



# Reaxys 化學資料庫 教育訓練

[www.reaxys.com](http://www.reaxys.com)

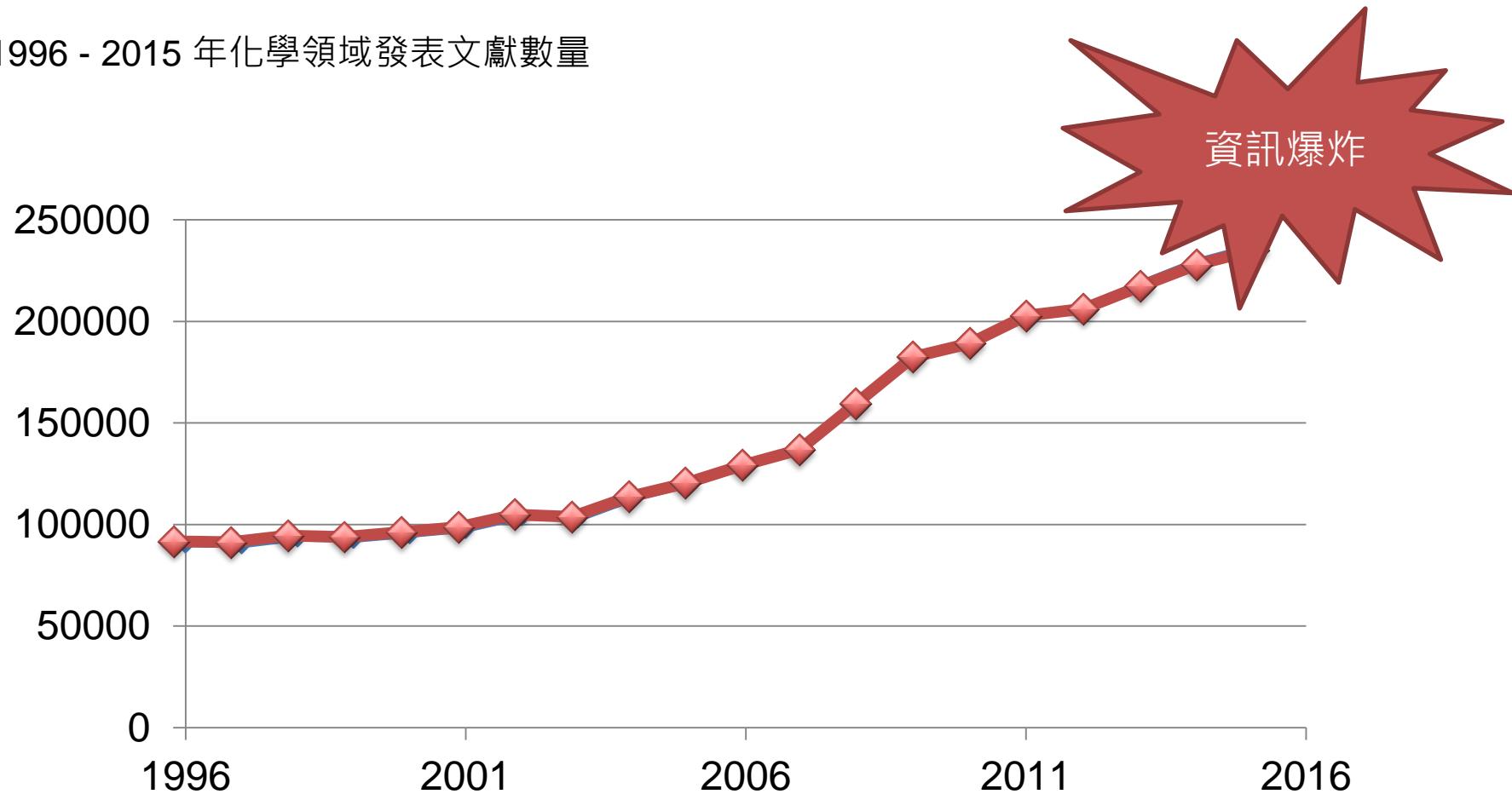
梁成芝 Olivia Liang  
[\[o.liang@elsevier.com\]\(mailto:o.liang@elsevier.com\)](mailto:o.liang@elsevier.com)

201610

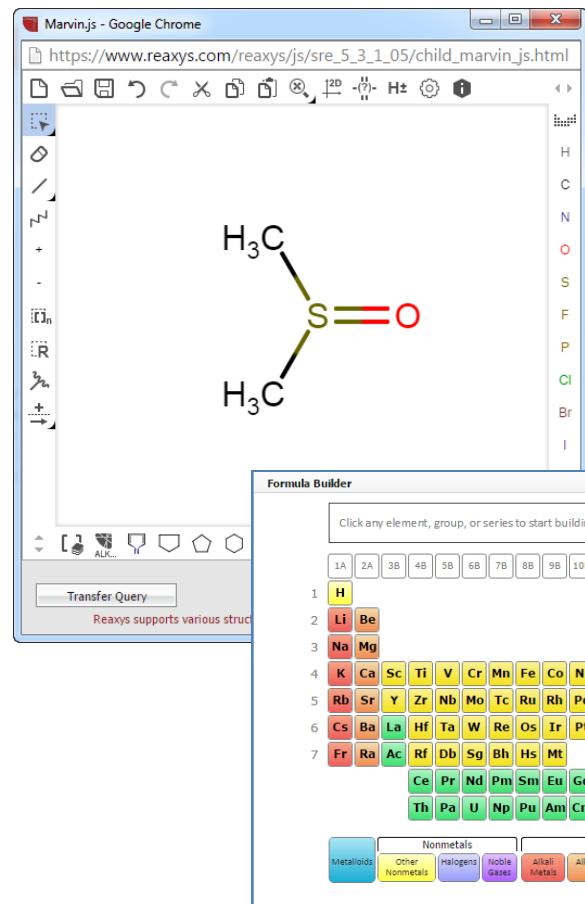
Olivia Liang

# 資訊爆炸的年代，是否有更好的選擇？

1996 - 2015 年化學領域發表文獻數量



# 更化學的搜尋方法



# Reaxys 可以用來搜尋哪些資料？

一般資料庫無法搜尋特定數值範圍的化學特性或實驗數據

搜尋結果

反應  
(Reactions)

化合物  
(Substances)

文獻  
(Citations)

