

# 掌握化學未來的關鍵 工具：Reaxys 全方位 版助您突破研究

Taiwan Customer Success

2026



Advancing human progress together

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### 核心內容

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# Welcome to Reaxys

# 歡迎來到 Reaxys

## 化學數據與 AI 加速研發

Reaxys 是一個綜合性的化學資料庫與化學搜尋引擎，整合了超過十億個涵蓋化合物、反應式、文件、專利及生物活性等領域的化學數據。

探索化學、規劃合成路線並驗證跨領域的證據，包括：

- **產業：**製藥、生物技術、合同研究組織 (CRO) 和合同開發與製造組織 (CDMO)、化學品與材料、能源、工程與技術。
- **學術與政府：**大學、政府機構、研究所及實驗室。

立即前往 Reaxys

### 企業級隱私與安全

您在 Reaxys 中的所有操作均為[私密](#)、[安全](#)且經過加密。您的提示詞絕不會被儲存或用於訓練任何大型語言模型。

了解更多關於 [Elsevier](#) 如何[確保](#)在每一個[步驟](#)中保障[隱私](#)與[安全](#)的資訊。



### 隨時掌握 Reaxys 最新動態

[發布說明](#) [說明](#)  
[2026 路線圖](#)



可信賴的數據、技術與專業知識，支持化學研究



# 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)



### Patent Database

105 patent offices in  
170 patent classes



### Predictive Retrosynthesis

AI based



### Reaxys AI Search

AI based

### Substance Database

>350m substances



### Chemical Reaction Database

71m reactions

### 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:

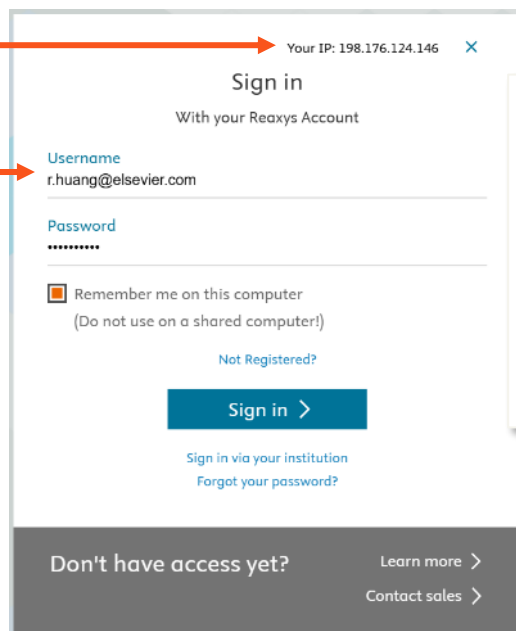
- 我研究的化合物有哪些特性被報導過?
- 有哪些其他化合物曾經報導過類似的特性?
- 這個材料自己合成可行嗎? 用買的省下的時間划算嗎?
- 有哪些類似的結構可能可以讓我參考?
- 這是一個值得投入時間與金錢的藥物靶點嗎?

# 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。



The image shows the Reaxys 'Sign in' page. At the top, it says 'Your IP: 198.176.124.146' with a close button. Below is the heading 'Sign in With your Reaxys Account'. There are input fields for 'Username' (containing 'r.huang@elsevier.com') and 'Password' (masked with dots). A checkbox labeled 'Remember me on this computer (Do not use on a shared computer!)' is present. Below the fields is a blue 'Sign in >' button. At the bottom of the form area, there are links for 'Not Registered?', 'Sign in via your institution', and 'Forgot your password?'. A dark grey footer contains the text 'Don't have access yet?' and links for 'Learn more >' and 'Contact sales >'.

新用戶註冊

Not Registered?

Sign in >

Sign in via your institution

[Forgot your password?](#)

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。

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。

# 檢索介面介紹

**1 Quick search:** 使用關鍵字、結構或自然語言搜尋，產出 AI 摘要。

**2 Query builder:** 結構式、物理性質等方面的布林邏輯加成檢索。對搜尋歷史進行加成檢索。

**3 Results:** 搜尋結果。對資訊進行優先排序。

**4 Retrosynthesis:** 逆向合成路線搜尋。

**5 搜尋欄位:** 可用自然語言搜尋。

**6 批次導入結構進行搜尋。**

**7 繪出結構或反應是搜尋。**

**8 搜尋紀錄、新知通報、客戶支援中心。**

Discover the *most relevant insights* with keywords, everyday language and AI summaries.

Search Reaxys [Learn how it works](#) [New](#) [Import](#)

Substance Molecular Formula, e.g. Pt(PPh3)3

AND

[Draw Structure / Reaction](#)

Search

Latest content update: 16. April 2026 [↗](#)

356M Substances • 74M Reactions • 126M Documents • 49M Patents • 51M Bioactivities

# 核心功能

## Quick search 快速搜尋

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## 自然語言搜尋

Search Reaxys

[Learn how it works](#)

New

[Import](#)

How do the main polyphenolic components in matcha (such as catechins) influence its antioxidant activity?



**Quick Search 中的 AI 驅動自然語言搜尋與摘要。**

NLQ 理解結合關鍵字邏輯來檢索並排序文件。符合條件的搜尋會從最高排名的多達 20 份文件的標題與摘要中生成引用摘要。

**搜尋結果**

排序後的文件結果引用摘要行內引用 → 參考預覽 → 摘要 / 全文

**適用情境**

- 快速篩選主題
- 深入閱讀前的證據初篩
- 建立引用起點資料集

**驗證資料來源**

- 開啟行內引用 → 參考預覽 → 摘要 / 全文
- 驗證後篩選 (篩選器會改變文件集，可能隱藏摘要)

**注意**

- 摘要僅出現在符合條件的 Quick Search 文件搜尋中，不適用於結構化或混合查詢，或查詢建構器搜尋。

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## 索引關鍵字搜尋

Search Reaxys [Learn how it works](#) [New](#) [Import](#)

oxe

**Chemical Names**

- oxepan-2-one
- oxetan-3-on

使用索引欄位與實體擷取進行高精度搜尋。關鍵字邏輯匹配索引的元資料及擷取的化學術語。結果以結構化集合形式呈現（文件、物質、反應、商業物質），並在可用時提供相關標的與生物活性證據的連結。

## 搜尋結果

- 依查詢類型結構化結果集
- 篩選（限制/排除）與排序功能
- 連結紀錄及證據對象

## 適用情境

- 搜尋精確詞彙及已知實體
- 標識符密集的查詢（名稱、專利及 CAS 編號）
- 受控回溯及可重現的檢索

## 驗證資料來源

- 使用篩選器，然後開啟連結的記錄與資料來源
- 使用「查詢建構器中的編輯」來明確設定欄位邏輯

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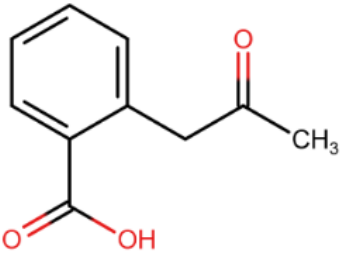
個人化設定

## 繪製結構/反應式

Search Reaxys [Learn how it works](#) [New](#) [Import](#)

"carbon dioxide" [×](#)

AND



As drawn [✎](#)

The image shows a chemical structure editor interface. At the top, there is a search bar with the text "carbon dioxide" and a close button. Below the search bar, the word "AND" is displayed. The main area shows a chemical structure of 2-(4-oxocyclohex-2-en-1-yl)acetic acid, which consists of a cyclohexene ring with a ketone group at the 4-position and an acetic acid group at the 1-position. The structure is enclosed in a dashed blue box with a close button. At the bottom left, there is a label "As drawn" with a pencil icon.

使用 Marvin JS 或 ChemDraw JS 工具繪製結構或反應進行化學原生檢索。Reaxys 可透過精確匹配、子結構匹配或相似性匹配，並將結果連結至反應、文件（包括專利）、目標與生物活性證據（如有），以及商業可得性。

## 搜尋結果

- 連結至證據的物質和反應結果集
- 連結至文件（包括專利）、目標與生物活性證據及商業可得性的樞紐連結
- 篩選和排序功能以篩選候選項目

## 適用情境

- 類比與架構探索
- 反應模式與條件探索
- 使用可用性訊號進行製造或購買決策

## 驗證資料來源

- 開啟連結的反應步驟/條件及來源記錄
- 根據性質與證據驗證相似性匹配

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**Quick Search** 是開始 Reaxys 搜尋的最快方法。選擇查詢類型，然後執行文字或結構搜尋，以獲得可排序的結果，也可以進一步篩選並匯出。

### 搜尋流程

1. 從上方選單選擇 Quick Search。
2. 匯入已保存的查詢：重新載入已保存的搜尋。
3. 輸入自然語言查詢、關鍵字（例如 CAS 和專利號碼）。
4. 結構式搜尋：使用繪圖工具繪製或貼上化學結構或反應。Reaxys 支援 Marvin JS 和 ChemDraw。
5. 執行搜尋：快速搜尋支援物質、反應和文件搜尋。符合條件的文件搜尋啟用時，可能會顯示引用摘要。



**進階用戶技巧：**結合文字詞彙與結構，然後依溶劑或產率篩選，以快速收斂。這樣可以減少雜訊，同時提升您匯出分析的資料集品質。

The screenshot shows the Reaxys Quick Search interface. At the top, there's a navigation bar with 'Quick search' highlighted. Below it, the main heading is 'Explore Chemistry with Reaxys'. A sub-header says 'Discover substances, reactions, documents and bioactivity data with our powerful integrated databases'. The main search area has a text input field with the placeholder 'Substance Properties, e.g. solubility of vitamin D3'. Above the input field, there's a 'Search Reaxys' label and a 'Learn how it works' link. To the right of the input field, there's a 'New' button and an 'Import' button. Below the input field, there's a 'Draw Structure / Reaction' button. At the bottom, there's a 'Search' button. The interface also displays statistics: '356M Substances', '74M Reactions', '126M Documents', '49M Patents', and '51M Bioactivities'. A 'Feedback' button is at the bottom right.

