



ELSEVIER

## Reaxys 化學資料庫介紹

如何聰明的搜尋化學資料節省時間

**Ryan Huang 黃恪涵**

Life Science Solutions – Elsevier

[r.huang@elsevier.com](mailto:r.huang@elsevier.com)





ELSEVIER

OUR SHARED PURPOSE

TO ACCELERATE  
SCIENCE TO  
IMPROVE HEALTH

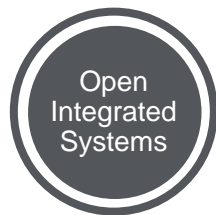
A Knowledge & Information  
Analytics Company



OUR PROMISE

Partners in propelling research  
and innovation forward to  
transform the way you bring  
new medicines to the world

OUR KEY DIFFERENTIATORS



140+

years of scientific  
knowledge curated as  
semantically rich content to  
enable tomorrow's medical  
breakthroughs

RELX

\$1.4bn  
on technology annually

~30,000  
employees

Serving customers in  
180+  
countries

Partnering with

90%

of top Pharma  
companies

# Reaxys 全國學術授權版本



NAR Labs 財團法人國家實驗研究院

科技政策研究與資訊中心

Science & Technology Policy Research and Information Center

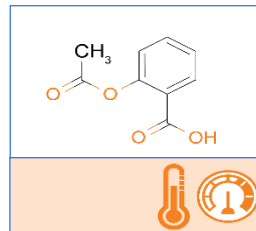
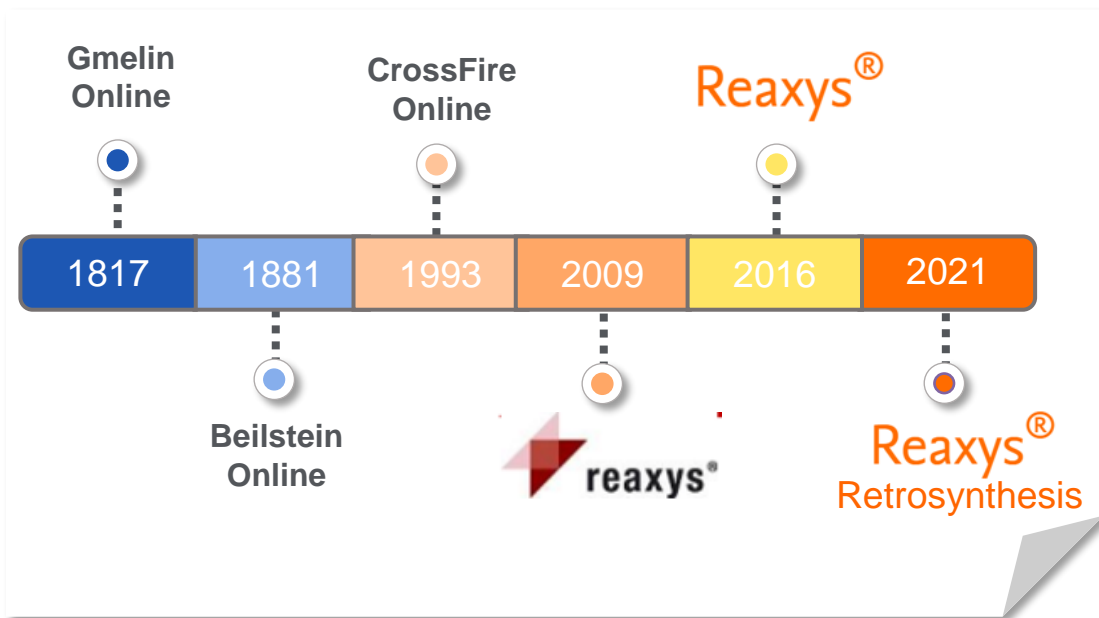
- 科技部科政中心贊助，授權設有化學、應化、藥學等大專院校限研究、教學使用
- 免費教育推廣、技術支援、網路自學資源
- Webinars網路會議分享化學研究新知
- 4/6 亞太區使用者大會



# Agenda

1. Reaxys是甚麼?
2. Reaxys如何取得?
3. 基本介面導覽
4. 如何學習結構搜尋? 
5. 如何學習搜尋物質的化學性質? Video by Professor Damon Ridley
6. 命名反應的手機APP  
7. 甚麼是逆合成?AI工具的演進
8. 網路自我學習資源 Youtube
9. 化學供應商資料庫

# Reaxys是充滿歷史與先進的化學資料庫



**>118 Million**  
有機、無機及有  
機金屬物質  
**>500 Million**  
公開實驗數據  
(物性、光譜、  
生物活性等)



**>49 Million**  
化學反應(反應條件、  
溶劑、催化劑及產  
率等)



**>54 M 文獻記錄**  
**>16,000 期刊, 專利**  
涉及有機化學, 材料  
化學, 生物醫藥, 地  
球科學, 工程等多種  
領域

# Reaxys提供關鍵的實驗數據，讓研究人員回答重要的研究問題

Journals, patents,  
conference  
proceedings



人工閱讀、擷取重要的”實驗數據  
結構、物理特性、光譜、製備反應、生物活性(藥物毒  
性、藥物靶點蛋白、藥物活性、細胞、動物試驗)

## 回答關鍵的研究問題:

- 具有美白功能的天然萃取物質有哪些?證據在哪裡?實驗室萃取的X物質是有人報導過的嗎?
- 能夠有抗病毒活性的化合物長甚麼樣子? 我們實驗室的化合物值得拿來發展藥物嗎?
- 我的研究所題目有人做過類似的實驗嗎?有其他的應用被發表嗎?
- 我要合成一個目標分子才能繼續做實驗?怎麼辦?該怎麼找參考文獻?

# 如何連上Reaxys

在學校IP範圍內，打開瀏覽器鍵入 <http://www.reaxys.com>

Reaxys® Quick search History Alerts Ryan Huang Import

點擊X跳過註冊視窗

**Welcome to Reaxys**

Ready to take the shortest path from chemistry question to relevant answer? Reaxys gives you the best means to explore the world of chemistry.  
To learn more visit our [support hub page](#).

**Create your account or sign in to access all these features!**

- Create alerts & save searches
- Reduce timeouts
- Customize structure editor settings and layout

No Thanks Sign-in Register

Content Overview | Latest update: 11. September 2019 >

118M 49M 59M 37M 1.5M  
Substances

Reaxys使用瀏覽器Cookies來強化您的使用體驗



ELSEVIER

# Reaxys 介面導覽

學習展示要點





# 快速搜尋 – 研究學習的第一步

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang



Search substances, reactions, documents and bioactivity data

Import

in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Search Reaxys

Find >

Substance Effect, e.g. anticoagulant

AND



Draw

- 關鍵字查詢文獻
- 關鍵字查詢物質

結構編輯器

- 如何畫結構搜尋物質
- 如何搜尋核心骨架、相似結構 (Scaffold, Core structure)
- ChemDraw相容 (複製&貼上)

Content Overview | Latest update: 29. September

157M

56M

68M

Substances

Reactions

Documents

ELSEVIER

Copyright © 2021 Elsevier Life Sciences IP Limited.

Remote access

Terms and Conditions

Privacy policy

About content

RELX Group™

Feedback



ELSEVIER

# 預覽頁面

Reaxys®

[Quick search](#)

[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)



















Ryan Huang 



Results for Simvastatin

New  Edit 

實驗數據

	323	Substances	Structure :  as drawn <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> ▾	<a href="#">View Results</a> >
	37,538	Documents	Titles, Abstracts, Keywords : "Simvastatin" <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> ▾	<a href="#">View Results</a> >
	3	Commercial Substances	Structure :  as drawn <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> ▾	<a href="#">View Results</a> >
	22	Targets	Target(s) : hmg-coa reductase <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> ▾	<a href="#">View Results</a> >
	70	Reactions	Reaction Query :  as drawn <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> ▾	<a href="#">View Results</a> >

生物靶點

反應、合成方法



ELSEVIER

# 進階搜尋 Query Builder

- 天然萃取物搜尋
- NMR圖譜的搜尋
- 有機反應條件的進階搜尋

Reaxys

Quick search **Query builder** Results Retrosynthesis History Alerts

Ryan Huang

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Patent Assignee Structure Molecular Formula CAS RN TI, AB & KW

Structure

Nc1ccncc1

As drawn

AND

NMR Spectroscopy  Find any Show fields (Description...Original Text)

Search fields

Fields Forms History

Topics and Keywords

Identification

Physical Properties

Spectra

MedChem

Other

Reactions

Bibliography

AND  
OR  
NOT

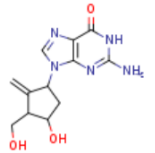
自行組合搜尋條件 (例如結合結構+NMR圖譜)

超過百種搜尋條件

# 逆合成面板 (規劃合成路徑、合成材料與反應條件)

Reaxys® Quick search Query builder Results **Retrosynthesis** History Alerts Ryan Huang

Draw new structure

No.	Date/Time	Project name		No. of routes
5581	30 Sep 2021 11:22	Project #5581		Predicted <span style="width: 100px; height: 10px; background-color: #90EE90; display: inline-block;"></span> In progress Published <span style="border: 1px solid blue; border-radius: 50%; padding: 2px 5px;">1</span> <a href="#">View &gt;</a>
5319	29 Sep 2021 05:43	Project #5319		Predicted <span style="width: 100px; height: 10px; background-color: #ccc; display: inline-block;"></span> Published <span style="border: 1px solid blue; border-radius: 50%; padding: 2px 5px;">4</span> <a href="#">View &gt;</a>

找到文獻報導的合成計畫

- 如何查詢、比較合成計畫
  - 自訂合成計畫
  - 預估合成計畫的成本
  - 學習利用AI工具來輔助設計創新化合物的合成策略
  - 儲存、資料匯出
- (需登入個人帳號)



ELSEVIER

# Quick Search

關鍵字查詢文獻



# Quick Search 關鍵字查詢文獻

Reaxys

Quick search Query builder <sup>New</sup> Results Synthesis planner History Alerts

Ryan Huang

Search for 184475-35-2 [Import](#)

Search Reaxys

184475-35-2 [Find >](#)

Documents, e.g. published by Schrock

AND

Draw

**鈣鈦礦太陽能電池**  
**Perovskite Solar Cell**

Content Overview | Latest update: 11. September 2019 >

118M	49M	59M	37M	1.5M
Substances	Reactions	Documents	Bioactivities	Targets

# Quick Search 關鍵字查詢文獻

Reaxys

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang  

Results for Perovskite solar cell



New  Edit 



14,952

Documents

Titles, Abstracts, Keywords : "Perovskite", "solar", "cell"