## 化學反應資料庫

收錄 > 4,100 萬筆  
單一或多步驟化學反應

## 化合物資料庫

收錄 > 2,650 萬種  
有機、無機、有機金屬  
化合物

## 文獻資料庫

收錄 > 5,200 萬筆資料  
來自 >16,000 種期刊及主要  
專利局

## 特性資料庫

收錄 > 5 億筆實驗數據  
> 500 種欄位  
來自 > 130 個研究子領域

可直接瀏覽 281 本化學  
期刊及專利全文中的合成  
材料方法

可搜尋數值範圍。  
例如：沸點 = 100 °C 或沸  
點 > 100 °C 的所有化合物

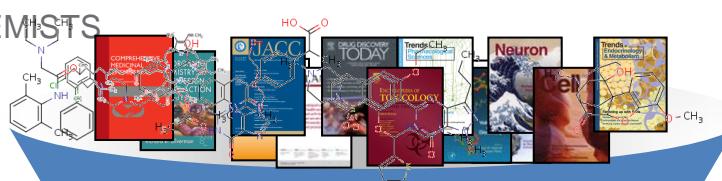
# Reaxys 與 SciFinder 收錄內容比較



# Reaxys 化學及藥物化學資料庫

我們的目標是為您節省更多時間

CATALOGUED AND TAXONMISED BY CHEMISTS FOR CHEMISTS



涵蓋 16,000 期刊及三大專利局

從 1771 年開始收錄

分類整理各種數據

高度相關的答案  
RELEVANT ANSWERS

各種數據分門別類整理成表格

Structure	Structure/Compound Data	N° of preparations All Preps   All Reactions	Available Data	Target	N° of ref.
	<p><b>Chemical Name:</b> propene</p> <p><b>Reaxys Registry Number:</b> 1696878 <b>CAS Registry Number:</b> 107-13-1 <b>Type of Substance:</b> organic <b>Molecular Formula:</b> C<sub>3</sub>H<sub>6</sub> <b>Linear Structure Formula:</b> C<sub>2</sub>H<sub>5</sub>CH<sub>3</sub> <b>Molecular Weight:</b> 42.0806 <b>InChI Key:</b> QQONPFFTQHPHPA-UHFFFAOYSA-N</p>	2624 prep out of 7655 reactions.	Hit Data (67) Druglikeness Bioactivity Identification Physical Data (1078) Spectra (1078) Ecological Data (60) Use/Application (29) Natural Product (4)	Show Targets	9151
<b>Chemical Names and Synonyms</b>					
propene, 1-propene, propylene					
<b>± IR Data</b> <b>± IR Spectroscopy ( 67 Hits out of 67 view all )</b>					
Description (IR Spectroscopy)	Solvent (IR Spectroscopy)	Temperature (IR Spectroscopy)	Comment (IR Spectroscopy)	Reference	
Bands	gaseous matrix			Maior, Guenther; Lautz, Christian Angewandte Chemie - International Edition, 1999, vol. 38, # 13-14 p. 2038 - 2041 Title/Abstract Full Text View citing articles Show Details	
Spectrum	gas	26.9 °C	3500 - 500 cm <sup>−1</sup> (-1)	Street, Gellman Journal of Physical Chemistry B, 1997, vol. 101, # 8 p. 1389 - 1395 Title/Abstract Full Text View citing articles Show Details	
Spectrum	solid matrix	-262.2 °C	3300 - 800 cm <sup>−1</sup> (-1)	Rowland, Brad; Hess, Wayne P. Journal of Physical Chemistry A, 1997, vol. 101, # 43 p. 8049 - 8056 Title/Abstract Full Text View citing articles Show Details	
Bands	solid matrix	-262.2 °C	3086 - 916 cm <sup>−1</sup> (-1)	Rowland, Brad; Hess, Wayne P. Journal of Physical Chemistry A, 1996, vol. 100, # 43 p. 8049 - 8056 Title/Abstract Full Text View citing articles Show Details	
Spectrum	solid matrix	-261.2 °C	3200 - 400 cm <sup>−1</sup> (-1)	Radziszewski, Juliusz G.; Downing, John W.; Gudipati, Murthy S.; Balaji; Thielstrup, Erik W.; Michl, Josef Journal of the American Chemical Society, 1996, vol. 118, # 42 p. 10275 - 10284 Title/Abstract Full Text View citing articles Show Details	
Bands	solid matrix	-261.2 °C	3075 - 578 cm <sup>−1</sup> (-1)	Radziszewski, Juliusz G.; Downing, John W.; Gudipati, Murthy S.; Balaji; Thielstrup, Erik W.; Michl, Josef Journal of the American Chemical Society, 1996, vol. 118, # 42 p. 10275 - 10284 Title/Abstract Full Text View citing articles Show Details	
<a href="#">Show next 20</a> <a href="#">Show next 47</a>					
<a href="#">Druglikeness</a> <a href="#">Bioactivity</a> <a href="#">Identification</a> <a href="#">Physical Data</a> <a href="#">Spectra</a> <a href="#">Ecological Data</a> <a href="#">Use/Application</a> <a href="#">Natural Product</a>					

# 各種資料分門別類整理為表格，並抽出重要數據

表格中的文字皆可分類搜尋

▲ IR Spectroscopy ( 67 Hits out of 67 [view all](#) )

Description (IR Spectroscopy)	Solvent (IR Spectroscopy)	Temperature (IR Spectroscopy)	Comment (IR Spectroscopy)	Reference
Bands	nasenous matrix			<a href="#">Maier, Guenther, Lautz, Christian</a>

▲ Physical Data

▼ Melting Point (10)

▲ Boiling Point (3)

Boiling Point	Pressure (Boiling Point)	Reference
1950 °C		<b>Pourbaix, M.</b> Bulletin des Societes Chimiques Belges, 1944 , vol. 53, p. 159 - 164 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Zn: SVol., 235, page 802 - 803 <a href="#">Full Text</a> <a href="#">Show Details</a>
1731 °C	600 Torr	<b>Lemarchands, M.; Jacobs, M.</b> Bulletin de la Societe Chimique de France, 1935 , vol. 2, p. 479 - 487 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Zn: SVol., 235, page 802 - 803 <a href="#">Full Text</a> <a href="#">Show Details</a>
2350 °C	760 Torr	<b>Hagenbach; Langbein</b> Arch. Sci. Phys. Nat., 1919 , vol. 1, p. 48 - 48 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Gmelin Handbook:</b> Zn: MVol., 43, page 126 - 128 <a href="#">Full Text</a> <a href="#">Show Details</a>

10284  
[Title/Abstract](#) [Full Text](#) [View citing articles](#) [Show Details](#)

