

# 掌握化學未來的關鍵 工具：Reaxys 全方位 版助您突破研究

Customer Success

2025

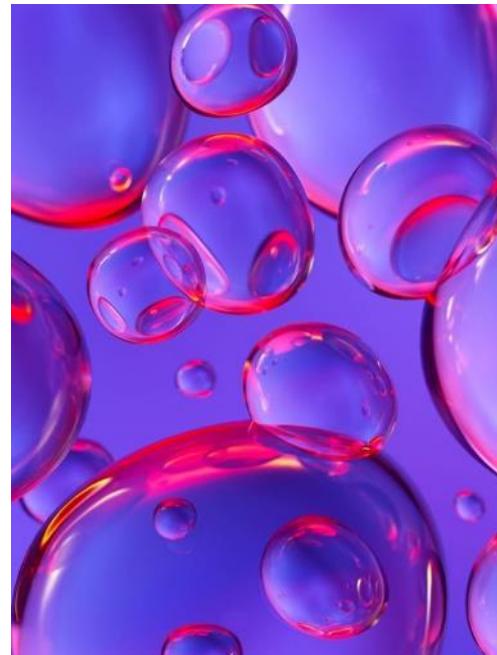


Advancing human progress together



# 課程內容

- 1 Reaxys RAE 介紹
- 2 檢索介面導覽
- 3 搜尋結果種類
- 4 Retrosynthesis AI: 探索及預測合成途徑
- 5 個人化設定及管理
- 6 線上自我學習及用戶資源



查詢資料時，您會先從哪一個平台開始搜尋？

請將最符合您答案的數字打在聊天室中！

1

Google  
Scholar

2

PubChem

3

ChatGPT/Other  
GenAI Tools

4

Reaxys

5

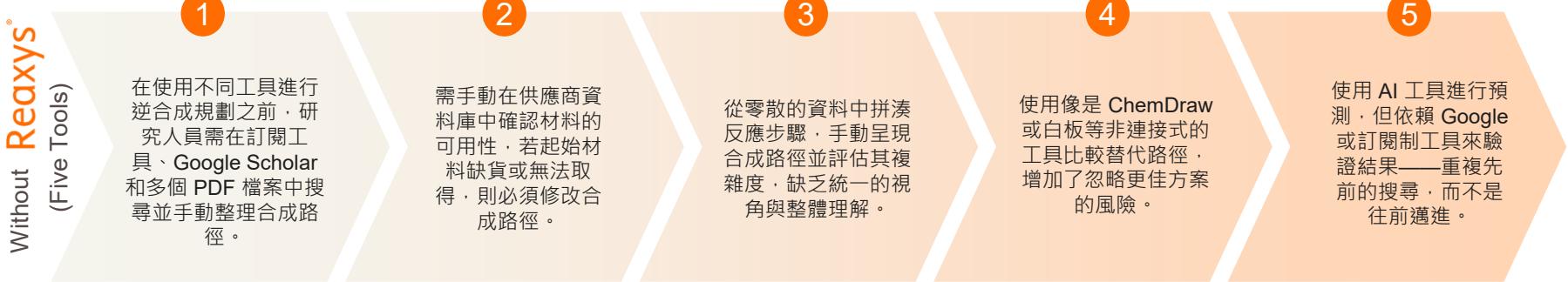
Scopus/WoS

6

SciFinder

# 訂閱制資料庫常常是碎片化工作流程中的第五個步驟

研究人員相信自己已經具備相關工具，但每一個「簡單」的搜尋背後都藏著一段繁雜、多工具交織的流程。在進行搜尋之前，他們其實已經在其他地方完成了一部分準備工作：



訂閱資料庫

# 但你只需用 Reaxys 搜尋一次，就能獲得所需的資料。

在其他地方需要五個工具的操作，使用Reaxys只需五個點擊。

使用Reaxys的研究人員不需在不同平台、PDF或預測引擎間跳轉。每一個關鍵的合成決策——從已出版與預測的合成路徑到材料成本與實驗證明——都在一個統一的體驗中呈現。

Reaxys®

1

在同一個視圖中查看已發表、預測及自訂的合成路徑。

2

評估合成所需起始材料的市售可用性。

3

查看合成計劃中步驟的數量，以便更快地優先選擇較短的合成路徑。

4

輕鬆預覽合成路徑的多樣性，透過路徑拓撲結構快速掌握。

5

發現真實的預測步驟範例，這是唯一提供已發表範例並將其與合成路徑連結在單一視圖中的化學資料庫。

Reaxys® + Scopus® + ScienceDirect

若需要，Reaxys 可無縫擴展至 Scopus 或 ScienceDirect，實現從搜尋到資料來源、從洞察到輸出的連貫體驗。

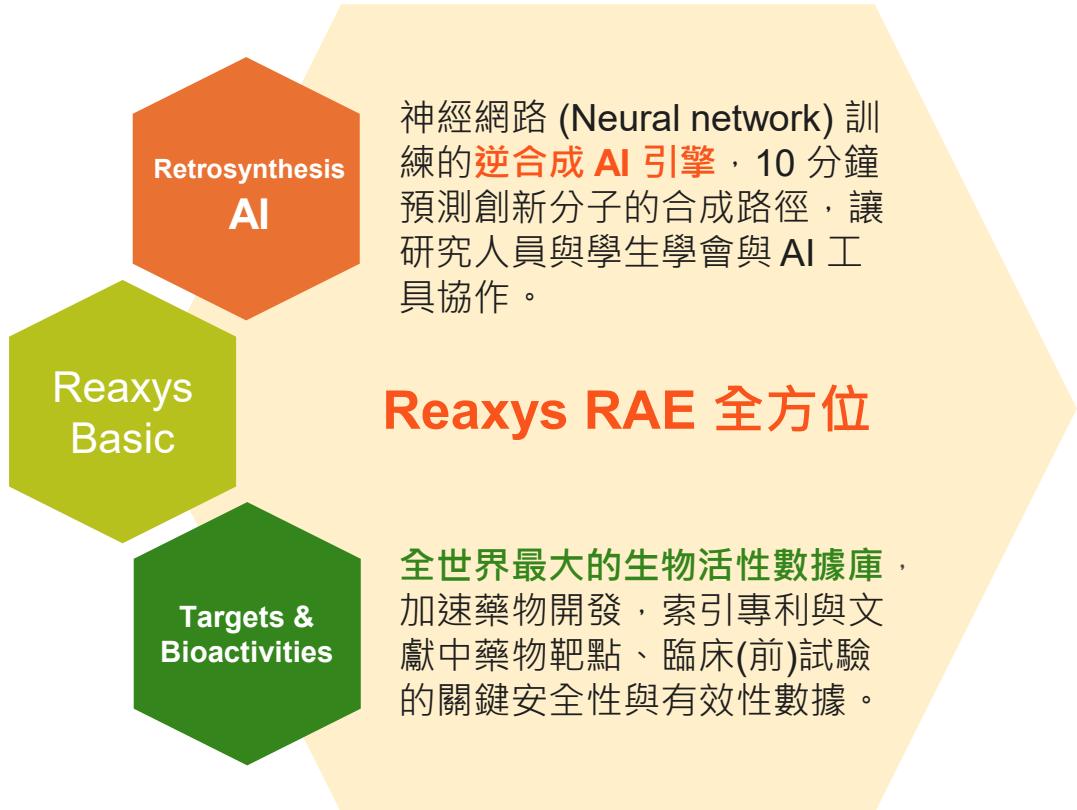
# Reaxys RAE

介紹

# Reaxys 全方位 (RAE) 版與 Reaxys 基本 (Basic) 版差異

## Reaxys Basic Edition

- 有機、無機、有機金屬物理化學特性、實驗量測數據，保留文獻出
- 反應式、產率、試劑與催化劑，保留詳細文獻出處
- 化學研究、藥物開發最快、最詳盡的專利收集與專利空  
間中文譯本
- 獨家商用材料資料庫



# Reaxys Academic Edition

## 涵蓋的範圍

Reaxys 是最大型收錄經實驗驗證  
(非計算) 之物質性質與反應數  
據的資料庫，以化學為組織原則  
呈現。



**Bibliographic Database**  
>121m records  
(from 19k+ journals)



**Substance Database**  
>350m substances



**Patent Database**  
105 patent offices in  
170 patent classes



**Chemical Reaction Database**  
71m reactions



**Predictive Retrosynthesis**  
AI based



**Reaxys AI Search**  
AI based



**Property Database**  
>500m experimental  
properties in >500 fields  
in >130 subject areas



**Target Database**  
43k targets

Reaxys 人工整理了科學文獻、專利資料中關鍵的實驗數據，讓您有更豐富的資料查詢方法

Journals, patents,  
conference  
proceedings



化合物結構, 物理化學特性  
(>500 種), 反應式, 反應條件  
實驗材料方法

### 回答關鍵的研究問題:

- 我研究的化合物有哪些特性被報導過?
- 有哪些其他化合物曾經報導過類似的特性?
- 這個材料自己合成可行嗎?用買的省下的時間划算嗎?
- 有哪些類似的結構可能可以讓我參考?
- 這是一個值得投入時間與金錢的的藥物靶點嗎?

# Reaxys 全國授權本連線說明

- 連線網址：[www.reaxys.com](http://www.reaxys.com)
- 登入帳號：自2025年月起，服務採雙認證模式連線，使用者需於學校機構授權網路範圍，以學校 Email自行註冊Reaxys帳號，登入帳號以連線。

請確認位於校內或機構網路範圍

請使用機構 Email、目前不支援免費信箱帳號。

Your IP: 198.176.124.146

Sign in  
With your Reaxys Account

Username: r.huang@elsevier.com

Password:

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

Not Registered?

Sign in >

Sign in via your institution

Forgot your password?

Don't have access yet? Learn more > Contact sales >

新用戶註冊

Not Registered?

Sign in >

Sign in via your institution

Forgot your password?

Elsevier 旗下 ScienceDirect、Scopus、Embase 等資料庫帳號與 Reaxys 互通，若您曾申請過相關帳號，可點擊忘記密碼重新找回帳號。

台灣大多數學校並不支援機構登入，請嘗試上述雙認證連線。

# Reaxys RAE 檢索介面導覽

# 檢索介面介紹

The screenshot shows the Reaxys search interface with the following numbered callouts:

- 1 Quick search: 關鍵字檢索 (Key search)
- 2 Query builder: 結構式搜尋 (Structure search)
- 3 Results: 搜尋結果 (Search results)
- 4 Retrosynthesis: 逆向合成路線搜尋 (Retrosynthesis)
- 5 History: 搜尋歷史 (Search history)
- 6 Alerts: 瀏覽提示 (Alerts)
- 7 Reaxys AI Search: AI 搜尋功能 (Reaxys AI Search)

The sidebar on the right includes:

- 使用者偏好設定與登出 (User preferences and login)
- 常見問題、技術訓練、影片、支援中心 (FAQ, Technical training, Videos, Support center)
- Import (批次導入結構) (Import (Batch import structure))

Key interface elements include:

- Reaxys logo
- Quick search bar: Substance Molecular Formula, e.g. Pt(PPh<sub>3</sub>)<sub>3</sub>
- Find button
- AND operator
- Draw button (Chemical structure input)
- Chemical structure search (反應式、結構式) (Reaction式、Structure)
- Reaxys AI Search Beta button
- Help and Support icons (Question mark and SS)

# Reaxys AI Search



Reaxys AI Search

Welcome to the new Reaxys AI Search Beta

A faster and more intuitive search experience.

What is your research question?

Type your query



[Learn how it works >](#)

## Search Examples

[How to retain blueberry puree anthocyanin levels under high pressure processing?](#)

[Development of conductive polymers enhancing their applications in flexible electronics](#)

[The application of PVA in antibiofouling coatings](#)

[What are the key challenges in Mn based catalysts for VOCs removal?](#)

[Can carbon dioxide capture and hydrogen production operate simultaneously?](#)

[Siloxane blend with polycarbonate for flame retardants](#)

Use Reaxys [Quick Search](#) or [Query Builder](#) if you're looking for:

- Molecular formula, SMILES and CAS numbers
- Patent number
- Author name
- Structures and Specific datapoints: What is the melting point of lamotrigine?
- Reactions and conditions: "suzuki cross coupling reaction" in toluene

# Reaxys serves a varying profile of chemist



I am a chemist where I mainly search using structures



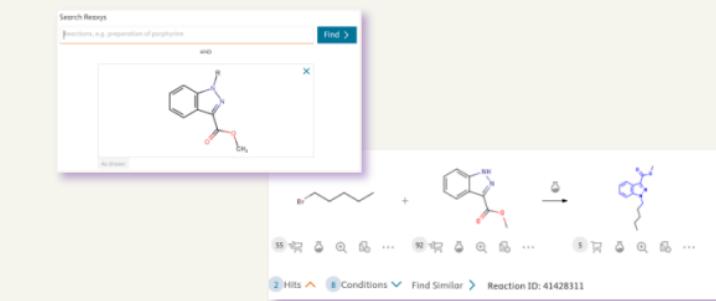
I am a chemist where I search using structures and text



I am a chemist where I search using **text** because structure searches are difficult or not possible

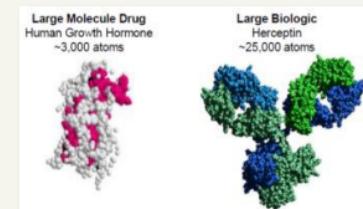
## Structure search:

- Search for substances, reaction, properties that have been extracted by structure through structure or text search queries



## Text search:

- Use of natural language querying for information retrieval
- Text search supports interdisciplinary fields where chemistry is combined with other subjects, e.g. material science, chemical engineer, polymer scientist etc.



Large molecule researchers require text search for information retrieval

**Sample query from chemical engineer:**  
*"Wastewater treatment physical processes"*

**Sample query from material scientist:**  
*"Advances in hair fibre reinforcement techniques"*

# Discoverability: 使用自然語言查詢進行搜尋

**Reaxys AI search (beta version)**  
讓使用者可以透過自然語言搜尋化學文獻。搜尋結果來自於Reaxys索引的所有文件的標題與摘要。

Reaxys AI Search 主要優勢：

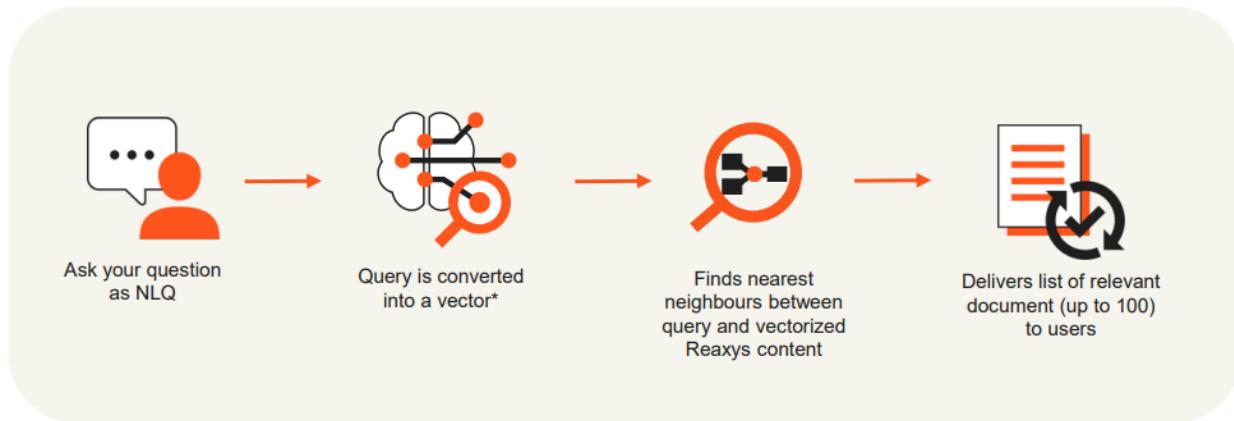
- 支援化學與其他學科結合的跨領域領域，例如聚合物、化學工程、材料科學等。
- 具有彈性的查詢功能，能夠處理拼寫錯誤、單數與複數、縮寫以及同義詞。

The screenshot shows the Reaxys AI Search interface. At the top, there is a navigation bar with 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', 'Alerts', and a 'Reaxys AI Search' button with a 'Beta' label. A red box highlights the 'Reaxys AI Search' button. Below the navigation bar, a banner says 'Discover a more intuitive way to search — with Reaxys AI Search Beta'. The main search results page has a header 'Benefits of using Single-Crystal Cathode Particles in lithium-ion batteries'. It shows '100+ Documents found'. A red box highlights the 'View in Reaxys.com' link next to the 'All' checkbox. Below the results, there are two entries. The first entry is for a paper titled 'Single-crystal high-nickel layered cathodes for lithium-ion batteries: advantages, mechanism, challenges and approaches' (2022, Score: 0.999707). The second entry is for a paper titled 'Pulse High Temperature Sintering to Prepare Single-Crystal High Nickel Oxide Cathodes with Enhanced Electrochemical Performance' (2023, Score: 0.999528). Both entries include an 'Abstract' section and a 'Was this relevant to the question?' button.