Edit in Query Builder  Create Alert 

Preview Results 

View Results 



27,489

Documents

Titles, Abstracts, Keywords : "Perovskite", "solar"

Edit in Query Builder  Create Alert 

Preview Results 

View

**“Perovskite Solar Cell”**  
利用前後””限制搜尋範圍

Reaxys

Quick search



Query builder

Results

Retrosynthesis

History

Alerts

Ryan Huang  

Results for "Perovskite solar cell"



New  Edit 



6,561

Documents

Titles, Abstracts, Keywords : "Perovskite solar cell"

Edit in Query Builder  Create Alert 

Preview Results 

View Results 



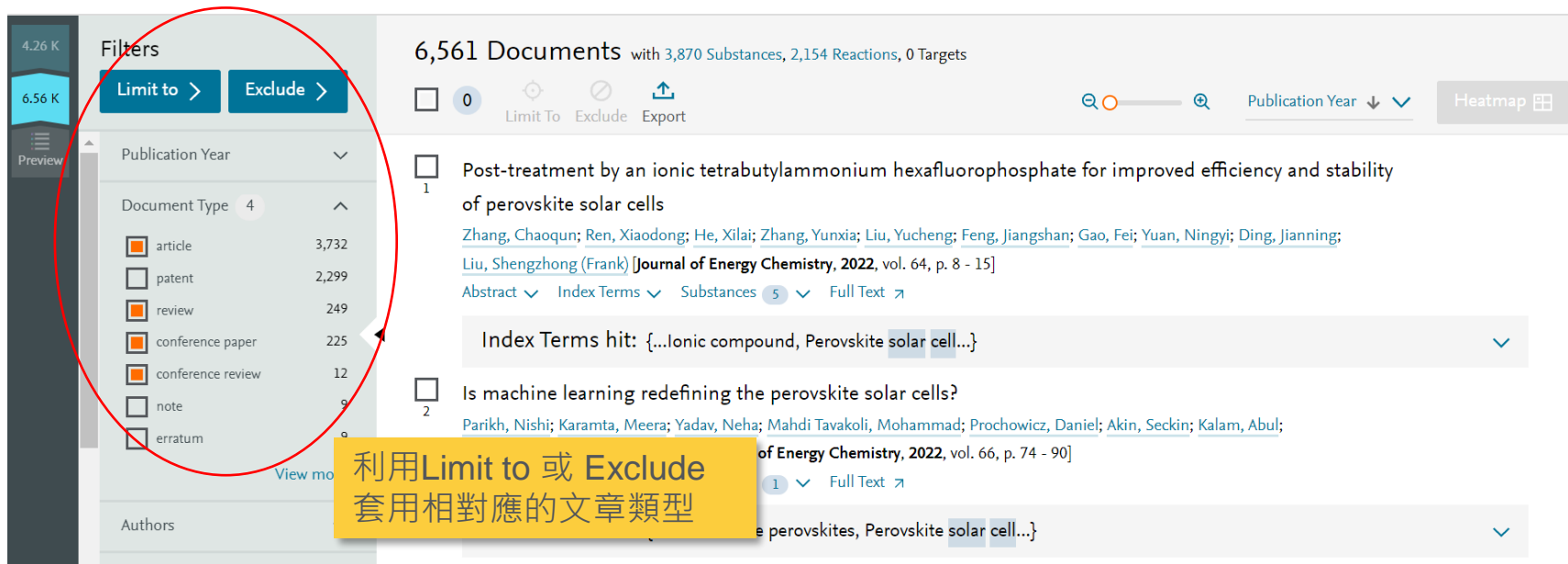
# Quick Search 關鍵字查詢文獻

- 文章類型篩選 (Reaxys包含學術期刊與全世界105個專利局化學專利資料)

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  



The screenshot shows the Reaxys search results interface. On the left, a sidebar contains filters for 'Publication Year' and 'Document Type'. The 'Document Type' filter is expanded, showing options like 'article' (3,732), 'patent' (2,299), 'review' (249), 'conference paper' (225), 'conference review' (12), 'note' (9), and 'erratum' (0). A red circle highlights this sidebar. The main content area shows 6,561 documents with 3,870 substances, 2,154 reactions, and 0 targets. Two search results are visible, each with an 'Index Terms hit' box. A yellow callout box with the text '利用Limit to 或 Exclude 套用相對應的文章類型' (Use Limit to or Exclude to apply corresponding document types) points to the 'Limit to' and 'Exclude' buttons in the filters sidebar.

4.26 K  
6.56 K  
Preview

Filters

Limit to > Exclude >

Publication Year

Document Type 4

- article 3,732
- patent 2,299
- review 249
- conference paper 225
- conference review 12
- note 9
- erratum 0

View more

Authors

6,561 Documents with 3,870 Substances, 2,154 Reactions, 0 Targets

0 Limit To Exclude Export

Publication Year Heatmap

1 Post-treatment by an ionic tetrabutylammonium hexafluorophosphate for improved efficiency and stability of perovskite solar cells  
Zhang, Chaoqun; Ren, Xiaodong; He, Xilai; Zhang, Yunxia; Liu, Yucheng; Feng, Jiangshan; Gao, Fei; Yuan, Ningyi; Ding, Jianing; Liu, Shengzhong (Frank) *Journal of Energy Chemistry*, 2022, vol. 64, p. 8 - 15  
Abstract Index Terms Substances 5 Full Text

Index Terms hit: {...Ionic compound, Perovskite solar cell...}

2 Is machine learning redefining the perovskite solar cells?  
Parikh, Nishi; Karamta, Meera; Yadav, Neha; Mahdi Tavakoli, Mohammad; Prochowicz, Daniel; Akin, Seckin; Kalam, Abul; ... *Journal of Energy Chemistry*, 2022, vol. 66, p. 74 - 90  
1 Full Text

perovskites, Perovskite solar cell...



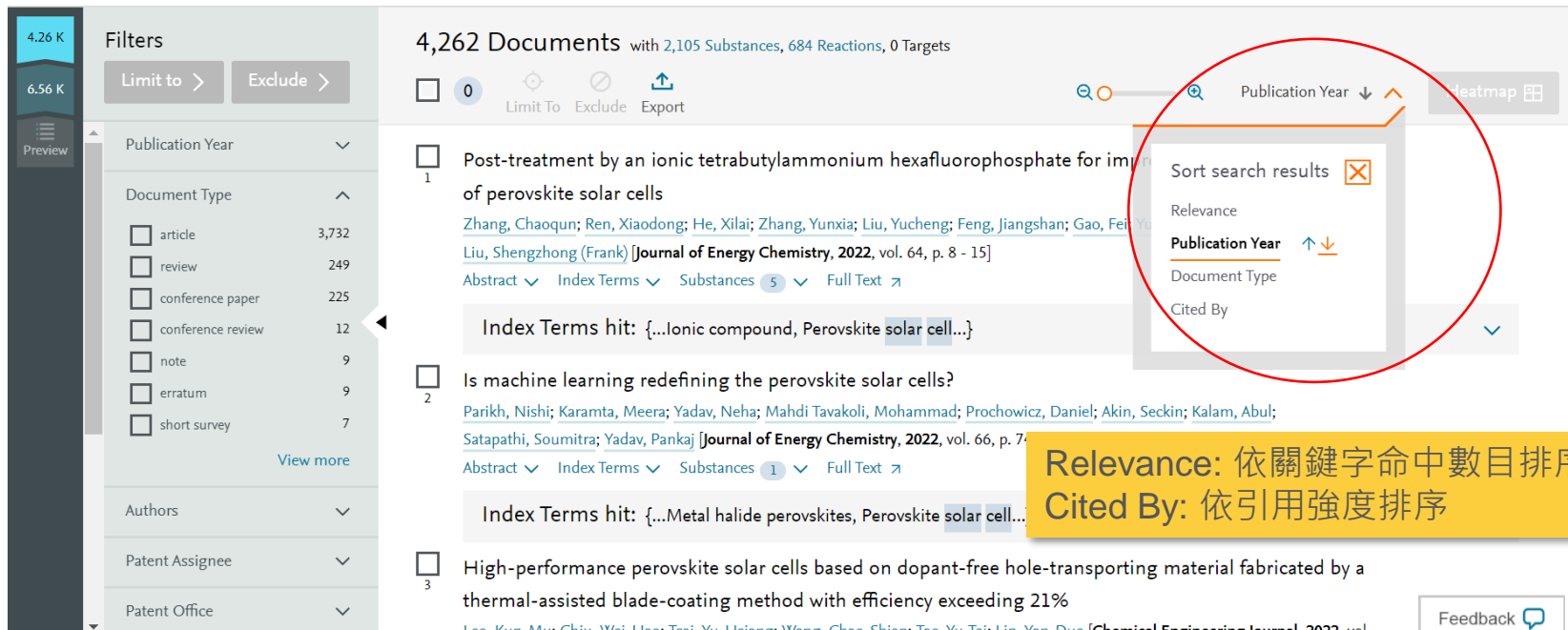
# Quick Search 關鍵字查詢文獻

## - 文章排序

Reaxys®

Quick search Query builder **Results** Retrosynthesis History Alerts

Ryan Huang  




4,262 Documents with 2,105 Substances, 684 Reactions, 0 Targets

0 Limit To Exclude Export

Publication Year ↓

Heatmap


Sort search results 

- Relevance
- Publication Year** ↑↓
- Document Type
- Cited By

1 Post-treatment by an ionic tetrabutylammonium hexafluorophosphate for improved performance of perovskite solar cells  
Zhang, Chaoqun; Ren, Xiaodong; He, Xilai; Zhang, Yunxia; Liu, Yucheng; Feng, Jiangshan; Gao, Fei; Yu, Shengzhong (Frank) [Journal of Energy Chemistry, 2022, vol. 64, p. 8 - 15]  
Abstract Index Terms Substances 5 Full Text  
Index Terms hit: {...Ionic compound, Perovskite solar cell...}

2 Is machine learning redefining the perovskite solar cells?  
Parikh, Nishi; Karamta, Meera; Yadav, Neha; Mahdi Tavakoli, Mohammad; Prochowicz, Daniel; Akin, Seckin; Kalam, Abul; Satapathi, Soumitra; Yadav, Pankaj [Journal of Energy Chemistry, 2022, vol. 66, p. 7-12]  
Abstract Index Terms Substances 1 Full Text  
Index Terms hit: {...Metal halide perovskites, Perovskite solar cell...}