# 多元搜尋方式 -- 超過 400 種欄位可獨立或合併搜尋。

例如：搜尋包含34個碳，旋光度=18.2的所有化合物

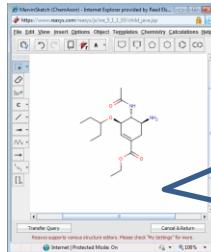
關鍵字

**Ask Reaxys**

Smart searching with Ask Reaxys. See examples >

**Citation Basic Index**

結構



- 支援 9 種繪圖軟體
- 強大衍生物搜尋功能
- Marvin JS 免安裝 JAVA

物質特性、實驗數據種類及其數值範圍

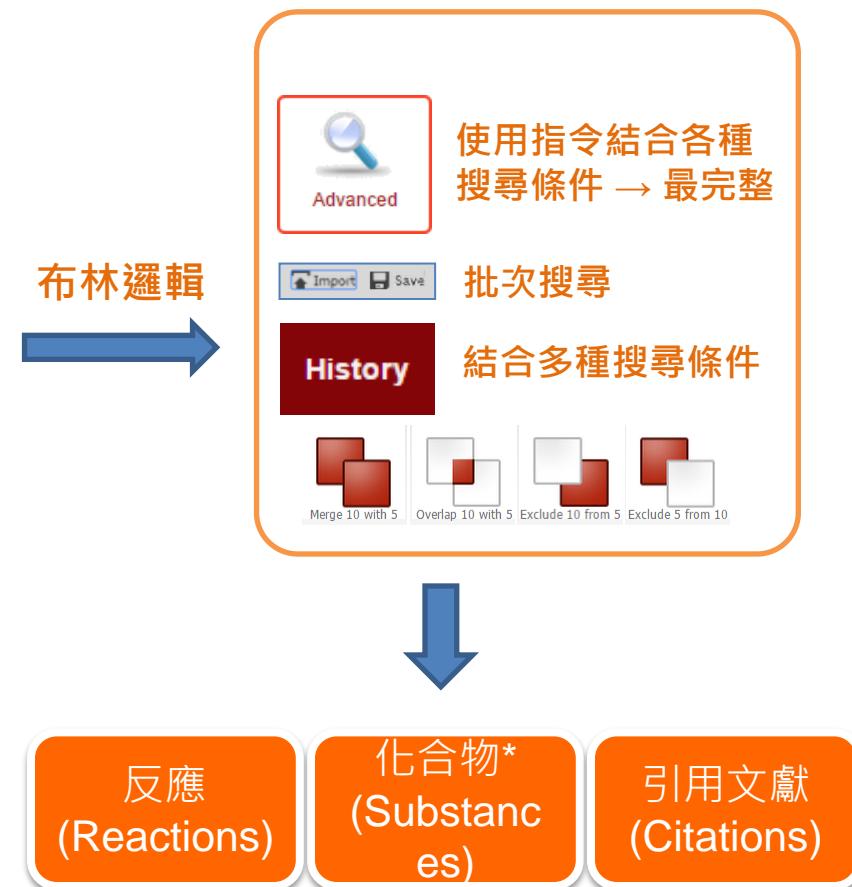
**Physical Data**

Optical Rotatory Power (deg)  =

Show AND Buttons

Optical Rotatory Power (deg)  =

分子式、合金、及其它 > 500 種欄位搜尋



# 反應搜尋結果

## 儲存勾選的反應資料

## 排序

# 搜尋結果 – substances

Bioactivities (0)	Reactions (35)	Substances (9)	Targets (0)	Citations (77)	go to Page <input type="text"/>  Page 1 of 1  
    	  	Sort by <b>No of References</b>   Display as:   <input type="checkbox"/> Exclude GOSTAR data			
Structure	Structure/Compound Data	Nº of preparations All Preps   All Reactions	Available Data	Target	Nº of ref.
AgInS <sub>2</sub>    <a href="#">Synthesize</a>   <a href="#">Hide Details</a> <a href="#">Find similar</a>	<p><b>Chemical Name:</b> silver indium disulfide</p> <p><b>Reaxys Registry Number:</b> 15946194 <b>Type of Substance:</b> Solid solution <b>Molecular Formula:</b> AgInS<sub>2</sub> <b>Linear Structure Formula:</b> AgInS<sub>2</sub> <b>Molecular Weight:</b> 266.82 <b>InChI Key:</b> RDYBAOKQJVXEPR-UHFFFAOYSA-N</p>	19 prep out of 22 reactions.	Druglikeness Identification Physical Data (88) Spectra (15) Use/Application (1) Quantum Chemical Data (4)	<a href="#">Show Targets</a>	62
<b>Chemical Names and Synonyms</b> silver indium disulfide					
<b>Druglikeness</b> <b>Identification</b> <b>Physical Data</b> <b>Melting Point (5)</b>					
Melting Point	Reference				
871.84 °C	<b>Bodnar'; Korzun; Yasyukevich</b> Russian Journal of Inorganic Chemistry, 1998 , vol. 43, # 5 p. 771 - 774 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> <b>Bodnar; Yasyukevich; Korzun; Karoza</b> Journal of Materials Science, 1998 , vol. 33, # 1 p. 183 - 188 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>				
977 °C	<b>Mal'sagov, A. U.</b> Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 22 - 29 <a href="#">Full Text</a> <a href="#">Show Details</a>				
872 °C	<b>Bodnar', I. V.; Orlova, N. S.</b> Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 330 - 335 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 382 - 387 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Bodnar, I. V.; Korzun, B. V.; Chernyakova, A. P.</b> Physica Status Solidi A: Applied Research, 1987 , vol. 101, p. 409 - 420 <a href="#">Full Text</a> <a href="#">Show Details</a>				

