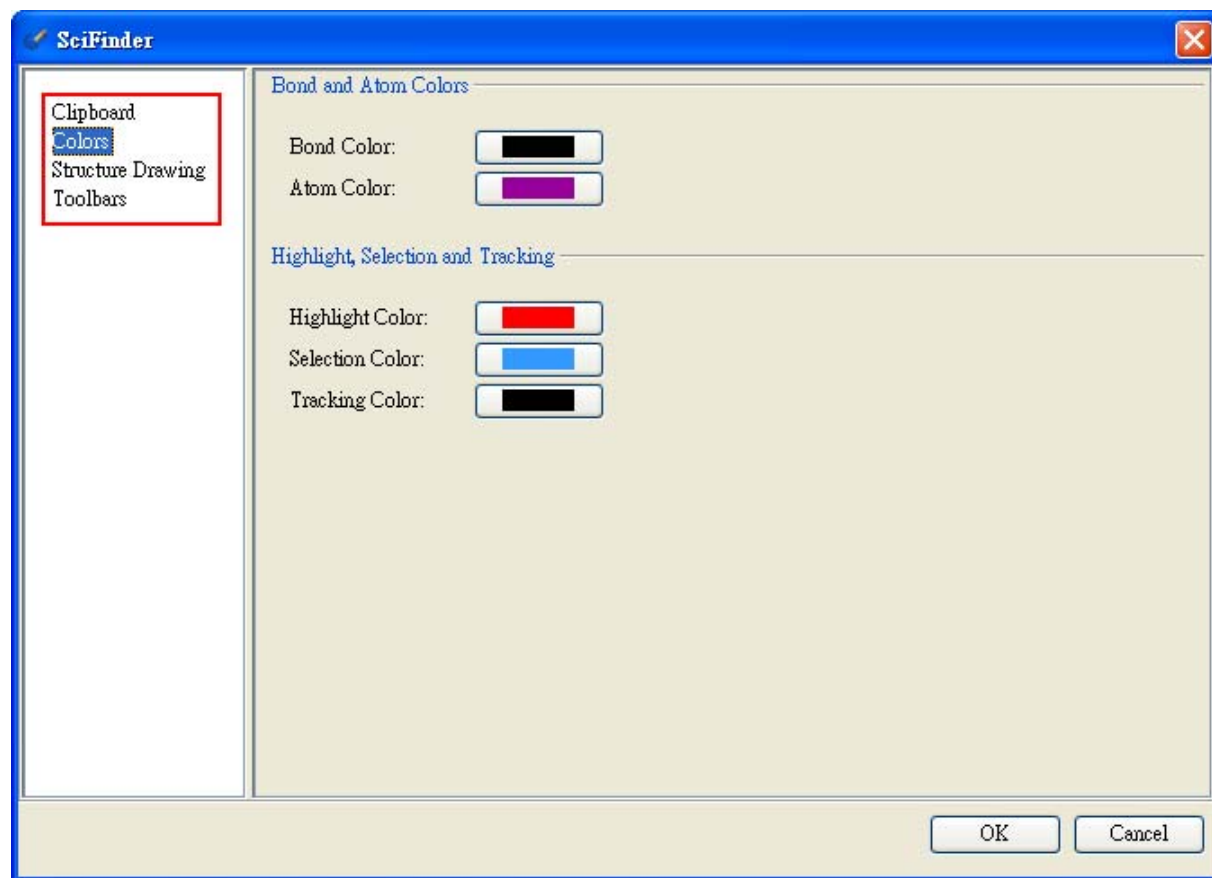


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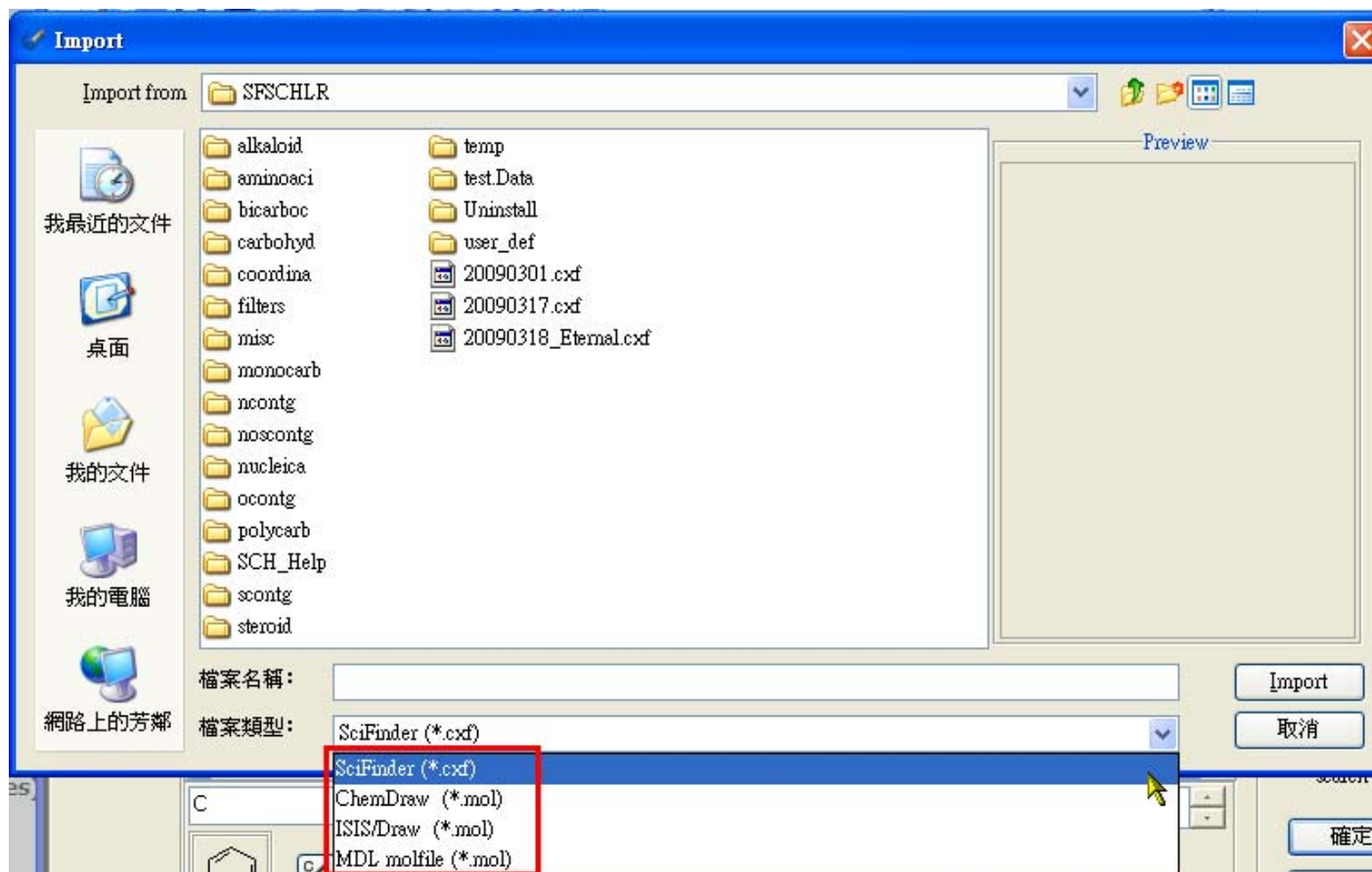
The screenshot displays the 'Structure editor' window. The central workspace shows a chemical structure of a benzothiazole derivative with an R<sub>1</sub> substituent. The left sidebar contains various drawing tools, with a search icon (magnifying glass) and a box containing '1-4' highlighted by a red arrow. A yellow text box points to this icon, stating: 'Repeating Tool及VAP功能，針對複雜結構式的查詢，或幫助設計開發新化合物。' The right sidebar features a section titled 'Get substances that match your query using:' with three radio button options: 'Exact search', 'Substructure search' (which is selected and highlighted by a red box and a red arrow), and 'Similarity search'. Below these options are '確定' (OK) and '取消' (Cancel) buttons. At the bottom of the window, there is a toolbar with element symbols (C, H, O, S, N, P, Cl, Br, F, I, Si) and a 'Scale' field set to 100. The status bar at the very bottom indicates 'Formula not available'.



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Substance Detail：更清楚易懂的排列方式，讓研究人員快速掌握物質的相關性質與連結相關資訊。

Substance Detail

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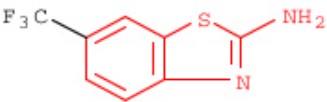
8151.

CAS Registry Number: 777-12-8

C<sub>8</sub> H<sub>5</sub> F<sub>3</sub> N<sub>2</sub> S

2-Benzothiazolamine, 6-(trifluoromethyl)-

Benzo[1,2-c]thiazole, 2-amino-6-(trifluoromethyl)- (6CI,7CI,8CI); 2-Amino-6-(trifluoromethyl)benzo[1,2-c]thiazole; 2-Amino-6-trifluoromethyl-1,3-benzothiazole; 6-(Trifluoromethyl)-1,3-benzothiazol-2-ylamine; 6-Trifluoromethylbenzo[1,2-c]thiazol-2-ylamine



~44 References

Document Types: Journal, Patent