詳情請參閱 [Release Notes](#)

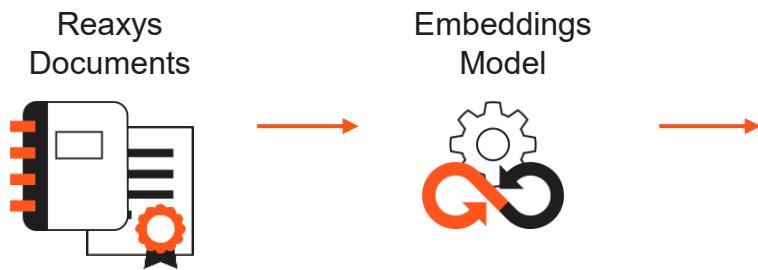
# How does Reaxys AI search work?

Reaxys AI is based on vector search, which is a technique to find similar items by comparing numerical representations ("vector") of content like text, images, or molecules. The upcoming Reaxys AI search focuses on vectorized text only.

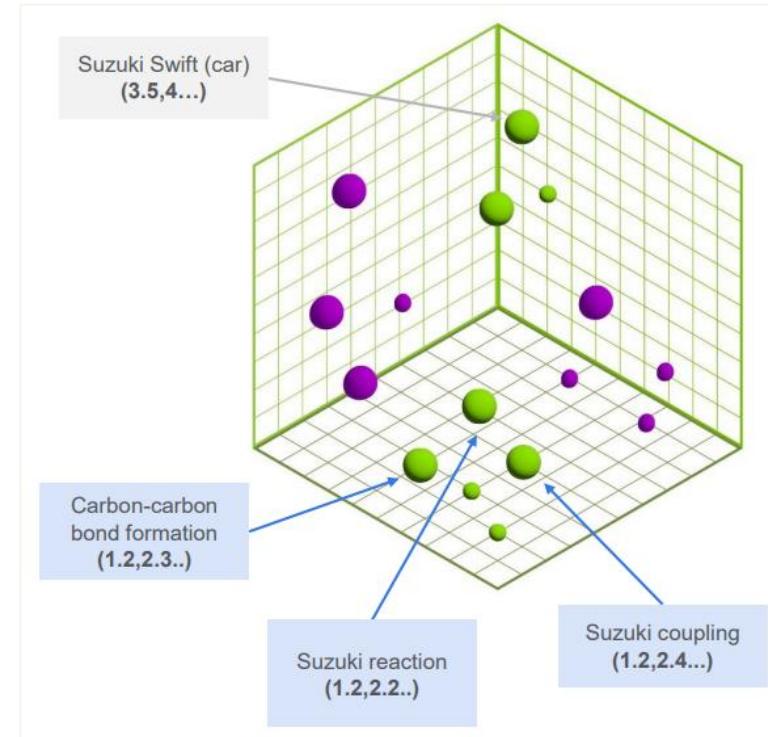


- ✓ BERT model is trained to answer chemistry-related questions with full Reaxys data (Title and Abstracts)
- ✓ Reviews more relevant results for natural language query
- ✓ Leverages strength of both vector & keyword-based search

# What is Reaxys Semantic Search?



- Textual content from journal articles and patents (abstracts, patent claims, full text) can be transformed into vectors, represented as numerical values
- This numerical representation of this complex text is represented as points in a multidimensional vector space. The embedding model ensures that text with a similar meaning sits in close proximity in the vector space



# Reaxys AI Search Demo

Which metal-organic frameworks are most effective for encapsulating anticancer drugs like doxorubicin?

What is your research question?  
Which metal-organic frameworks are most effective for encapsulating anticancer drugs like doxorubicin? 🔍

Learn how it works >

100 Documents found

All [Export as CSV file](#) [View in Reaxys.com](#)

**1 Encapsulation, Release, and Cytotoxicity of Doxorubicin Loaded in Liposomes, Micelles, and Metal-Organic Frameworks: A Review**  
[2022]  
Score: 0.999667

**Abstract:**  
Doxorubicin (DOX) is one of the most widely used anthracycline **anticancer drugs** due to its high efficacy and evident antitumoral activity on several cancer types. However, its **effective** utilization is hindered by the adverse side effects associated with its administration, the detriment to the patients' quality of life, and general toxicity to healthy fast-dividing cells. Thus, delivering DOX to the tumor site encapsulated inside nanocarrier-based systems is an area of research that has garnered colossal interest in targeted medicine. Nanoparticles can be used as vehicles for the localized delivery and release of DOX, decreasing the effects on neighboring healthy cells and providing more control over the drug's release and distribution. This review presents an overview of DOX-based nanocarrier delivery systems, covering loading methods, release rate, and the cytotoxicity of liposomal, micellar, and metal organic frameworks (MOFs) platforms.

You can Review AI search results, or pass it to Reaxys.com for further filtering

The screenshot shows the Reaxys AI Search interface. At the top, there's a search bar with the query "Which metal-organic frameworks are most effective for encapsulating anticancer drugs like doxorubicin?". Below the search bar, a message says "You can Review AI search results, or pass it to Reaxys.com for further filtering". The main area displays "100 Documents found" with a list of results. The first result is highlighted with a yellow box and an arrow pointing down to the Reaxys interface. The Reaxys interface shows the search results with the same document at the top. The sidebar on the left contains various filters: Publication Year, Document Type, Authors of Scientific Documents, Current Affiliation, Inventors of Patents, Current Patent Assignee, Patent Office, Journal Title, Substance Classes, Reaction Classes, Index Terms (List), and Index Terms (ReaxysTree). The results list includes the following documents:

- 1 Encapsulation, Release, and Cytotoxicity of Doxorubicin Loaded in Liposomes, Micelles, and Metal-Organic Frameworks: A Review [2022] Cited 240 times
- 2 Coordination polymer particles as potential drug delivery systems [2010] Cited 98 times
- 3 Unusual microporous polycatenane-like metal-organic frameworks for the luminescent sensing of  $\text{Ln}^{3+}$  cations and rapid adsorption of iodine [2012] Cited 177 times
- 4 Peptide targeted lipid nanoparticles for anticancer drug delivery [2012] Cited 533 times
- 5 Lipid nanocapsules: A new platform for nanomedicine [2009]

At the bottom right of the Reaxys interface, there's a "Beta" badge, a help icon, and a "Sort by Relevance" dropdown.

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# Reaxys AI Search 搜尋結果

[Go back to main search](#)

What is your research question?

How to retain blueberry puree anthocyanin levels under high pressure processing?



[Learn how it works](#) >

## 100 Documents found

All [Export as CSV file](#) [View in Reaxys.com](#)

[Method for processing dried blueberry fruit having high anthocyanin content](#)

1 CN104642949, [2015]

Score: 0.997681

**Abstract:**

The invention discloses a method for **processing a dried blueberry fruit having high anthocyanin content**. The method comprises the following steps: step (1) screening fresh **blueberry** fruits, washing and removing water; step (2) dewaxing the **blueberry** which is treated in the step (1), cooling and removing water; step (3) firstly performing an osmotic dehydration treatment and then performing a heat pump-hot wind united drying treatment; step (4) cooling the dried **blueberry** fruits to room temperature, making sure that the retained amount of an **anthocyanin** type substance in the dried **blueberry** fruits is above 800mg/100g. By controlling the **processing** parameters such as pH and temperature that influence the stability of the **anthocyanin**, a vertical stacked hydrophobic structure is formed by utilizing copigmentation and union of molecules, so that hydration of the **anthocyanin** type substance is inhibited; the structural stability of the **anthocyanin** type substance is improved by modification effect of an intra-molecular structure which has reactions such as glycosylation and acylation, and thus the stability of the **blueberry anthocyanin** is improved, and the loss of the **blueberry anthocyanin** during **processing** is reduced.

Was this relevant to the question?

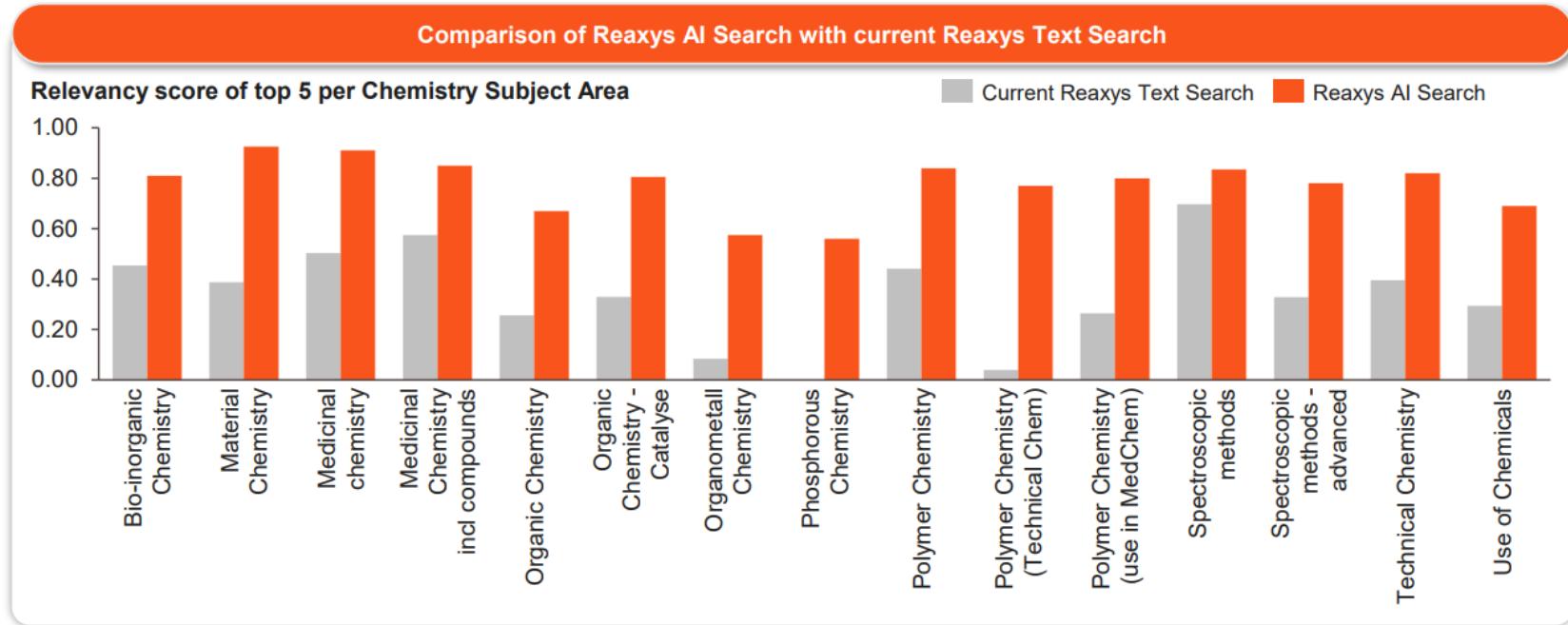
[Effects of high hydrostatic pressure and thermal processing on anthocyanin content, polyphenol oxidase and  \$\beta\$ -glucosidase activities, color, and antioxidant activities of blueberry \(\*Vaccinium Spp.\*\) puree](#)

2 [2021]

Score: 0.995587

Did the results answer your question? [Yes](#) [No](#)

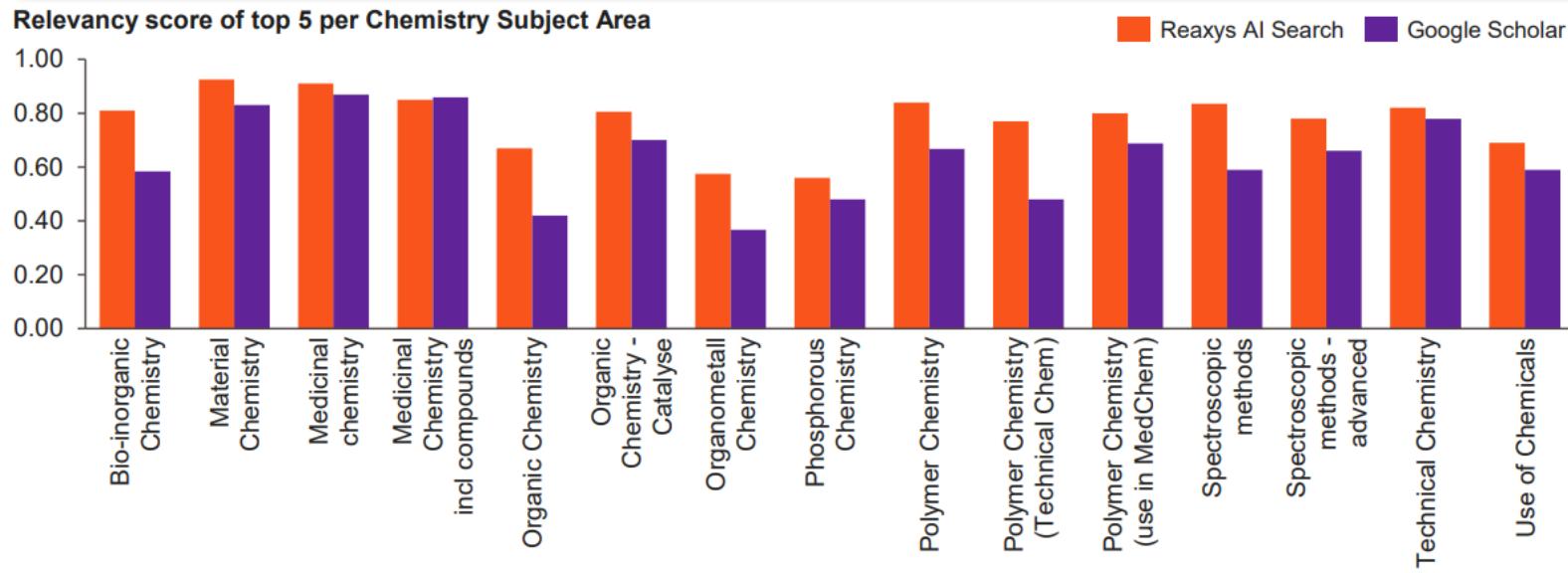
# Internal evaluation – Significant improvement vs. current Reaxys text search: Relevancy score increased from 38% to 81%