# 搜尋結果 -- Citations

Bioactivities (0)		Reactions (35)		Substances (9)		Targets (0)		Citations (77)			
										go to Page <input type="text"/> Page 1 of 9	
								<input style="border: none; padding: 0; margin: 0;" type="button" value="Sort by"/> <span style="font-size: 1.2em;">▼</span> <span style="font-size: 1.2em;">▲</span>		<input type="checkbox"/> Exclude GOSTAR data	
		<input type="checkbox"/> Limit to <input type="checkbox"/> Exclude <input type="checkbox"/> Export <input type="checkbox"/> Print <input type="checkbox"/> Zoom in <input type="checkbox"/> Zoom out <input type="checkbox"/> Hide									
1	Thermodynamic Stability of n-AgInSe <sub>2</sub> in Photoelectrochemical Cells	Bicelli, Luisa Peraldo	1988	Journal of Physical Chemistry, 1988, vol. 92, # 24 p. 6991 - 6997 <a href="#">Full Text</a> <a href="#">View citing articles</a>							Times cited
	<span style="color: red;">▼</span> <b>Title/Abstract</b> <span style="color: red;">▼</span> <a href="#">Show All Substances (5)</a> <span style="color: red;">▼</span> <a href="#">Hit Substances in this article (1 out of 5)</a>										
2	Photoelectrochemical study on the ternary semiconductors AgInS <sub>2</sub> and AgInSe <sub>2</sub>	Odenweller; Grabner	1988	Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics, 1988, vol. 92, # 11 p. 1330 - 1334 <a href="#">Full Text</a> <a href="#">View citing articles</a>							7
	<span style="color: red;">▼</span> <b>Title/Abstract</b> <span style="color: red;">▼</span> <a href="#">Show All Reactions (2)</a> <span style="color: red;">▼</span> <a href="#">Show All Substances (6)</a> <span style="color: red;">▼</span> <a href="#">Hit Substances in this article (1 out of 6)</a>										
3	Solvothermal reaction route to nanocrystalline semiconductors AgMS <sub>2</sub> (M = Ga, In)	Hu, Junqing; Lu, Qingyi; Tang, Kaibin; Qian, Yitai; Zhou, Guien; Liu, Xianming	1999	Chemical Communications, 1999, # 12 p. 1093 - 1094 <a href="#">Full Text</a> <a href="#">View citing articles</a>							40
	<span style="color: red;">▼</span> <b>Title/Abstract</b> <span style="color: red;">▼</span> <a href="#">Show All Reactions (2)</a> <span style="color: red;">▼</span> <a href="#">Show All Substances (6)</a> <span style="color: red;">▼</span> <a href="#">Hit Substances in this article (1 out of 6)</a>										
4	A simple route to synthesize MInS <sub>2</sub> (M = Cu, Ag) nanorods from single-molecule precursors	Cui, Yong; Ren, Jin; Chen, Gang; Qian, Yitai; Xie, Yi	2001	Chemistry Letters, 2001, # 3 p. 236 - 237 <a href="#">Full Text</a> <a href="#">View citing articles</a>							28

# Reaxys 搜尋結果分析及輸出

分析篩選搜尋結果，並輸出報告與同儕分享討論

搜尋結果

反應  
(Reactions)

化合物\*  
(Substances)

引用文獻  
(Citations)

合成路徑規畫

Synthesis Plans

資料庫連結



篩選功能：Analysis View 及 28 種 Filter

Filter by:  
Substructure

包裝價格資料

多元資料儲存或輸出方式

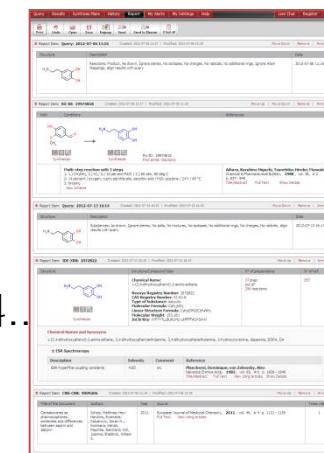
Report

檔案格式：E-mail、HTML網頁、PDF

可儲存：搜尋條件、化合物、反應、文獻、合成路徑

優點：適合儲存少量資料、操作簡便、格式簡明、保留超連結

- 彙整各種搜尋結果
- 一鍵 e-mail 分享



檔案格式：PDF、XML、Word、Excel、電子實驗記錄本、書目資料...

可儲存：化合物、反應、文獻、合成路徑

優點：可大量輸出搜尋結果、多種檔案格式可與進階分析軟體相容

Export

# New Reaxys 2016.10 更新

新版網頁 [new.reaxys.com](http://new.reaxys.com)

- 內容擴充
  - 加入亞洲專利 (日本、韓國、中國、臺灣)
  - 摘錄 281 本期刊與專利的合成材料方法
  - 摘錄更多實驗數據內容，由 400 本擴充為 16000 本期刊
- 介面更新
  - 依據使用頻率重新調整介面

\* 新版將與舊版並行至少半年

# 首頁 Quick Search

關鍵字搭配結構搜尋是使用頻率最高的搜尋方式

Reaxys

Quick search   Query builder   Results   Synthesis planner   History   Olivia Liang   ?

Search substances, reactions, citations and bioactivity data

輸入關鍵字搜尋

Substance Property, e.g. solubility of vitamin D3

Search >

AND

Create Structure or Reaction Drawing

繪製結構

REAXYS Version 1

Feedback

# 進階搜尋 – Query Builder

整合超過 400 個欄位

The screenshot shows the Reaxys Query Builder interface. The top navigation bar includes 'Quick search', 'Query builder' (which is underlined, indicating the active tab), 'Results', 'Synthesis planner', and 'History'. The top right shows a user profile for 'Olivia Liang'.

**3. 搜尋** (Search Substances) is highlighted in red. The search bar contains the text 'Search Substances >'. Below the search bar are four search icons: 'Structure', 'Molecular Formula', 'CAS', and 'Doc. Index'.

**2. 輸入條件 :** (Input Conditions) is highlighted in red. The search criteria are:

- Boiling Point = 100
- NOT (Boiling Point, Torr) = Pressure (Boiling Point), Torr
- Molecular Formula is H2O

**1. 搜尋欄位** (Search Fields) is highlighted in red. The sidebar on the right lists search fields under 'Basic Indexes', 'Identification', and 'Physical Properties'. The 'Boiling Point' field is expanded, showing sub-fields: Melting Point, Boiling Point, Sublimation, Refractive Index, and Density.

# 化學反應搜尋結果

Reaxys

Quick search    Query builder    Results    Synthesis planner    History    Olivia Liang

83 Reactions out of 72 Documents containing 96 Substances

Back to Results Preview

0 selected: Limit To Export Reaxys Ranking

Yield

- >95 - 100 2
- >80 - 85 1
- >75 - 80 1
- >30 - 35 2
- >15 - 20 1
- (no entry given) 76

Reagent/Catalyst

- hydrogenchloride 9
- oxygen 7
- lithium hydroxide 7
- n-ethyl-n,n-diisopropylamine 0
- lithium bromide 5
- cu(ii) perchlorate 5
- ascorbic acid powder 5

1

Find Similar Reactions

Yield	Conditions	Reference
99%	With hydrogenchloride; hydrogen palladium on activated charcoal In ethanol under 760 Torr for 24h Ambient temperature	Kohno; Sasa; Murahashi - Bulletin of the Chemical Society of Japan, 1990, vol. 63, # 4, p. 1252 - 1254