1. Quick search

2. Search Reaxys

3. Substance Properties, e.g. solubility of vitamin D3

4. Draw Structure / Reaction

5. Search

Latest content update: 16 April 2026

356M Substances • 74M Reactions • 126M Documents • 49M Patents • 51M Bioactivities

Feedback

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**AI 摘要:** 混合檢索 ( 語義 + 關鍵詞 ) 對最相關的論文/專利進行排序。從最多20 個結果的標題和摘要生成結構化摘要，並附有可追溯的引用來源。

### 搜尋流程

1. 輸入自然語言問題 ( 或關鍵字 ) 以開始快速搜尋的文件搜尋。
2. 在結果預覽頁面，選擇標示為「Includes Summary AI」的結果集，然後點擊 View Results → Summary AI。

1

Search Reaxys



Learn how it works

New

Import

How do the main polyphenolic components in matcha (such as catechins)

2

Results for

New

Edit query

How do the main polyphenolic components influence its antioxidant activity?

Includes Summary AI

100

Documents

Structure : as drawn

Titles, Abstracts, Keywords : "main", polyphenolic, "components", matcha, "catechins", "influence", "antioxidant activity"

Create Alert

Edit in Query Builder

Preview Results

View Results

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驗證（可追溯至來源）：閱讀摘要，然後點擊編號引用 → 打開 Reference Preview → 跳轉至文件詳情 / 摘要 / 完整文本進行驗證 → 匯出。

注意：應用篩選條件會改變文件集，可能會隱藏摘要。返回原始未篩選結果以恢復摘要。



進階用戶技巧：先用日常語言來界定主題範圍，然後使用關鍵詞來提高精確度。透過在結果列表視圖中打開引用的文件來驗證陳述。所有用戶互動均為私密，且不會將數據用於訓練外部模型。

Summary

AI +

2

Influence of Main Polyphenolic Components (Catechins) on Matcha's Antioxidant Activity

Key Points from Context

- **Catechins** are major polyphenolic compounds in matcha and are recognized for their strong antioxidant properties. Their structure, particularly the presence of galloyl and pyrogallol groups, is crucial for their antioxidant activity. The more galloyl groups present, the higher the antioxidant activity observed in catechins and their derivatives (1).
- **Synergistic Effects:** Catechins can act synergistically with other polyphenols and compounds in matcha, enhancing overall antioxidant activity. This synergy is especially notable among different catechin types (e.g., EGCG, EGC, ECG, EC) (2).
- **Antioxidant Mechanisms:** Catechins act as antioxidants by scavenging free radicals, chelating metal ions, and regenerating other antioxidants like  $\alpha$ -tocopherol (vitamin E). Their effectiveness is linked to their chemical structure, particularly the number and position of hydroxyl groups (3).
- **Contribution to Antioxidant Activity:** Studies show that catechins, especially epigallocatechin gallate (EGCG), are significant contributors to the antioxidant activity of tea, including matcha. EGCG often exhibits higher antioxidant activity than other catechins (4).
- **Stability and Bioavailability:** Catechins are sensitive to storage conditions and digestion, which can reduce their content and antioxidant activity in matcha over time or after ingestion (5); (6).
- **Other Polyphenols:** While catechins are important, other polyphenols (e.g., chlorogenic acid, rutin, quercetin) also contribute to matcha's antioxidant capacity, but catechins are among the most potent (6).

Conclusion

Catechins are the main polyphenolic components in matcha responsible for its strong antioxidant activity. Their effectiveness is determined by their chemical structure, especially the presence of galloyl and pyrogallol groups. Catechins act through multiple mechanisms, including free radical scavenging and metal chelation, and their antioxidant effects are enhanced by synergistic interactions with other polyphenols. However, their stability can be affected by storage and digestion, which may reduce their contribution over time (1) (3) (4) (2) (5) (6).

All statements are supported by the provided context.



References



資料來源

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## 實際操作練習題

Search Reaxys

[Learn how it works](#)

New

[Import](#)

What are the benefits of drinking matcha?



AND



Draw Structure / Reaction

Search

## Quick search 快速搜尋

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**結構編輯器**允許您繪製、貼上或生成分子或反應式，以化學結構搜索。將結構轉換為查詢，以檢索匹配的物質或反應，供審查和導出。

## 搜尋流程

1. **選擇結構編輯器**：選擇 MarvinJS 或 ChemDrawJS (預設值：建議使用 MarvinJS)。
2. **從名稱輸入結構名稱**：輸入化學名稱、CAS-RN、InChIKey 或 SMILES，自動生成結構 (見 2a)。
3. **繪製結構**：使用繪圖工具創建或修改您的結構或反應。



詳細說明：[How to create a Structure Drawing in Reaxys](#)

The screenshot illustrates the 'Structure editor selected' interface, which is set to MarvinJS. The workflow is numbered 1 through 3:

- 1**: The 'Structure editor selected' dropdown is set to MarvinJS.
- 2**: The 'Insert structure from name' button is highlighted.
- 2a**: A dialog box titled 'Create structure template from name' is shown. It contains a search input field with the placeholder 'Enter a chemical name, CAS-RN, InChIKey or SMILES'. Below the input field, a dropdown menu is open, showing options: 'is', 'starts with', 'ends with', and 'contains'. The 'is' option is selected.
- 3**: The 'Structure editor' toolbar is highlighted, showing various drawing tools.

At the bottom of the interface, there are buttons for 'Clear', 'Cancel', and 'Transfer to query'.

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## 搜尋流程

4. 應用搜尋修改：選擇互變異構體、立體構型、同位素或自由基來擴展搜尋範圍。
5. **Transfer to Query**：點擊「轉移至查詢」以將結構加入搜尋並優化搜尋參數。
6. 從名稱建立結構：使用結構範本產生精確或部分匹配。



進階用戶技巧：從名稱或識別碼生成結構，然後在 Transfer to Query 之前進行審核。

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

Insert structure from name

4

Marvin JS  
by Chemaxon

5

Clear Cancel Transfer to query

## Quick search 快速搜尋

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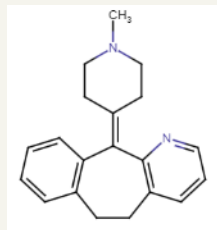
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我感興趣的結構



Azatadine  
CAS# 3964-81-6

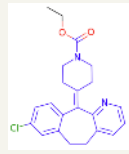
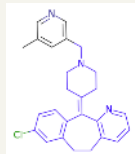
## As drawn

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

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## 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

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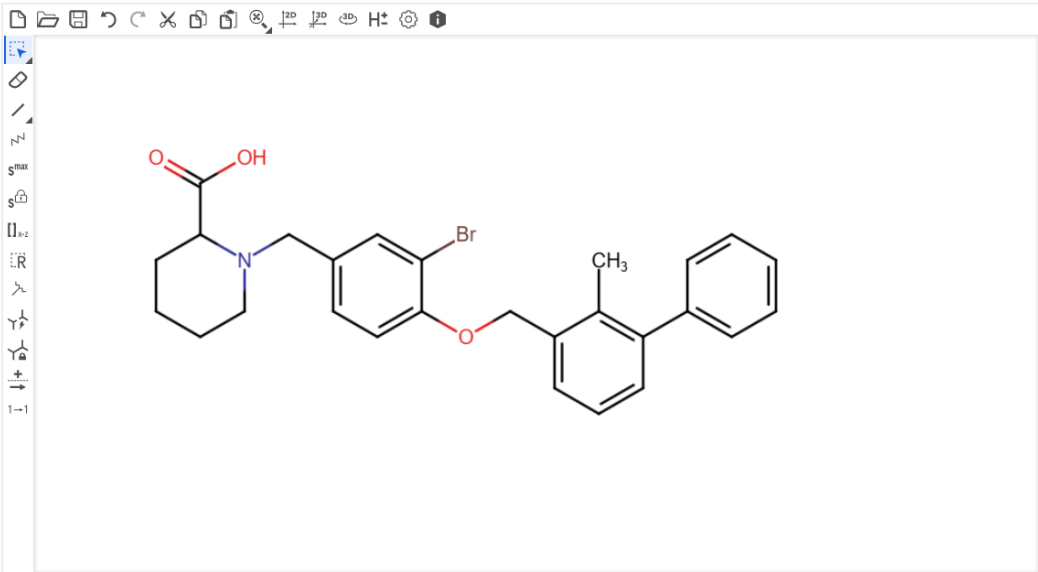
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## 實際操作練習題

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

Clear  Cancel  Transfer to query 

Feedback 

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結果預覽顯示查詢、返回的類別以及頂級結果的預覽。打開「View Results」以篩選、檢查關聯數據，並僅導出所需的數據集。

## 搜尋流程

1. **查詢顯示**：查看您執行的查詢，包括文字條件及任何結構指示。
2. **新建或編輯**：選擇「New」開始新的搜尋，或選擇「Edit query」修改當前查詢。
3. **結果**：查看返回的結果類型，例如文件、化合物、目標或商業化合物。
4. **預覽結果**：快速預覽特定結果類型的熱門項目。
5. **查看結果**：打開完整結果列表，進行篩選、匯出及詳細審查。



**進階用戶技巧**：在範圍界定主題時，請先從文獻開始。如果顯示摘要，請先閱讀摘要以了解概況，然後通過打開引用的參考資料來驗證關鍵陳述。當需要字段級精確度時，請使用「Query Builder」功能。

Results for "aspirin"

1

2

New Edit query

1,023

Substances

Structure : as drawn

Create Alert Edit in Query Builder

4

Preview Results

View Results

500,565

Documents

Structure : as drawn

Titles, Abstracts, Keywords : "aspirin"