CAplus Role	Patents	Nonpatents
Biological study	✓	✓
Preparation	✓	✓
Properties		✓
Reactant or reagent	✓	✓
Uses	✓	✓

Predicted Properties: Biological   Chemical   Density   Lipinski and Related   Spectra   Structure-related   Thermal

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(4)	
Bioconcentration Factor	1.78	pH 2 Temp: 25 °C	(4)	
Bioconcentration Factor	12.4	pH 3 Temp: 25 °C	(4)	

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Document Types: Conference, Diss Report

CAplus Role	Patents	Nonpatent		
Analytical study	✓	✓		
<b>Biological study</b>	✓	✓		
Combinatorial study	✓	✓		
Formation, nonpreparative	✓	✓	✓	
Miscellaneous			✓	
Occurrence		✓		
Preparation	✓	✓	✓	✓
Process	✓	✓		✓
Properties		✓		✓
<b>Prophetic in patents</b>	✓			
Reactant or reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

Create Keep Me Posted Substance Identifier "500-22-1" > substances (1) > 500-22-1 > get references (178)

### References

178 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags

Select All Deselect All Sort by: Accession Number

1. Hair dyes containing an indolium derivative and a carbonyl compound

By Gross, Wibke; Oberkobusch, Doris; Nemitz, Ralph  
 From Ger. Offen. (2009), DE 102008062234 A1 20091015. Language: German, Database: CAPLUS

The invention concerns hair dyes that contain (a) at least one indolium deriv. of the general formula  
 Thus 1-[3-(diethoxyphosphorylpropyl)-2,3,3-trimethyl]-3H-indolium bromide was synthesized from 2 acid diethylester. A two component hair dye contained (gel1): 10 mmol of the synthesized dye, Natrosol 10 mmol reactive carbonyl compd., Natrosol HR 250 2 g, sodium hydroxide (50% soln.) q.s.; water to of 1:1; the pH was set with ammonia and tartaric acid resp.