Full Text Cited 11 times Show details

Exports Feedback

# Autoplan 合成路徑規劃

Reaxys

Synthesis Planner Edit 

Autoplan 1 5 

1 Plan 1

2 Plan 2

3 Plan 3

4 Plan 4

5 Plan 5

+ Create new

Quick

Plan 1

Import

Conditions

Preparation - 2

Yield	Conditions	Reference
14%	With oxygen; Cu(II) perchlorate; ascorbic acid powder In water; acetone at 60°C for 24h	Aihara, Kazuhiro; Higuchi, Tsunehiko; Hirobe, Masaaki - Chemical & Pharmaceutical Bulletin, 1988, vol. 36, # 2, p. 837 - 840

Full Text  Show details 

Preparation - 3

Yield	Conditions	Reference

82%

14%

1f

1

lg

1g

67%

3

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1

2

3

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# Reaxys Demo & Case Study



# Ask Reaxys

分子式  $\text{AgInS}_2$

Reaxys is changing! Join one of our webinars tomorrow to find out how. [Register here](#) X

 Anonymous user (198.176.84.34)

[Query](#) [Results](#) [Synthesis Plans](#) [History](#) [Report](#) [My Alerts](#) [My Settings](#) [Help](#) [Register](#) [Login](#) ▼

 Import  Save

## Ask Reaxys

Search

Smart searching with Ask Reaxys. [See examples >](#)

Reactions



Substances, Names, Formulas



Medicinal Chemistry



Literature



ReaxysTree



Start by specifying common ID fields such as CAS Registry number and more.

You can also search directly by these common property groups:

 Physical  Spectra  Natural Product  Advanced

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<https://www.reaxys.com/reaxys/secured/search.do#>

# 搜尋結果 – substances

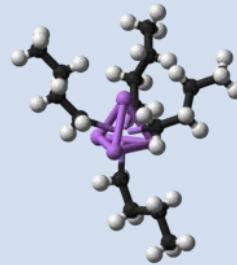
Bioactivities (0)	Reactions (35)	Substances (9)	Targets (0)	Citations (77)	go to Page <input type="text"/> Page 1 of 1
		Sort by <input style="border: 1px solid black; padding: 2px 10px;" type="button" value="No of References"/> Display as: <input type="checkbox"/> Exclude GOSTAR data			
Structure	Structure/Compound Data	Nº of preparations All Preps   All Reactions	Available Data	Target	Nº of ref.
AgInS <sub>2</sub>   <a href="#">Synthesize</a>   <a href="#">Hide Details</a> <a href="#">Find similar</a>	<p><b>Chemical Name:</b> silver indium disulfide</p> <p><b>Reaxys Registry Number:</b> 15946194  <b>Type of Substance:</b> Solid solution  <b>Molecular Formula:</b> AgInS<sub>2</sub>  <b>Linear Structure Formula:</b> AgInS<sub>2</sub>  <b>Molecular Weight:</b> 266.82  <b>InChI Key:</b> RDYBAOKQJVXEPR-UHFFFAOYSA-N</p>	19 prep out of 22 reactions.	Druglikeness Identification Physical Data (88) Spectra (15) Use/Application (1) Quantum Chemical Data (4)	<a href="#">Show Targets</a>	62
<b>Chemical Names and Synonyms</b> silver indium disulfide					
<b>Druglikeness</b> <b>Identification</b> <b>Physical Data</b> <b>Melting Point (5)</b>					
Melting Point	Reference				
871.84 °C	<b>Bodnar', Korzun; Yasyukevich</b> Russian Journal of Inorganic Chemistry, 1998 , vol. 43, # 5 p. 771 - 774 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> <b>Bodnar; Yasyukevich; Korzun; Karoza</b> Journal of Materials Science, 1998 , vol. 33, # 1 p. 183 - 188 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>				
977 °C	<b>Mal'sagov, A. U.</b> Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 17 - 20 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 22 - 29 <a href="#">Full Text</a> <a href="#">Show Details</a>				
872 °C	<b>Bodnar', I. V.; Orlova, N. S.</b> Inorganic Materials (Transl. of Neorg. Mater.), 1989 , vol. 25, p. 330 - 335 Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, 1989 , vol. 25, p. 382 - 387 <a href="#">Full Text</a> <a href="#">Show Details</a> <b>Bodnar, I. V.; Korzun, B. V.; Chernyakova, A. P.</b> Physica Status Solidi A: Applied Research, 1987 , vol. 101, p. 409 - 420 <a href="#">Full Text</a> <a href="#">Show Details</a>				

# 不同研究領域，適合不同的搜尋方式

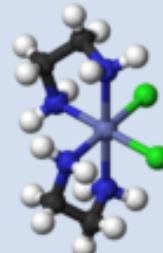
Found in REAXYS SUBSTANCE RECORDS  
... and ...



CLASSIC ORGANICS



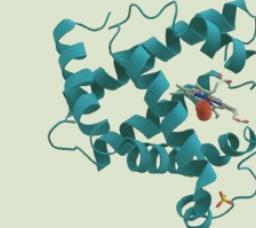
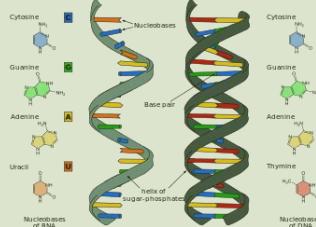
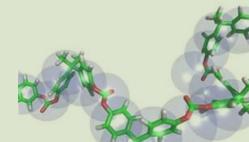
ORGANOMETALLICS  
COORDINATION  
COMPOUNDS



CLASSIC INORGANICS

Found in KEYWORDS in REAXYS BIBLIOGRAPHIC  
RECORDS

POLYMERS



NUCLEIC ACIDS &  
PROTEINS



ALLOYS & METALS



CERAMICS



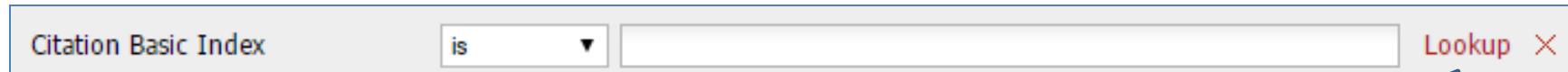
搜尋化合物 Substances

搜尋文獻 Literature

# 關鍵字文獻搜尋 – 結合多個關鍵字

使用 Citation Basic Index 欄位或 Advanced Search

可使用多種指令  
結合關鍵字



## 布林邏輯 Boolean operators

- AND 涵蓋所有關鍵字
- OR 涵蓋任一關鍵字
- NOT 不涵蓋指定關鍵字

## 鄰近搜尋指令 Proximity Operators

- Next 兩個相鄰關鍵字依指定順序排列
- Near 兩個關鍵字無須依指定順序排列

## 其它搜尋指令

- 通用字元 \* 可加在單字的左右側，用來搜尋不完整單字 (例如 cataly\* 可找到 catalyst, catalysis 等)
- 括弧 () 優先運算括弧內指令
- 空格 = AND
- ; = OR
- - 連接詞彙 (例如 low-density)