Disclaimer: Reaxys text search wasn't built for natural languages queries

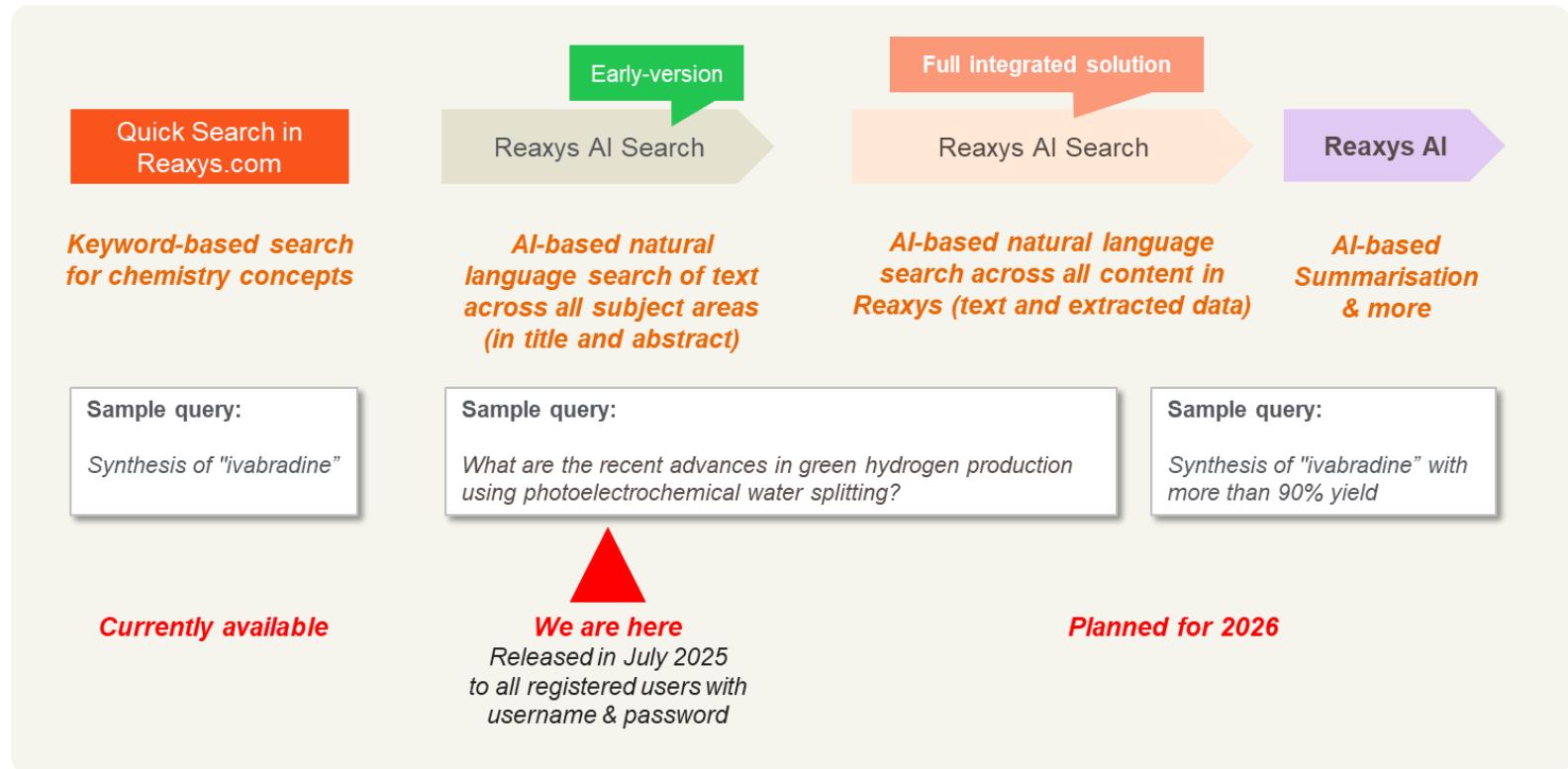
# Internal evaluation – Reaxys AI Search is also better than Google Scholar

Comparison of Reaxys AI Search and Google Scholar



Relevancy score top 5 results: **Reaxys AI Search 81% vs. Google Scholar 64%**

# Reaxys AI Search 未來發展



# Quick Search 多元搜尋指令

## 化合物搜尋

Search Reaxys

XFind >

Substance Properties, e.g. solubility of vitamin D3

## 化學性質搜尋

Search Reaxys

XFind >

Substance Effect, e.g. anticoagulant

## 逆合成搜尋

Search Reaxys

XFind >

Substance CAS Registry Number, e.g. 102625-70-7

## 化學作用搜尋

Search Reaxys

XFind >

Reactions, e.g. phosphorylation

## 文獻搜尋

Search Reaxys

XFind >

Documents, e.g. Tetrahedron, 2014, 70, 2343

# 天然萃取物檢索:鬼針草 (Bidens Pilosa)



Photo by [An Hoàng](#) on [Unsplash](#)

ELSEVIER

**Question:** 探索藥用植物萃取物的生活性應用，已發表文獻中有哪些 Substances 紀錄？

## 方法一:

1. 檢索 *Bidens Pilosa* 的文獻
2. 取得文獻中人工提取的 Substances 清單

## 方法二:

1. 利用進階搜尋工具 Isolated from natural source

# 結構編輯器介面

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Structure editor selected: MarvinJS ChemDrawJS

可直接輸入結構名稱

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

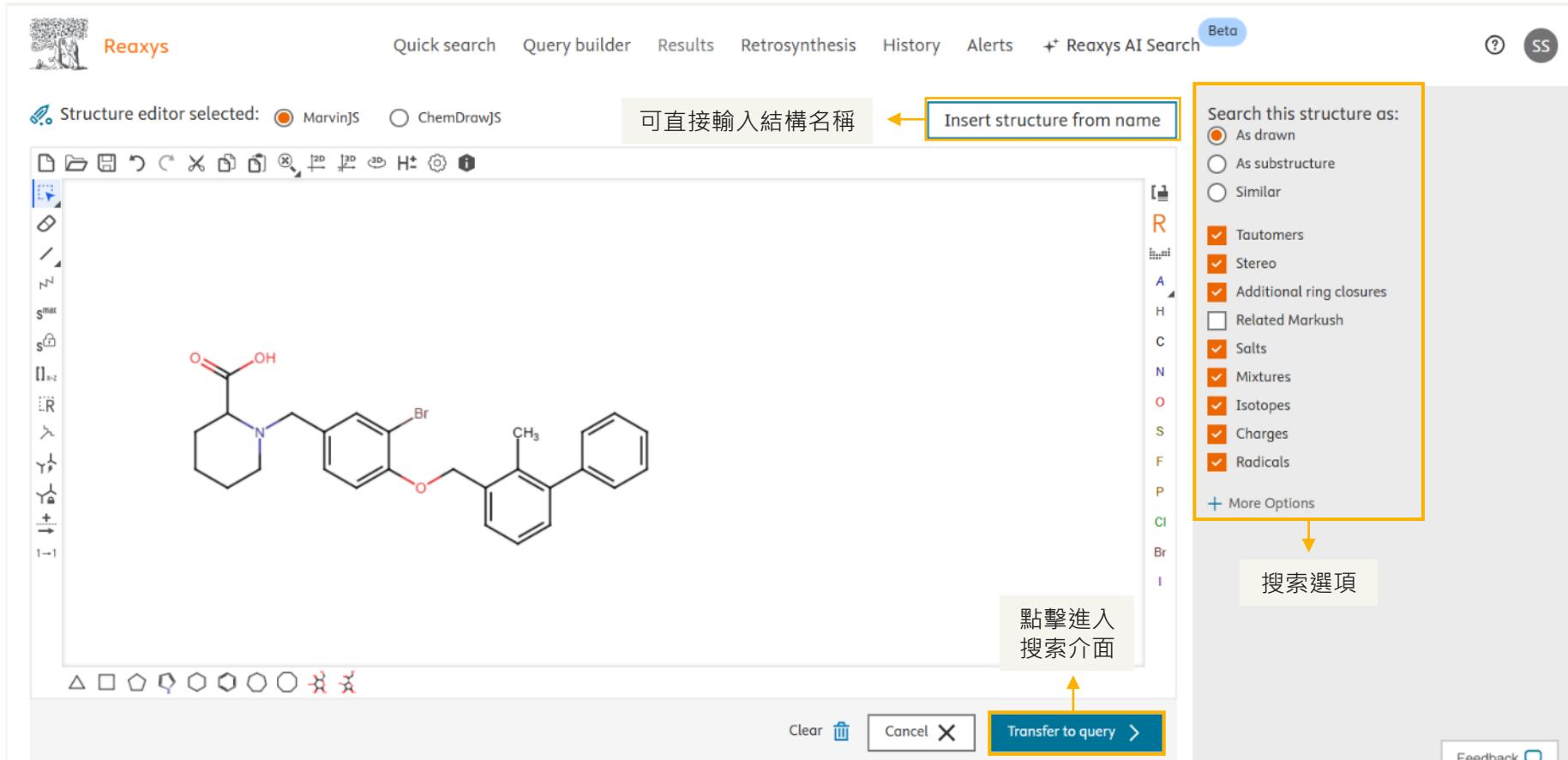
+ More Options

點擊進入  
搜索選項

點擊進入  
搜索介面

Transfer to query >

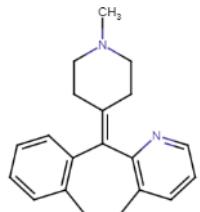
Feedback



Chemical structure: CC1=CC=C(C=C1)C2=C(C=C(C=C2)Oc3cc(Br)cc(CN4CCCCC4C(=O)O)cc3)C(C)=C

# Reaxys 三種結構搜尋與怎麼用

我感興趣的結構



Azatadine  
CAS# 3964-81-6

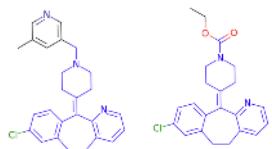
As drawn

尋找跟我畫的  
**「一模一樣」**  
結構

針對已知的藥物、已發表的結構想查詢物理化學性質、生醫活性應用製備方法、研究背景。

As substructure

含有相同**「核心結構」**的一群衍生物



研究新的化合物，從已經發表的結構找線索，例如優化前導化合物 (lead compound)

Similar

**「結構類似」**的化合物提供不同程度的結構變化

# 結構編輯器搜尋選項

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
- Radicals

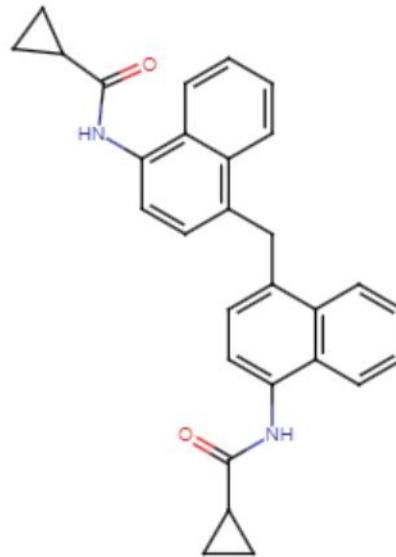
[+ More Options](#)

- **As drawn:** 按照繪製的結構
- **As substructure:** 部分結構
  - **On all atoms:** 搜索所有原子的子結構
  - **On heteroatoms:** 只在雜園子上進行結構搜索
- **Similar:** 類似的化合物與反應

- **Tautomers:** 同分異構體
- **Stereo:** 立體異構體
- **Additional ring closures:** 額外的環形閉合
- **Related Markush:** 相關的 Markush 資料
- **Salts:** 鹽類
- **Mixtures:** 混合物
- **Isotopes:** 同位素
- **Charges:** 帶電分子
- **Radicals:** 自由基

# 示範: 結構探索

我有一個實驗室感興趣的結構，是沒有人發表過的，如何從有**相似化學結構**的文獻中，找尋可以參考應用、關鍵的實驗數據。



# Query builder 檢索介面

The screenshot shows the Reaxys Query builder interface. At the top, there is a navigation bar with 'Quick search', 'Query builder' (underlined), 'Results', 'Retrosynthesis', 'History', 'Alerts', '+ Reaxys AI Search' (Beta), and a user icon. Below the navigation bar are buttons for 'Import', 'Save Options', 'Reset Query', and 'Delete Query'. To the right, there are search buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A search bar labeled '6' is at the top right. On the left, there are search fields for 'Melting Point' (with dropdowns for '=', 'is', and 'Find Any'), 'Measurement pX', and 'Reagent/Catalyst'. Each field has a search icon. On the right, there is a sidebar with tabs for 'Fields' (selected), 'Forms', and 'History'. The 'Fields' tab contains numbered callouts 7, 8, and 9, each with a description: 7 for 'Fields', 8 for 'Forms', and 9 for 'History'. Below the sidebar, there are sections for 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'Target and Bioactivity', 'Other', 'Reactions', 'Bibliography', 'PubChem', and 'Commercial Substances'. A 'Feedback' button is at the bottom right.

1 Current Patent Assignee

2 Structure: 結構式繪圖畫面

3 Molecular formula: 分子式搜尋

4 CAS RN: CAS 代號

5 TI, AB & KW: 標題 · 摘要 · 關鍵字

6 Search: 化學條件項目搜尋欄位

7 Fields: 化學條件項目

8 Forms: 調用你自己創造的檢索公式或嘗試我們為您建立的公式範本

9 History: 搜尋歷史也可用於建構檢索公式

# Query builder 檢索介面

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

可以保存創建的檢索公式

Search in: Reactions > Targets > Substances > Documents >

選擇反應式、蛋白靶點、物質或文獻搜索

Import Save Options Reset Query Delete Query

Melting Point: 50 - 50.1 (is acetic acid)

Sublimation

Reactive Index

AND

OR AND NOT NEAR NEXT PROXIMITY

Measurement pX: Measurement pX

Reagent/Catalyst: Reagent/Catalyst

Identification

Physical Properties

Melting Point

Boiling Point

Sublimation

Reactive Index

Density

Adsorption

Association

Autoignition

Azeotropes

Feedback

## Query builder: 實驗數據檢索

### Question:

實驗室需尋找加熱至約 60 度可昇華的材料，然而利用 Google 取得的資訊雜訊太多，如何從實驗數據搜尋符合的材料再連結至相關文獻

利用進階搜尋工具「**Sublimation**」

# Query builder: 實驗數據檢索

The screenshot shows the Reaxys Query builder interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis, History, Alerts, and Reaxys AI Search (Beta). Below the tabs, there are search buttons for Reactions, Targets, Substances (highlighted in orange), and Documents. On the left, there are import and export options: Import, Save Options, Reset Query, and Delete Query. Below these are search filters: Current Patent Assignee, Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main search area shows a search for 'sublimation' in the 'Substances' category. The search results panel on the right shows '1' result for 'Sublimation' (highlighted in orange) and '2' results for 'Enthalpy of Sublimation'.

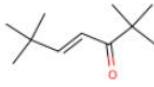
- 1 以關鍵字搜尋 Sublimation
- 2 左鍵點選 Sublimation
- 3 點擊 Show fields 顯示數據欄位

- 4 輸入溫度區間 55-65
- 5 可輸入 760 (torr) 或保持空白
- 6 點選 Substances 資料類型

# Query builder: 實驗數據檢索

2 Substances out of 52 Documents, containing 65 Reactions, 0 Targets Sort by No of References

0 selected Limit To Exclude Export Preparations Grid Bioactivity Visualization

1   
(E)-2,2,6,6-tetramethylhept-4-en-3-one  
(CH3)3CCHCHCOC(CH3)3 168.279 1904245 20859-13-6

[Hit Data - 1](#) [Druglikeness](#) [Spectra - 25](#) [Preparations - 14](#) >  
[Identification](#) [Physical Data - 12](#) [Reactions - 62](#) >  
[Documents - 44](#) >

2 ...

Hit Data - 1 系統會將 Sublimation 資料標示於 Hit Data >>  
Sublimation - 1 hits out of 1 方便比較並列出文獻出處 Show/Hide columns

Sublimation, °C	Pressure (Sublimation), Torr	Reference
55	760	Overman,L.E.; Clizbe,L.A.; Freerks,R.L. [Journal of the American Chemical Society, 1981, vol. 103, p. 2807] <a href="#">Full Text</a> ↗ <a href="#">Cited 69 times</a> ↗ <a href="#">Details</a> >

# 反應式搜尋

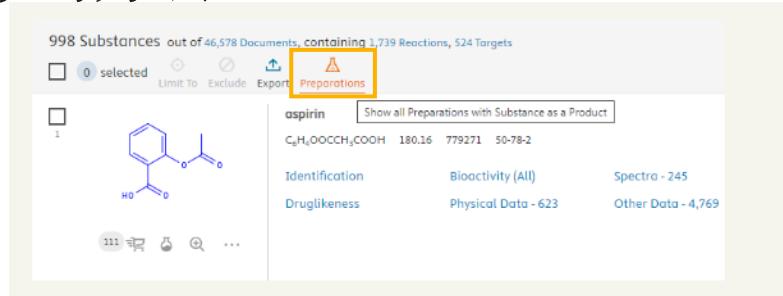
How to search chemical reactions

ELSEVIER

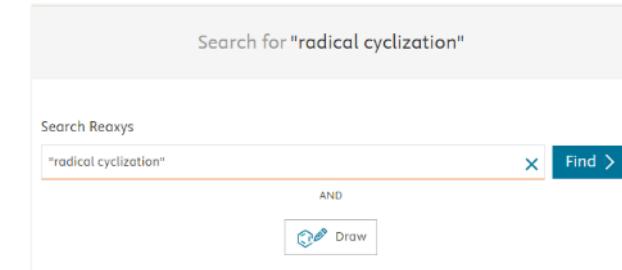
# 尋找反應式 (Chemical equation) 的方法

## 1. 已知物質的製備方式

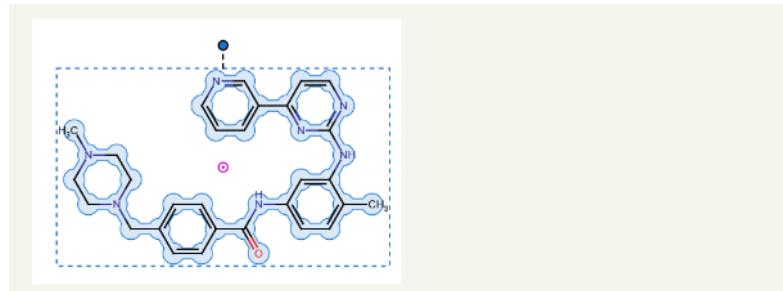
(從 substance 介面連結  
preparations)