專利中屬於可預測性的物質。

Substance Detail：經由系統推導演算所預測的物質特性包含NMR光譜，並已完整分類。可點選預測性光譜圖(見下頁)。

Predicted Properties: [Biological](#) [Chemical](#) [Density](#) [Lipinski and Related](#) [Spectra](#) [Structure-related](#) [Thermal](#)

Biological Properties	Value	Conditions	Notes	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(50)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(50)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(50)	
Bioconcentration Factor	1.25	pH 4 Temp: 25 °C	(50)	
Bioconcentration Factor	1.55	pH 5 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 6 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 7 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 8 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 9 Temp: 25 °C	(50)	
Bioconcentration Factor	1.59	pH 10 Temp: 25 °C	(50)	

Chemical Properties	Value	Conditions	Notes	Top
Koc	1.0	pH 1 Temp: 25 °C	(50)	
Koc	1.88	pH 2 Temp: 25 °C	(50)	
Koc	13.2	pH 3 Temp: 25 °C	(50)	

Lipinski and Related Properties	Value	Conditions	Notes	Top
Freely Rotatable Bonds	1		(50)	
H Acceptors	2		(50)	
H Donors	0		(50)	
H Donor/Acceptor Sum	2		(50)	
logP	0.568±0.258	Temp: 25 °C	(50)	
Molecular Weight	107.11		(50)	

Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum <span style="color: red; font-weight: bold;">NEW</span>	<a href="#">See spectrum</a>		(51)	
Proton NMR Spectrum	<a href="#">See spectrum</a>		(51)	

Substance Detail : Carbon-13 NMR光譜，由  
ACD/Labs以軟體推導演算得出。

Carbon-13 NMR Spectrum

Print

Spectrum ID

500221-CNMR

Nucleus

$^{13}\text{C}$

Standard

Tetramethylsilane (75-76-3)

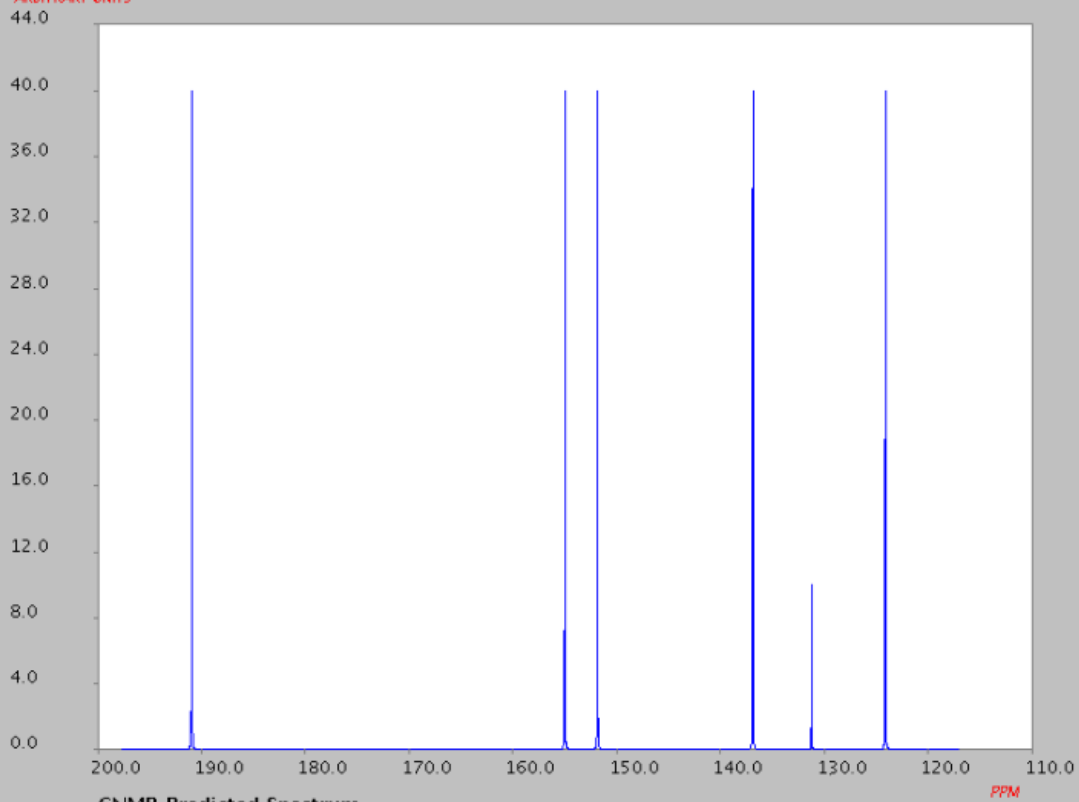
Temperature

25 °C

Source

Predicted NMR data calculated  
using Advanced Chemistry  
Development, Inc. (ACD/Labs)  
Software V9.07 (© 1994-2009  
ACD/Labs)

ARBITRARY UNITS



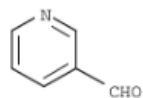
CNMR Predicted Spectrum

PPM

CAS Registry Number: 500-22-1

$\text{C}_6\text{H}_5\text{NO}$

3-Pyridinecarboxaldehyde



Substance Detail：經由實驗所得到的物質特性包含各式光譜圖，並已完整分類。可點選各類型的光譜圖參考(見下頁)。

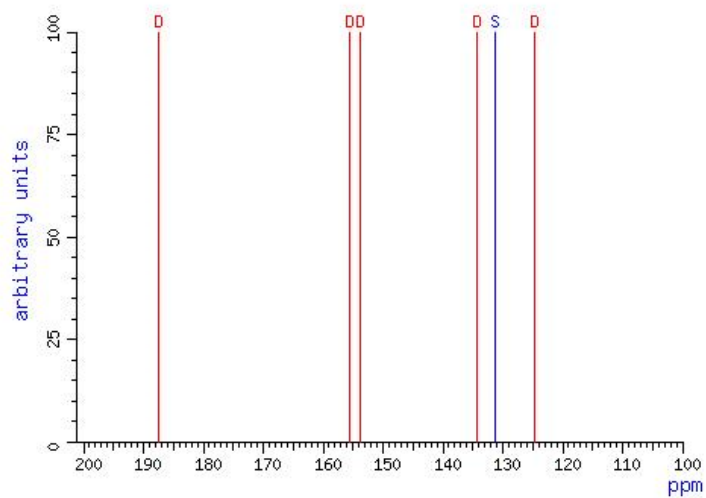
Experimental Properties: [Biological](#) [Chemical](#) [Optical and Scattering](#) [Spectra](#) [Thermal](#)