# 小分子化合物文獻搜尋結果

## 乙烯裂解廠

Citation Basic Index is 'ethylene cracker plant'

Select index items and click 'Transfer'

Reaxys

Search for:

ethylene cracker (8)  
ethylene cracker byproducts (1)  
ethylene cracker complex (1)  
ethylene cracker feed (3)  
ethylene cracker feedstock (1)

Economic optimization of a thermal cracker via model predictive control technology Savu, Andreea R.; Muntean, Ionut; Lazea, Gheorghe; Agachi, Paul-Serban 2011 2011 19th Mediterranean Conference on Control and Automation, MED 2011, 2011, art. no. 5983153, p. 819 - 824   1

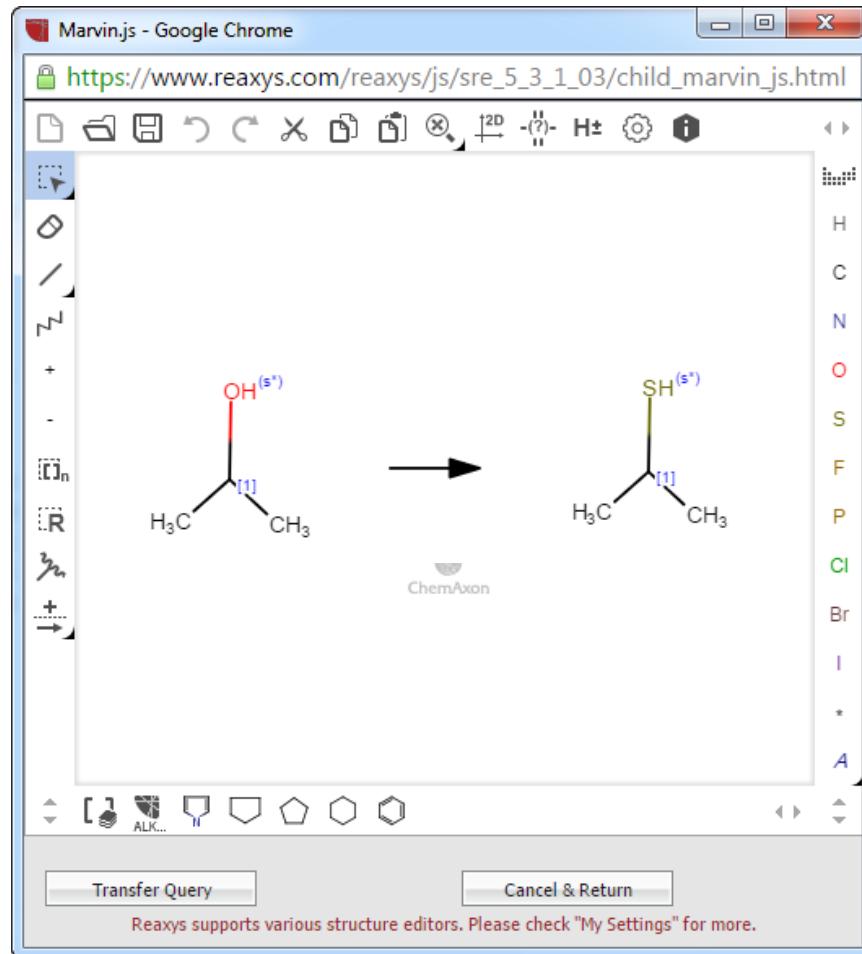
**▲ Title/Abstract**  
Economic optimization of a thermal cracker via model predictive control technology  
An **ethylene plant** is one of the largest chemical plants and **ethylene** is industrially obtained through thermal cracking of hydrocarbons. The cracking furnace is the heart of such an installation and the frequent changes in feed mix, quality and prices; and the demand for its olefin products are influencing directly the production efficiency. Each reactant in the feed produces a certain distribution of products and in order to satisfy the demand constraints at the lowest cost; one needs to optimize the amounts of each reactant.

**Keywords:**  
**Author:** economic optimization; **ethylene plant**; hydrocarbon pyrolysis; MPC; **thermal cracker**  
**Compendex Free Language:** Economic optimization; **Ethylene plants**; hydrocarbon pyrolysis; MPC; **Thermal cracker**  
**Compendex Descriptor:** Chemical plants; Cracking (chemical); **Ethylene**; Hydrocarbons; Model predictive control; Optimization; Petroleum chemistry  
**Compendex Mainhead:** Predictive control systems  
**Reaxys Terms:** cracking; thermal cracking

Transfer

# 繪圖軟體 – Marvin JS

Reaxys 共支援 9 種繪圖軟體，包含常用的 Chemdraw, Accelrys, Marvinsketch 等



- 豐富的功能協助您搜尋各種衍生物與反應類型
  - 限定特定位置的鍵結、原子、或官能基種類，並具備多種彈性選項
  - R-group 功能
  - Substitution 限定特定原子是否接上官能基或接上鍵結的數量
  - Position variation bond 限定指定鍵結或官能基可能連接的多個位置
- 無須 Java 支援
- 可從 ChemDraw 複製貼上
- 繪製完畢的結構可存成去背圖檔，並可調整檔案大小

原廠線上教學短片

<https://docs.chemaxon.com/display/docs/Video+Tutorials+JS>

## Reaction 搜尋結果

找到 1205 筆反應

Reactions (1205) Substances (1918) Citations (474) go to Page  Page 1 of 134

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Reaxys-Ranking ▾

Yield Conditions References

1

Rx-ID: 1786437

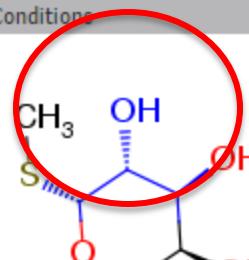
Rx-ID: 1786437

Synthesize Find similar Synthesize Find similar Rx-ID: 1786437 Find similar reactions