3 High-performance perovskite solar cells based on dopant-free hole-transporting material fabricated by a thermal-assisted blade-coating method with efficiency exceeding 21%  
Lee, Kun-Mu; Chiu, Wei-Hao; Tei, Yu-Heian; Wang, Chao-Shan; Tao, Yu-Tai; Lin, Yen-Duo [Chemical Engineering Journal, 2022, vol. 428, p. 132-141]  
Abstract Index Terms Substances 1 Full Text

Feedback 

Relevance: 依關鍵字命中數目排序  
Cited By: 依引用強度排序

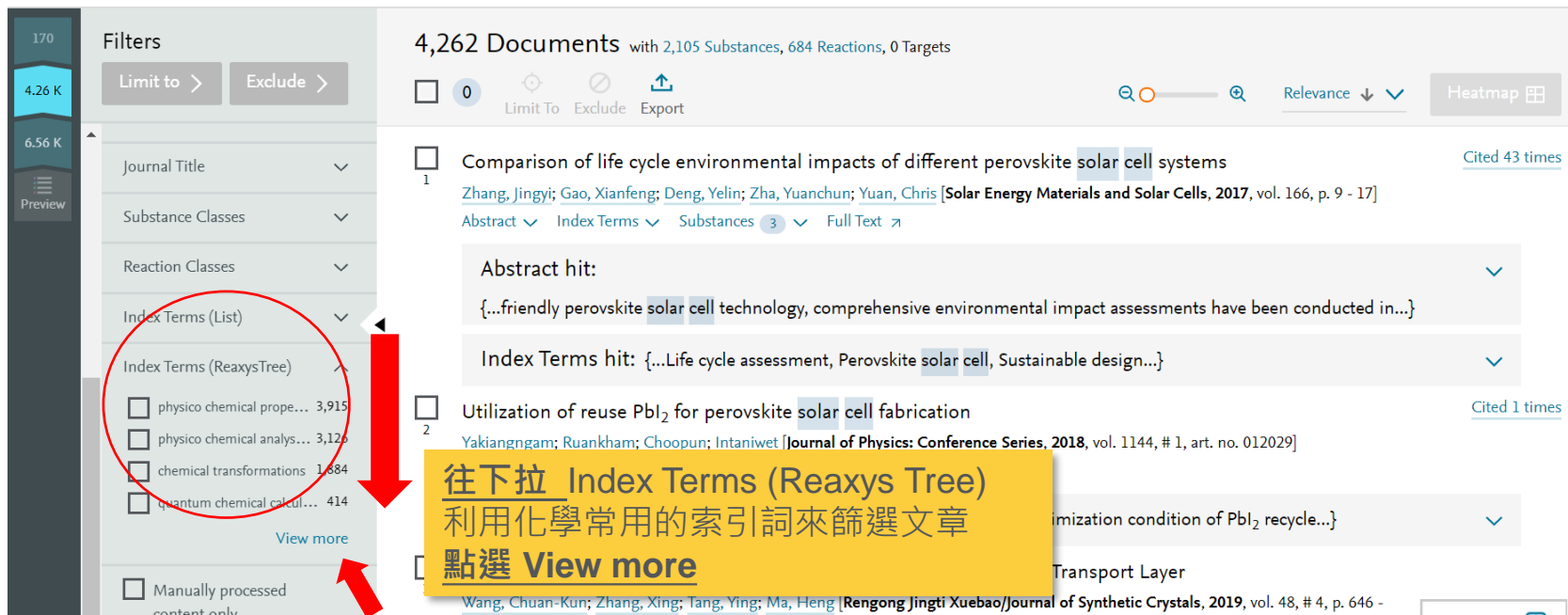
# Quick Search 關鍵字查詢文獻

## - 索引詞篩選 (Index Terms Reaxys Tree)

Reaxys®

Quick search Query builder **Results** Retrosynthesis History Alerts

Ryan Huang  



170

4.26 K

6.56 K

Preview

Filters

Limit to > Exclude >

Journal Title

Substance Classes

Reaction Classes

Index Terms (List)

Index Terms (ReaxysTree)



- physico chemical prope... 3,915
- physico chemical analys... 3,126
- chemical transformations 1,884
- quantum chemical calcul... 414

View more

Manually processed content only

4,262 Documents with 2,105 Substances, 684 Reactions, 0 Targets


0 Limit To Exclude Export

Relevance  Heatmap 


1 Comparison of life cycle environmental impacts of different perovskite solar cell systems [Cited 43 times](#)

[Zhang, Jingyi; Gao, Xianfeng; Deng, Yelin; Zha, Yuanchun; Yuan, Chris](#) [Solar Energy Materials and Solar Cells, 2017, vol. 166, p. 9 - 17]

[Abstract](#) [Index Terms](#) [Substances](#) (3) [Full Text](#) [↗](#)


Abstract hit: 

{...friendly perovskite solar cell technology, comprehensive environmental impact assessments have been conducted in...}

Index Terms hit: {...Life cycle assessment, Perovskite solar cell, Sustainable design...} 

2 Utilization of reuse PbI<sub>2</sub> for perovskite solar cell fabrication [Cited 1 times](#)

[Yakiangngam; Ruankham; Choopun; Intaniwet](#) [Journal of Physics: Conference Series, 2018, vol. 1144, # 1, art. no. 012029]

optimization condition of PbI<sub>2</sub> recycle...} 

Transport Layer

[Wang, Chuan-Kun; Zhang, Xing; Tang, Ying; Ma, Heng](#) [Rengong Jingti Xuebao/Journal of Synthetic Crystals, 2019, vol. 48, # 4, p. 646 -

# Quick Search 關鍵字查詢文獻

## - 索引詞篩選 (Index Terms Reaxys Tree)

Index Terms (ReaxysTree) 3221

- Index Terms (ReaxysTree) 4,262
  - physico chemical properties 3,915
    - electrical property 3,461
      - permittivity 719
      - electrical conductivity 329
      - piezoelectricity 48
      - photovoltaic effect 3,221
      - photoelectricity 545
      - resistivity 252
      - ferroelectricity 202
      - photoconductivity 104
      - thermoelectricity 56

Selected search items:

photovoltaic effect

Index Terms (ReaxysTree) 170

- Index Terms (ReaxysTree) 4,262
  - physico chemical properties 3,915
  - physico chemical analysis methods 3,126
    - spectroscopical analysis 2,433
    - separation method 1,652
    - crystal structure determination 1,255
    - microscopy 946
      - scanning probe microscopy 796
      - electron microscopy 242
        - transmission electron microscopy 170
        - scanning electron microscopy 66
      - optical microscopy 31
    - electro analytical method 287

Selected search items:

transmission electr...



ELSEVIER

# Quick Search

## 結構搜尋



# Quick Search 結構搜尋

Reaxys®

Quick search


Query builder

Results

Retrosynthesis


History

Alerts

Ryan Huang 



Search substances, reactions, documents and bioactivity data

Import 

in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Search Reaxys

Find >


Substance Effect, e.g. [anticoagulant](#)

AND


 Draw

Content Overview | Latest update: 29. September 2021 >


157M

 Substances


56M

 Reactions

68M

 Documents

41M

 Bioactivities




ELSEVIER

# MarvinJS 結構編輯器

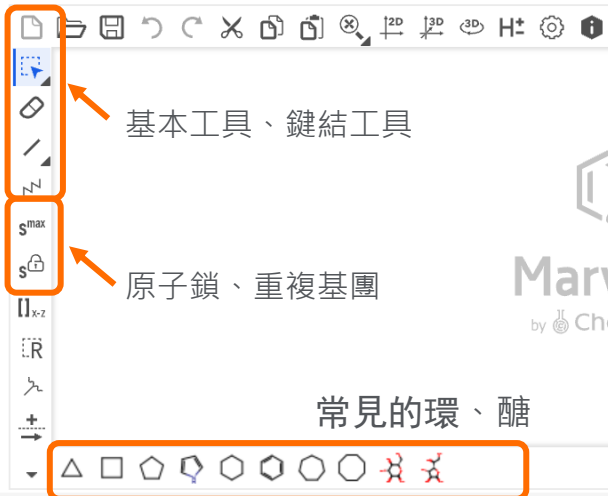
Reaxys<sup>®</sup>

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >



基本工具、鍵結工具

原子鎖、重複基團

常見的環、醣

元素週期表與  
原子列表

原子屬性  
定義工具



R  
A  
H  
C  
N  
O  
S  
F

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear 

Cancel 

Transfer to query >

# 絕對結構搜尋 As drawn

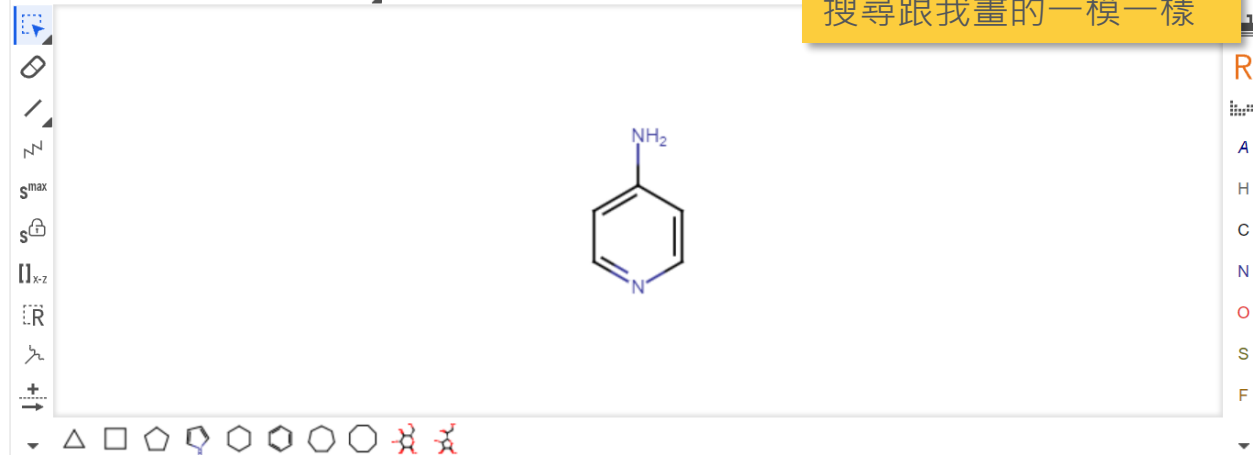
Reaxys<sup>®</sup>

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >





搜尋跟我畫的一模一樣

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

容許：  
異構物  
鹽  
同位素  
離子型態  
混合物


Clear  Cancel  Transfer to query >



# 相似結構搜尋 As substructure

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >

Search this structure as:

- As drawn
- As substructure
- On all atoms
- On heteroatoms

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

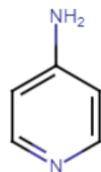
Salts

Mixtures

Isotopes

Charges

我畫的結構為核心結構  
在“所有氫原子沒有畫出  
來的地方”容許取代基



Clear 

Cancel 

Transfer to query >



# 相似結構搜尋 $S^{\text{lock}}$ & $S^{\text{max}}$

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang

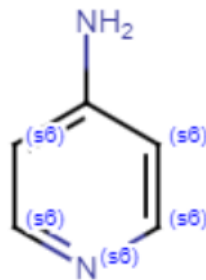
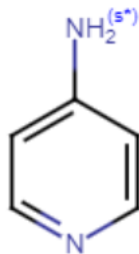
Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >

Search this structure as:

- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts

$S^{\text{max}}$   
  $S^{\text{lock}}$   
  $S^{\text{lock}}$   
  $S^{\text{lock}}$   
  $S^{\text{lock}}$



用 As substructure 開放所有位置取代基  
搭配  $S^{\text{lock}}$  把不要的地方鎖起來

用 As drawn  
搭配  $S^{\text{max}}$  把發生取代的地方打開

Clear

Cancel

Transfer to query >


Charges



# 不定位鍵的使用

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >

Search this structure as:

As drawn

As substructure

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

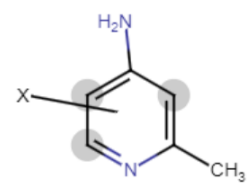
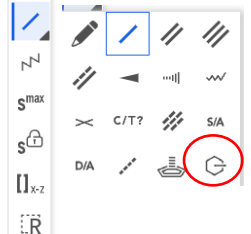
Charges

Radicals



+ More options

1

4



1. 點選選擇工具
2. 按住鍵盤Shift
3. 左鍵選擇不定位鍵可以出現的位置
4. 選擇不定位鍵

Clear  Cancel  Transfer to query >

[\(151\) Reaxys 結構編輯器 - 不定位鍵 - YouTube](#)



# 更多關於結構編輯器的進階技巧

[\(151\) Reaxys 結構編輯器 - 縮寫官能基團 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 原子屬性列表 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - G 任意官能基工具定義 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - R 基團與末端定義工具 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 原子列表與原子列表非 - YouTube](#)

[\(151\) Reaxys 結構編輯器 - 鹽類與同位素 - YouTube](#)



# 訂閱Elsevier Taiwan 自學線上資源

YouTube TW taiwan elsevier

Elsevier Taiwan 台灣愛思唯爾  
782 位訂閱者 · 202 部影片  
台灣愛思唯爾，旗下商品(包括系統)之活動、教學及宣傳影片。

訂閱

Elsevier Taiwan  
416 位訂閱者 · 235 部影片  
Elsevier 是一家全球首創經營科學、技術和醫學資訊產品及出版服務的出版商，透過與世界各國的科技與醫學機構的合作，每年...

已訂閱

Reaxys - 基本介紹  
觀看次數：10次 · 1 週前  
Elsevier Taiwan  
本影片作者為Sam Yu - Elsevier 大中華區Reaxys 專業講師如您對Reaxys 的搜尋有任何問題，歡迎與我們...

YouTube TW taiwan elsevier

Reaxys 線上教育訓練  
22 部影片 · 觀看次數：9次 · 昨天更新

本系列影片作者為 Sam Yu - Elsevier 大中華區 Reaxys 專業講師。如您對 Reaxys 的搜尋有任何問題，歡迎與我們聯繫  
taiwan.marketing@elsevier.com

Elsevier Taiwan 已訂閱

- 1 Reaxys - 基本介紹  
Elsevier Taiwan 4:56
- 2 Reaxys - 快速搜尋  
Elsevier Taiwan 11:38
- 3 Reaxys - 進階搜尋  
Elsevier Taiwan 8:15
- 4 Reaxys - 註冊個人帳號  
Elsevier Taiwan 14:46
- 5 Reaxys 結構編輯器 - 基本介紹  
Elsevier Taiwan 2:42

Reaxys 結構編輯器 - 不定位鍵

無廣告、持續更新中



<https://www.youtube.com/playlist?list=PLBSTWuNnJAl4laTo5zNkqaJ9va-LUtj0>



# 應用案例- 新穎性搜尋Novelty Search

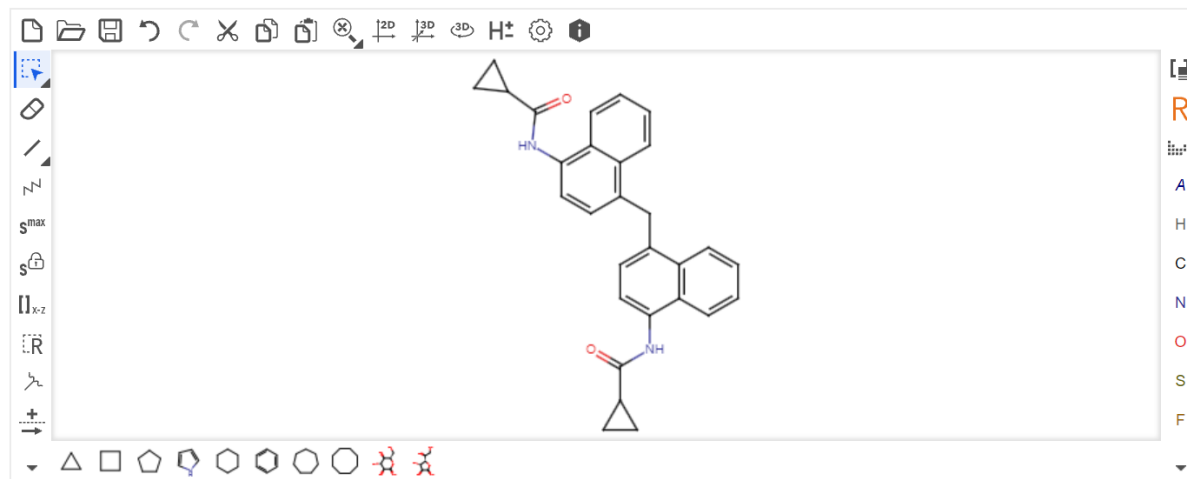
Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang  

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >



Search this structure as:

- As drawn
- As substructure
- Similar
  - Tautomers
  - Stereo
  - Additional ring closures
  - Related Markush
  - Salts
  - Mixtures
  - Isotopes
  - Charges
  - Radicals



O=C(NC1=CC=C(CC2=C3C=CC=CC3=C(NC(=O)C3CC3)C=C2)C2=C1C=CC=C2)C1CC1



ELSEVIER

# Substance Page

物質數據整理



# 預覽頁面選擇Substances

## Results for Simvastatin

New Edit

	323	Substances	Structure :  as drawn Edit in Query Builder  Create Alert	Preview Results	<b>View Results &gt;</b>
	37,538	Documents	Titles, Abstracts, Keywords : "Simvastatin" Edit in Query Builder  Create Alert	Preview Results	View Results >
	3	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert	Preview Results	View Results >

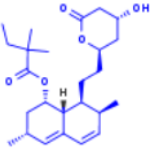
# Reaxys人工擷取重要的實驗數據，並保留原始文獻出處

## - 物理性質、光譜

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Search Sort by No of References Grid Heatmap

1



**simvastatin**  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 123049-81-0, 79902-63-9

Identification

Druglikeness

Bioactivity (All)

Physical Data - 94

Spectra - 96

Other Data - 3,152

Preparations - 49 >

Reactions - 161 >

Targets - 165 >

Documents - 12,211 >

這個物質有哪些物理特性已經被報導過了？



# Reaxys人工擷取重要的實驗數據，並保留原始文獻出處

## - 物理性質、光譜

Solubility, g·l <sup>-1</sup>	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					water, soluble in organic solvents	<a href="#">[Macromolecular Bioscience, 2014, vol. 14, # 11, p. 1530 - 1506]</a> Full Text ↗ Cited 27 times ↗ Details > Abstract >
6.73904	in pure solvent		aq. phosphate buffer	supporting information		<a href="#">Chung, Sanny S. W.; Cuellar, Rebecca A. D.; Wang, Xiangyuan; Reczek, Peter R.; Georg, Gunda I.; Wolgemuth, Debra J.[ACS Medicinal Chemistry Letters, 2013, vol. 4, # 5, p. 446 - 450]</a> Full Text ↗ Cited 8 times ↗ Details > Abstract >
15	in solution	25	aq. phosphate buffer			<a href="#">Ambike, Anshuman A.; Mahapatra, Sankar K.; Ghosh, Sankar K.[Journal of Pharmaceutical Sciences, 2005, vol. 22, # 6, p. 990 - 998]</a> Full Text ↗ Cited 149 times ↗ Details > Abstract >
7.3E-05	in pure solvent	25	H2O			<a href="#">Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350]</a> Full Text ↗ Details > Abstract >
79.55	in pure solvent	25	propan-2-ol			<a href="#">Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350]</a> Full Text ↗ Details > Abstract >
19.09	in pure solvent	25	diethyl ether			<a href="#">Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002, vol. 25, # 3, p. 346 - 350]</a> Full Text ↗ Details > Abstract >

提供原始文獻連結

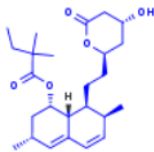
# Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 專利出處、純化方法、專利名稱

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations 🔍 🔍 Sort by No of References ↓ Grid Heatmap

1



[View related Markush](#)

**simvastatin**  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 123049-81-0, 79902-63-9

Identification Bioactivity (All) Spectra - 96

Druglikeness Physical Data - 94 Other Data - 3,152

Preparations - 49 >

Reactions - 161 >

Targets - 165 >

Documents - 12,211 >

這個物質是否有相關的專利文件報導?