Biological Properties	Value	Conditions	Notes	Top
LC50	See full text		(41) CAS	
LC50	See full text		(42) CAS	
Median Lethal Dose(LD50)	900 mg/kg	Organism: mouse Route: intravenous	(12) CAS	
Chemical Properties	Value	Conditions	Notes	Top
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(1) CAS	
Solubility	See full text		(41) CAS	
Optical and Scattering Properties	Value	Conditions	Notes	Top
Refractive Index	1.5507	Wavlen: 589.3 nm; Temp: 20 °C	(49) CAS	
Refractive Index	1.5475	Wavlen: 589.3 nm; Temp: 20 °C	(3) CAS	
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(25) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(26) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(27) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(27) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(27) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(28) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(28) WSS	
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(29) AIST	
Carbon-13 NMR Spectrum	See full text		(30) CAS	
Carbon-13 NMR Spectrum	See full text		(31) CAS	
Carbon-13 NMR Spectrum	See full text		(32) CAS	
Carbon-13 NMR Spectrum	See full text		(33) CAS	
Carbon-13 NMR Spectrum	See full text		(34) CAS	

Substance Detail：右側顯示來源資料。

### Carbon-13 NMR Spectrum

Print



#### Spectrum ID

CNCC-78983-177P

#### Nucleus

<sup>13</sup>C

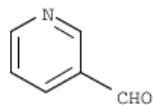
#### Source

Spectral data were obtained from Wiley Subscription Services, Inc. (US)

CAS Registry Number: 500-22-1

C<sub>6</sub> H<sub>5</sub> N O

3-Pyridinecarboxaldehyde





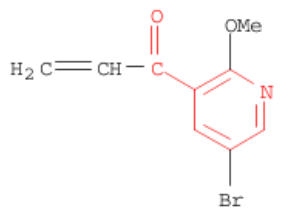
New features : 若物質檢索有多筆資料，  
可透過Refine功能”Property Value”進行篩  
選。(見下頁)

Substances Get References Get Reactions Get Commercial Sources

443473 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [50] 1 2 3 4 5 6 ... 8870 View: [grid icons]

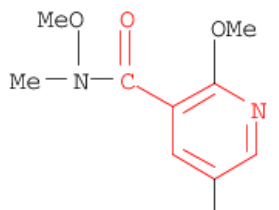
1. Substance Detail  
1190130-57-4



C<sub>9</sub> H<sub>8</sub> Br N O<sub>2</sub>  
2-Propen-1-one, 1-(5-bromo-2-methoxy-3-pyridinyl)-

~0 References  
Reactions  
Commercial Sources

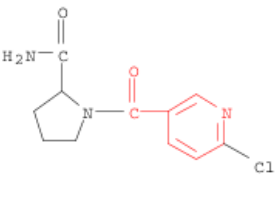
2. Substance Detail  
1190128-69-8



C<sub>9</sub> H<sub>11</sub> Br N<sub>2</sub> O<sub>3</sub>  
3-Pyridinecarboxamide, 5-bromo-N,2-dimethoxy-N-methyl-

~0 References  
Reactions

3. Substance Detail  
1190111-05-7



C<sub>11</sub> H<sub>12</sub> Cl N<sub>3</sub> O<sub>2</sub>  
2-Pyrrolidinecarboxamide, 1-[(6-chloro-3-pyridinyl)carbonyl]-

~0 References  
Reactions  
Commercial Sources  
Regulatory Information

Analysis **Refine**

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value **NEW**
- Reference Availability
- Atom Attachment

Select Properties

Refine：透過指定分子量的大小來限縮檢索結果。

**Refine by Property Value**

1. Select one or more properties. Click each property to display value options.

2. Specify values and limits.

**Properties - 1 selected**

**Experimental**

- Boiling Point
- Melting Point

**Predicted**

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Acceptor/Donor Sum
- Koc
- logD
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility

**Values - Predicted Molecular Weight**

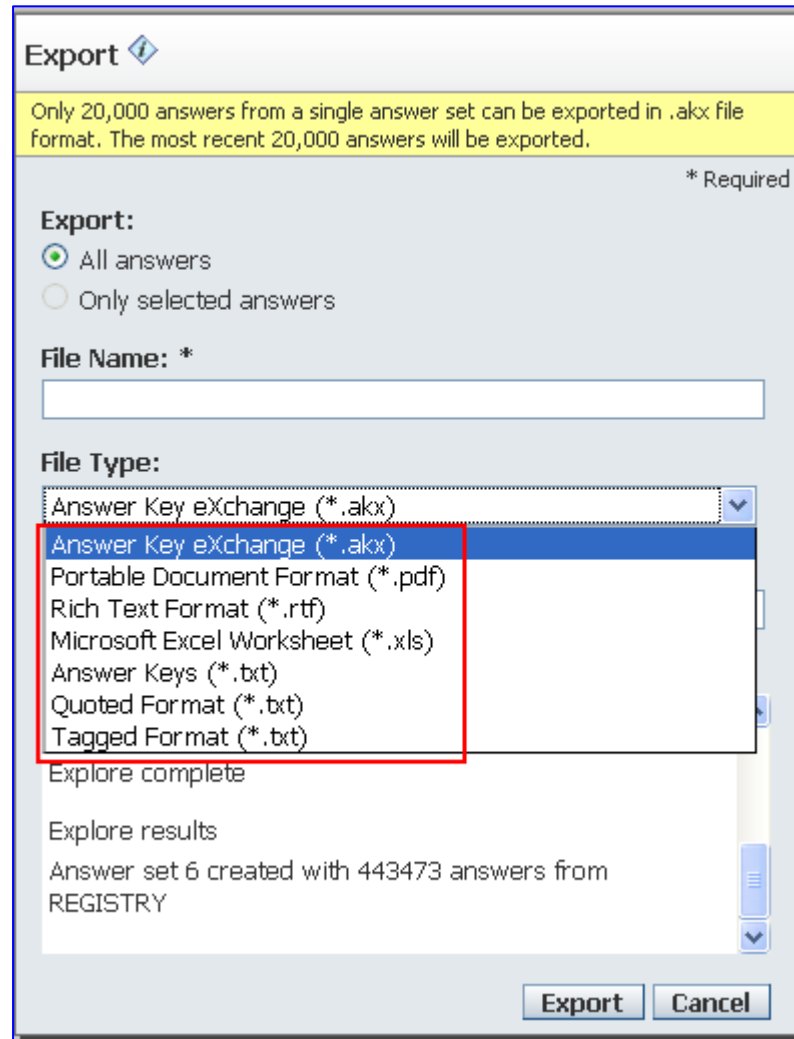
Specify range:

to

Min: 0.0 Max:

Include substances with no value for the specified properties

Export檔案支援多種格式，如  
akx, pdf, rtf, xls, txt。



# 反應檢索:

Explore References

Explore Substances

Explore Reactions

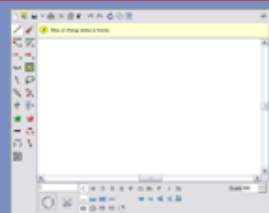
新增Solvent選擇功能，可依需求設計反應條件。點選小圖後出現畫板，較物質檢索多出5個專屬按鍵，下方有限制條件區可供設定。

Explore Reactions

Reaction Structure

Reaction Structure

Search



Click image to draw or import structure

新增Solvent選擇功能，可依需求設計反應條件。

Solvents

Select Solvents **NEW**

Number of Steps

Examples: 1, 1 - 3, 1 -, - 3

Classification(s)

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial

Source(s)

- Any source
- Patents only
- Sources other than patents

Publication Year(s)

Examples: 1995, 1995 - 1999, 1995 -, - 1995

Draw or change atoms or bonds.

新增快捷鍵，可快速轉換至物質檢索。

反應相關功能鍵。

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

確定

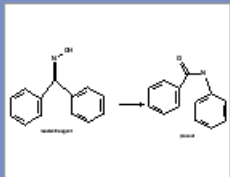
取消

承接軟體版強大的工具列設計理念，方便使用者更輕鬆的選擇功能。


The screenshot displays the 'Reaction editor' window. The main workspace shows a chemical reaction: a reactant (a benzene ring attached to a carbon atom which is double-bonded to a nitrogen atom with a hydroxyl group) reacting to form a product (a benzene ring attached to a carbon atom which is double-bonded to a nitrogen atom attached to another benzene ring). The interface includes a toolbar on the left with various drawing tools, a search bar at the bottom with the formula C13H11NO and a 'query' option, and a right-hand panel with search filters. A yellow box highlights the search bar area with the text: '可使用精確方式或相關衍生物進行查詢，以增加檢索數量。' (Use precise methods or related derivatives for search to increase the number of search results). A red box highlights the search filter options: 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures' (which is selected). Below these are '確定' (OK) and '取消' (Cancel) buttons. The status bar at the bottom shows the formula C13H11NO and the number 197.24.

進行檢索之前，可選擇特定 Solvents以限縮檢索結果。

Reaction Structure 



Click image to change structure or view detail

Search type:   Allow variability only as specified  
 Substructure

Search

Solvents 

 Close **NEW**

### Solvent Hierarchy

[\[View solvent list\]](#)

850 Selected [Select All](#) [Deselect All](#)

- Ionic liquids
  - Imidazolium derivatives
  - Nonimidazolium derivatives
- Nonpolar solvents
  - Aliphatic compounds
  - Aromatic compounds
  - Silanes
- Polar solvents
  - Polar solvents, aprotic
  - Polar solvents, protic
- Supercritical fluids

Find:  [↓Next](#) [↑Previous](#)

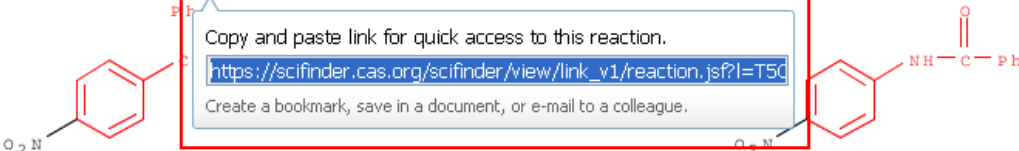
簡潔的檢索結果瀏覽頁面，自動完成分析統計；Link功能快速複製與分享重要檢索結果。

Reactions Get References

**145 Reactions** 0 Selected Keep Selected Remove Selected Link功能，快速複製與分享重要檢索結果。 Save Print Export

Select All Deselect All | Sort by: Accession Number | Answers per Page [15] 1 2 3 4 5 6 ... 10 | Display: [Icons]

1. Reaction Detail Link Similar Reactions NEW



Copy and paste link for quick access to this reaction.  
[https://scifinder.cas.org/scifinder/view/link\\_v1/reaction.jsf?l=T5c](https://scifinder.cas.org/scifinder/view/link_v1/reaction.jsf?l=T5c)  
Create a bookmark, save in a document, or e-mail to a colleague.