Create Alert Edit in Query Builder

Includes Summary AI

Preview Results

View Results

180

Commercial Substances

Structure : as drawn

Create Alert Edit in Query Builder

Preview Results

View Results

5

## Top 3 results



113

aspirin

 $C_9H_8O_4$  180.16 779271 50-78-2

Identification

Druglikeness

Bioactivity (All)

Physical Data - 635

Spectra - 264

Other Data - 4,800

Preparations - 112

Reactions - 1,745

Targets - 529

Documents - 49,518

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搜尋預覽結果分類

1,023

Substances

Structure :  as drawn

Create Alert  Edit in Query Builder 

實驗數值與參考出處

Preview Results 

View Results

500,565

Documents

Structure :  as drawn

Titles, Abstracts, Keywords : "aspirin"

Create Alert  Edit in Query Builder 

文獻、專利

Preview Results 

View Results

180

Commercial  
Substances

Structure :  as drawn

Create Alert  Edit in Query Builder 

供應商資訊

Preview Results 

View Results

305

Reactions

Reaction Query :  as drawn

Create Alert  Edit in Query Builder 

合成方法

Preview Results 

View Results

84

Targets

Target(s) : adenosine a2a receptor

Create Alert  Edit in Query Builder 

蛋白、可用藥靶點與化  
合物交互作用的數據

Preview Results 

View Results

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結果頁面是您使用篩選工具、排序和列選項來聚焦搜尋。打開連結的化合物、反應式、藥物靶點和文獻，然後匯出乾淨的資料集。

## 搜尋流程

1. 結果內容：查看當前類別和資料庫的結果集及數量
2. 篩選面板：使用篩選條件句交結果。使用「限制於」或「排除」來包含或移除符合條件的結果。
3. 結構縮圖：預覽結果列表中每個的結構。
4. 變更資料庫範圍：使用下拉選單切換 Reaxys 及其他資料庫。
5. 結果工具：當有提供時，使用頁內工具，如結果內搜索、網格視圖或生物活性可視化。

The screenshot shows the Reaxys Quick search results page. The interface includes a top navigation bar with tabs for Quick search, Query builder, Results, and Retrosynthesis. Below the navigation bar, the search results are displayed for 'Reaxys - 1,023' substances. The page is divided into several sections:

- 1. Results Content:** The top section shows the search results for 'Reaxys - 1,023' substances, with a total of 1,023 substances out of 50,555 documents, containing 1,905 reactions and 550 targets.
- 2. Filter Panel:** A sidebar on the left contains a 'Filters' section with various criteria for refining the search results, including By Structure, Measurement pX, Targets, Parameters, Substance Classes, Molecular Weight, Number of Fragments, Availability, Available Data, Document Type, Publication Year, Current Patent Assignee, and LogP.
- 3. Structure Thumbnails:** The main results area displays chemical structures as thumbnails, each accompanied by its name and chemical formula.
- 4. Database Range:** The top of the results section shows the current database range, 'Reaxys - 1,023', with options to switch to 'Commercial Substances - 180' or 'PubChem - 1,156'.
- 5. Results Tools:** The bottom right of the results area contains a 'Results' section with options to 'Zoom structures', 'Grid', and 'Bioactivity Visualization'.

## 個人化設定

**進階用戶技巧：**先從廣泛範圍開始，然後逐漸縮小。使用「限制於」來聚焦最相關的結果，並使用「排除」來移除不需要的類別。在匯出之前，打開連結的反應、目標或文件以驗證證據。

**Reaxys**

Quick search   Query builder   Results   Retrosynthesis

Search > [Preview results](#) > 1.02 K Substances

Reaxys - 1,023   Commercial Substances - 180   PubChem - 1,156

## 1,023 Substances

out of 50,555 Documents, containing 1,905 Reactions, 550 Targets

Save search   Create alert   Edit in Query Builder

**Filters**

- By Structure
- Measurement pX
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Available Data
- Document Type
- Publication Year
- Current Patent Assignee
- LogP

0 selected Limit To Exclude Export Preparations

|   |  |                                                                                                                                                                   |                                                            |                                                                                                                                                |
|---|--|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 |  | <b>aspirin</b><br>$C_9H_8OOCCH_3COOH$ 180.16 779271 50-78-2<br><br>Identification<br>Druglikeness<br>Bioactivity (All)                                            | Physical Data - 635<br>Spectra - 264<br>Other Data - 4,800 | <a href="#">Preparations - 112</a><br><a href="#">Reactions - 1,745</a><br><a href="#">Targets - 529</a><br><a href="#">Documents - 49,518</a> |
| 2 |  | <b>calcium O-acetylsalicylate</b><br>$2C_9H_7O_3 \cdot [Ca^{2+}]$ 398.382 3755901 69-46-5<br><br>Identification<br>Druglikeness                                   | Physical Data - 2<br>Other Data - 20                       | <a href="#">Preparations - 5</a><br><a href="#">Reactions - 9</a><br><a href="#">Documents - 245</a>                                           |
| 3 |  | <b>lysine Acetylsalicylate</b><br>$C_{24}H_{32}O_{10} + C_{12}H_{19}N_2O_2$ 326.349 5690287 62952-06-1<br><br>Identification<br>Druglikeness<br>Bioactivity (All) | Physical Data - 5<br>Spectra - 2<br>Other Data - 59        | <a href="#">Preparations - 1</a><br><a href="#">Reactions - 1</a><br><a href="#">Documents - 177</a>                                           |

Sort by No of References

Zoom structures Grid Bioactivity Visualization

Limit to Exclude

Feedback

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**篩選工具**會根據每種類型的結果進行調整，讓您能夠根據重要欄位進行篩選。物質專注於屬性，商業物質則關注供應商資料，而反應則著重於條件和實驗細節。

### 篩選工具

**化合物結果：**依據結構、分子量、pH值、可得性、發表年份及專利受讓人進行篩選。

- 商業物質結果：**依據供應商、庫存、價格、純度、所在地及包裝尺寸進行篩選。
- 反應式：**依據條件、試劑、催化劑及溶劑進行篩選；切換單步反應或實驗程序。

1

Filters

By Structure

Measurement pX

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Available Data

Document Type

Publication Year

Current Patent Assignee

Limit to

Exclude

Clear

2

Filters

Molecular Weight

Number of Fragments

Availability

Commercial Suppliers

Supplier Preferences

Supplier Geolocation

Usage Classification

Package Size

Currency

Price

Purity

Limit to

Clear

3

Filters

By Structure

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Reactant Availability

Reaction Classes

Document Type

Publication Year

☐ Single step reactions only

Limit to

Exclude

Clear

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## 篩選工具

1. **藥物靶點結果**：根據物種、目標類型、測量和參數等目標屬性進行篩選。
2. **文獻結果**：根據出版年份和文件類型進行篩選，並依據書目、專利及化學領域如專利局、索引詞和物質類別進行細化。



**進階用戶技巧**：先使用「限制條件」和「排除條件」，然後再添加一個高影響力的化學過濾器。

1

Filters |←

✓ Targets

✓ Target Species

✓ Target Type

✓ Measurement pX

✓ Parameters

✓ Substance action on target

✓ Document Type

✓ Publication Year

✓ Current Patent Assignee

Limit to

Exclude

Clear

2

Filters |←

Search within results

✓ 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)

Limit to

Exclude

Clear

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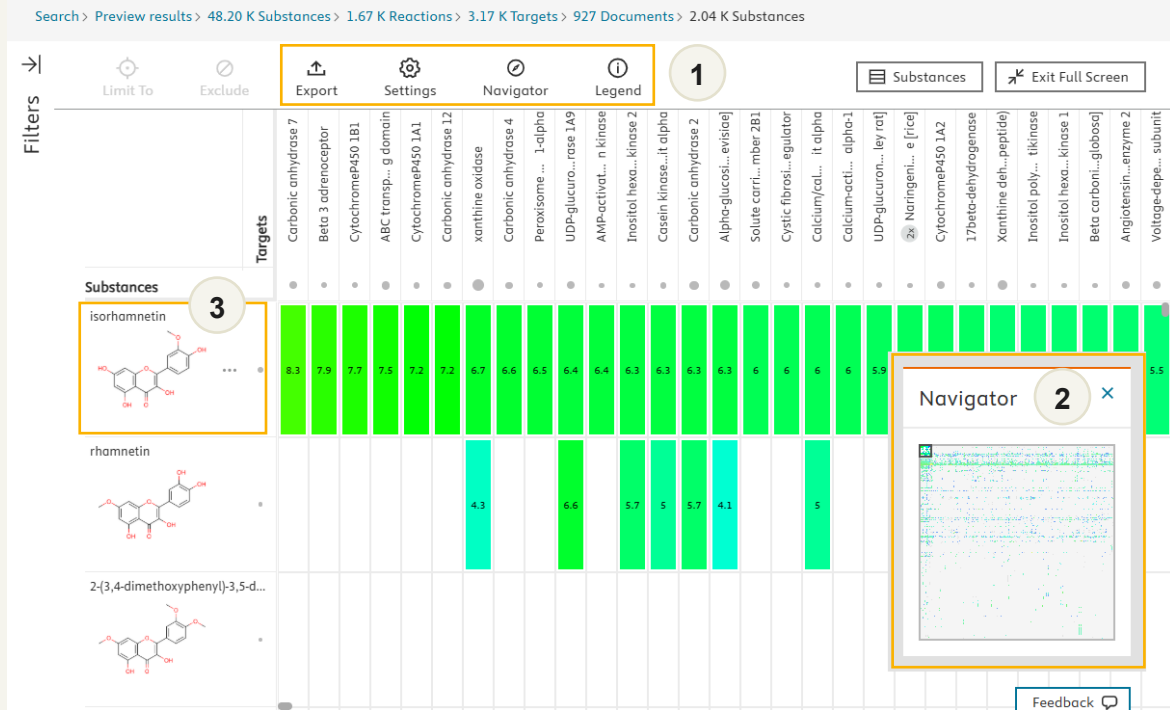
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**生物活性視覺圖:** 在一個視圖中比較不同物質和目標的生物活性。可視化生物活性輪廓，以評估結構-活性關係 (SAR)、效力及目標選擇性。矩陣顯示各物質和目標的標準化 [pX值](#)。