## 2. 關鍵字檢索 (例：radical cyclization)、命名反應式 (例：Suzuki coupling)



## 3. 直接畫出反應式 (完整、半個反應式)



# 尋找反應式的方法: 已知物質的製備方式

998 Substances out of 46,578 Documents, containing 1,739 Reactions, 524 Targets

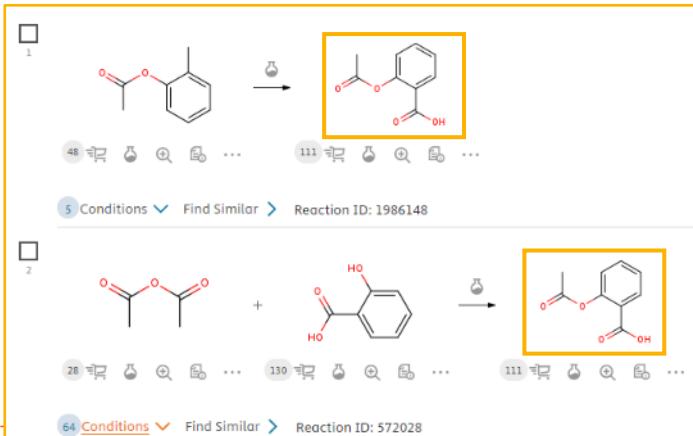
0 Limit To Exclude Export Preparations No of References Grid Bioactivity Visualization

aspirin  
C6H4OOCCH3COOH 180.16 779271 50-78-2

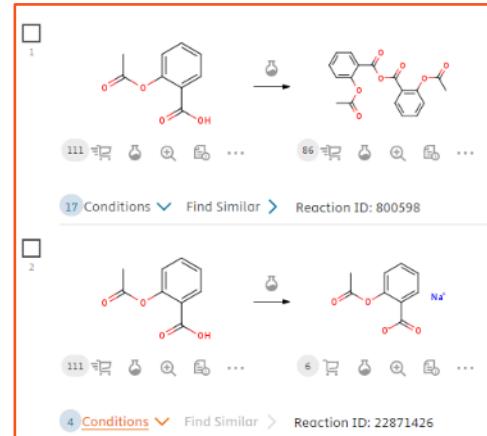
Identification Physical Data - 623  
Druglikeness Spectra - 245  
Bioactivity (All) Other Data - 4,769

Preparations - 109 >  
Reactions - 1,582 >  
Targets - 506 >  
Documents - 45,581 >

## Preparations 指出現在產物 (Product)



## Reactions 產物或起始物 (Reactants or Products)



# 尋找反應式的方法: 關鍵字檢索

Search for "radical cyclization"

Search Reaxys

"radical cyclization" X Find >

AND

Draw

Results for "radical cyclization" New Edit

75	Reactions	Condition : radical cyclization	Preview Results	<span style="background-color: #ff7043; color: white; padding: 5px 10px;">View Results &gt;</span>	
	75	Reactions	Condition : radical cyclization	Preview Results	<span style="background-color: #ff7043; color: white; padding: 5px 10px;">View Results &gt;</span>
	9,499	Documents	Titles, Abstracts, Keywords : "radical cyclization"	Preview Results	<span style="background-color: #ff7043; color: white; padding: 5px 10px;">View Results &gt;</span>

[Edit in Query Builder](#)  [Create Alert](#)

[Edit in Query Builder](#)  [Create Alert](#)

# 尋找反應式的方法: 關鍵字檢索

Reaxys®

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

Stephanie Su  

75 Reactions out of 86 Documents, containing 232 Substances, 44 Targets

0 Limit To Exclude Export Hide Conditions   Reaxys Ranking

1 

1 Hits  9 Conditions  Find Similar > Reaction ID: 8578406

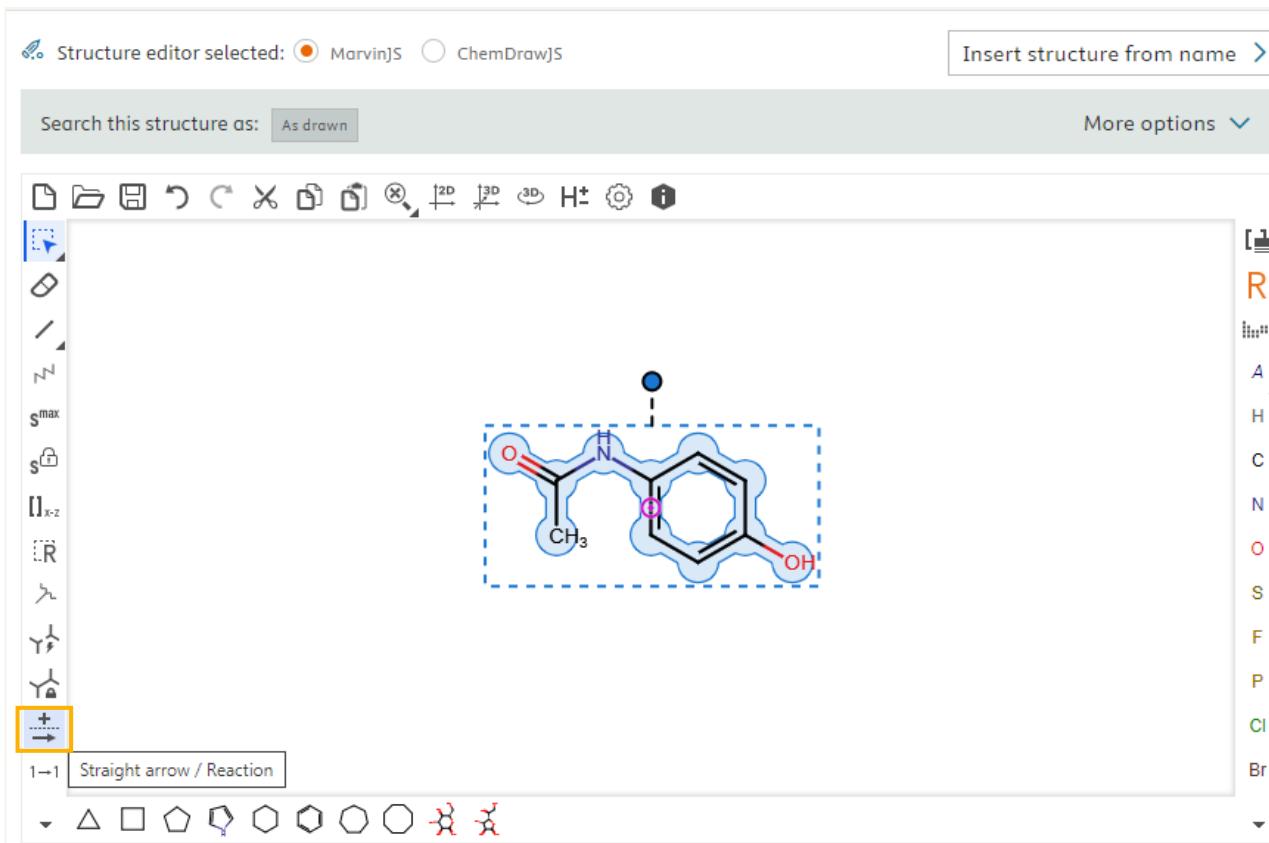
Conditions	Yield	Reference
With 2,2'-azobis(isobutyronitrile); tri-n-butyl-tin hydride In toluene for 4h; Cyclization; radical cyclization; Heating;	68%	Orito, Kazuhiko; Uchiito, Shiro; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao [Organic Letters, 2000, vol. 2, # 3, p. 307 - 310] Full Text  Cited 77 times  Details  Abstract 

2 

40 

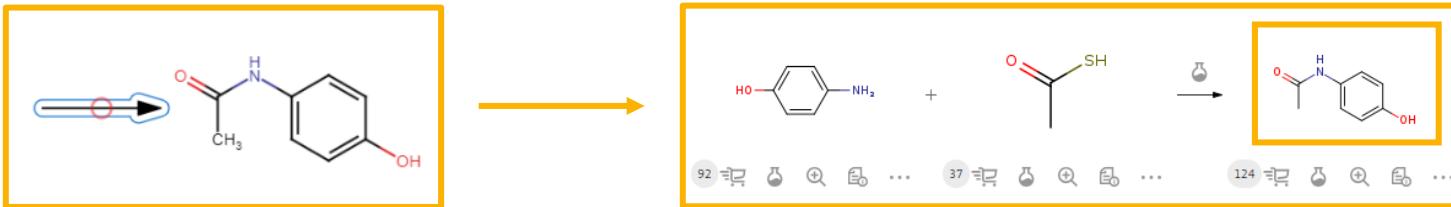
Feedback 

## 尋找反應式的方法: 繪製反應式

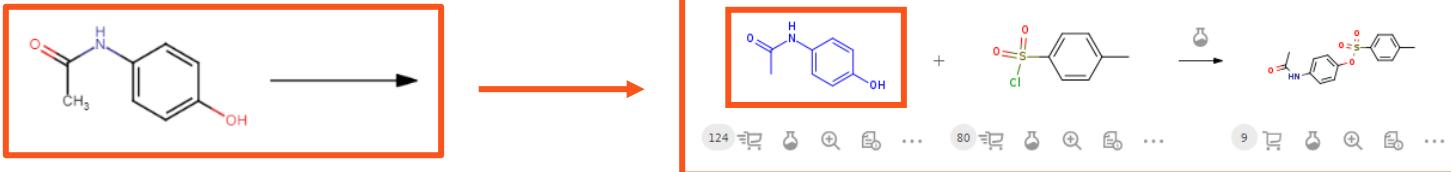


# 尋找反應式的方法: 繪製反應式

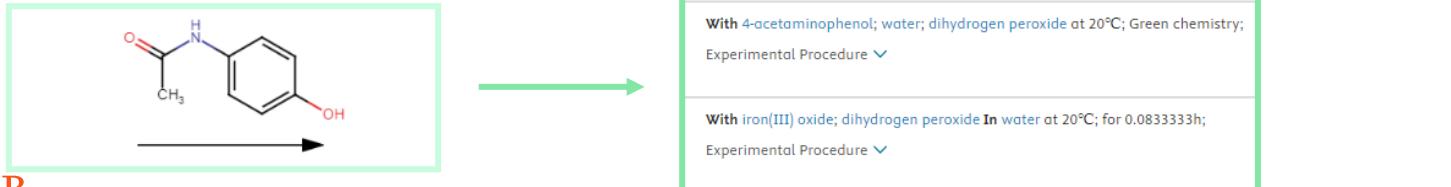
產物: 箭頭在左



起始物: 箭頭在右



催化劑或溶劑: 箭頭在下



# 進階反應式檢索: Query builder

利用 **Query builder** 進一步「加工」搜尋條件



3,532 Reactions Reaction Query : as drawn Preview Results ▾ View Results >

9,368 Reactions Reaction Query : average similarity; included: tau-tomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Preview Results ▾ View Results >

將搜尋結果複製到進階搜尋 **Query Builder** 增加搜尋條件

# 進階反應式檢索: Query builder

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Search in: **Reactions >** Targets > Substances > Documents >

Import Save Options Reset Query Delete Query

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

Structure

As drawn

CC(=O)Nc1ccc(O)cc1

**AND**

Reaction Data & Condi... is **microbiolog\***

**小提示:** 利用 contains 與結合萬用字元「\*」來進行自首搜尋。

reaction

Reaxys

- Reaction Data & Conditions
- Solvent (Reaction Details)
- Time (Reaction Details)
- Temperature (Reaction Details)
- Product XRN (Reaction)
- Product XRN (Reaction Details)
- Product (Reaction Details)

Feedback

# 搜尋結果種類

Types of search results

# 搜尋預覽介面

Search Reaxys

Caffeine

1,554 Substances

Structure : as drawn

Edit in Query Builder Create Alert

Preview Results View Results >

161,183 Documents

Structure : as drawn

Titles, Abstracts, Keywords : "caffeine"

Edit in Query Builder Create Alert

Preview Results View Results >

174 Commercial Substances

Structure : as drawn

Edit in Query Builder Create Alert

Preview Results View Results >

Search Reaxys

Caffeine preparation

431 Reactions

Reaction Query : as drawn

Edit in Query Builder Create Alert

Preview Results View Results >

Search Reaxys

"adenosine a2a receptor"

83 Targets

Target(s) : adenosine a2a receptor

Edit in Query Builder Create Alert

Preview Results View Results >

實驗數值與參考出處

文獻、專利

供應商資訊

合成方法

蛋白、可用藥靶點與化合物交互作用的數據

# Substances: 化合物搜尋結果

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Sort by No of References ↴ ↵

Filters

48,007 Substances out of 2,546 Documents, containing 97,217 Reactions, 83 Targets

0 selected Limit To Exclude Export Preparations 4

Grid Bioactivity Visualization 5

1

2

3

4

5

6

7

8

Preparations - 208 >  
Reactions - 1,646 >  
Targets - 1,616 >  
Documents - 69,689 >

Preparations - 139 >  
Reactions - 1,454 >  
Targets - 361 >  
Documents - 60,555 >

Preparations - 94 >  
Reactions - 535 >  
Targets - 788 >  
Documents - 60,364 >

Feedback

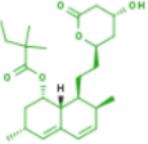
1. 瀏覽搜索結果的軌跡  
2. 過濾功能  
3. 資料庫切換  
4. 顯示化合物製備方法  
5. 生物活性熱圖分析  
6. 商業試劑資訊  
7. 化合物的合成規劃  
8. 化合物的地物理化學實驗數值、光譜、生物活性數據與合成方法

Chemical structures and data for three substances:

- 1. quercetol**  
Chemical structure: (HO)2C6H3C9H2O[O](OH)3  
Properties: 302.24, 317313, 117-39-5  
Data: Identification, Bioactivity (All), Other Data - 5,272  
Druglikeness, Physical Data - 1,297  
Bioactivity (Hit Data), Spectra - 1,993
- 2. 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione**  
Chemical structure: C5H(CH3)3O2N4  
Properties: 194.193, 17705, 58-08-2  
Data: Identification, Bioactivity (All), Other Data - 1,701  
Druglikeness, Physical Data - 804  
Bioactivity (Hit Data), Spectra - 297
- 3. 27**  
Chemical structure: C2  
Properties: 1d, 2d, 3d, Bi

# 詳細的化合物數據

1



80    ...

simvastatin  
C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> 418.574 4768037 

Identification    
Druglikeness  Other Data - 3,543

Preparations - 52 >  
Reactions - 210 >  
Targets - 204 >  
Documents - 17,282 >

▲ Bioactivity (All)

- ▼ In vitro: Efficacy - 3757
- ▼ In vivo: Animal Model - 2171
- ▼ Metabolism - 547
- ▼ Pharmacokinetic - 2767
- ▼ Toxicity/Safety Pharmacology - 1325

▲ Physical Data - 102

- ▼ Melting Point - 15
- ▼ Density - 5
- ▼ Association (MCS) - 10
- ▼ Chromatographic Data - 12
- ▼ Circular Dichroism - 1

▲ Spectra - 133

- ▼ NMR Spectroscopy - 61
- ▼ IR Spectroscopy - 18
- ▼ Mass Spectrometry - 28
- ▼ UV/VIS Spectroscopy - 21
- ▼ Raman Spectroscopy - 3
- ▼ Fluorescence Spectroscopy - 2

- **Preparations:** 製備反應 (作為產物)
- **Reactions:** 包含此化合物的所有反應
- **Targets:** 與此化合物有活性證據的靶點蛋白
- **Documents:** 參考文獻

# Bioactivity (all): 生物活性數據介面

bioactivity (All)

In vitro: Efficacy - 3757

Quantitative Results

- pX 值: 數字越大活性越高
- Action on target: 作用機制
- Value (quant)/Unit: 實驗數值
- Target: 活性蛋白靶點

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Tissue/Organ	Cell	Dose	Effect	Concomitants	Reference
11.9	activation percentage (relative to control + more)		44	%				Hep-G2 cell line	10E-7 $\mu$ M			Other compound: Geranylgeranyl pyrophosphate	Current US2017, Full Text
11.3	activation percentage (relative to control + more)		210	%				Hep-G2 cell line	10E-5 $\mu$ M			Other compound: Geranylgeranyl pyrophosphate	Current US2017, Full Text
10.9	activation percentage (relative to control + more)		46	%				Hep-G2 cell line	10E-6 $\mu$ M			Other compound: Geranylgeranyl pyrophosphate	Current US2017, Full Text
10	Ki (inhibition constant)	=	0.1	nM		Radioligand (/ligand)	3-hydroxy-3-methylglutaryl-coenzyme A reductase:Wild						Riganti, Bosia, A Chemis Full Text