搜尋涵蓋此結構的專利結構式

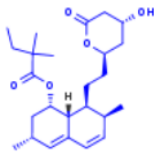
# Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

## - 合成反應 & 購物車

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Sort by No of References Grid Heatmap

1



**simvastatin**  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 123049-81-0, 79902-63-9

Identification	Bioactivity (All)	Spectra - 96
Druglikeness	Physical Data - 94	Other Data - 3,152

- Preparations - 49
- Reactions - 161
- Targets - 165
- Documents - 12,211

這個物質哪裡買？  
多少錢？

我該如何合成這個化合物？

# Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

## - 生物活性應用

熱圖分析

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References

Grid Heatmap

**simvastatin**  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 123049-81-0, 79902-63-9

Identification  
Druglikeness  
Bioactivity (All)  
Physical Data - 94  
Spectra - 96  
Other Data - 3,152  
Preparations - 49  
Reactions - 161  
Targets - 165  
Documents - 12,211

- 有哪些生物活性已經被報導過？
- 是否有毒性？有哪些實驗已經證實？
- 如果我要進行細胞試驗？有哪些細胞株已經測試過？從哪個濃度開始較為適當？
- 有哪些蛋白質被報導與此物質有作用？

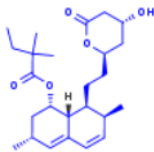
# Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處

- 天然萃取物、應用

323 Substances out of 12,342 Documents, containing 177 Reactions, 175 Targets Reaxys - 323

0 selected Limit To Exclude Export Preparations Sort by No of References Grid Heatmap

1



**simvastatin**  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 123049-81-0, 79902-63-9

Identification Bioactivity (All)  
Druglikeness Physical Data - 94

Spectra - 96  
Other Data - 3,152

Preparations - 49  
Reactions - 161  
Targets - 165  
Documents - 12,211

**Other Data - 3152**

- ✓ Use - 3149
- ✓ Isolated from Natural Source - 1

化合物的用途？  
從天然物萃取的證據？

# 如何訓練學生學習用資料庫尋找化學關鍵資訊



ELSEVIER

About Elsevier

Products & Solutions

Services

Shop & Discover

Search



↓ [Download the infographic](#) for practical insights about this topic, or watch the full webinar below to hear Professor Damon Ridley, a recognized expert in chemical information retrieval, share his views on the challenges of finding properties of substances and how Reaxys and other chemistry databases enable this type of search.



[Finding physical and chemical properties of substances in Reaxys and other chemistry databases – Webinar and Infographic \(elsevier.com\)](#)



ELSEVIER



ELSEVIER

# Reactions Search

反應式查詢



# 您可以用各種方式搜尋Reaction

1. 從物質資訊頁面連結到製備方式
2. 關鍵字搜尋、命名反應搜尋 (例如 Suzuki coupling)
3. 畫出反應式搜尋





# 方法一、由物質頁面連結到製備方式 Preparation

1

**BPA**  
O=C(O)C(C)(C)C1=CC=C(O)C=C1 228.291 1107700 80-05-7

Identification      Physical Data - 346  
Druglikeness      Spectra - 139  
Bioactivity (All)      Other Data - 470

Preparations - 98 >  
Reactions - 1,366 >  
Targets - 157 >  
Documents - 13,432 >

只出現在產物

可出現在產物或起始物

99 Reactions out of 236 Documents containing 132 Substances, 436 Targets

Reaxys - 99

0 selected Limit To Exclude Export Syn-Plan Show Conditions

Sort by Reaxys Ranking

1

4 Conditions Find Similar Reaction ID: 46083924

2

1 Conditions Find Similar Reaction ID: 44100782

1,402 Reactions out of 1,138 Documents containing 1,923 Substances, 1,080 Targets

Reaxys - 1,402

0 selected Limit To Exclude Export Syn-Plan Show Conditions

Sort by Reaxys Ranking

1

8 Conditions Find Similar Reaction ID: 70732

2

4 Conditions Find Similar Reaction ID: 46083924

# 方法二、直接輸入反應關鍵字或是命名反應

Reaxys®

[Quick search](#)


[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

Ryan Huang 



Search for "radical cyclization"

Import 

Search Reaxys

"radical cyclization"



Find >

Reactions, e.g. [Suzuki coupling](#)

AND



Draw


[Content Overview](#) | Latest update: 31. August 2020 >


118M


49M


59M

37M

 Substances

 Reactions

 Documents

 Bioactivities

ELSEVIER

Copyright © 2020 Elsevier Life Sciences IP Limited.

[Terms and Conditions](#)

[Privacy policy](#)

[About content](#)

[Performance Page](#)

Cookies are used by this site. To decline or learn more, visit our [Cookies page](#)

 RELX Group™

Feedback 



10.03.2022

ELSEVIER

# 方法二、直接輸入反應關鍵字或是命名反應

Reaxys

[Quick search](#)


[Query builder](#)

[Results](#)

[Synthesis planner](#)

[History](#)











[Alerts](#)

Ryan Huang 



Results for "radical cyclization"

New  Edit 

	75	Reactions	Condition : radical cyclization <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> 	<a href="#">View Results</a> 
	6,113	Documents	Titles, Abstracts, Keywords : "radical cyclization" <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a> 	<a href="#">View Results</a> 



10.03.2022

# 方法二、直接輸入反應關鍵字或是命名反應


Reaxys<sup>®</sup>


Quick search Query builder Results Synthesis planner History Alerts


Ryan Huang  


75 Filters


Limit to > Exclude >


By Structure 


Yield 


Reagent/Catalyst 


Solvent 


Catalyst Classes 


Solvent Classes 

Product Availability 

Reactant Availability 

Reaction Classes 






Document Type 

Publication Year 




Single step reactions only

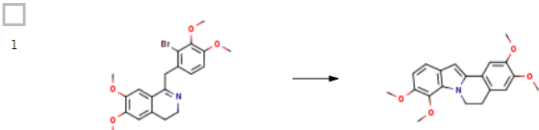
Experimental procedure only


75 Reactions out of 86 Documents containing 232 Substances, 40 Targets




0 selected     

Limit To Exclude Export Syn-Plan Hide Conditions

  Sort by Reaxys Ranking 

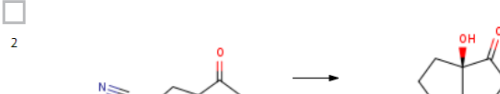
1 




1 Hits  9 Conditions  Find Similar > Reaction ID: 8578406 

Conditions	Yield	Reference
With 2,2'-azobis(isobutyronitrile); tri-n-butyl-tin hydride In toluene for 4h; Cyclization; radical cyclization; Heating;	68%	Orito, Kazuhiko; Uchiito, Shiho; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao [Organic Letters, 2000, vol. 2, # 3, p. 307 - 310] Full Text <a href="#">↗</a> Cited 62 times <a href="#">↗</a> Details <a href="#">&gt;</a> Abstract <a href="#">&gt;</a>

[+ Show all conditions](#) 1 hit out of 1

2 

[Feedback](#) 



10.03.2022

ELSEVIER

# 方法三、結構編輯器畫反應式

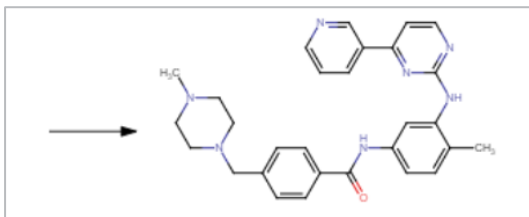
Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Structure editor selected:  MarvinJS  ChemDrawJS Insert structure from name >

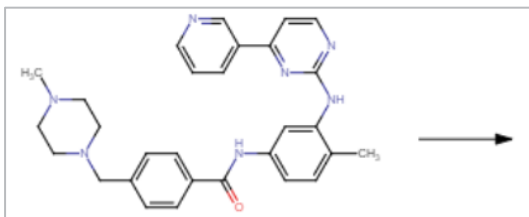
1-1 反應箭頭

Clear Cancel Transfer to query >

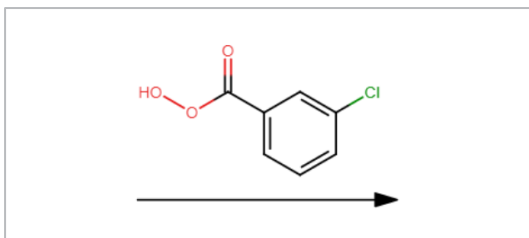
# 方法三、結構編輯器畫反應式



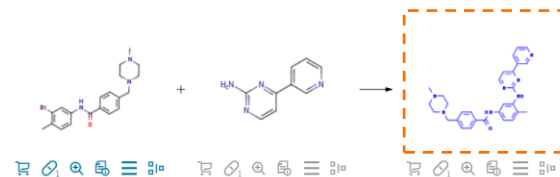
箭頭在左  
產物



箭頭在右  
起始物



箭頭在下  
催化劑或溶劑



Conditions Find Similar Reaction ID: 29521413

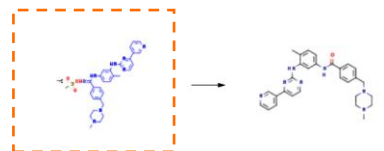
Conditions

With tris(dibenzylideneacetone)dipalladium<sup>0</sup> chloroform complex; 2,2'-bis-(diphenylphosphino)-1,1'-binaphthyl; sodium t-butanol In 5,5-dimethyl-1,3-cyclohexadiene at 140°C; for 5h; Temperature;

Yield

Reference

92% Kang, Julie; Lee, Jun Young; Park, Jeong-Hoon; Chang, Dong-Jo [Journal of labelled compounds and radiopharmaceuticals, 2020, vol. 63, # 4, p. 174 - 182]  
Full Text Details Abstract



Conditions Find Similar Reaction ID: 32441176

Conditions

With ammonia In water; isopropyl alcohol at 20°C; for 4h; pH=7.6 - 8.5;

Experimental Procedure

Yield

Reference

93% KRKA, D. D., NOVO MESTO; BENKIC Primož; TIHI Jaroslav; PECAVAR Anica; GERMAN Tamara; VREČER Franc; VAJS Anamarija; SKRABANJA Vida  
WO2011/157450, 2011, A1  
Location in patent: Page/Page column 19  
Full Text Details Abstract

With dihydrogen peroxide; methyltrioxorhenium(VII) In dichloromethane; water at 15°C; for 5h;  
Experimental Procedure

Yield

Reference

100% METHYLGENE INC.  
WO2005/92899, 2005, A1  
Location in patent: Page/Page column 73  
Full Text Details Abstract

With 3-chloro-benzenecarboxylic acid In dichloromethane at 20°C; Inert atmosphere;