Yield	Conditions	References
94%	With Lawesson's reagent in toluene 0.5 h; Heating;	<b>Nishio, Takehiko</b> Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1993, # 10 p. 1113 - 1118 Title/Abstract Full Text View citing articles Show Details
94%	With Lawesson's reagent in toluene 0.5 h; Heating;	<b>Nishio, Takehiko</b> Journal of the Chemical Society, Chemical Communications, 1989, # 4 p. 205 - 206 Title/Abstract Full Text View citing articles Show Details
94%	With Lawesson's reagent; water in toluene T=50°C;	<b>Ohno, Michihiro; Miyamoto, Mitsuko; Hoshi, Kazuhiro; Takeda, Takahiro; Yamada, Naohiro; Ohtake, Atsushi</b> Journal of Medicinal Chemistry, 2005, vol. 48, # 16 p. 5279 - 5294 Title/Abstract Full Text View citing articles Show Details

# 若不使用 atom mapping

找到 3158 個反應，但官能基的位置可能不同

Yield	Conditions	References
 94%	<p>With methanol; sodium methylate T=20°C; 0.33333 h; Show Experimental Procedure</p>	<p>Meiji Seika Kaisha, Ltd. Patent: EP1970377 A1, 2008 ; Location in patent: Page/Page column 48 ;</p>
	 Synthesize  Find similar	 Synthesize  Find similar
		<a href="#">Rx-ID: 27887377</a> <a href="#">Find similar reactions</a>

# 合金搜尋

輸入元素成份搜尋合金、陶瓷複合材料  
例如鈦合金 Ti-6Al-4V、貴金屬催化劑 Pd/C、  
陶瓷材料Yttria(y2o3)/Zirconia Ceramics (ZrO2)

Alloy

合金成分	合金比例(範圍)
Component Formula	Percentage
Ti Fe or Fe2O3	Number or range: 20 or 20-40
Al	
V	
Percentage Type: <input type="button" value="▼"/>	Additional Components: <input type="checkbox"/> 是否允許含有其他成分

合金成分比例單位

# 分子式搜尋

不完整分子式，例如只知道包含 34 個碳，輸入 C34\*

多種分子數量組合，例如  $\text{Fe}_x\text{O}_y$ ,  $X=2,3$   $Y=2-4$

不同元素比例固定，例如  $\text{C}_n\text{H}_{2n}$ ,  $n=2-4$

**Formula Builder**

Molecular Formula: **Fe[2-3]** X Use this Formula

1A	2A	3B	4B	5B	6B	7B	8B	9B	10B	1B	2B	3A	4A	5A	6A	7A	8A	
1	H																He	
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg																
4	K	Ca	Sc	Ti	V	Cr	Mn	<b>Fe</b>	Co									
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh									
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir									
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									
			Ce	Pr	Nd	Pm	Sm	Eu										
			Th	Pa	U	Np	Pu	Am										

Selected Element definition:

Fe

2

3

Charge(s)

Count(s)

**Add**

**7 Nitrogen**  
**N**

Configuration [He] 2s<sup>2</sup> 2p<sup>3</sup>  
Isotopes <sup>14</sup>N <sup>15</sup>N  
Density (kg/m<sup>3</sup>) 1.251

**14.0067**

0 ▲ more element(s)  
▼ with arbitrary count  
Any more  
elements with any counts

Special groups:

Me
Et
Ph

Note: it's also possible to enter

- ranges or enumerations defined via variables, e.g.  $\text{Fe}_x\text{O}_y$ ,  $x=2,3$   $y=2-4$
- Arithmetic terms, e.g.  $\text{C}_n\text{H}_{2n+2}$   $n=3,4,5$

Metalloids
Nonmetals
Other Nonmetals
Halogens
Noble Gases
Alkali Metals
Alkaline Earth Metals
Lanthanoids
Transition Metals
Post Transition Metals

# 分子式搭配其它欄位搜尋

分子式：氧化鋯  $\text{ZrO}[1-2]$

用途：牙科材料

**Molecular Formula**

Molecular Formula  [Lookup](#) [X](#) [Formula Builder](#)

**Use/Application**

Use Pattern  [Lookup](#) [X](#)

[Show AND Buttons](#)

Structure	Structure/Compound Data	Nº of preparations <a href="#">All Preps</a>   <a href="#">All Reactions</a>	Available Data	Target	Nº of ref.
$\text{O}_2\text{Zr}$   <a href="#">Synthesize</a>   <a href="#">Hide Details</a> <a href="#">Find similar</a>	<p><b>Chemical Name:</b> zirconium oxide</p> <p><b>Reaxys Registry Number:</b></p> <p><b>CAS Registry Number:</b> 744</p> <p><b>Type of Substance:</b> Glass or compoundSolid solution</p> <p><b>Molecular Formula:</b> <math>\text{O}_2\text{Zr}</math></p> <p><b>Linear Structure Formula:</b></p> <p><b>Molecular Weight:</b> 123.223</p> <p><b>InChI Key:</b> YYTCNKUFARLLT</p> <p><b>Chemical Names and Synonyms</b></p> <p>zirconium oxide, zirconia, <math>\text{ZrO}_2</math>, zirconium oxide meso</p> <p><b>Hit Data</b></p> <p>Use ( 53 Hits out of 515 <a href="#">view all</a> )</p>	<p>Use Pattern</p> <p>conventional particulate filler for fiber-reinforce composites used for <a href="#">dental</a> applications</p> <p>conventional particulate filler for fiber-reinforce composites used for <a href="#">dental</a> appliances</p> <p>conventional particulate filler for fiber-reinforce composites used for <a href="#">dental</a> cavity fillings</p> <p>conventional particulate filler for fiber-reinforce composites used for <a href="#">dental</a> core composites</p> <p>conventional particulate filler for fiber-reinforce composites used for <a href="#">dental</a> provisional crown and bridge composites</p>	<p>Reference</p> <p>STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract <a href="#">Full Text</a> <a href="#">Show Details</a></p> <p>STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract <a href="#">Full Text</a> <a href="#">Show Details</a></p> <p>STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract <a href="#">Full Text</a> <a href="#">Show Details</a></p> <p>STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract <a href="#">Full Text</a> <a href="#">Show Details</a></p> <p>STICK TECH OY Patent: WO2008/917 A1, 2008 ; Title/Abstract <a href="#">Full Text</a> <a href="#">Show Details</a></p>		

# 物化特性搜尋範例

搜尋包含34個碳，旋光度=18.2，且萃取自天然物的所有化合物

搭配分子式搜尋  
C34\* 表示此分子含有34個碳，其餘未知

Molecular Formula

Molecular Formula  Lookup Formula Builder

Physical Data

Optical Rotatory Power (deg) =

Show AND Buttons

選擇旋光度  
optical rotatory power (deg)  
選擇 = 輸入 18.2

Natural Product

Isolation from Natural Pro...  exists

Show AND Buttons

天然物來源

Add to Query: Structure Molecular Formula Alloy Add/Remove Fields...