Show/Hide columns 

Show/Hide columns

- pX
- Parameter
- Value (qual)
- Value (quant)
- Unit
- Biological Species
- Action on target
- Target
- (Clinical) findings / disease
- Tissue/Organ
- Cell
- Bioassay
- Dose
- Effect
- Concomitants
- Metabolites
- Reference

更多的參數  
預設隱藏

Reset to default >  Apply > 

ELSEVIER

# Bioactivity Visualization: 生物活性視覺化分析



# 生物活性視覺化分析篩選工具

Filters

Limit to > Exclude >

By Structure

Measurement pX

Parameters

Targets

Target Species

Target Type

Substance action on target

Molecular Weight

Effect

Document Type

Publication Year

Current Patent Assignee

ELSEVIER

Limit To  Exclude  Export  Settings  Navigator  Legend 

以次結構篩選

pX值篩選

實驗數值類型 (IC50 ; Quantatative ; Cmax 、 Tmax)

蛋白靶點

蛋白靶點物種

蛋白靶點類型 (野生型 ; 突變型)

化合物作用機轉

分子量篩選

生物活性效益

文獻類型

發表年份

目前專利授予者

3-hydroxy-3-met...fowleri]  
3-hydroxy-3-met... 1 [rat]  
3x 5'-AMP-acti... [mouse]  
3x 5'-AMP-acti... hamster]  
5'-AMP-activate... it alpha  
ABC transpor...member 2  
ABC transpor...member 3  
ABC transpor...member 6  
ABC transport...ily MRP4  
ABC transport...g domain  
Acetylcholinest... peptide)  
Actin  
Activating mole...rotein 1  
Acyl-CoA (8-3)-desaturase  
Acyl-CoA 6-desaturase  
Adapter molecule crk  
Adenomatous p... sis coli

5.3 1 5.7 4.7

# Reactions: 反應式搜尋結果

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

1,646 Reactions out of 913 Documents, containing 2,012 Substances, 3,050 Targets

0 selected Limit To Exclude Export Hide Conditions

Sort by Reaxys Ranking 2

1. 匯出按鈕  
2. 搜尋結果的排序推薦  
3. 文獻出處、引用強度、原文連結  
4. 詳細實驗步驟

1

109 31 49

17 Conditions Find Similar Reaction ID: 429107

Conditions In propan-2-one

Yield 96% Reference Shi, Ya-Juan; Gao, Jian-Wei; Liu, Chen-Fu [Journal of Molecular Structure, 2022, vol. 1268, art. no. 133674] Full Text Cited 6 times Details Abstract

85% Tatsuzaki, Jin; Ohwada, Tomohiko; Otani, Yuko; Inagi, Reiko; Ishikawa, Tsutomu [Beilstein Journal of Organic Chemistry, 2018, vol. 14, p. 3112-3121] Full Text Cited 7 times Details Abstract

4

Methylation of quercetin (2) with the Me<sub>2</sub>SO<sub>4</sub>/KOH/DMSO system (run 2 in Table 2): QPE [2-(3,4-Dimethoxyphenyl)-3,5,7-trimethoxy-4H-1-benzopyran-4-one] (1)

To a suspension of powdered KOH (1.66 g, 29.7×10<sup>-3</sup> mol) in DMSO (8 mL) was slowly added quercetin (2, 1 g, 3.3×10<sup>-3</sup> mol), followed by Me<sub>2</sub>SO<sub>4</sub> (2.5 mL, 26.4×10<sup>-3</sup> mol), with control of the temperature to less than 10 °C (CAUTION: The reaction is exothermic). The resulting dark brown solution was stirred at rt for 2 h, during which time the color changed to light brown. The reaction was quenched with H<sub>2</sub>O (80 mL), and the resulting suspension was extracted with EtOAc (50/20/20 mL). The EtOAc solution was successively washed with 5% NaOH aq (10 mL×4), H<sub>2</sub>O (10 mL×3), and brine (10 mL), dried over sodium sulfate, and evaporated under reduced pressure to give QPE (1) as a light brown solid (1.05 g), which was homogeneous on TLC and showed a single peak at the same retention time as that of an authentic sample. Recrystallization from MeOH gave colorless prisms, mp 147–149 °C [lit. mp 136–137 °C [34]; mp 151 °C [39]; mp 151.2 °C [51]; <sup>1</sup>H NMR δ 3.88 (s, 3H, OMe), 3.90 (s, 3H, OMe), 3.95 (s, 9H, OMe×3), 6.34 (d, J = 2.2 Hz, 1H, 6- or 8-H), 6.49 (d, J = 2.2 Hz, 1H, 6- or 8-H), 6.97 (d, J = 8.4 Hz, 1H, 5'-H), 7.71 (dd, J = 8.4, 2.0 Hz, 1H, 6'-H), 7.72 (s-like, 1H, 2'-H); <sup>13</sup>C NMR δ 55.9, 56.1, 56.3, 56.6, 60.1, 92.7, 96.0, 109.8, 111.2, 111.8, 121.8, 123.8, 141.4, 149.0, 151.2, 152.6, 159.0, 161.3, 164.1, 174.1

3

# 反應式搜尋結果篩選工具

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

結構

產率

試劑 · 催化劑

溶劑

催化劑類別

溶劑類別

產物的可能性

反應物的可能性

反應類別

來源種類 (文獻 · 專利)

出版年份

縮小到只有一步反應

縮小到只包含實驗性術語的名單

可展開查看篩選細項

Solvent Classes

- Low boiling (<100°C) 17
- Inorganic 9
- Protic 8
- Green 8
- Aprotic apolar 1
- Aprotic dipolar 1
- Red 1

[View more](#)

- 每個專案的細目可以通過點擊展開
- 這些專案按照案件數量的順序進行排序
- 可以透過輸入數位或單位詞來過濾專案

Solvent Classes 26

- Solvent Classes
  - Low boiling (<100°C) 21
  - Inorganic 17
  - Protic 9
  - Green 8
  - Aprotic apolar 8
  - Aprotic dipolar 1
  - Red 1

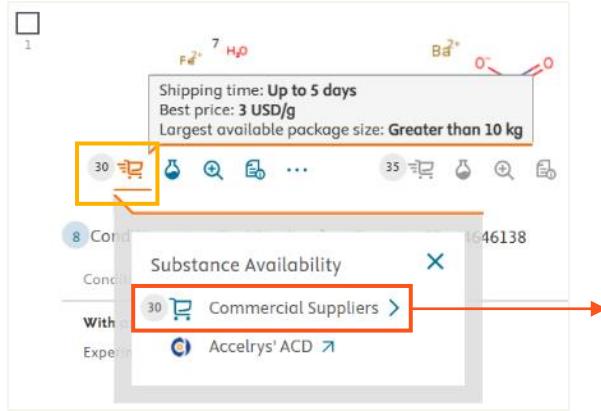
Selected search items:  
[Inorganic](#) [Low boiling \(<100°C\)](#)

More +

Limit to > Exclude >

# 商業試劑目錄資訊

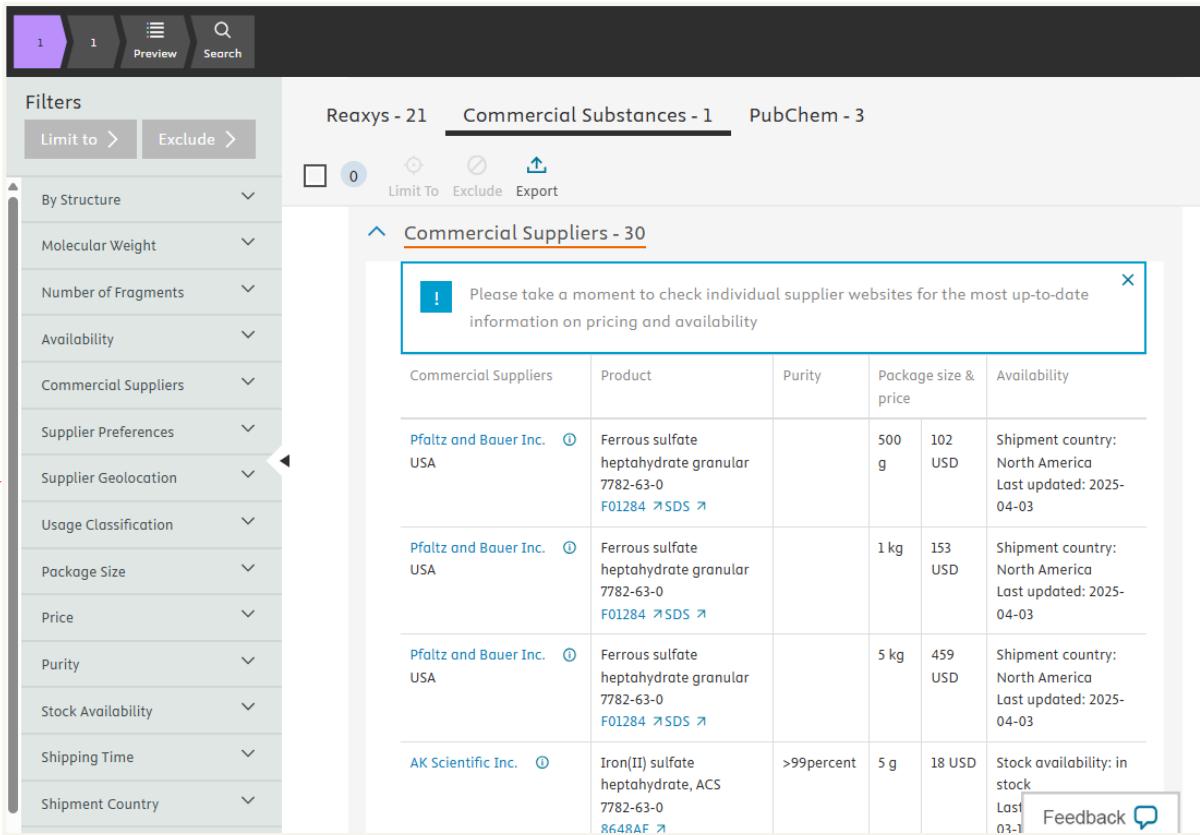
滑鼠滑至購物車上方會自動顯示最佳價格，  
購物車旁的數字代表全球有多少供應商供應此材料。



Shipping time: Up to 5 days  
Best price: 3 USD/g  
Largest available package size: Greater than 10 kg

30  Commercial Suppliers 

- 可以檢查供應商、商品編號、純度、包裝大小、價格和交貨日期。篩選功能使您將搜索範圍縮小到特定供應商
- 篩選設定也依供應商相關資訊而定義



1 1 Preview Search

Filters

Limit to > Exclude >

By Structure  
Molecular Weight  
Number of Fragments  
Availability  
Commercial Suppliers  
Supplier Preferences  
Supplier Geolocation  
Usage Classification  
Package Size  
Price  
Purity  
Stock Availability  
Shipping Time  
Shipment Country

Reaxys - 21 Commercial Substances - 1 PubChem - 3

0 Limit To Exclude Export

Commercial Suppliers - 30

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

Commercial Suppliers	Product	Purity	Package size & price	Availability
Pfaltz and Bauer Inc. USA	Ferrous sulfate heptahydrate granular 7782-63-0 F01284  		500 g 102 USD	Shipment country: North America Last updated: 2025-04-03
Pfaltz and Bauer Inc. USA	Ferrous sulfate heptahydrate granular 7782-63-0 F01284  		1 kg 153 USD	Shipment country: North America Last updated: 2025-04-03
Pfaltz and Bauer Inc. USA	Ferrous sulfate heptahydrate granular 7782-63-0 F01284  		5 kg 459 USD	Shipment country: North America Last updated: 2025-04-03
AK Scientific Inc. USA	Iron(II) sulfate heptahydrate, ACS 7782-63-0 864RAF  	>99percent	5 g 18 USD	Stock availability: in stock Last updated: 2025-03-11

Feedback 

# 文獻專利搜尋結果

49,338 Documents with 26,579 Substances, 9,947 Reactions, 8 Targets

0 selected Limit To Exclude Export

Sort by Relevance  Bioactivity Visualization 

Relevance  
Publication Year  
Document Type  
Cited By

1 Iron control in nitrate hydrometallurgy by (auto)decomposition of iron(II) nitrate  
van Weert; Shang [Hydrometallurgy, 1993, vol. 33, # 3, p. 255 - 271]  
Abstract  Index Terms  Full Text  Cited 21 times

Abstract hit: {...in the nitrate system. Iron(III) nitrate leaching of metallic iron or reactive iron...}

Index Terms hit: {...Iron control, Iron(II) nitrate, Nitrate hydrometallurgy...}

2 Effect of ferric iron and nitrate on hydrogen sulfide control in lab-scale reactors  
Yang, Zhi; Zhu, David Z.; Yu, Tong; Shypanski, Adam; Zhang, Guijiao; Zhou, Yongchao [Environmental science : water research and technology, 2021, vol. 7, # 10, p. 1806 - 1818]  
Abstract  Index Terms  Substances  4  Full Text  Cited 9 times

Abstract hit: {...force mains. Ferric iron and nitrate were added into two of the four...}

Index Terms hit: {...inhibition, iron, kinetics...}

3 The anaerobic oxidation of methane in paddy soil by ferric iron and nitrate, and the microbial communities involved  
Luo, Dan; Meng, Xiangtian; Zheng, Ningguo; Li, Yaying; Yao, Huaiying; Chapman, Stephen J. [Science of the Total Environment, 2021, vol. 788, art. no. 147773]  
Abstract  Index Terms  Substances  1  Full Text  Cited 73 times

來自 Scopus 的引用次數，可點擊查看引用該文章的參考文獻列表

Feedback 

# 文獻專利搜尋結果篩選工具

Filters

Limit to > Exclude >

出版年份

Document Type

Authors of Scientific Documents

Current Affiliation

Inventors of Patents

Current Patent Assignee

Patent Office

Journal Title

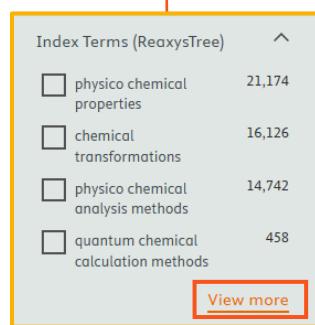
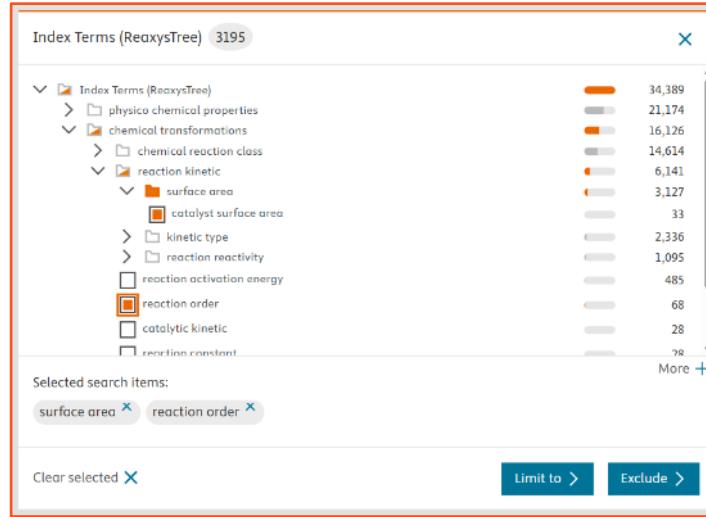
Substance Classes

Reaction Classes

Index Terms (List)

Index Terms (ReaxysTree)

Manually curated content only



用常見的化學概念來整理索引詞

以「**催化劑表面積**」catalyst surface area 的文獻為例：點擊 View more > chemical transformations > reaction kinetic > surface area > catalyst surface area

# Reaxys 資料庫中的資料互相串連

取得研究咸豐草的一千篇文獻中被我們**人工索引**的化合物清單。

↓

2,190 Documents with 4,317 Substances, 346 Reactions, 6 Targets

0 selected    Limit To    Exclude    Export

Sort by Publication Year Bioactivity Visualization

1 Changes in plant diversity and community attributes of coal mine affected forest in relation to a community reserve forest of Nagaland, Northeast India

Semy, Khikeya; Singh, Maibam Romeo [*Tropical Ecology*, 2024, vol. 65, # 1, p. 16 - 25]