Yield

100% Roudesly, Fares; Veiros, Luis F.; Oble, Julie; Poli, Giovanni [Organic Letters, 2018, vol. 20, # 8, p. 2346 - 2350]

Full Text Cited 19 times Details Abstract

# 方法三、結構編輯器畫反應式

## - 指定反應中心

Reaxys

Quick search Query builder Results Retrosynthesis History

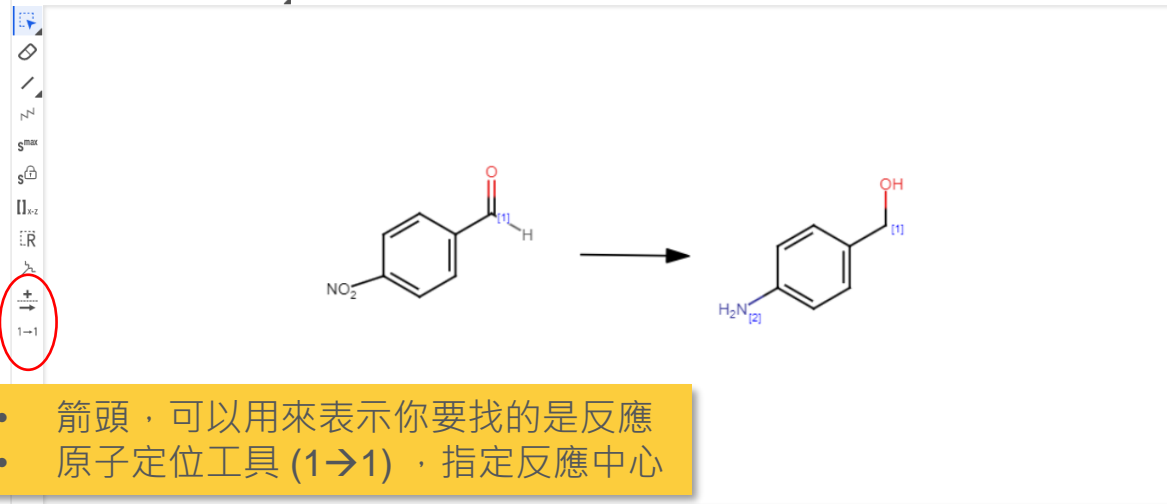
Register >

Sign in



Structure editor selected:  MarvinJS  ChemDrawS

Insert structure from name >



[R]  
[A]  
[H]  
[C]  
[N]  
[O]  
[S]  
[F]  
[P]  
[Cl]  
[Br]  
[I]

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals
- + More options

- 箭頭，可以用來表示你要找的是反應
- 原子定位工具 (1→1)，指定反應中心



Clear

Cancel

Transfer to query >

# 方法三、結構編輯器畫反應式

- 記得探索左邊的反應過濾器

The screenshot displays the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results' (highlighted), 'Retrosynthesis', 'History', and 'Alerts'. The user 'Ryan Huang' is logged in. The main content area shows '11,489 Reactions out of 6,833 Documents, containing 12,995 Substances, 2,202 Targets'. A 'Show Conditions' button is circled in red, with a yellow callout box containing the text '隱藏實驗條件'. The left sidebar contains a 'Filters' panel with various categories: 'By Structure', 'Yield', 'Reagent/Catalyst', 'Solvent', 'Catalyst Classes', 'Solvent Classes', 'Product Availability', 'Reactant Availability', 'Reaction Classes', 'Document Type', and 'Publication Year'. The 'Solvent', 'Product Availability', and 'Publication Year' filter categories are circled in red. A yellow callout box points to these categories with the text '篩選研究主題有興趣的催化劑/溶劑/反應類型'. At the bottom of the filters, two checkboxes are circled in red: 'Single step reactions only' and 'Experimental procedure only'. A yellow callout box points to these checkboxes with the text '篩選有實驗材料方法的反應式'. The main reaction list shows three entries, each with a chemical structure and a 'Reaction ID'. The first reaction is labeled '1' and has a 'Reaction ID: 601797'. The second reaction has a 'Reaction ID: 608056' and '511 Conditions' listed below it.





# 方法三、結構編輯器畫反應式

## - 利用進階搜尋 (Query Builder來限制反應條件)

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' are in the center. On the right, the user's name 'Ryan Huang' and a profile icon are visible. Below the navigation, there are buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar includes 'Import', 'Save', 'Reset form', and 'Delete all'. The main workspace shows a chemical reaction: benzaldehyde (a benzene ring with an aldehyde group) reacting to form benzyl alcohol (a benzene ring with a primary alcohol group). Below the reaction, the text 'As drawn' is present. On the left side of the workspace, there are buttons for 'AND' and 'PROX'. The 'Group 1' section contains two search filters: 'Yield (numerical)' with a value of '96' and a greater-than-or-equal-to operator, and 'Time (Reaction Details)' with a value of '0.25' and a less-than-or-equal-to operator. On the right side, a sidebar menu lists search fields: 'Fields', 'Forms', and 'History'. Under 'Fields', there are expandable categories: 'Reaxys', 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', 'Bibliography', 'PubChem', and 'Commercial Substances'.

- 時間單位為Hr
- 同一個資料格裡面必須用 Proximity (相鄰)串在一起

[\(152\) Reaxys 反應式搜尋 - 如何定義反應條件 - YouTube](#)

# 使用Query Builder 搜尋使用”特定催化劑”的反應式

Query > Forms > Reactions

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

Search in: **Reactions** Targets Substances Documents

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Search fields and forms Fields **Forms** History

Reaxys Forms

- Bibliography
- Natural Products
- Physical Data
- Reactions**
- Spectra
- Substances
- Patents
- Reaxys MedChem Forms

Reactions

- Structure
- AND Reaction Data & Condi... is Reaction Data & Conditions
- AND Reagent/Catalyst is Reagent/Catalyst**
- AND Yield (numerical) = Yield (numerical)
- AND Solvent (Reaction Det... is Solvent (Reaction Details)
- AND Time (Reaction Details) = Time (Reaction Details)
- AND Temperature (Reaction... = Temperature (Reaction Details)
- AND Pressure (Reaction De... = Pressure (Reaction Details), Torr

◇ Reagent/Catalyst contains Pd(OAc)<sub>2</sub>

◇ Yield (numerical) ends with is Yield (numerical)

◇ Solvent (Reaction Det... contains Solvent (Reaction Details)

◇ Time (Reaction Details) starts with Time (Reaction Details)

◇ Temperature (Reaction Details) is Temperature (Reaction Details)

◇ Pressure (Reaction Details) is Pressure (Reaction Details), Torr

或使用自由字元\*來增加搜尋效率  
例如：  
Pd\*  
Pd\*Pt

# 免費的有機反應APP – 你需要知道的命名反應都在這裡

ReactionFlash® gives access to over 1,000 Named Reactions, their mechanisms and examples published in peer-reviewed literature.

Developed in collaboration with the renowned research group of Prof. Dr. Carreira of ETH Zurich.

Available for free on:



自學

實驗室  
查詢

闖關



[ReactionFlash - Need to know everything about named reactions? \(elsevier.com\)](https://www.elsevier.com)



ELSEVIER

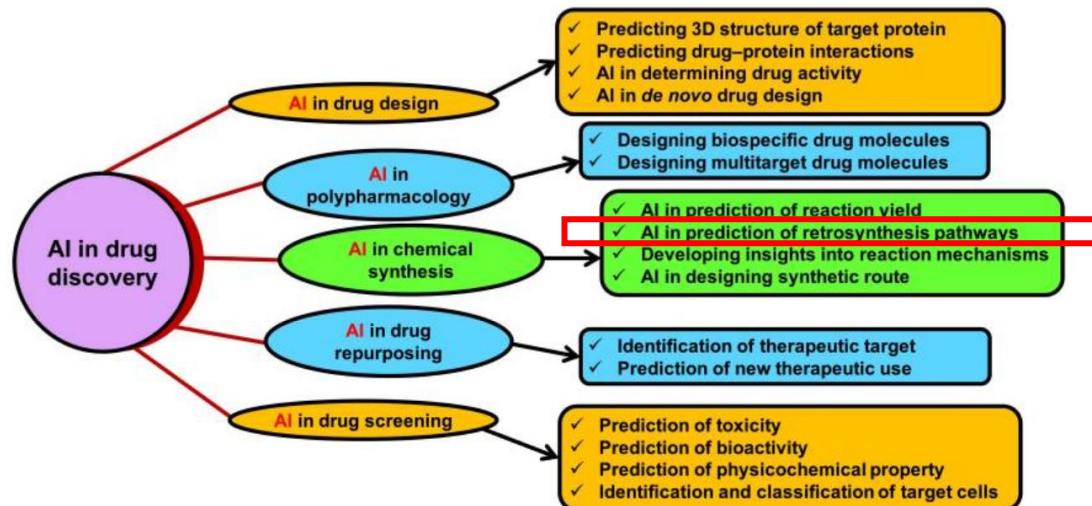
# Reaxys Retrosynthesis Page

逆合成工具



# Reaxys retrosynthesis要解決的問題

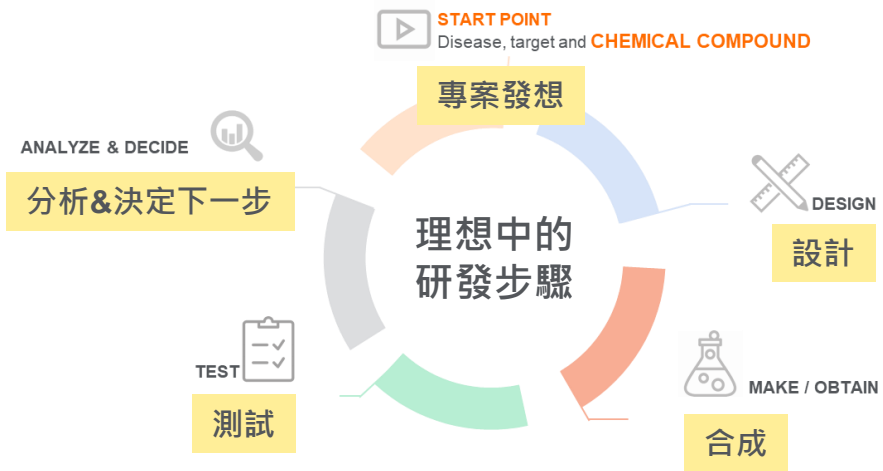
- 如何有效率的合成目標分子



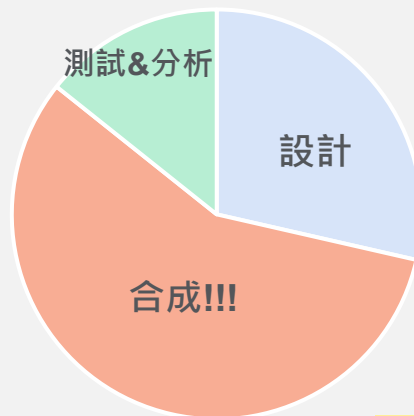
Drug Discovery Today



# 合成步驟正在拖慢你的腳步



## 現實狀況



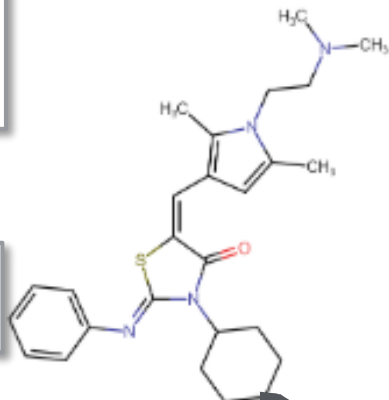
合成是瓶頸步驟  
花了>50%的時間

能不能有電腦輔助的工具來加快合成的步驟?