使用匯出、設定、導航器及圖例來調整視圖並提取 pX數據，以便分析和報告。

## 搜尋流程

1. 使用匯出、設定、導航器和圖例來配置視圖並匯出 pX 值。
2. 使用導航器面板在大型矩陣中移動。
3. 將滑鼠懸停在物質或目標上，以查看結構和識別碼。



|     |  |                             |
|-----|--|-----------------------------|
|     |  | 3x 5'-AMP-acti... [mouse]   |
|     |  | 3x 5'-AMP-acti... hamster]  |
| 1   |  | 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    |
| 5.7 |  | Acetylcholinest... peptide) |
|     |  | Actin                       |
|     |  | Activating mole...rotein 1  |
|     |  | Acyl-CoA (8-3)-desaturase   |
|     |  | Acyl-CoA 6-desaturase       |
|     |  | Adapter molecule crk        |
| 4.7 |  | Adenomatus p... sis coli    |

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## 匯出流程

1. 從結果中開啟匯出視窗：訪問匯出選項。
2. 選擇格式：挑選檔案格式。
3. 定義範圍：匯出所有結果、選取結果或自訂範圍。
4. 選擇要匯出的資料：全選資料、僅 ID、僅命中或特定欄位。
5. 其他選項：包含結構或描述以豐富報告內容。
6. 開始匯出：點擊匯出以啟動，隨時可取消。

The screenshot displays the 'Export substances' dialog box in Reaxys. The dialog is titled 'Export substances Reaxys' and includes a close button (X). It is divided into several sections:

- 1. Choose a format:** A dropdown menu is set to 'PDF/Print'. An arrow points from this section to a separate window showing the available export formats.
- 3. Range:** A dropdown menu is set to 'Range (e.g. 1-2, 1-10)'. Below it, a table shows 'From 1' and 'To 9'.
- 4. Export:** Radio buttons are used to select the data to export. 'All available data' is selected. Other options include 'Identification data only', 'Hit data only', and 'Choose specific data'.
- 5. Additional options:** Checkboxes for 'Include structures' (checked) and 'Include a description in the document' (unchecked).
- 6. Export >** A button to initiate the export process.

A separate window on the right shows the available export formats: PDF/Print, XML, Microsoft Word, Microsoft Excel, Tab-delimited text, Electronic Lab Notebook, RD File, SD/Molfile, and Smiles. The 'PDF/Print' option is highlighted.

At the bottom of the dialog, a message states: 'This is export attempt 1 out of 25 for today. Disclaimer: please refer to our [Terms and Conditions](#) before downloading data.'

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## 搜尋記錄

1. **歷史標籤**：點擊歷史以訪問最近的和已保存的搜尋。
2. **最近查詢**：顯示您當前會話中的查詢和操作。
3. **已保存的查詢**：顯示先前會話中保存的查詢（參見插圖E）。
4. **編輯和重用**：點擊編輯查詢、保存、提醒或查看以修改或重用最近的搜尋。
5. **已保存查詢選項**：從已保存列表中編輯、重新命名或刪除查詢。



**進階用戶技巧**：將關鍵查詢保存以便快速調用，減少重複操作並提升研究效率。

The screenshot displays the Reaxys Quick search interface. At the top, the Reaxys logo is on the left, and navigation tabs for 'Quick search', 'Query builder', 'Results', and 'Retrosynthesis' are in the center. On the right, there are icons for a search history (1), notifications, help, and a user profile (SS). Below the navigation bar, the 'History' section is active, showing a timeline with 'Recent' and 'Saved' tabs. The 'Recent' tab is selected, showing a list of search results. The first result is '2044 Substances' from 'Today 15:27', with a context switch from 926 Documents. It has buttons for 'Edit Query', 'Save', and 'View'. The second result is '927 Citations' from 'Today 15:19', with a context switch from 3175 Targets. The third result is '3175 Tgitems' from 'Today 15:19', with a context switch from 1671 Reactions. Below the 'Recent' tab, the 'Saved' tab is selected, showing a list of saved queries. The first saved query is '1023 Substances' from 'Today 14:48', titled 'Aspirin'. It has buttons for 'Edit Query', 'Delete', 'Rename', 'Alert', and 'View'. Below the saved query, there is a 'Quick Search' section with the query '"aspirin" AND' and a chemical structure of Aspirin.

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## 建立新知通報

1. 從結果預覽或歷史記錄中點擊建立通報。
2. 輸入通報名稱以組織主題（例如，分子、競爭對手、專案）。
3. 新增收件人：您的電子郵件會自動加入；如有需要，可加入其他人。
4. 設定頻率/時間：選擇每週、雙週、每月或資料庫更新後發送。
5. 設定觸發條件：在文件更新或首次出現時觸發通報。（可選：排除結果為零的通報）
6. 自訂通報內容：選擇資料來源（例如 Reaxys）及包含項目（標題、摘要、命中詳情）。進階通報請先使用查詢建構器。
7. 啟用通報：點擊建立以完成設定並接收通知。

**1** Create Alert

Query: Quick Search: ""aspirin"" AND

**2** Alert name: Aspirin

Send alerts to: s.sul@elsevier.com

**3** Add another email

**4** Frequency: Every week on: Friday

Send alert: Upon first appearance in the database

☐ Do not send alerts with zero results

**6** 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.

**7**

> Cancel > Create

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## 管理新知通報

1. 點擊主導覽列中的「Alert」以檢視及管理您已儲存的警示。
2. **Alerts** 依照最新到最舊的順序顯示，包含查詢類型（化合物、反應式、藥物靶點、文獻、商業化合物）、建立日期、資料庫及通知名稱的詳細資訊。
3. **先前結果**：使用下拉選單中的結果來檢視警示的早期版本，方便識別新增內容。
4. **編輯設定**，例如名稱和頻率。若要更改查詢，請在查詢建構器中修改，然後建立新的通知。



**進階用戶技巧：**根據研究需求設定提醒頻率 - 每週接收最新消息，每月掌握趨勢

Reaxys Quick search Query builder Results Retrosynthesis

Alerts

Substances Aspirin - in Reaxys  
Since Apr 17, 2026 Quick Search: "&quot;aspirin&quot; AND

Results from: No alert results

Edit Delete

Substances alert1 - in Reaxys  
Since May 29, 2025 Quick Search: "&quot;simvastatin&quot; AND

Results from: Oct 16, 2025 1 hits

Edit Delete

## Quick search 快速搜尋

選擇搜尋模式

總覽

AI 強化文獻探索與摘要

結構編輯器

搜尋結果

匯出及搜尋紀錄

建立及管理新知通報

個人化設定

個人設定可調整 Reaxys 預設值，以符合您的搜尋方式、規劃路徑及結果顯示。設定您的結構編輯器、自動規劃限制及結果顯示，讓使用過程保持一致。

1. 登入 Reaxys: 點擊您的名字或人物圖示登入，然後選擇「個人檔案」。
2. 點擊「Account」以編輯用戶名、電子郵件和密碼。進入「偏好設定」以調整查詢設定。

 Reaxys Quick search Query builder Results Retrosynthesis    

Profile

2 Account Profile Preferences

Username

s.su1@elsevier.com

Email

s.su1@elsevier.com 

Password

\*\*\*\*\* 

## Quick search 快速搜尋

選擇搜尋模式

總覽

AI 強化文獻探索與摘要

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個人化設定

個人設定可調整 Reaxys 預設值，以符合您的搜尋方式、規劃路徑及結果顯示。設定您的結構編輯器、自動規劃限制及結果顯示，讓使用過程保持一致。

1. 在結構編輯器中，選擇 MarvinJS 或 ChemDrawJS 作為您偏好的編輯器，並修改相關設定（例如：包含/排除互變異構體、鹽類）。
2. 在逆合成設定中，選擇自動生成的計劃數量及最大步驟數。
3. 選擇每頁顯示的結果數量。



進階用戶技巧：設定您偏好的結構編輯器和異構體設定一次，然後在各個專案中保持一致，這樣比較和匯出時才能保持一致性。

1

Default structure/reaction editor settings [Reset to default](#)

Structure Editor ChemAxon's MarvinJS [✎](#)

Search structure as As drawn [✎](#)

Preferences [✎](#)

- Include Tautomers
- Include Stereo
- Include Additional ring closures
- Include Salts
- Include Mixtures
- Include Isotopes
- Include Charges
- Include Radicals

2

Synthesis Planner [Reset to default](#)

Published Default Settings [✎](#)

- Number of full routes to create = 10
- Max. alternative branches = 5
- Max. number of steps = 10
- Stop searching if building block is commercially available
- Default yield for reactions without a given yield = 20%

Predicted Default Settings [✎](#)

- 15 steps per route (up to)
- Stereochemistry supported
- Regioselectivity ignored
- RCS: delivery time up to 10 days
- RCS: no price limit
- Processing time = Standard

3

Results per page [✎](#)

Number of results per page 15

## Query builder

總覽

分析專利擁有權

**Query Builder** 透過拖放欄位和布林邏輯，建立精確的多參數搜尋。結合化學、生物活性及專利欄位，鎖定您所需的紀錄並重複使用查詢。

## 搜尋流程

1. **開啟查詢建構器**：從頂部導航啟動或使用編輯查詢來自訂您的搜尋。
2. **拖放新增欄位**：結合化學、生物及專利欄位（例如：熔點、CAS 編號、專利受讓人）。
3. **結合科學與知識產權數據**：尋找具有已知合成路徑且未被競爭對手申請專利的高效化合物。



**進階用戶技巧**：結合當前專利受讓人與生物活性及合成領域，以尋找具效力且可合成的候選物，並及早篩選所有權。

The screenshot shows the Reaxys Query Builder interface. At the top, there's a navigation bar with 'Quick search', 'Query builder' (highlighted with a circled '1'), 'Results', and 'Retrosynthesis'. Below this is a toolbar with icons for save, copy, undo, and redo. A circled '3' highlights the 'Add' icon (a plus sign in a square). To the right, a sidebar (highlighted with a circled '2') contains a search box and a list of fields categorized under 'Fields', 'Forms', and 'History'. The 'Fields' category is selected, showing a list of fields including 'Reaxys', 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'Target and Bioactivity', 'Other', and 'Reactions'. The main area shows two query boxes. The first box contains 'Melting Point' with a 'Find Any' checkbox and a 'Show fields' dropdown menu showing '(Melting Point, °C, Solvent)'. Below this is an 'AND' connector. The second box contains 'Boiling Point' with a 'Find Any' checkbox and a 'Show fields' dropdown menu showing '(Boiling Point, °C, Pressure, Torr)'. At the bottom, there's a 'Search in:' section with buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A 'Feedback' button is located at the bottom right of the sidebar.