Abstract Index Terms Substances Full Text

Abstract hit: {...Ageratum conyzoides, **Bidens pilosa** and Drymaria cordata were prominently distributed in CMAF while...}

2 Phytoremediation of Heavy Metal Contaminated Soil Using **Bidens pilosa**: Effect of Varying Concentrations of Sophorolipids

Shah, Vijendra; Dani, Pooja; Daverey, Achlesh [*Applied Biochemistry and Biotechnology*, 2024, vol. 196, # 5, p. 2399 - 2413]

Abstract Index Terms Substances Full Text

Abstract hit: {...soil using **Bidens pilosa**. The results showed that increasing concentrations of SL increased...}

Index Terms hit: {...**Author keyword:** **Bidens pilosa**, Biosurfactant...}

3 Effect and mechanism of Qing Gan Zi Shen decoction on heart damage induced by obesity and hypertension

Zhang, Shujie; Liu, Zitian; Zhang, Han; Zhou, Xiaonian; Wang, Xiuming; Chen, Yan; Miao, Xiaofan; Zhu, Yao; Jiang, Weimin [*Journal of Ethnopharmacology*, 2024, vol. 319, art. no. 117163]

Abstract Index Terms Full Text

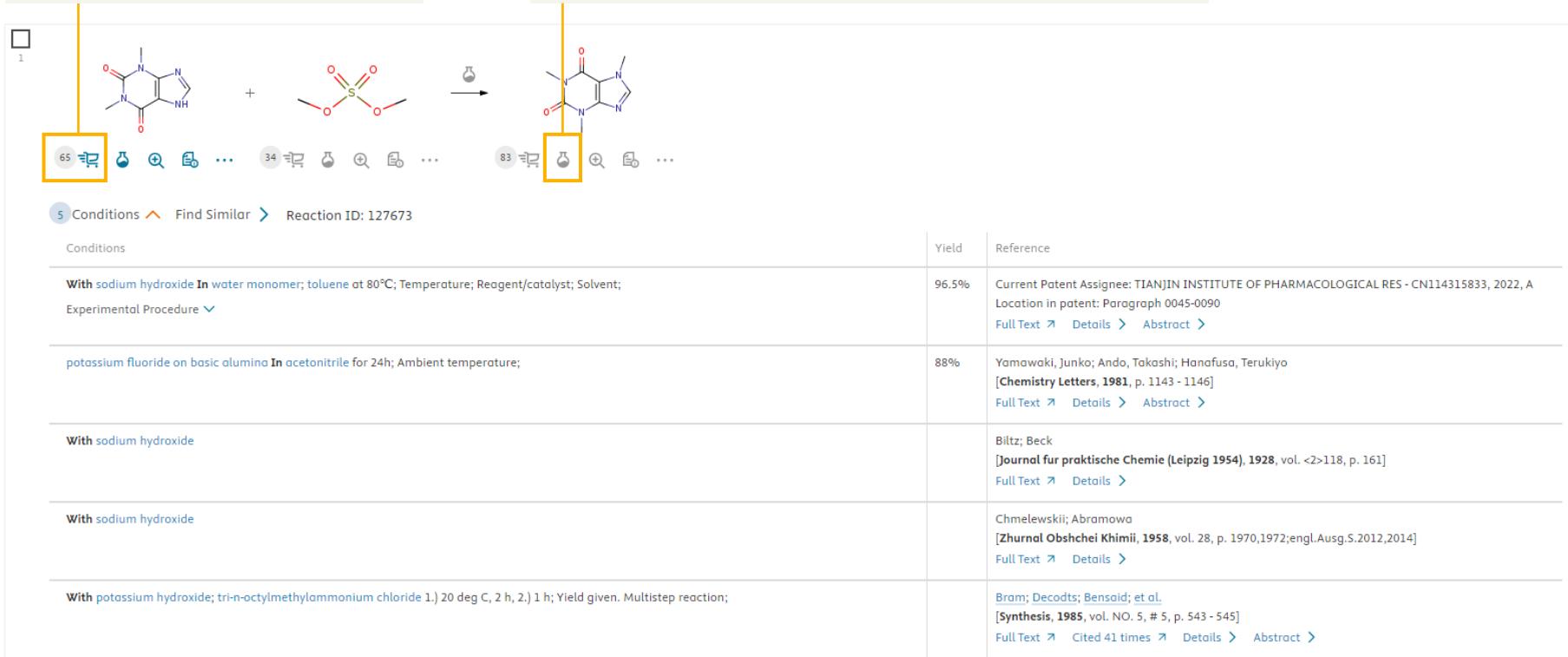
Index Terms hit: {...wheat germ agglutinin, **Bidens pilosa** extract, unclassified drug...}

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# Reaxys 資料庫中的資料互相串連

從購物車連結到商用資料庫去評估實驗的成本

你可以從反應式的查詢結果再連結到物質資料庫，查詢這個產物的光譜數據。



1

65 34 83

5 Conditions Reaction ID: 127673

Conditions	Yield	Reference
With sodium hydroxide In water monomer; toluene at 80°C; Temperature; Reagent/catalyst; Solvent; Experimental Procedure	96.5%	Current Patent Assignee: TIANJIN INSTITUTE OF PHARMACOLOGICAL RES - CN114315833, 2022, A Location in patent: Paragraph 0045-0090 <a href="#">Full Text</a> <a href="#">Abstract</a>
potassium fluoride on basic alumina In acetonitrile for 24h; Ambient temperature;	88%	Yamawaki, Junko; Ando, Takashi; Hanafusa, Terukiyo [Chemistry Letters, 1981, p. 1143 - 1146] <a href="#">Full Text</a> <a href="#">Abstract</a>
With sodium hydroxide		Biltz; Beck [Journal fur praktische Chemie (Leipzig 1954), 1928, vol. <2>118, p. 161] <a href="#">Full Text</a>
With sodium hydroxide		Chmielewskii; Abramowa [Zhurnal Obshchei Khimii, 1958, vol. 28, p. 1970,1972;engl.Ausz.S.2012,2014] <a href="#">Full Text</a>
With potassium hydroxide; tri-n-octylmethylammonium chloride 1.) 20 deg C, 2 h, 2.) 1 h; Yield given. Multistep reaction;		Bram; Decodts; Bensaid; et al. [Synthesis, 1985, vol. NO. 5, # 5, p. 543 - 545] <a href="#">Full Text</a> Cited 41 times <a href="#">Abstract</a>

# 藥物靶點與 藥物設計

Drug Targets and Drug Design

ELSEVIER

# 活性化合物的設計與優化

## 任務

- 建立 Structure-Activity Relationships (SAR) 並辨認哪些結構特徵促進高活性和低活性
- 識別與化合物結構相似的化合物潛在非靶標活性
- 合理化並優化化合物系列的藥物代謝、藥物動力學和毒性特性

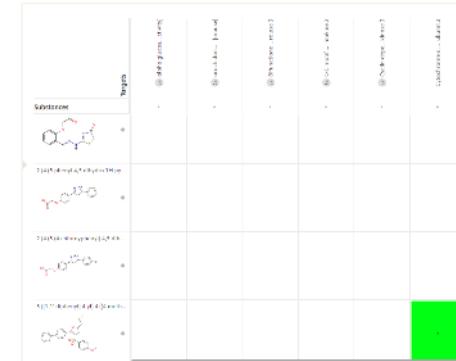
## Reaxys 如何協助

- 提供完整的生物活性 (bioactivity) 資訊，以幫助建立已知的結構-活性關係 (Structure-Activity Relationships)、藥物代謝藥物動力學 (DMPK) 和吸收、分佈、代謝、排泄及毒性 (ADME-Tox) 特性
- 提供生物活性熱圖，使結構及其對各種靶標的生物活性值能快速高效地展示

▲ [Toxicity/Safety Pharmacology - 81](#)

Quantitative Results

pX	Parameter	Value (quant)	Unit	Action on target	Target
8.11	IC50	7.7	nM		
8.11	IC50	7.8	nM		
8	IC50	10	nM	Inhibitor	Bcr-ABL p210 (T315A):Wild



# 活性化合物的設計與優化

## 任務

- 建立 Structure-Activity Relationships (SAR) 並辨認哪些結構特徵促進高活性和低活性
- 識別與化合物結構相似的化合物潛在非靶標活性
- 合理化並優化化合物系列的藥物代謝、藥物動力學和毒性特性



## Reaxys 如何協助

- 提供完整的生物活性 (bioactivity) 資訊，以幫助建立已知的結構-活性關係 (Structure-Activity Relationships)、藥物代謝藥物動力學 (DMPK) 和吸收、分佈、代謝、排泄及毒性 (ADME-Tox) 特性
- 提供生物活性熱圖，使結構及其對各種靶標的生物活性值能快速高效地展示



49m  
bioactivity  
data points



8.6m  
substances with  
bioactivity data



44k  
biological  
targets



6.6m  
essays with  
additional insights



26k  
cell lines from  
102k species

## Question:

如何快速地取得靶點訊息並評估結構活性分析？

### 感興趣的靶點：

JAK3 (Tyrosine-protein Kinase JAK3)

與 JAK3 有 interaction 的 substances 有哪些？

結構特徵？高活性的有哪些？

# 藥物靶點檢索

從 Reaxys 獨特的靶點分類樹(Reaxystree) 找到相對應的關鍵字，可以確保相關的同義詞都涵蓋在搜尋範圍內

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Discover a more intuitive way to search — with Reaxys AI Search Beta.

Search for tyrosine-protein Kinase JAK3 Import

Search Reaxys

tyrosine-protein Kinase JAK3 Find >

Target Names tyrosine-protein kinase jak3

47 Targets Target(s) : tyrosine-protein kinase jak3 Preview Results View Results

67,068 Substances Target(s) : tyrosine-protein kinase jak3 Preview Results View Results

17,186 Documents Titles, Abstracts, Keywords : "tyrosine-protein kinase jak3" Preview Results View Results

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# 藥物靶點檢索

## 利用生物活性專屬的過濾工具

Filters 

105 Substances out of 3 Documents, containing 209 Reactions, 2 Targets

0 selected Limit To Exclude Export Preparations

By Structure 

Measurement pX 2

>12-13 2

>11-12 105

(no entry given) 105

Targets 

Parameters 

Substance Classes 

Molecular Weight 

Number of Fragments 

Availability 

Available Data 

Document Type 

Publication Year 

Current Patent Assignee 

LogP 

H Bond Donors 

tasocitinib

C<sub>18</sub>H<sub>20</sub>N<sub>6</sub>O 312.374 11647225 

Identification Bioactivity (All) Other Data - 1,104

Druglikeness Physical Data - 33

Bioactivity (Hit Data) Spectra - 39



**Bioactivity (Hit Data)**



**In vitro: Efficacy - 1**

**Quantitative Results**

pX	Parameter	Value (quant)	Unit	Target
11.1	IC50	7.308E-06	μM	Tyrosine-protein kinase JAK3 [human]:Wild/Tyrosine-protein kinase JAK1 [human]:Wild/Tyrosine-protein kinase JAK2 [human]:Wild



Bioactivity (All)

Preparations - 105 >

Reactions - 314 >

Targets - 668 >

Documents - 1,863 >

Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

**Bioactivity Visualization Settings**

Value of X-axis Targets

Value of Y-axis Substances 

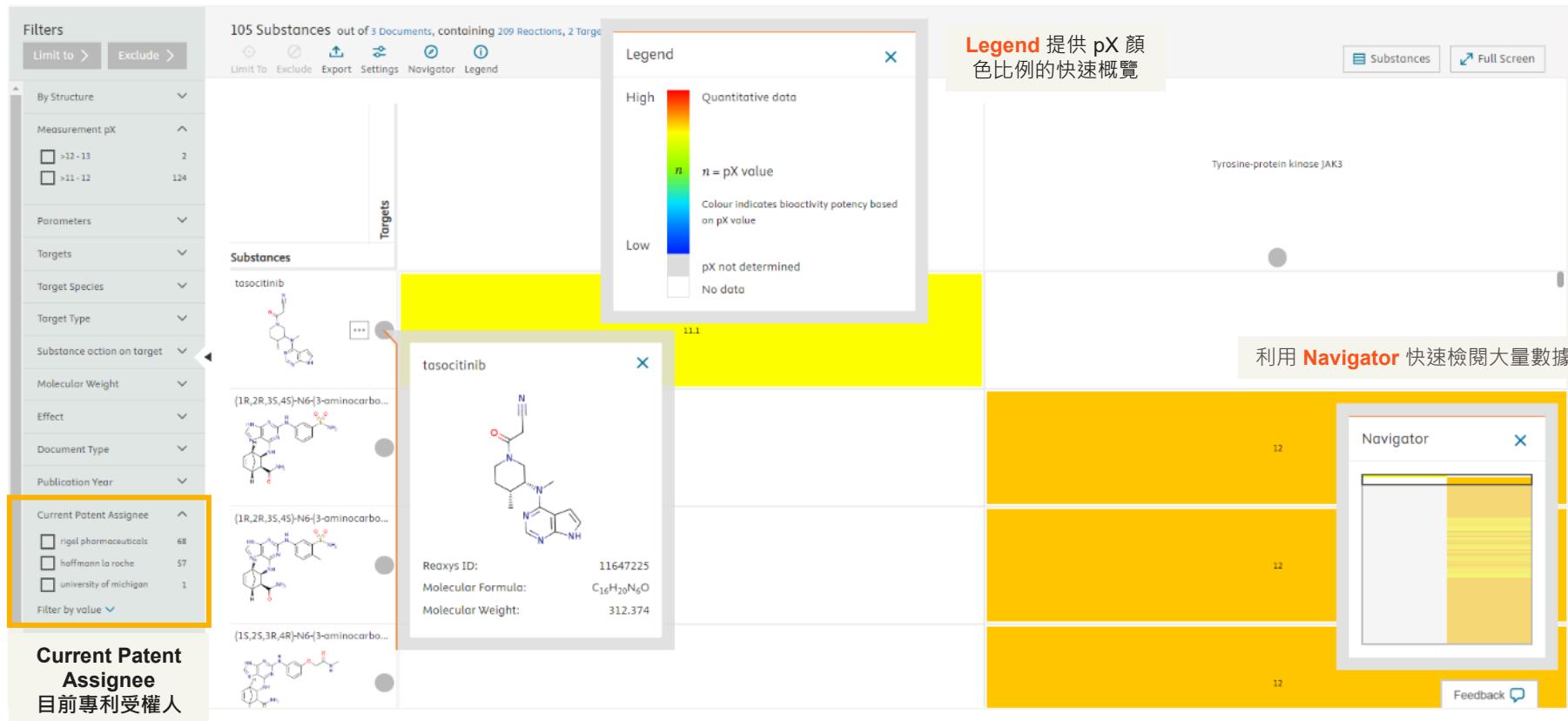
Value of Cells

Show substances

Display mode

Always show set

# 藥物靶點檢索: 使用熱圖視覺化分析



# 藥物靶點檢索: 匯出 SAR 資料做更多分析

Reaxys

Quick search Query builder Results Refersynthesis History Alerts

105 Substances out of 10 documents, containing 20% Reactions

Substances Targets

Export Substances

Export substances and bioactivities

Choose a format: Microsoft Excel New Layout

- Microsoft Excel New Layout (selected)
- Microsoft Excel
- Tab-delimited text
- XML
- SD/Molfile

Range:

Export:

Additional options:  Include structures

Disclaimer: please refer to our Terms and Conditions before downloading data.

Export >

Tyrosine-protein kinase JAK3

Navigator

# 逆合成 AI 工具

Retrosynthesis AI

ELSEVIER

# Retrosynthesis AI: 探索合成途徑

The screenshot shows the Reaxys search interface with the Retrosynthesis AI feature highlighted. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (which is selected and highlighted in orange), 'History', 'Alerts', and 'Reaxys AI Search Beta'. A search bar at the top asks '繪製你的目標分子，尋找完整的合成路徑 (Complex molecules)'. Below the search bar, there is a 'Discover a mo' button and a 'Search Beta.' button. The main search area is titled 'Search substances, reactions, documents and bioactivity data' and includes an 'Import' button. The search form has a 'Search Reaxys' label, a search input field with placeholder 'Documents, e.g. published by Schrock', and a 'Find >' button. Below the search input is an 'AND' operator and a 'Draw' button, which is highlighted with a yellow box. To the right of the 'Draw' button is a box labeled '尋找單步驟的反應' (Search for single-step reactions). At the bottom, there is a 'Content Overview' section with statistics: 350M Substances, 71M Reactions, 122M Documents, 47M Patents, and 49M Bioactivities. The Elsevier logo is in the bottom left, and the RELX logo is in the bottom right. A feedback button is also present in the bottom right corner.