# 新分子的合成路徑是如何以人工設計的?

- Thinking chemistry
- 搜尋可以參考的反應式
- 搜尋可以參考的起始材料
- 上實驗桌

- Thinking chemistry
- 上實驗桌



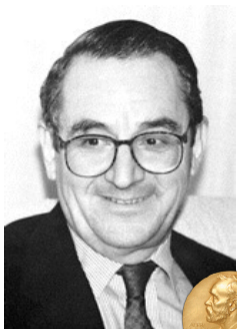
- ✓ 拓展更多可行的合成策略/合成材料
- ✓ 節省查詢時間
- ✓ 加速學習曲線

The screenshot shows the Reaxys search interface. At the top, there are navigation tabs: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". A yellow smiley face with a tear is in the top right corner. Below the navigation, it says "Results for" followed by a search icon. The main content area displays four search categories, each with a count of 0 and a search icon:

- Substances**: Structure : as drawn. Edit in Query Builder. Create Alert.
- Targets**: Structure : as drawn. Edit in Query Builder. Create Alert.
- Substances**: Structure : average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals. Edit in Query Builder. Create Alert.
- Reactions**: Reaction Query : as drawn. Edit in Query Builder. Create Alert.

# 諾貝爾獎得主EJ Corey以電腦輔助化學合成規劃

The roots of Computer Aided Synthesis Planning



EJ Corey  
Nobel prize 1990



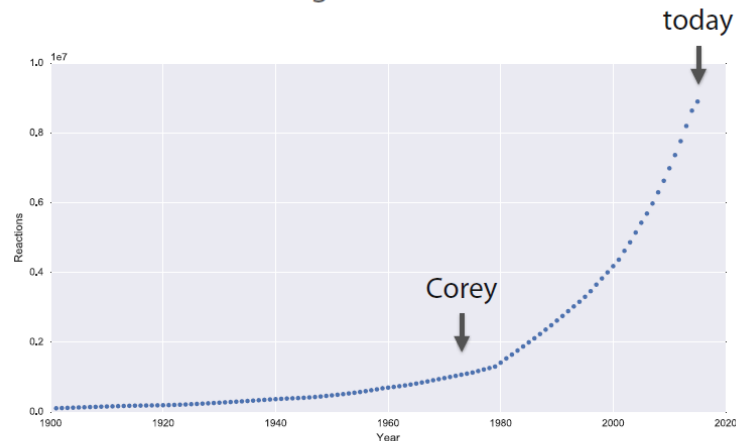
Vleduts (1963), Corey (1968)

Write down all of chemical  
knowledge in logic form

**Great for humans!  
Not so much for  
machines...**

Vléduts, G. *Inform. Storage Retrieval* 1, 117–146 (1963).  
Corey, *The Logic of Chemical Synthesis*

Manual coding cannot work on scale



❖ chemical knowledge grows exponentially,  
doubles every decade

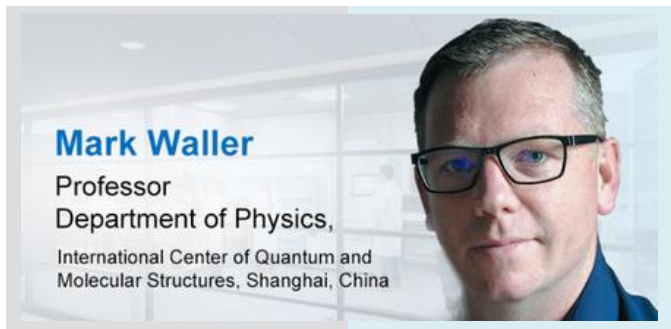
兩個超越90年代的成功障礙：

1. 電腦的硬體尚未發展到可以解決預測化學合成的計算規模。
2. 以人工編寫合成規則，需要大量的時間且跟不上新反應發表的速度。



# Reaxys使用的策略

—結合 高品質的Reaxys reactions資料 與 神經網路 (Neural Network) 3N-MCTS 科技



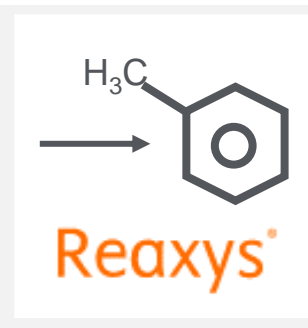
## NEWS

### AI in Action: Neural networks learn the art of chemical synthesis

Robert F. Service

+ See all authors and affiliations

Science 07 Jul 2017:  
Vol. 357, Issue 6346, pp. 27  
DOI: 10.1126/science.357.6346.27



3N-MCTS : 3 layers Neural Network - Monte-Carlo-Tree-Search

# 簡單的介面，只要10分鐘的預測時間

—只要畫出目標分子，Reaxys 15M的反應式做後盾

Reaxys

Quick search Query builder Results Retrosynthesis History Peter van Straaten

1 selected Export Compare Legend Show Costs

No.	Buildingblocks to target	No. of steps	Route overview	Confidence	
1		7 steps		0.867	Tree view > Table view >
2		4 steps		0.867	Tree view > Table view >
		5 steps		0.8	Tree view > Table view >
		4 steps		0.6	Tree view > Table view >
		5 steps		0.576	Tree view > Table view >
		5 steps		0.3	Tree view > Table view >

Results per page 60 1 >

- 1 同時呈現文獻發表的合成路徑與AI預測路徑進行比較
- 2 AI會確定合成路徑起點是買的到的商用材料
- 3 以合成路徑長短排序
- 4 以圖形讓你判斷合成策略的複雜度
- 5 內建的評分系統輔助您判斷AI的可信度

# 簡單的介面，只要10分鐘的預測時間

—只要畫出目標分子，Reaxys 15M的反應式做後盾

Reaxys 15M Retrosynthesis interface showing a predicted reaction route and detailed reaction information.

8: Export button

6: Reaction scheme

7: Experimental procedure

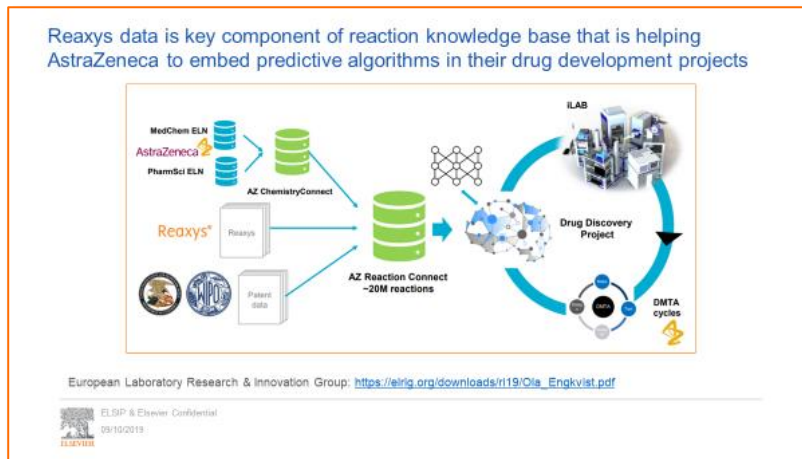
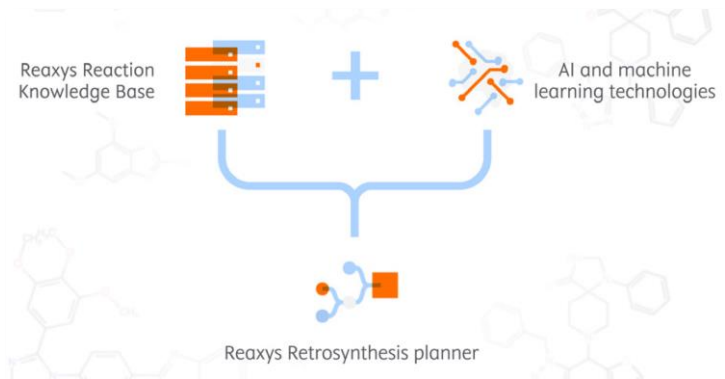
8: Export button

6 自動搜尋呈現文獻中“相似”的反應，畫面(左側)呈現預測路徑，(右側)呈現 Reference 路徑，讓您輕鬆判斷可行性

7 提供完整的實驗材料方法 Experimental Procedure 讓您參考如何規劃實驗細節

8 各種輸出格式，PDF 並支援各式電子實驗記錄

# 知名研究團隊的AI進展



Elsevier collaboration with leading academics and the use of Reaxys data powers the most significant developments in predictive retrosynthesis algorithms

**Waller Lab – Predictive Retrosynthesis**

Game Changer: Scientist Mark Waller  
Next level with AI Driven Synthesis

Planning chemical syntheses with deep neural networks and symbolic AI

AI in Action: Neural networks learn the art of chemical synthesis

Reaxys Data

Reaxys

- >12.5M reactions data
- Organic, single step reactions
- Harmonized, curated and AI/ML ready data

Reaxys empowers cutting edge research at MIT

Connor Coley

ELSP & Elsevier Confidential  
09/10/2019

Reaxys data is helping Jensen group transform the design of industrial processes for chemical and drug manufacturing

**MIT Jensen Research Group**  
MIT Department of Chemical Engineering

Route selection

- Retrosynthetic planning
- Condition recommendation
- Pathway evaluation

Process development

- Specification of residence times, concentrations
- Module selection

Reaction execution

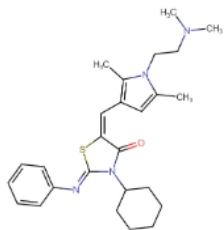
- Recipe-driven synthesis
- Robotic reconfiguration
- Process monitoring

Published reactions → Commercially available compounds → Synthetic route

From 12.5 million published single-step reactions tabulated in the Reaxys database, they prepared a library of **163,723 rules**. Transformations with **stereochemistry** were included in the rules.