## Query builder

總覽

分析專利擁有權

## 搜尋流程

- 儲存、重複使用及設定提醒：儲存查詢以供日後使用，並針對新資料（物質、反應、專利）設定提醒。
- 布林邏輯及其他運算子：使用AND、OR、NOT，以及鄰近、文字和比較運算子，來擴大、縮小或限定您的查詢——非常適合精煉結構活性關係（SAR）或專利篩選。



**進階用戶技巧：**結合目前專利受讓人、生物活性及合成領域，加速發現具高效力且可合成的化合物，這些化合物未被專利申請，幫助您開啟嶄新且具創新潛力的機會。

Reaxys

Quick search Query builder Results Retrosynthesis

Close Panel >>

Search fields and forms

Fields Forms History

Reaxys

Topics and Keywords

Identification

Physical Properties

Spectra

Target and Bioactivity

Other

Reactions Feedback

Search in: Reactions > Targets > Substances > Documents >

選擇反應式、藥物靶點、物質或文獻搜索

4

5

Melting Point Find Any Show fields (Melting Point, °C, Solvent)

Boiling Point Find Any Show fields (Boiling Point, °C, Pressure, Torr)

## Query builder

總覽

實際操作練習題

## 實際操作練習題

 **Reaxys**

Quick search Query builder Results Retrosynthesis

📄 Import

💾 Save Options

↺ Reset Query

🗑 Delete Query

🏠 Structure

📊 Molecular Formula

⌘ CAS RN

🔍 TI, AB & KW

⋮ Substance Properties & Comments

is ▼

catechin

✕ 🔍 🗑

AND ▼

⋮ Isolated from Natural Source

☐ Find Any

Hide fields ▲

🗑

is ▼

matcha

✕ 🔍

Search in: 

Reactions >

Targets >

Substances >

Documents >

Close Panel >>

nat

✕

Reaxys ▲

🔍 Enthalpy of Hydrogenation

⋮

🔍 Target Nature

⋮

🔍 Isolated from Natural Source

⋮

🔍 Concentration in the Environment

⋮

🔍 Bioaccumulation, Biomagnification and Biomonitoring

⋮

🔍 Natural Products

⋮

Feedback 🗨

## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

已發表的逆合成法尋找與 Reaxys 反應證據相關的文獻路徑。可繪製一種物質並運行合成，以逐步比較路徑、條件和引用來源。

## 搜尋流程

1. 前往逆合成頁面，繪製或匯入您感興趣的化合物。
2. 設定已發表合成路徑的搜尋參數。此功能適用於所有擁有 Reaxys 帳號的使用者。
3. 如果您的機構有權限使用預測逆合成模組，您還會看到選擇「預測路徑」的選項。
4. 點擊『Synthesize』：根據您的結構執行查詢，以生成可用的逆合成路徑。

The screenshot displays the Reaxys Retrosynthesis interface. At the top, the Reaxys logo and navigation tabs (Quick search, Query builder, Results, Retrosynthesis) are visible. Below the navigation bar, the 'Structure editor selected' section shows 'MarvinJS' and 'ChemDrawJS' options. The main workspace contains a chemical structure of a substituted benzene ring with a carboxylic acid group and a methyl group, highlighted by a dashed blue box. To the right of the workspace is a 'Parameters' panel with various search settings. The 'Predicted' section is active, showing 'Length of routes' set to 15 and 'Max. Number of steps' set to 15. The 'Stereo and Regioselectivity' section has 'Ignore stereochemistry' and 'Only regioselective reactions' options. The 'Starting materials settings' section includes 'Max. Shipping time' and 'Max. Price per gram' options. At the bottom, there is a 'Synthesize' button and a 'Feedback' button.

1. Insert structure from name >

2. Parameters

3. Predicted

General Intermediates

Length of routes

Max. Number of steps: 15 (2-15)

First disconnect only

Stereo and Regioselectivity

Ignore stereochemistry

Only regioselective reactions

Starting materials settings

Reaxys Commercial Substances (RCS)

Max. Shipping time

up to 10 days any

Max. Price per gram: any (\$/g)

4. Synthesize >

## Retrosynthesis 逆合成

## Published &amp; Predicted 發表及預測逆合成

## 分析結果

## 如何調整逆合成分析參數 Predicted

## 基本設定

☒ Predicted ⓘ

General

Intermediates

Length of routes ⓘ

☒ Max. Number of steps: 15 (2-15)

☐ First disconnect only

Stereo and Regioselectivity ⓘ

☐ Ignore stereochemistry

☐ Only regioselective reactions

Starting materials settings ⓘ

Reaxys Commercial Substances (RCS)

Max. Shipping time ⓘ

☒ up to 10 days

☐ any

Max. Price per gram: any (\$/g) ⓘ

Processing time ⓘ

☒ Standard

☐ Extended

Powered by iktos ⓘ

- **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 ⓘ

General

Intermediates

Enter intermediates ⓘ

Include substructures (up to 10)

Enter SMILES ⓘ

Exclude substructures (up to 10)

Enter SMILES ⓘ

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)

## Retrosynthesis 逆合成

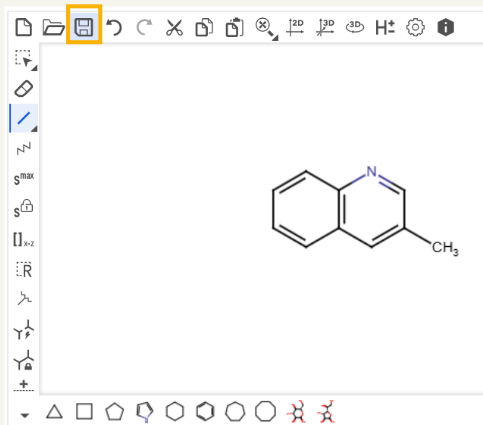
Published &amp; Predicted 發表及預測逆合成

分析結果

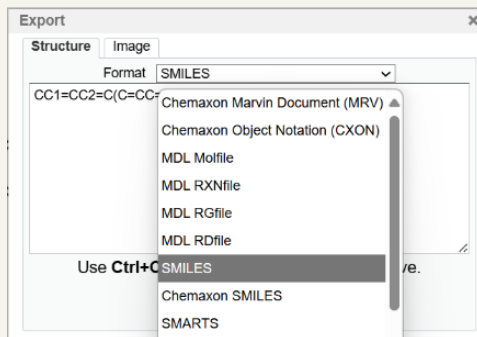
## 將中間產物結構轉為 SMILES 格式

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



| Structure              | Image  | Win+句號 |
|------------------------|--------|--------|
| Format                 | SMILES |        |
| CC1=CC2=C(C=CC=C2)N=C1 |        |        |
| 表情圖示                   |        |        |
| 語音輸入                   |        |        |
| 剪下                     |        |        |
| 複製                     |        |        |
| 貼上                     |        |        |

## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

## 如何調整逆合成分析參數 Published

## Parameters

Standard processing time

No intermediates defined

Powered by **iktos** Edit ☒ Published ⓘ

Length &amp; depth of synthesis plans ⓘ

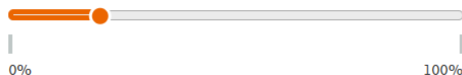
☒ Full routes: 10 ▼☐ Last step only

Branches per step: 5 ▼

Max. number of steps: 10 ▼

Stop searching if building block is commercially available ☒ Yes ☐ No

Assumed yield for reactions without a given yield



- **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 step:** 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

## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

## 如何更精準地控制 AI 的合成規劃策略

**不使用** Atom lock 標記

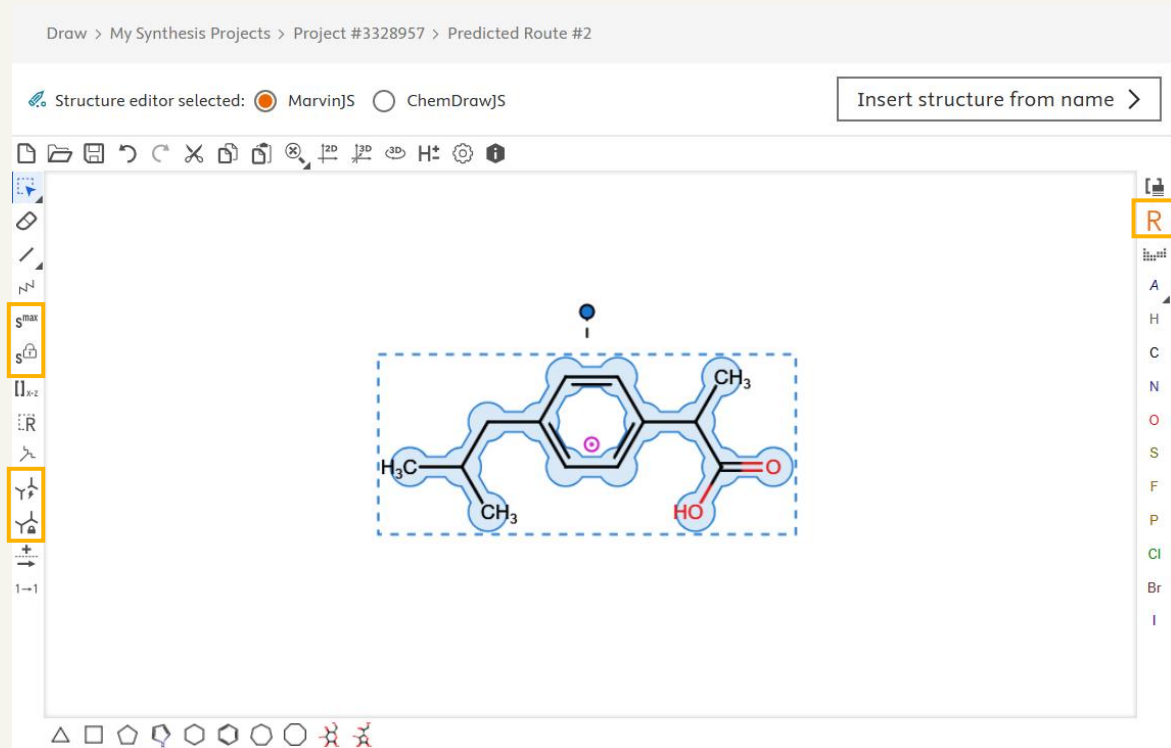
目標分子需繪製完整，**不使用** Generics group，例用“ALT”來代表 Akyl group



**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



## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

## 搜尋流程

- 逆合成計劃已新增至您的專案頁面：需登入以儲存、重新訪問或追蹤逆合成工作流程的進展。
- 分析合成路徑：在結構化且互動的視圖中檢視完整的反應步驟、中間體及實驗條件。



**進階用戶技巧：**使用已發表的路線來進行經文獻驗證的合成路徑。遇到合成瓶頸嗎？試試預測路線（需訂閱），探索機器建議的新穎替代方案。

Reaxys Quick search Query builder Results Retrosynthesis

Draw > My Synthesis Projects

0 selected Delete **4** Draw Structure

|                          | Number  | Date        | Project name     | Target Molecule |  | Number of routes                                                                   |
|--------------------------|---------|-------------|------------------|-----------------|--|------------------------------------------------------------------------------------|
| <input type="checkbox"/> | 3693707 | 17 Apr 2026 | Project #3693707 |                 |  | <div>Predicted </div> <div>Published <b>10</b></div> <div><b>5</b> View &gt;</div> |
| <input type="checkbox"/> | 3328957 | 19 Nov 2025 | Project #3328957 |                 |  | <div>Predicted <b>13</b></div> <div>Published <b>1</b></div> <div>View &gt;</div>  |
| <input type="checkbox"/> | 3314346 | 13 Nov 2025 | Project #3314346 |                 |  | <div>Predicted <b>23</b></div> <div>Published <b>5</b></div> <div>View &gt;</div>  |

Feedback

## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

## 分析預測逆合成結果

1. 切換已發表與預測的合成路徑：使用導航按鈕在不同的合成方案間切換。
2. 檢視每個步驟的實驗條件：查看反應產率、溫度、溶劑及文獻參考資料。
3. 取得實驗操作流程：當可用時，開啟完整操作流程以便複製或評估反應。



學習資源：[預測逆合成簡易操作指南 - Iktos](#)

The screenshot displays the Reaxys Retrosynthesis interface. At the top, the Reaxys logo and navigation tabs (Quick search, Query builder, Results, Retrosynthesis) are visible. The breadcrumb trail indicates the current project: Draw > My Synthesis Projects > Project #3328957 > Predicted Route #2. The interface features a series of navigation buttons (Export, Legend, Rotate, Fit view, Copy route, Zoom in, Zoom out) and a set of colored boxes representing different reaction steps. A green box labeled 'Predicted route #2' is highlighted. The main reaction scheme shows a predicted step (labeled 'Predicted Step 1') involving the reaction of a cyclopentanecarboxylic acid derivative (labeled 110) and a dimethylaminopropyl carbodiimide derivative (labeled 90) to form a complex product (labeled 52). The right panel displays the experimental conditions for the selected reaction (Reaction ID: 1819113), including reagents (hydrogen chloride, sodium hydroxide, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride), solvents (dioxane, H<sub>2</sub>O), temperature (RT, 4 h), and yield (given). A feedback button is located at the bottom right.

## Retrosynthesis 逆合成

Published &amp; Predicted 發表及預測逆合成

分析結果

## 分析預測逆合成結果

4. 切換佈局或使用適合檢視：切換垂直/水平佈局，並縮放以便更輕鬆查看複雜路徑。
5. 匯出合成路線：下載結構圖和實驗數據，或直接匯出至 ChemDraw 以便實驗室規劃或協作。
6. 直接在樹狀視圖中查看/輸入多步驟方案，以更快展開路線。



**進階用戶技巧：**安插一個反應步驟，以聚焦並調整路徑以符合您的特定合成目標。

Retrosynthesis 逆合成

Published & Predicted 發表及預測逆合成

分析結果

實際操作練習題

查詢 Oseltamivir 已發  
表及預測逆合成路徑

## Conditions Navigator

操作步驟

Workflow 工作流程

1. 繪製您的目標反應。
2. Reaxys 會找出相似的已發表反應。
3. 檢視彙整後的反應條件與佐證資料。
4. 探索官能基行為與相關反應。

The screenshot displays the Reaxys Conditions Navigator interface. At the top, the Reaxys logo is on the left, and navigation links for Quick search, Query builder, Results, Retrosynthesis, and Conditions navigator (marked as 'New') are on the right. A dark banner below the navigation bar reads 'Reaxys Conditions Navigator' with a sub-link 'Learn how it works >'. Below the banner, a breadcrumb trail shows 'Draw > My Conditions Projects'. The main workspace is titled 'Structure editor selected: MarvinJS ChemDrawJS'. A toolbar at the top of the workspace contains various drawing tools. On the left, a vertical sidebar lists chemical elements (R, H, C, N, O, S, F, P, Cl, Br, I). The central workspace shows a chemical reaction being drawn, labeled with a large '1' in a circle. The reaction involves 3-chloropyridine reacting with 4-methoxyphenylboronic acid to form 4-(3-pyridyl)anisole. At the bottom of the workspace, there are icons for geometric shapes and a '1-1' ratio indicator. The bottom right of the interface includes 'Clear', 'Cancel', and 'Search conditions >' buttons, along with a 'Feedback' link.

## Conditions Navigator

操作步驟

Workflow 工作流程

1. 繪製您的目標反應。
2. **Reaxys** 會找出相似的已發表反應。
3. 檢視彙整後的反應條件與佐證資料。
4. 探索官能基行為與相關反應。

 **Reaxys**

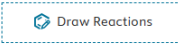
Quick search   Query builder   Results   Retrosynthesis   Conditions navigator New

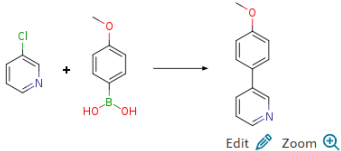
   

Draw > My Conditions Projects

### Reaction Conditions Navigator

Reagent, catalyst and solvent conditions extracted from published Reaxys reactions - for a reaction you draw, a Retrosynthesis step, or a Reaxys search result.

☐ 0 selected  Delete 

|                          | Project name   | Date  | Source                                                                                                | Input reaction                                                                                                                                                                                                                                                           | Results                                                                            |
|--------------------------|-------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
| <input type="checkbox"/> | Project 27972  | 6 October 2026                                                                          |  My drawn reaction | <br>Edit  Zoom  | <div>Condition sets 20</div> <div>Examples found 471</div> <div>2 Conditions</div> |