NOTE: solid-supported catalyst, regioselective, silica-supported dichlorophosphate prepared and used as catalyst, microwave irradiation (445W), 100% selectivity at 70% conversion, Beckmann rearrangement, catalyst recyclable, green chemistry-solvent, Reactants: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1

Silica-supported dichlorophosphate catalyzed Beckmann rearrangement and dehydration of oximes under microwave irradiation  
By Li, Zheng and Lu, Zhong  
From Letters in Organic Chemistry, 5(6), 495-501; 2008

檢索結果自動分析 "Catalyst" -

**Analysis** Refine

Analyze by: Catalyst

Click bar to view only those reactions within the current answer set

SiO <sub>2</sub>	18
ClSO <sub>3</sub> H	10
POCl <sub>3</sub>	7
HgCl <sub>2</sub>	5
PCl <sub>3</sub>	5
16385-59-4	3
CF <sub>3</sub> SO <sub>3</sub> H	3
InCl <sub>3</sub>	2
ZnCl <sub>2</sub>	2

可依照不同需求進行排序，以及調整文獻/反應的筆數(one reaction per reference)。

Reactions Get References

145 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Accession Number

- Accession Number
- Number of Steps
- Percent Yield
- Publication Year

Answers per Page [15] 1 2 3 4 5 6 ... 10 Display:

1. Reaction Detail

O=[N+]([O-])c1ccc(cc1)C(=N)O  $\xrightarrow{\text{C:POCl}_3, \text{C:SiO}_2, \text{S:THF}, 6 \text{ min}}$  O=[N+]([O-])c1ccc(cc1)NC(=O)c2ccccc2

NOTE: solid-supported catalyst, regioselective, silica-supported dichlorophosphate prepared and used as catalyst, microwave irradiation (445W), 100% selectivity at 70% conversion, Beckmann rearrangement, catalyst recyclable, green chemistry-solvent, Reactants: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1

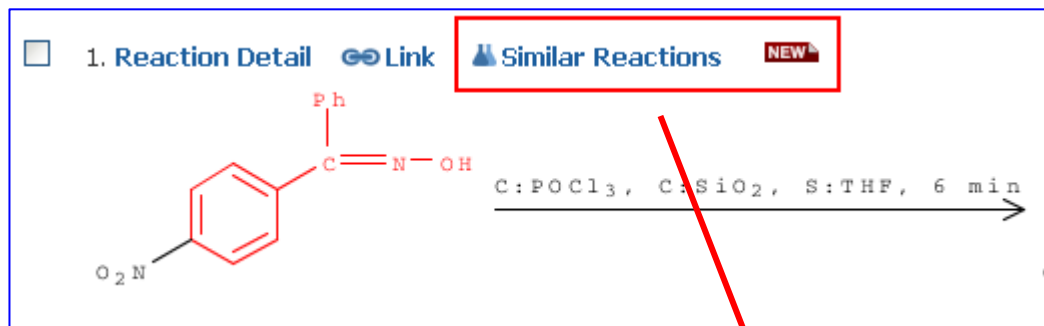
Silica-supported dichlorophosphate catalyzed Beckmann rearrangement and dehydration of oximes under microwave irradiation  
By Li, Zheng and Lu, Zhong  
From Letters in Organic Chemistry, 5(6), 495-501; 2008

可依不同需求進行排序。

調整文獻/反應的筆數。



新功能: Similar Reaction, 可依照相似程度不同(筆數多寡), 勾選適合的相似反應。



Get Similar Reactions ⓘ

Retrieve similar reactions from:

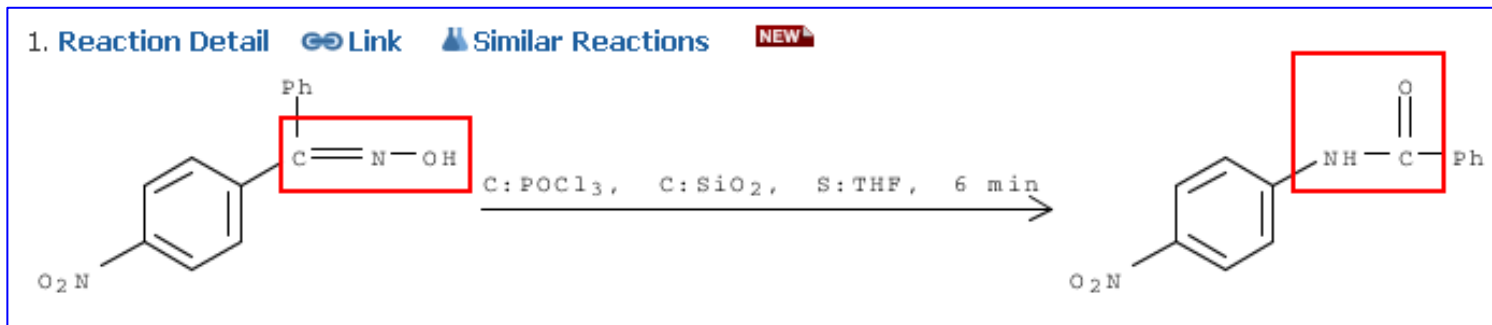
- All reactions
- Current answer set

Include this level of similarity:

- Broad** - Reaction centers only (908)
- Medium** - Reaction centers plus adjacent atoms and bonds (224)
- Narrow** - Reaction centers plus extended atoms and bonds (167)

Get Reactions Cancel

執行similar reaction結果。



直接點選感興趣物質，可再進行相關查詢。

The screenshot shows a search result for a chemical compound. The compound is 4-nitrobenzamide, represented by a benzene ring with a nitro group (O<sub>2</sub>N) and an amide group (-NH-C(=O)-Ph). A context menu is open over the structure, listing various options for further exploration. The menu items are:

- Reactions
- References
- Substance Detail
- Commercial Sources
- Regulatory Information
- Explore by Chemical Structure
- Explore Reactions

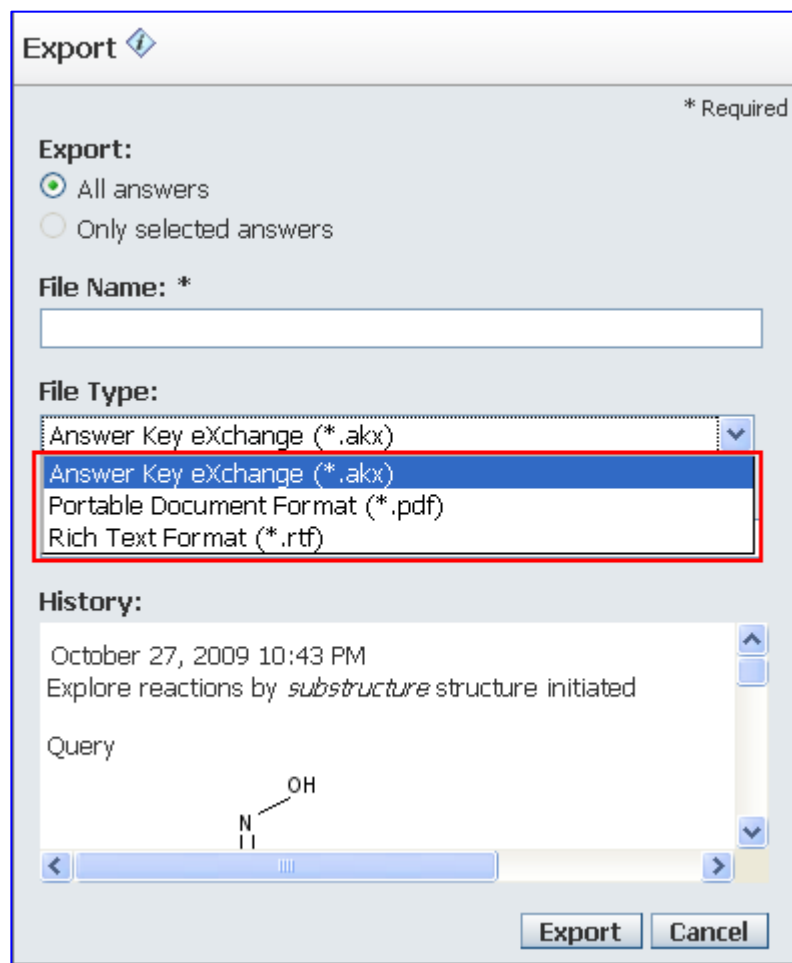
The 'Reactions' option is highlighted, and a sub-menu is visible to its right, listing roles:

- Product
- Reactant
- Reagent
- Reactant or Reagent
- Catalyst
- Solvent
- Any role

Below the search result, there is a snippet of text: "Silica-supported catalyst, microwave irradiation, Beckmann rearrangement".

and dehydration of oximes under microwave irradiation

Export檔案支援多種格式，如  
akx, pdf, rtf。



## 其他常用功能:

**Answer Sets:** 可對2個以上的答案群集進行 combine 功能。

**History:** 可下載最新10筆檢索歷程，方便研究人員熟悉檢索策略。

**KMP results:** 檢索結果更新通知功能設定。

Saved Answer Sets    Help  
 Keep Me Posted Results    History  
 My Connections    Preferences

可個別以“文獻”、“物質”、“反應”進行2個以上答案群集的combine功能。

Saved Answer Sets    Combine Answer Sets

References (55)     Substances (10)     Reactions (3)

55 Answer Sets    3 Selected    Delete Selected

Reference Answer Set Details	Date Saved
<input checked="" type="checkbox"/> IPAMA_CY with Ak repeat_patent (18) Combine with tyrosinase and dopamine Combine Reference Answer Sets "IPAMA_CY with Ak repeat_patent"	Edit     Link    Oct 20, 2009
<input checked="" type="checkbox"/> IPAMA_CY with Ak repeat_patent (4) By dopamine Opened saved answer set "IPAMA_CY with Ak repeat_patent" remove 0 references (485) > refine "dopamine"	Oct 20, 2009
<input checked="" type="checkbox"/> IPAMA_CY with Ak repeat_patent (14) By tyrosinase Opened saved answer set "IPAMA_CY with Ak repeat_patent" remove 0 references (485) > refine "tyrosinase"	Oct 20, 2009
<input type="checkbox"/> IPAMA_CY based_patent (53) Combine with tyrosinase and dopamine Combine Reference Answer Sets "IPAMA_CY based_patent" (53) > remove 0 references (53)	Oct 20, 2009
<input type="checkbox"/> IPAMA_CY based_patent (19) By dopamine Chemical Structure substructure > substances (11890) > get references (4882) > refine "Patents only" (2488) > remove 106 references (2382) > refine "dopamine" (19)	Edit     Link    Oct 20, 2009

**Combine Answer Sets**

Select an option for combining the selected saved answer sets:

**Combine**    Include all references from all selected answers

**Intersect**    Include only references that appear in all selected sets

Saved Answer Sets | Help  
Keep Me Posted Results | **History**  
**NEW** My Connections | Preferences

可下載最新10筆歷程並以  
Word程式開啟，方便研究  
人員了解檢索策略。

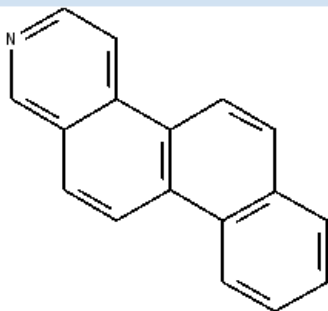
## History

Print Export

Session began October 27, 2009 at 8:20 PM

Explore substances by *substructure* structure initiated  
Query

October 27, 2009 8:26 PM



Explore complete

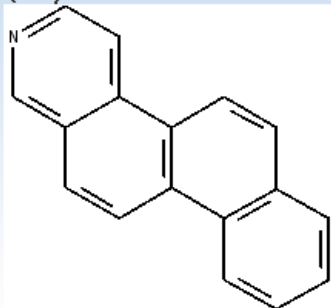
Explore results

Answer set 1 created with 2 answers from REGISTRY

Detailed display from Answer set 1 of 472986-99-5

Explore substances by *substructure* structure initiated  
Query

October 27, 2009 8:28 PM



## Previous Sessions

- SFSessionHistory-2009-10-27\_101211.rtf
- SFSessionHistory-2009-10-23\_040541.rtf
- SFSessionHistory-2009-10-23\_040401.rtf
- SFSessionHistory-2009-10-22\_011910.rtf
- SFSessionHistory-2009-10-20\_235046.rtf
- SFSessionHistory-2009-10-20\_233906.rtf
- SFSessionHistory-2009-10-20\_201623.rtf
- SFSessionHistory-2009-10-20\_200924.rtf
- SFSessionHistory-2009-10-20\_105129.rtf
- SFSessionHistory-2009-10-20\_052239.rtf

Saved Answer Sets	Help
Keep Me Posted Results	History
<b>NEW</b> My Connections	Preferences

可隨時對KMP更新通知進行調整，如 **Edit/Link/Combine/Delete**。

Keep Me Posted

11 Profiles      0 Selected      Delete Selected Profiles

Profiles and Results	Status	Created	Expires
<input type="checkbox"/> org. solar cell in NCTU ▶ Search Strategy: Select All   Deselect All Results <input type="checkbox"/> Oct 24, 2009 (1)	<input type="button" value="Edit"/>	Enabled	Oct 9, 2009    Oct 7, 2010

Selected Results:



使用完畢記得點選“Sign Out”登出，  
以免影響其他人使用權益。

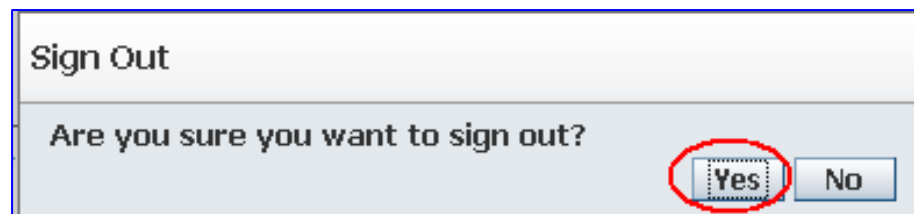


SciFinder®

Explore References   Explore Substances   Explore Reactions

Sign Out

Create Keep Me Posted   Reaction Structure substructure with limiters > reactions (145) > similar reactions (908)



Sign Out

Are you sure you want to sign out?

Yes No

## 當發現Web版連線速度變慢時...

- 與網管人員確認Web版伺服器不要設定防火牆

port: 443 IP: 134.243.5.42

- 更新 瀏覽器或JAVA(結構/反應畫板需要)版本
- 關閉 不必要的程式或網頁
- 改用其他瀏覽器, 如: FireFox, Safari, Chrome

# 透過線上學習更多關於Web版的檢索技巧



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Meeting Center | Training Center | **Event Center** | Support Center | More Services | My WebEx | Log In

## All e-Seminars

Product: Category: Language:

All All All

All event times in:

Date & Time	Event	Category	Subcategory
<b>October 2009</b>			
October 14, 2009 2:00 - 3:00 Taipei ST	<a href="#">SciFinder®: Exploring What's New with SciFinder®!</a>	Basic Orientation	Basic
October 28, 2009 1:00 - 2:00 Taipei ST	<a href="#">STN®: MARPAT® Searching on STN®: Why did I Get That?</a>	MARPAT®	Advanced
<b>November 2009</b>			
November 12, 2009 3:00 - 4:00 Taipei ST	<a href="#">SciFinder®: Exploring What's New with SciFinder®!</a>	Search Techniques, Miscellaneous Topics	Intermediate
November 12, 2009 22:00 - 23:00 Taipei ST	<a href="#">STN®: MARPAT® Searching on STN®: Why Did I Get That?</a>	MARPAT®	Advanced
November 17, 2009 19:00 - 20:00 Taipei ST	<a href="#">SciFinder®: Exploring What's New with SciFinder®!</a>	Search Techniques, Miscellaneous Topics	Intermediate
November 17, 2009 22:00 - 23:00 Taipei ST	<a href="#">SciFinder®: Exploring What's New with SciFinder®!</a>	Search Techniques, Miscellaneous Topics	Intermediate
November 18, 2009 10:00 - 11:00 Taipei ST	<a href="#">SciFinder®: Exploring What's New with SciFinder®!</a>	Search Techniques, Miscellaneous Topics	Intermediate

完成

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若您需要進一步資訊，請與我們連絡 ~

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