ELSP & Elsevier Confidential  
09/10/2019

# 人工查詢規劃逆合成路徑



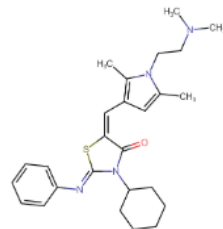
Reaxys

Quick search Query builder Results Synthesis planner History

Results for

0	Substances	Structure: as drawn
0	Targets	Structure: as drawn
0	Substances	Structure: average similarity, include absolute stereo, additional ring closures all isotopes, charges, radicals
0	Reactions	Reaction Query: as drawn

# 以數位工具輔助逆合成規劃路徑



一键推導

My Synthesis Projects

Show 10 entries

No.	Date/Time	Structure	Parameters	No. of Routes
4	23. Januar 2020 07:56		TypeOfPlan: FullRoute Diversity: high Used building blocks: SIAL, LN, RX, EM	8

View result > Edit Delete



1. Thinking about chemistry
2. Reaction & Literature Search
3. Start Material Search
4. Work at the Bench



- Thinking about chemistry
- Work at the Bench

# 登入Reaxys – 註冊免費帳號

Reaxys®

[Quick search](#) [Query builder](#) <sup>New</sup> [Results](#) [Synthesis planner](#) [History](#) [Alerts](#)

Ryan Huang  

Search for 184475-35-2

Import 

Search Reaxys

184475-35-2

如果要深入的使用Reaxys，可以免費申請Reaxys帳號：

- 更久的掛網時間
- 能夠匯出資料
- 儲存、管理搜尋結果
- 設定被動接收更新內容
- 可以有自己的 **Retrosynthesis** 面板

## Create account

Your IP: 198.176.125.21 

First Name

Last Name

Email address

Password

Confirm password

Remember me on this computer  
(Do not use on a shared computer!)

Stay informed about Elsevier products and services

I have read and agree to the [Registered User Agreement](#)

Register >

[Content Overview](#) | Latest update: 11. September 2019 >

118M [Substances](#) 49M [Reactions](#) 59M [Documents](#) 37M [Bioactivities](#) 1.5M [Targets](#)

ELSEVIER

Copyright © 2019 Elsevier Life Sciences IP Limited.

[Terms and Conditions](#) [Privacy policy](#) [About content](#) [Performance Page](#)

Cookies are used by this site. To decline or learn more, visit our [Cookies page](#)

RELX Group™

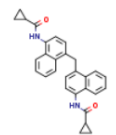




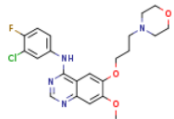



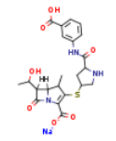



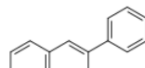


ELSEVIER

# 逆合成面板 (規劃合成路徑、合成材料與反應條件)

Reaxys

Quick search Query builder Results **Retrosynthesis** History Alerts

Ryan Huang  

No.	Date/Time	Project name		No. of routes
5623	01 Oct 2021 03:06	Project #5623	 Delete  Edit 	Predicted  In progress Published 0 View 
5622	01 Oct 2021 02:58	Project #5622	 Delete  Edit 	Predicted 13 Published 5 View 
5146	28 Sep 2021 08:01	Project #5146	 Delete  Edit 	Predicted 0 Published 4 View 
4556	17 Sep 2021 03:25	Project #4556	 Delete  Edit 	Predicted 18 Published 5

畫出專屬於你的結構

View the results

# 逆合成面板 (規劃合成路徑、合成材料與反應條件)

Reaxys®

Quick search Query builder Results **Retrosynthesis** History Alerts

Ryan Huang

Export Legend

Hide Reaxys Examples **Tree view** Table view

Output complete synthesis plan

Predicted route #1

Step 1 Step 2 Step 3 Step 4 Step 5

1

Reaction ID: 11291703

Conditions	Yield	Reference
With pyridine; dmap In 1,2-dichloro-ethane at 100°C; for 3h;		Jenkins, Tracy J.; Guan, Bing; Dai, Mingshi; Li, Gang; Lightburn, Thomas E.; Huang, Shan; Freeze, B. Scott; (...) Ocain, Timothy D.; Harriman, Geraldine C. [Journal of Medicinal Chemistry, 2007, vol. 50, # 3, p. 566 - 584] Full Text Cited 29 times Details Abstract

1 out of 1

The screenshot displays the Reaxys retrosynthesis software interface. At the top, there are navigation tabs for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user's name 'Ryan Huang' is visible in the top right. The main workspace shows a retrosynthetic analysis of a complex molecule, with the predicted route labeled 'Predicted route #1'. The route is broken down into five steps, with Step 1 being the primary focus. Step 1 shows the reaction of a starting material (a substituted benzamide derivative) with a cyclic ketone (cyclopropanone) to form the target molecule. The reaction conditions are listed as 'With pyridine; dmap In 1,2-dichloro-ethane at 100°C; for 3h;'. A reference is provided: 'Jenkins, Tracy J.; Guan, Bing; Dai, Mingshi; Li, Gang; Lightburn, Thomas E.; Huang, Shan; Freeze, B. Scott; (...) Ocain, Timothy D.; Harriman, Geraldine C. [Journal of Medicinal Chemistry, 2007, vol. 50, # 3, p. 566 - 584]'. The interface also includes an 'Export' button circled in red, a 'Legend' button, and a sidebar with 'Project #5623', 'My Synthesis Projects', and 'Draw' options. A yellow box highlights the 'Export' button with the text '輸出完整的合成計畫' (Output complete synthesis plan).





ELSEVIER

# Reaxys Commercial Substances

供應商物質資料庫



# 新增分類"Commercial Substances"於預視頁面

## - Quick Search輸入CAS#，或畫結構搜尋您要購買的物質

Reaxys®

Quick search


Query builder

Results

Synthesis planner

History














Alerts

Ryan Huang 



Results for "186519-92-6"

New  Edit 

	1	<b>Substances</b> CAS# : 186519-92-6 Edit in Query Builder  Create Alert 	<a href="#">Preview Results</a>  <a href="#">View Results</a> 
	0	<b>Documents</b> Titles, Abstracts, Keywords : "186519-92-6" Edit in Query Builder  Create Alert 	
	2	<b>Commercial Substances</b> CAS# : 186519-92-6 Edit in Query Builder  Create Alert 	<a href="#">Preview Results</a>  <a href="#">View Results</a> 



10.03.2022

# 物質頁面購物車新增分類”Commercial Substances”

- 或點擊右上方切換資料庫為Commercial Substances

Reaxys® Quick search Query builder **Results** Synthesis planner History Alerts Ryan Huang

1 Substances out of 5 Documents, containing 11 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References

Grid Heatmap

Reaxys - 1

Reaxys - 1

- Reaxys - 1
- Commercial Substances - 2
- eMolecules - 2
- LabNetwork - 0
- PubChem - 1
- SigmaAldrich - 1

4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid  
C<sub>7</sub>H<sub>4</sub>ClN<sub>3</sub>O<sub>2</sub> 197.581 14006617 186519-92-6

Identification  
Druglikeness  
Physical Data - 1  
Spectra - 2

Substance Availability

- Commercial Substances
- Accelrys' ACD
- CambridgeSoft ACX
- Sigma Aldrich
- eMolecules

化學品供應商資料庫

ELSEVIER

RELX Group™

Sciences IP Limited.  
Privacy policy About content Performance Page

Cookies are used by this site. To decline or learn more, visit our Cookies page



Reaxys Commercial Substances 為每一筆物質提供詳細的供應商列表(A)包括純度、價格、包裝及到貨時間。您可利用篩選工具(B)加速挑選過程，並點擊供應商商品頁面連結(C)造訪供應商網頁。

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

0 selected Limit To Exclude Export Sort by Commercial Substance ID ↑ Grid

Please take a moment to check individual supplier websites for the most up-to-date information on pricing and availability

Supplier (A)	Product	Purity	Package size & price		Availability
Enamine - USA USA	186519-92-6 EN300-152527 ↗		mg		Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Enamine - USA USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 EN300-152527 ↗	95%	500 mg	159 USD	Shipment time: 2-10 days Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Manchester Organics Ltd USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 F45799 ↗		1 g	994 USD	Shipment time: 12 weeks Tier Time: Tier 4 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	250 mg	134 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	1 g	241 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		10 g	670 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		50 g	2241 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01

Show Less ^

Feedback

(B)

# 其他自學線上資源

YouTube <sup>TW</sup>

Elsevier for Life Sciences  
459 位訂閱者

訂閱

首頁 影片 播放清單 頻道 討論 簡介

上傳 全部播放 排序依據

Video Title	Duration	Views	Time Ago
Searching Substance by Structure in Reaxys	2:03	88	1 個月前
Searching Substance by Name in Reaxys	2:35	94	1 個月前
Biology Knowledge Graph	0:37	180	2 個月前
PharmaPendium DDI Risk Calculator v2.0	12:43	39	2 個月前
Learn Chemistry: How to identify named reactions	3:28	84	3 個月前
Learn Chemistry: The Diels-Alder cycloaddition reaction	5:47	50	3 個月前
Welcome to Reaxys	2:29	398	3 個月前
Learn Reaxys : How to copy and paste a structure...	1:28	70	3 個月前
Learn Reaxys: Text Search	4:45	168	3 個月前
Learn Reaxys : An introduction to searching...	2:19	73	3 個月前
Learn Reaxys : An introduction to searching f...	2:19	119	3 個月前
Learn Reaxys : How to create a structure drawing...	2:01	67	3 個月前

## RxED Learning Chemistry with Reaxys ( English )



[\(152\) RxED: Learning Chemistry with Reaxys - YouTube](#)



ELSEVIER



邀請您填寫課後問卷~

歡迎來信留下您對Reaxys的所有問題~  
[r.huang@elsevier.com](mailto:r.huang@elsevier.com)