Conditions Navigator

操作步驟

Workflow 工作流程

- 1. 繪製您的目標反應。
- 2. Reaxys 會找出相似的已發表反應。
- 3. 檢視彙整後的反應條件與佐證資料。
- 4. 探索官能基行為與相關反應。

 Reaxys

Quick searchQuery builderResultsRetrosynthesisConditions navigator New



Draw > My Conditions Projects > Project 27972

3

Similar condition sets

| Rank   | Reagents & catalysts                                                                                 | Solvents                                        | Similarity level  | Median yield   | Number of reactions   | Functional group reactivity reference   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|-------------------------------------------------|------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| 1                                                                                                                                                                        | Pd(dppf)Cl <sub>2</sub> , sodium carbonate                                                           | tetrahydrofuran (THF), water (H <sub>2</sub> O) |  Tight            | 31%                                                                                                                                                                                  | 122 Examples                                                                                             | Aryl ether - reacted 3% unreacted 97% (total 193)<br>O-methyl ether - reacted 3% unreacted 97% (total 117)                 |
| 2                                                                                                                                                                        | potassium carbonate, tetrakis(triphenylphosphine) palladium(0) [Pd(PPh <sub>3</sub> ) <sub>4</sub> ] | tetrahydrofuran (THF), water (H <sub>2</sub> O) |  Tight            | 82%                                                                                                                                                                                  | 45 Examples                                                                                              | Aryl ether - reacted 2% unreacted 98% (total 1,798)<br>O-methyl ether - reacted 1% unreacted 99% (total 1,034)             |
| 3                                                                                                                                                                        | sodium carbonate, tetrakis(triphenylphosphine) palladium(0) [Pd(PPh <sub>3</sub> ) <sub>4</sub> ]    | ethanol, toluene, water (H <sub>2</sub> O)      |  Tight            | 59%                                                                                                                                                                                  | 44 Examples                                                                                              | Aryl ether - reacted 1% unreacted 99% (total 1,853)<br>O-methyl ether - reacted 0% unreacted 100% (total 1,335)            |
| 4                                                                                                                                                                        | Pd(dppf)Cl <sub>2</sub> , potassium carbonate                                                        | 1,4-dioxane, water (H <sub>2</sub> O)           |  Tight            | 80%                                                                                                                                                                                  | 37 Examples                                                                                              | Aryl ether - reacted 1% unreacted 99% (total 7,065)<br>O-methyl ether - reacted 0% unreacted 100% (total 4,642)            |
| 5                                                                                                                                                                        | potassium carbonate, tetrakis(triphenylphosphine) palladium(0) [Pd(PPh <sub>3</sub> ) <sub>4</sub> ] | 1,4-dioxane, water (H <sub>2</sub> O)           |  Tight            | 76%                                                                                                                                                                                  | 33 Examples                                                                                              | Aryl ether - reacted 1% unreacted 99% (total 4,594)<br>O-methyl ether - reacted 1% unreacted 99% (total 3,324)             |
| 6                                                                                                                                                                        | potassium carbonate, tetrakis(triphenylphosphine) palladium(0) [Pd(PPh <sub>3</sub> ) <sub>4</sub> ] | ethanol, toluene, water (H <sub>2</sub> O)      |  Tight            | 78%                                                                                                                                                                                  | 27 Examples                                                                                              | Aryl ether - reacted 1% unreacted 99% (total 1,798)<br>O-methyl ether - reacted 1% unreacted 99% (total 1,337)             |
|                                                                                                                                                                          | potassium carbonate,                                                                                 | 1,2-dimethoxyethane                             |                                                                                                      |                                                                                                                                                                                      |                                                                                                                                                                                             | Aryl ether - reacted 0% unreacted 100%  |

## Conditions Navigator

操作步驟

Workflow 工作流程

1. 繪製您的目標反應。
2. Reaxys 會找出相似的已發表反應。
3. 檢視彙整後的反應條件與佐證資料。
4. 探索官能基行為與相關反應。

Reaxys

Quick search Query builder Results Retrosynthesis **Conditions navigator** New

Draw > My Conditions Projects > Project 27972

**Condition summary** 4

**Top reagents & catalysts**

Tight 974 Medium 5682 Wide 33083

|                                                                                                      |     |
|------------------------------------------------------------------------------------------------------|-----|
| sodium carbonate                                                                                     | 444 |
| tetrakis(triphenylphosphine) palladium(0) (Pd(PPh <sub>3</sub> ) <sub>4</sub> )                      | 438 |
| potassium carbonate                                                                                  | 415 |
| Pd(dppf)Cl <sub>2</sub>                                                                              | 337 |
| palladium(II) acetate (Pd(OAc) <sub>2</sub> )                                                        | 128 |
| potassium phosphate                                                                                  | 121 |
| caesium carbonate                                                                                    | 87  |
| bis(triphenylphosphine) palladium(II) chloride (Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> ) | 48  |
| sodium bicarbonate (NaHCO <sub>3</sub> )                                                             | 31  |
| palladium bis[bis(diphenylphosphino)ferrocene] dichloride                                            | 25  |

**Top solvents**

Tight 974 Medium 5682 Wide 33083

|                                                                  |     |
|------------------------------------------------------------------|-----|
| water (H <sub>2</sub> O)                                         | 945 |
| 1,4-dioxane                                                      | 298 |
| tetrahydrofuran (THF)                                            | 271 |
| toluene                                                          | 270 |
| ethanol                                                          | 249 |
| N,N-dimethyl-formamide                                           | 108 |
| 1,2-dimethoxyethane (DME, glyme, monoglyme, dimethyl cellosolve) | 74  |
| acetonitrile                                                     | 47  |
| methanol                                                         | 35  |
| isopropyl alcohol (IPA)                                          | 23  |

## Conditions Navigator

操作步驟

Workflow 工作流程

Conditions Navigator 會在 Reaxys 中檢索相似反應，並以單一直觀的檢視呈現最相關、具文獻佐證的反應條件。它專為支援化學家的整個合成工作流程而設計，讓您在需要時更快、更輕鬆地尋找、比較並選擇反應條件。

您可在工作流程中的任何合適位置使用 Conditions Navigator：

1. 在 Conditions Navigator 頁籤中繪製目標反應，以找出相關且具文獻佐證的反應條件

The screenshot displays the Reaxys Conditions Navigator interface. At the top, the Reaxys logo is on the left, and navigation links for Quick search, Query builder, Results, Retrosynthesis, and Conditions navigator (highlighted with a 'New' tag) are on the right. A dark banner below the navigation bar reads 'Reaxys Conditions Navigator' with a sub-link 'Learn how it works >'. Below the banner, a breadcrumb trail shows 'Draw > My Conditions Projects'. The main workspace features a toolbar at the top with icons for file operations and a structure editor selector (MarvinJS is selected, ChemDrawJS is unselected). A text box on the right says 'Insert structure from name'. The central canvas shows a chemical reaction: 3-chloropyridine reacts with 4-methoxyphenylboronic acid to form 3-(4-methoxyphenyl)pyridine. The bottom of the interface includes a 'Clear' button, a 'Cancel' button, and a 'Search conditions >' button. A 'Feedback' link is located in the bottom right corner.

## Conditions Navigator

操作步驟

Workflow 工作流程

2. 使用 **Conditions** 或 **Similar Conditions**，從 **Reaxys** 反應檢索結果中探索並比較相符反應的反應條件。

Reaxys Quick search Query builder Results Retrosynthesis Conditions navigator New

Search > Preview results > 344.89 K Reactions

344,886 Reactions out of 78,811 Documents, containing 520,365 Substances, 15,886 Targets

Save search Create alert Edit in Query Builder

Filters |<

- By Structure
- Yield
- Reagent/Catalyst
- Solvent
- Catalyst Classes
- Solvent Classes
- Product Availability
- Reactant Availability
- Reaction Classes
- Document Type

0 selected Limit To Exclude Export

Sort by Reaxys Ranking

Zoom structures Hide Conditions

1

130 141 15

Hits/Conditions - 4 Find Similar **Explore conditions** Reaction ID: 32186243

| Conditions                                                                                                                                              | Yield | Reference                                                                                                                   |
|---------------------------------------------------------------------------------------------------------------------------------------------------------|-------|-----------------------------------------------------------------------------------------------------------------------------|
| With<br><b>(1,1'-bis(diphenylphosphino)ferrocene)palladium(II) dichloride</b><br>; potassium carbonate In 1,4-dioxane; water at 95°C; Inert atmosphere; | 94%   | Zhang, Rui; Wen, Kangmin; Dong, Guangbin<br><b>Chem</b> , 2025, vol. 11, # 8, art. no. 102622<br>Full Text Details Abstract |

Feedback

## Conditions Navigator

操作步驟

Workflow 工作流程

### 3. 在 Retrosynthesis 中使用，於規劃與優化合成路徑時評估反應條件

Reaxys Quick search Query builder Results Retrosynthesis Conditions navigator New

Draw > My Synthesis Projects > Project #4086543 > Published Route #1

Export Legend Published route #1 Hide conditions

Rotate Fit view Copy route Zoom in Zoom out

Step 1

☐ 0 selected ☐ View selected Explore conditions

|                            | Conditions                                                                                                                                  | Yield | Reference                                                                                                                                                                    |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|-------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <input type="checkbox"/> 1 | With sodium hydroxide; cobalt(II) acetate<br>In ethanol at 65°C; under 1520 Torr; for 4h; Irradiation;                                      | 99.3% | Kudo, Kiyoshi; Shibata, Tadashi; Kc Tsugunori; Mori, Sadayuki; Sugita, <b>Chemistry Letters</b> , 1987, p. 577 - 58 Full Text <a href="#">↗</a> Details <a href="#">&gt;</a> |
| <input type="checkbox"/> 2 | With sodium hydroxide; tetrabutylammonium bromide; dicobalt octacarbonyl<br>In water; benzene at 65°C; under 760 Torr; for 5h; Irradiation; | 96%   | Brunet, Jean-Jacques; Sidot, Christ Caubere, Paul <b>Tetrahedron Letters</b> , 1981, vol. 22, 1016 Full Text <a href="#">↗</a> Cited 45 times <a href="#">↗</a> D            |
| <input type="checkbox"/> 3 | With tetrabutylammonium bromide; dicobalt octacarbonyl In                                                                                   | 95%   | Brunet, Jean-Jacques; Sidot, Christ Caubere, Paul <b>Journal of</b> Feedback <a href="#">↗</a> , 198:                                                                        |

Chemical reaction scheme showing the synthesis of a naphthalene derivative. The starting materials are carbon monoxide (C≡O) and 1-bromonaphthalene. The reaction proceeds via a Published Step 1, yielding a naphthalene-1-carboxylic acid derivative with a 99.3% yield.

# 核心内容

化合物

反應式

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化合物結果顯示經過精選的化合物記錄，包含關鍵屬性和連結。從名稱或結構開始，進行篩選，打開相關的反應或文件，並匯出針對性的資料集。

### 搜尋流程

1. 從化學結構或名稱輸入開始。
2. 以物理化學性質篩選（例如，logP、分子量、溶解度）。
3. 切換供應商可用性以進行採購：查看與物質記錄相關的商業可用性。
4. 探索相關反應、目標和文獻。
5. 匯出或重複使用整理後的資料集。
6. 分析合成路線：在結構化且互動的視圖中，檢視完整反應步驟、中間體及實驗條件。

Reaxys

1 Quick search Query builder Results Retrosynthesis

Search > From history

4

1,023 Substances out of 50,555 Documents, containing 1,905 Reactions, 550 Targets

6 Save search Create alert Edit in Query Builder

Filters

- By Structure
- Measurement pX
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Available Data
- Document Type
- Publication Year

2

0 selected Limit To Exclude Export Preparations

Sort by No of References

Zoom structures Grid Bioactivity Visualization

5

1

aspirin

C6H4OOCCH3COOH 180.16 779271 50-78-2

Identification Physical Data - 635  
Druglikeness Spectra - 264  
Bioactivity (All) Other Data - 4,800

Preparations - 112  
Reactions - 1,745  
Targets - 529  
Documents - 49,518

3

2

calcium O-acetylsalicylate

2C9H7O4^{1-}Ca^{2+} 398.382 3755901 69-46-5

Identification Physical Data - 2  
Druglikeness Other Data - 20

Preparations - 5  
Reactions - 9  
Documents - 245

3

lysine Acetylsalicylate

C9H8O4^\*C9H14N3O2 326.349 5690287 62952-06-1

Identification Physical Data - 5

Feedback

化合物

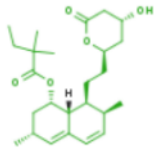
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## 化合物數據詳情



80    ...