新增其它欄位

# Reaxys 搜尋結果分析及輸出

分析篩選搜尋結果，並輸出報告與同儕分享討論

搜尋結果

反應  
(Reactions)

化合物\*  
(Substances)

引用文獻  
(Citations)

合成路徑規畫

Synthesis Plans

資料庫連結



篩選功能：Analysis View 及 28 種 Filter

Filter by:  
Substructure

包裝價格資料

多元資料儲存或輸出方式

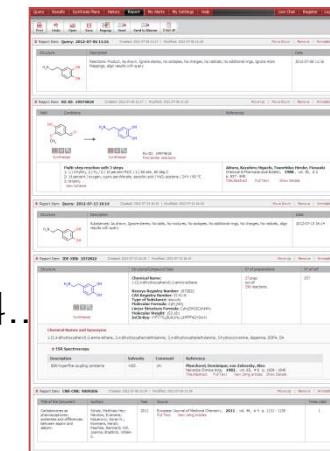
Report

檔案格式：E-mail、HTML網頁、PDF

可儲存：搜尋條件、化合物、反應、文獻、合成路徑

優點：適合儲存少量資料、操作簡便、格式簡明、保留超連結

- 彙整各種搜尋結果
- 一鍵 e-mail 分享



檔案格式：PDF、XML、Word、Excel、電子實驗記錄本、書目資料...

可儲存：化合物、反應、文獻、合成路徑

優點：可大量輸出搜尋結果、多種檔案格式可與進階分析軟體相容

Export

# Report – 快速比較多種反應式並與同儕分享

可儲存 XML 檔案或直接以 e-mail 分享搜尋結果

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Report Item: RX-ID: 27910026 Created: 2015-12-18 18:38 | Modified: 2015-12-18 18:42

Yield Conditions References

91% With 1,1'-carbonyldiimidazole; 4-(N,N-dimethylamino)pyridine in acetonitrile 5 - 6 h; Heating / reflux; Show Experimental Procedure

MATRIX LABORATORIES LTD Patent: WO2008/35378 A2, 2008 Location in patent: Page/Page column 6; Title/Abstract Full Text Show Details

Report Item: RX-ID: 29176469 Created: 2015-12-18 18:39 | Modified: 2015-12-18 18:42

Yield Conditions References

95% With ruthenium(IV) oxide; sodium periodate in dichloromethane; water; ethyl acetate T=40°C;

Yamamoto, Takeshi; Tokunaga, Etsuko; Nakamura, Shuichi; Shibata, Norio; Toru, Takeshi Chemical and Pharmaceutical Bulletin, 2010, vol. 58, # 1 p. 110 - 112 Title/Abstract Full Text View citing articles Show Details

Report Item: Synthesis Plan: Synthesis 8 Created: 2015-12-18 18:41 | Modified: 2015-12-18 18:42

Move Up | Move Down | Remove | Annotation

Hide Synthesis Plan

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可使用 autoplan 自動規劃、瀏覽反應條件、產量、包裝價格、並挑選符合需求的路徑輸出成報告

Report Item: Synthesis Plan: Synthesis 8    Created: 2015-12-18 18:41 | Modified: 2015-12-18 18:42    Move Up | Remove | Annotation

Hide Synthesis Plan

Hide Synthesis Details

Step	Yield	Conditions	References
1 Reaxys	34 mg	With ammonium cerium(IV) nitrate in acetonitrile T=20°C; 5 h;	<a href="#">Chang, Meng-Yang; Chang, Chung-Ho; Chen, Shui-Tein; Chang, Nein-Chen</a> <i>Journal of the Chinese Chemical Society</i> , 2002, vol. 49, # 3 p. 383 - 385 Title/Abstract   Full Text   View citing articles   Show Details
	34 mg	With ammonium cerium(IV) nitrate in water; acetonitrile 5 h;	<a href="#">Chang, Meng-Yang; Chen, Shui-Tein; Chang, Nein-Chen</a> <i>Synthetic Communications</i> , 2003, vol. 33, # 8 p. 1375 - 1382 Title/Abstract   Full Text   View citing articles   Show Details
2 Reaxys		With disodium hydrogenphosphate; sodium amalgam in methanol T=20°C; 1 h;	<a href="#">Chang, Meng-Yang; Chang, Chung-Ho; Chen, Shui-Tein; Chang, Nein-Chen</a> <i>Journal of the Chinese Chemical Society</i> , 2002, vol. 49, # 3 p. 383 - 385 Title/Abstract   Full Text   View citing articles   Show Details
		With sodium amalgam; sodium salt of phosphorous acid in methanol T=20°C; 1 h;	<a href="#">Chang, Meng-Yang; Chen, Shui-Tein; Chang, Nein-Chen</a> <i>Synthetic Communications</i> , 2003, vol. 33, # 8 p. 1375 - 1382 Title/Abstract   Full Text   View citing articles   Show Details

# Report – 透過 e-mail 快速分享搜尋結果

Report – 透過 e-mail 快速分享搜尋結果

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Bioactivities (206)		Reactions (11671)		Substances (94)		Targets (3)		Citations (12434)		go to Page	Page 1 of 1382	▶	▶
<input type="button" value="Limit to"/>	<input type="button" value="Exclude"/>	<input type="button" value="Export"/>	<input type="button" value="Print"/>	<input type="button" value="Zoom in"/>	<input type="button" value="Zoom out"/>	<input type="button" value="Hide"/>	Sort by	Relevance	<input type="button" value="▼"/>	<input type="button" value="▼"/>	<input type="checkbox"/> Exclude GOSTAR data		
1	Title of the Document	Authors	Year	Source								Times cited	
	Cleansing articles for skin and/or hair which also deposit skin care actives	The Procter and Gamble Company	2002	Patent: US6338855 B1, 2002 ; Patent Family: WO1998/18445 A1; WO1998/18446 A1; WO1998/52537 A1; WO1999/12519 A1; <a href="#">Full Text</a>									

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選擇檔案格式

Substances Grid  Substances Report Table  Substances Reactions Table

Choose format  PDF/Print  XML\*  RD File  
 Microsoft Word  Microsoft Excel\*  Electronic Lab Notebook

Literature Management Systems  
(e.g. ReferenceManager, EndNote etc.)

\* these export formats allow to export bioactivity data

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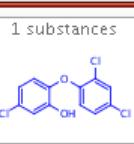
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Reaxys PubChem eMolecules

From History 1 substances

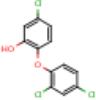


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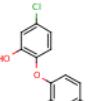
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