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Discover a mo

繪製你的目標分子，尋找完整的合成路徑 (Complex molecules)

Search Beta.

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances

Import

Search Reaxys

Documents, e.g. published by Schrock

Find >

AND

Draw

尋找單步驟的反應

Content Overview | Latest update: 18. August 2025 >

350M Substances 71M Reactions 122M Documents 47M Patents 49M Bioactivities

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RELX™

Feedback

# 繪製目標化合物的結構

需登入個人帳號以開啟 AI Predicted 選項

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts + Reaxys AI Search Beta

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Parameters

Predicted ⓘ  
15 steps per route (up to)  
Stereochemistry supported  
Regioselectivity ignored  
RCS: delivery time up to 10 days  
RCS: no price limit  
Standard processing time  
No intermediates defined  
Powered by iktos

Published ⓘ  
10 full routes (up to)  
5 branches per step (up to)  
10 steps per route (up to)  
Stop at commercial building blocks  
20% yield per step (assumed, if not published)

繪製 Retrosynthesis 的目標化合物「無須」添加反應式箭頭

CC1=CC=C(C=C1)C(C)C2=CC=C(C=C2)C3=CC=C(C=C3)C(C)C4=CC=C(C=C4)C5=CC=C(C=C5)C(C)C

**Predicted:** AI預測引擎會嘗試預測繪製分子的合成路徑，即便該分子無法找到任何參考資料。

**Published:** 當繪製的分子為 published 結構，Reaxys 呈現文獻中報導的合成路徑，若繪製的分子為 novel 分子，結果會顯示 0

進行分析

Clear  Cancel  Synthesize

Feedback

# 如何更精準地控制 AI 的合成規劃策略

The screenshot shows the Reaxys software interface. At the top, there is a navigation bar with links to 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (underlined), 'History', 'Alerts', and 'Reaxys AI Search'. Below the navigation bar is a toolbar with various icons for drawing and editing chemical structures. On the left, there is a sidebar with 'My Synthesis Projects' and a 'Draw' section. The main workspace shows a complex organic molecule with a hydroxyl group and a bromine atom. To the right of the molecule is a vertical column of synthesis planning tools, each with a small icon and a label: 'S<sup>max</sup>' (highlighted with a yellow box), 'S<sup>lock</sup>' (highlighted with a yellow box), 'R' (highlighted with a yellow box), 'Make/Break' (highlighted with a yellow box), and 'Protect (No change)' (highlighted with a yellow box). At the bottom of the workspace are buttons for 'Clear', 'Cancel', and 'Synthesize >'. The entire interface is set against a light gray background.

不使用 Atom lock 標記

目標分子需繪製完整，不使用 Generics group，例用“ALT”來代表 Akyl group

**Make/Break 工具：**每個目標分子可在一個鍵上標示 Make/Break，該鍵將被優先打斷，主導合成規劃策略

**Protect (No change) 工具：**每個目標分子可有數個鍵標示 Protect，該鍵將被保留於整個合成計畫，影響合成規劃策略

# 如何調整逆合成分析參數 Predicted

Predicted [\(i\)](#)

[General](#) [Intermediates](#)

Length of routes [\(i\)](#)

Max. Number of steps:  (2-15)

First disconnect only

Stereo and Regioselectivity [\(i\)](#)

Ignore stereochemistry

Only regioselective reactions

Starting materials settings [\(i\)](#)

Reaxys Commercial Substances (RCS)

Max. Shipping time [\(i\)](#)

up to 10 days  any

Max. Price per gram:  (\$/g) [\(i\)](#)

Processing time [\(i\)](#)

Standard  Extended

Powered by **iktos** 

## 基本設定

- **Length of routes:** 生成的路線的最大數目
- **Ignore stereochemistry:** 忽視立體化學選擇性
- **Only regioselective reactions:** 只選立體化學選擇性
- **Reaxys Commercial Substance:** 合成材料最長運送時間  
合成材料價格上限
- **Processing time:** AI 計算時間 (Standard 約 10 分鐘)  
若分子較複雜 Extended 設置可長達 30 分鐘，但有更高機會找出更多路徑

Predicted [\(i\)](#)

[General](#) [Intermediates](#)

Enter intermediates [\(i\)](#)

Include substructures (up to 10)  
 [\(i\)](#)

Exclude substructures (up to 10)  
 [\(i\)](#)

Powered by **iktos** 

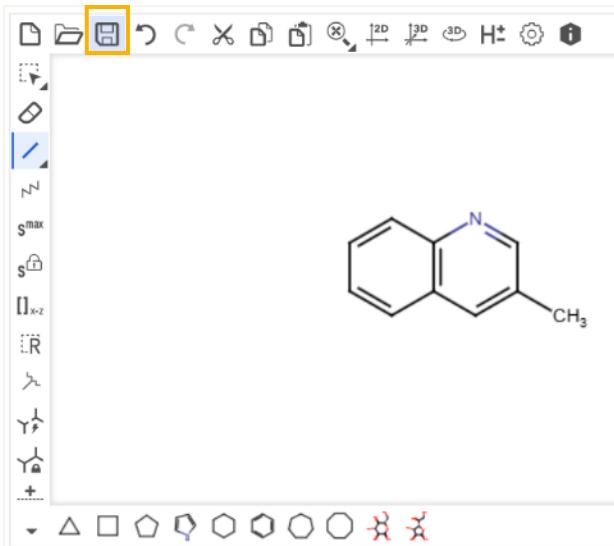
## 中間產物

- **Include substructures:** 可要求AI一定要採用某個化合物作為中間產物
- **Exclude substructures\*:** 可要求AI避免某個化合物作為中間產物  
\*(本功能需將結構預先轉換成 SMILES 格式，操作方法見下頁)

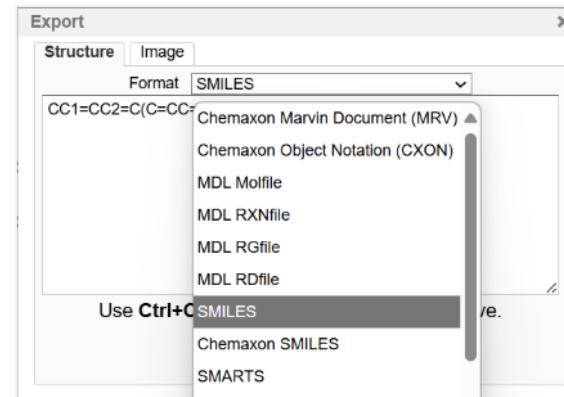
# 將中間產物結構轉為 SMILES 格式

1 用 Marvin JS 繪製想要轉換成 SMILES 的結構

2 點擊儲存



3 選擇 SMILES 格式



4 呈現的字串為 SMILES 格式，可反白複製



# 如何調整逆合成分析參數 Published

Parameters

Standard processing time  
No intermediates defined

Powered by iktos

Published

Length & depth of synthesis plans

Full routes: 10

Last step only

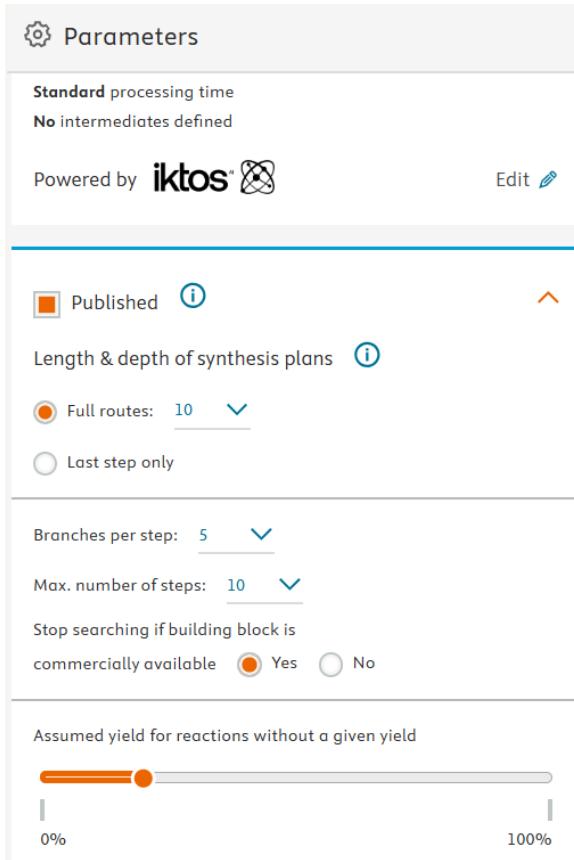
Branches per step: 5

Max. number of steps: 10

Stop searching if building block is commercially available

Assumed yield for reactions without a given yield

0% 100%



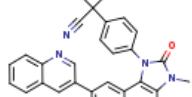
- Length & depth of synthesis plans: 生成的路線的最大數目
- Branches per step: 線上的最大分支數量
- Max. number of steps: 最大的步驟數
- Stop searching if building block is commercially available: 當歸因於一種商業化的化合物 時將停止分析 →建議關閉 (因為大分子有販售 )
- Assumed yield for reactions without a given yield: 設定各反應的允許產量

# 如何分析化合物搜尋結果中感興趣化合物的合成途徑

Reaxys - 115   Commercial Substances - 66   PubC

115 Substances out of 3,939 Documents, containing 143 Reactions, 33

0 selected   Limit To   Exclude   Export   Preparations

1    **2-methyl-2-[4-(3-methyl-1-phenylprop-1-ynyl)-1H-indol-3-yl]propan-1-one**  
C<sub>30</sub>H<sub>23</sub>N<sub>5</sub>O   469.546   12  
Identification  
Druglikeness  
Create synthesis Plan

2    **Synthesize**  
Find preparations  
Create retrosynthesis plans

自動將您查到的化合物帶入 Retrosynthesis 介面

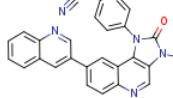
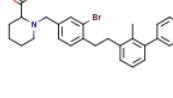
Reaxys®

Stephanie Su   ?

Quick search   Query builder   Results   **Retrosynthesis**   History   Alerts   Semantic Search Beta

Draw   My Synthesis Projects

0   Delete

No.	Date	Project name	Draw new structure	No. of routes	Predicted	Published
2891288	29 May 2025	Project #2891288		12	0 In queue	2
2891279	29 May 2025	Project #2891279		12	0 In progress	0 Click here for options

# 合成途徑開發的專案管理介面

The screenshot displays a software interface for managing synthesis projects. On the left, a sidebar shows 'My Synthesis Projects' with a 'Draw' button. The main area shows two projects:

- Project #2891288** (row 1):
  - Created on 29 May 2025.
  - Structure: A complex molecule with a central benzene ring substituted with a nitrile group, a phenyl ring, and a quinoline-like ring.
  - Route parameters (4):
    - 15 steps per route (up to)
    - 10 full routes (up to)
    - Stereochemistry supported
    - 10 steps per route (up to)
    - Regioselectivity ignored
    - 5 branches per step (up to)
    - RCS: delivery time up to 10 days
    - RCS: no price limit
    - Stop at commercial building blocks
    - Standard processing time
    - 20% yield per step (assumed, if not published)
    - No intermediates defined
  - Published routes: Predicted 13, Published 2.
- Project #2891279** (row 2):
  - Created on 29 May 2025.
  - Structure: A molecule with a central benzene ring substituted with a hydroxyl group, a phenyl ring, and a cyclohexane ring with a carboxylic acid group.
  - Route parameters (4):
    - 15 steps per route (up to)
    - 10 full routes (up to)
    - Stereochemistry supported
    - 10 steps per route (up to)
    - Regioselectivity ignored
    - 5 branches per step (up to)
    - RCS: delivery time up to 10 days
    - RCS: no price limit
    - Stop at commercial building blocks
    - Standard processing time
    - 20% yield per step (assumed, if not published)
    - No intermediates defined
  - Published routes: Predicted 1, Published 0. Click here for options.

1 點擊重新命名

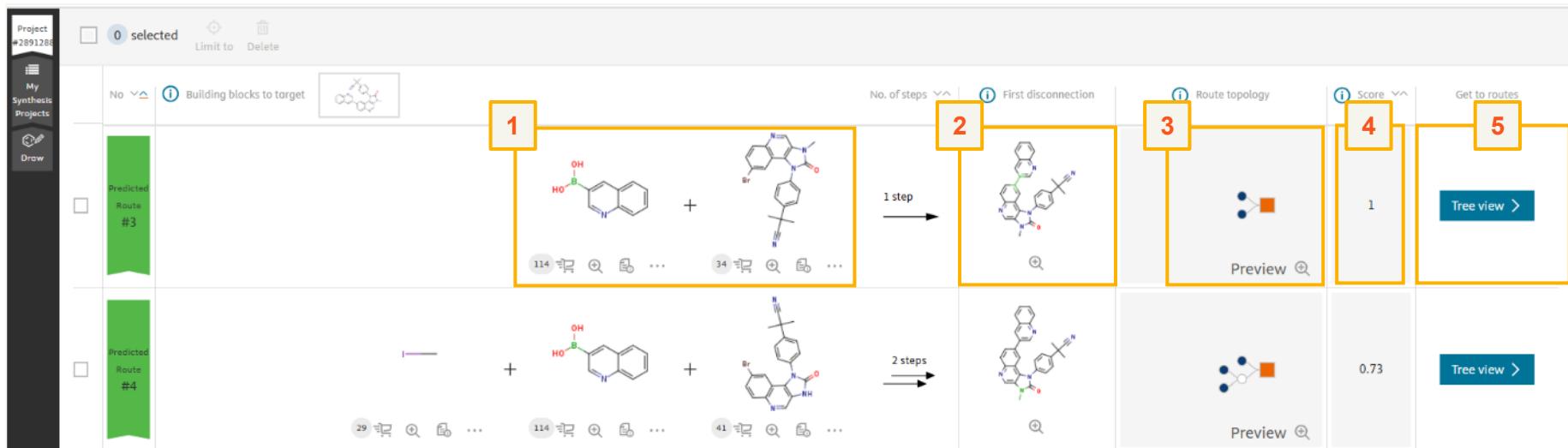
2 創建並分析一個新的結構

3 調整參數並重新分析或適度修改目標分子

4 預測及發表過的參數

5 確認路徑

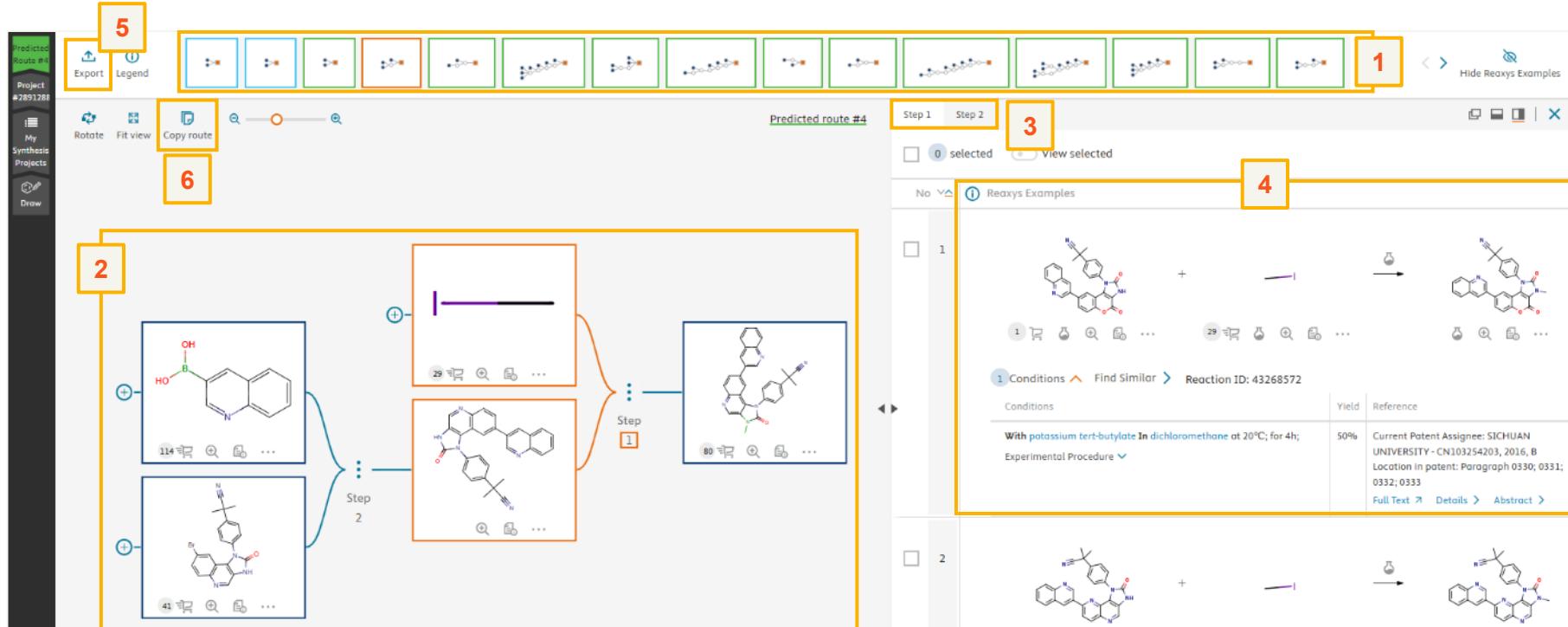
# 生成合成路線清單界面



- 1 該合成路徑需要的起始原料與材料金額
- 2 **First disconnection:** 第一個斷鍵位置
- 3 **Route topology:** 路徑長度與分支呈現，方便比較

- 4 **Confidence Score:** 評估該預測路徑的信賴度，從1分至0分。(1分很有可能，0分非常不可能)
- 5 **Get to routes:** 詳細路徑以樹狀路徑呈現

# 合成途徑的樹狀圖畫面



1. 切換至其他合成路徑
2. 預測路徑
3. 合成步驟切換
4. 相似反應的參考文獻
5. 匯出功能
6. 複製路徑可直接於 ChemDraw 貼上

# 個人化設定 及管理

ELSEVIER

## 匯出搜尋結果

Reaxys - 2,567 Commercial Substances

2,567 Substances out of 17,468 Documents, containing 0 selected Limit To Exclude Export Preparations

simvastatin C<sub>25</sub>H<sub>38</sub>O<sub>5</sub> Identification Druglike 3,541

80

**輸出介面設定:**

- 匯出形式，匯出範圍，匯出內容
- 選擇一個選項，然後點選匯出按鈕
- 每次輸出最多 5000 個項目
- 24 小時內最多 10 次

\*若您未登入且通過 IP 身分驗證，則無法匯出

Export substances Reaxys

Choose a format: PDF/Print

Range: Range (e.g. 1-2, 1-10) From 1 To 9

Export: All available data

Additional options:  Include structures  Include a description in the document

This is export attempt 1 out of 25 for today.  
Disclaimer: please refer to our [Terms and Conditions](#) before downloading data.

PDF/Print

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Tab-delimited text
- Electronic Lab Notebook
- RD File
- SD/Molfile
- Smiles

Include structures

Export >

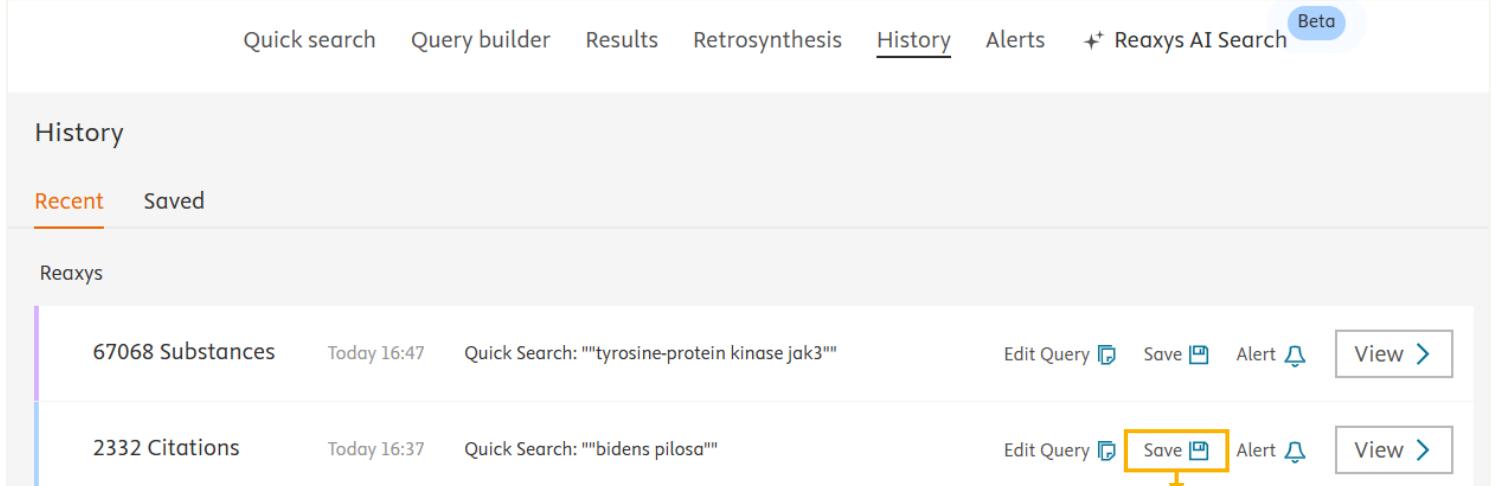
## 輸出介面設定:

- 匯出形式，匯出範圍，匯出內容
  - 選擇一個選項，然後點選匯出按鈕
  - 每次輸出最多 5000 個項目
  - 24 小時內最多 10 次

\*若您未登入且通過 IP 身分驗證，則無法匯出

ELSEVIER

# 儲存搜尋結果



The screenshot shows the Reaxys History page. At the top, there are navigation links: Quick search, Query builder, Results, Retrosynthesis, History (underlined), Alerts, and Reaxys AI Search (Beta). The History section is titled 'History' and has tabs for 'Recent' (selected) and 'Saved'. Below this, there are two search results for 'Reaxys':

- 67068 Substances (Today 16:47) - Quick Search: "tyrosine-protein kinase jak3" - Actions: Edit Query, Save, Alert, View
- 2332 Citations (Today 16:37) - Quick Search: "bidens pilosa" - Actions: Edit Query, Save, Alert, View

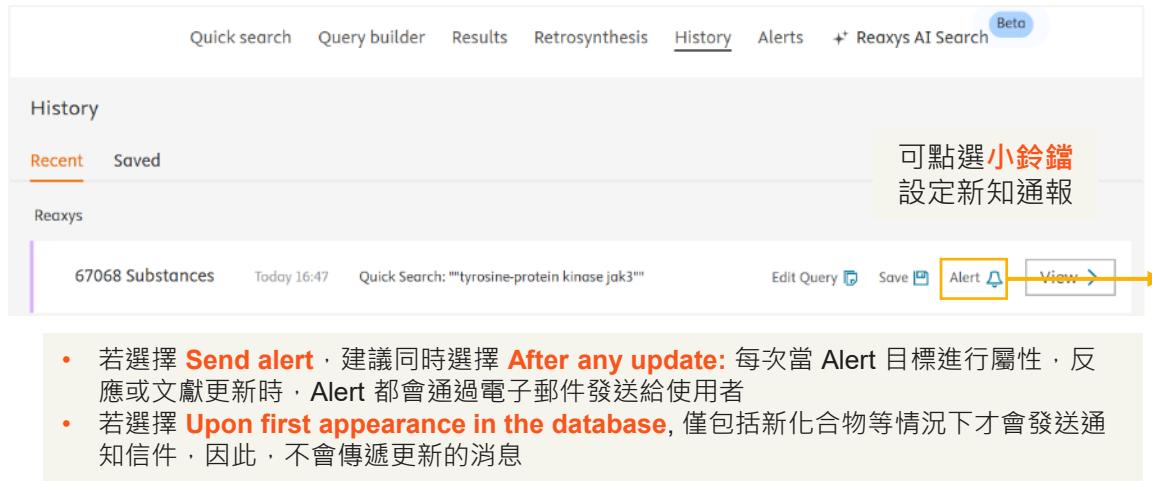
可於 **History** 頁面查看  
搜尋紀錄並設定儲存



# Alert: 設定新知通報

**Alert 會儲存您的搜尋指令，資料會定期自動提供符合指令的搜尋結果**

- 有助於當您想要在相同條件下檢查相關反應，物質和物理性質的資訊
- Alert 結果將會寄到註冊的電子郵件
- Alert 結果也可以分享給其他用戶



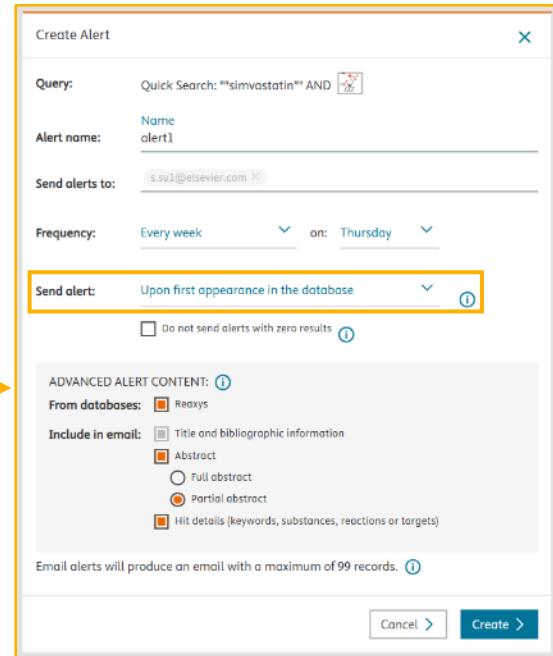
可點選 **小鈴鐺**  
設定新知通報

Recent Saved

67068 Substances Today 16:47 Quick Search: "tyrosine-protein kinase jak3"

Edit Query Save Alert View >

- 若選擇 **Send alert**，建議同時選擇 **After any update**：每次當 Alert 目標進行屬性，反應或文獻更新時，Alert 都會通過電子郵件發送給使用者
- 若選擇 **Upon first appearance in the database**，僅包括新化合物等情況下才會發送通知件，因此，不會傳遞更新的消息



Query: Quick Search: "simvastatin" AND

Alert name: alert1

Send alerts to: ssul@elsevier.com

Frequency: Every week on: Thursday

Send alert: Upon first appearance in the database

Do not send alerts with zero results

ADVANCED ALERT CONTENT:  From databases: Reaxys

Include in email:  Title and bibliographic information  Abstract  Full abstract  Partial abstract  Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records.

Cancel > Create >

# Alert: 管理新知通報

Quick search    Query builder    Results    Retrosynthesis    History    Alerts    + Reaxys AI Search    Beta

Alerts

Substances    alert1 - in Reaxys  
Since May 29, 2025    Quick Search: ""simvastatin""

**Edit Alert**

**Query:** Quick Search: ""simvastatin"" AND

**Alert name:** Name  
alert1

**Send alerts to:** s.su1@elsevier.com

**Frequency:** Every week  on: Thursday

**Send alert:** Upon first appearance in the database

Do not send alerts with zero results

**ADVANCED ALERT CONTENT:**

**From databases:**  Reaxys

**Include in email:**  Title and bibliographic information  
 Abstract  
 Full abstract  
 Partial abstract  
 Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records.

**Cancel >** **Save >**

from: No alert results  **Edit**  **Delete**

編輯新知  
通報設定

# 線上自我學習及 用戶資源

# Reaxys 學院: 線上學習與認證平台

## Reaxys Academy

加入我們為學生和教育工作者提供的自訂進度線上化學培訓。了解如何使用 Reaxys 加深您對分析、有機和無機化學的理解。



### Reaxys 101

預估完成時間：30-45 分鐘

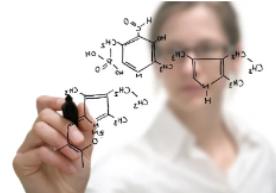
這個自訂進度課程非常適合圖書館員、教育工作者、研究員和學生，可簡單了解 Reaxys，也能提升自己的技能和對研究平台 Reaxys 的理解。



### Reaxys 化學 101

預估完成時間：45-60 分鐘

這門自訂進度課程展示了 Reaxys 能拓展各層級學生對於化學的了解，從大學生到研究生，甚或更高的層級。

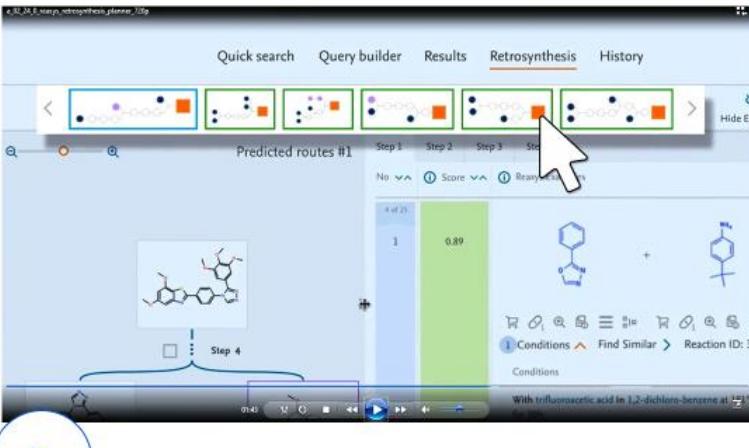


開始測驗

# 預測逆合成

## Reaxys 預測逆合成加速逆合成分析和預測 (網址)

Get a video overview of Predictive Retrosynthesis



The screenshot shows the Reaxys Retrosynthesis interface. At the top, there are tabs for Quick search, Query builder, Results, Retrosynthesis (which is underlined), and History. Below the tabs, there are several small chemical structures representing different retrosynthetic steps. A cursor is hovering over the Step 3 icon. The main area displays a list of predicted routes, with the first route highlighted in green. The route shows a target molecule being broken down into two fragments: a benzene ring and a substituted cyclohexane. Below the list, there is a section for 'Conditions' and a 'Reaction ID: 3'. At the bottom of the interface, there is a play button icon.

### 觀看 Reaxys 預測逆合成短片

過去，逆合成分析只能完全依靠化學家的專業知識和時間，但是，Reaxys 預測逆合成卻改變了這個模式，並贏得獎項。本產品將人工智慧應用於世界最大的化學反應資料庫，提供強大的預測路徑，從而增強你的知識水準。運用 Reaxys 預測逆合成，能以更快的速度，獲得更廣泛的分子答案。

# 用戶資源

## 線上講座

### Big data in chemistry

- [A universal approach to reaction informatics](#)
- [Understanding the history of chemical space through big data](#)
- [Reaction condition prediction using Reaxys: from raw data to best-in-class model](#)
- [Charting the chemical reaction space for DNA-encoded library design](#)

### Reaxys Predictive Retrosynthesis

- [Reaxys Predictive Retrosynthesis — speed matters](#)
- [AI-enabled predictive retrosynthesis tool to advance drug discovery](#)
- [Next generation synthesis planning using AI for chemists](#)

## 線上資源

### [Chemistry & Bioactivity data factsheet](#)

Chemistry & Bioactivity data from  
Reaxys®



### [Reaxys Quick reference guide](#)

# Reaxys®

Quick reference guide

### [Bioactivity Visualization](#)

# Reaxys® Medicinal Chemistry

# Reaxys 用戶資源



Reaxys 用戶資源

Reaxys 將超過 10 億個化學資料點與人工智慧結合，支援藥物發現、化學研發和學術創新。化學家可以快速取得相關專利、物質特性和生物活性資訊，以及獲獎的逆合成工具。

[Reaxys.com](https://www.reaxys.com)

用戶資源

使用連線須知

Reaxys 帳號登入機制會於 2025 年 7 月 1 日正式實施，未註冊用學校機構註冊帳號用戶將無法登入使用 Reaxys。

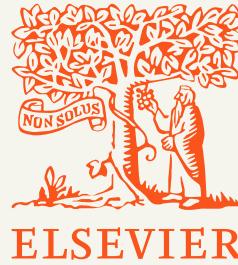
由於 RAE 允許使用者將自己的分子(目標分子)上傳進行 AI 預測，所得之 AI 預測結果(相應的合成計畫)會加密保存在使用者的 Reaxys 個人帳號內。是故能有更好的保護，同時避免非法授權者違法行為影響資料庫系統的穩定性，使用方式將採雙認證機制：

IP + 個人帳號登入 [www.reaxys.com](https://www.reaxys.com)

個人帳號：

- 第一次使用者，請於單位IP範圍內，前往 [www.reaxys.com](https://www.reaxys.com)，點選 Register，以學校機構的 email 申請。
- 若過往已於 Reaxys Basic Edition 或其他 Elsevier 資料庫 (ScienceDirect, Scopus, Embase, Engineering Village 等) 申請過帳號，但非以學校機構的 email 申請，則請循第一次使用者方式重新申請；若現有帳號已經是以學校機構的 email 申請，即可直接使用。





Advancing human progress together