**simvastatin**

$C_{25}H_{38}O_5$  418.574 4768037  [Retrieve CAS RN](#)

[Identification](#) [Bioactivity \(All\)](#) [Spectra - 133](#)

[Druglikeness](#) [Physical Data - 102](#) [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

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## 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

Show/Hide columns ▾

| 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 µM |        | Other compound: Geranylgeranyl pyrophosphate | Current US2017 Full Text          |
| 11.3 | activation percentage (relative to control + more |              | 210           | %    |                    |                       |                                                      |              | Hep-G2 cell line | 10E-5 µM |        | Other compound: Geranylgeranyl pyrophosphate | Current US2017 Full Text          |
| 10.9 | activation percentage (relative to control + more |              | 46            | %    |                    |                       |                                                      |              | Hep-G2 cell line | 10E-6 µM |        | 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

- ☒ 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 &gt;

Apply &gt;

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反應式結果顯示實驗報告的轉化情況，包括條件、產率及參考文獻。可依試劑、溶劑、產率及溫度篩選和排序，以選擇可行的路徑。

## 搜尋流程

1. 繪製或匯入目標分子。
2. 打開反應標籤以探索所有可行的合成轉化。
3. 根據試劑、催化劑、溶劑、產率和溫度進行篩選。
4. 依據反應產率或實驗條件進行排名。
5. 匯出路線候選，然後在引用的程序和條件中驗證可行性。



**進階用戶技巧：**從產量和關鍵條件開始，然後開啟實驗程序以確認範圍，最後再匯出路徑或比較替代方案。

Reaxys

1 Quick search Query builder Results Retrosynthesis

Search > From history > 1.91 K Reactions

2 1,905 Reactions out of 50,555 Documents, containing 1,023 Substances, 550 Targets

Save search Create alert Edit in Query Builder

Filters

- By Structure
- Yield
- Reagent/Catalyst
- Solvent
- Catalyst Classes
- Solvent Classes
- Product Availability
- Reactant Availability
- Reaction Classes
- Document Type
- Publication Year

3

4 Sort by Reaxys Ranking

5

18 Conditions Find Similar Reaction ID: 800598

Conditions

| Conditions                                                                        | Yield | Reference                                                                                                                                                                                                                      |
|-----------------------------------------------------------------------------------|-------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| With dicyclohexyl-carbodiimide In dichloromethane at 20°C; Experimental Procedure | 100%  | Current Patent Assignee: UNIVERSITY OF GEORGIA - WO2015/89389, 2015, A1<br>Location in patent: Paragraph 0098<br>Full Text Details Abstract                                                                                    |
| With dicyclohexyl-carbodiimide In dichloromethane at 20°C;                        | 73%   | Khoury, Aleen; Sakoff, Jennette A.; Gilbert, Jayne; Scott, Kieran F.; Karan, Shawan; Gordon, Christopher P.; Aldrich-Wright, Janice R.<br>Pharmaceutics, 2022, vol. 14, # 4, art. no. 787<br>Full Text Cited 23 times Feedback |

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## 反應式結果篩選工具

Filters

⏮

By Structure

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Reactant Availability

Reaction Classes

Document Type

Publication Year

☐ Single step reactions only

Limit to

Exclude

Clear

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

文獻種類 (論文，專利)

出版年份

縮小到只有一步反應

## 可展開查看篩選細項

^ Solvent Classes

☐ Low boiling (<100°C)

170,660

☐ Aprotic dipolar

131,653

☐ Red

128,072

☐ Green

110,688

☐ Protic

105,508

☐ Aprotic apolar

103,416

☐ Yellow

100,353

☐ High boiling (>150°C)

59,815

☐ Middle boiling(100°C - 150°C)

46,560

☐ Inorganic

2,473

View more >

- 每個篩選細項可以通過點擊展開
- 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 251210

×

✓ Solvent Classes

215,324

Low boiling (<100°C)

170,660

☒ dichloromethane

76,357

☒ tetrahydrofuran

69,719

☒ water

53,544

☒ methanol

51,590

☐ ethanol

31,438

☐ acetonitrile

21,946

☐ ethyl acetate

11,555

☐ acetone

11,386

☐ diethyl ether

10,508

☐ hexane

7,777

☐ chloroform

6,263

Selected search items:

dichloromethane × water × tetrahydrofuran × methanol ×

More +

Clear selected ×

Limit to >

Exclude >

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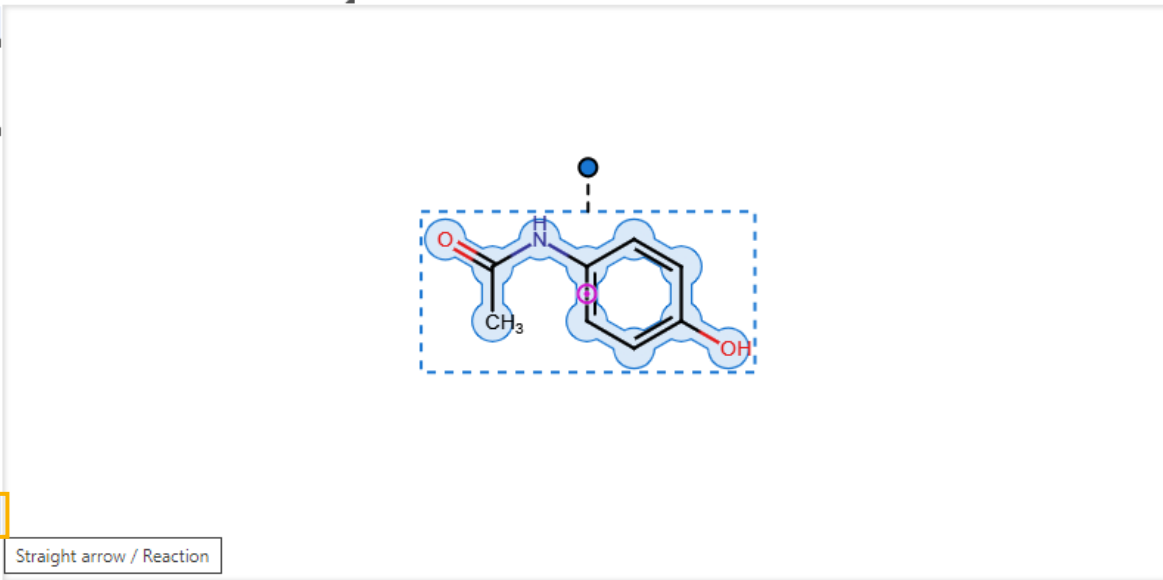
## 搜尋反應式的方法: 繪製

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

Insert structure from name &gt;

Search this structure as: As drawn

More options v



加入反應箭頭

1→1 Straight arrow / Reaction



化合物

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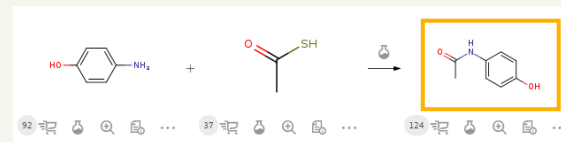
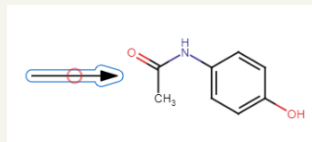
文獻

專利

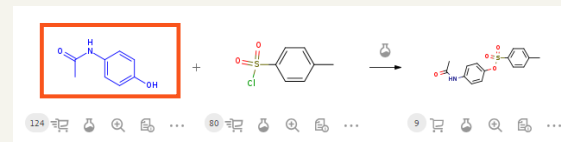
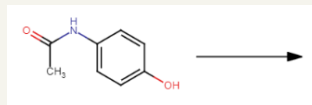
生物活性

## 搜尋反應式的方法: 繪製

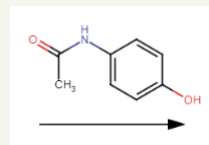
產物:  
箭頭在左



起始物:  
箭頭在右



催化劑或溶劑:  
箭頭在下



Conditions

With 4-acetaminophenol; water; dihydrogen peroxide at 20°C; Green chemistry; Experimental Procedure [▼](#)

With iron(III) oxide; dihydrogen peroxide In water at 20°C; for 0.0833333h; Experimental Procedure [▼](#)

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## 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                                                                                                                                      | <a href="#">Preview Results</a>  | <a href="#">View Results</a>  |
| Edit in Query Builder  Create Alert  |       |           |                                                                                                                                                                                                                                                  |                                                                                                                     |                                                                                                                  |
|                                                                                                                         | 9,368 | Reactions | Reaction Query :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals | <a href="#">Preview Results</a>  | <a href="#">View Results</a>  |
| Edit in Query Builder  Create Alert  |       |           |                                                                                                                                                                                                                                                  |                                                                                                                     |                                                                                                                  |

將搜尋結果複製到進階搜尋 **Query Builder** 增加搜尋條件

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## 進階反應式檢索: Query builder

Import

Save Options

Reset Query

Delete Query

Structure

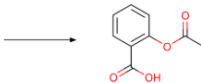
Molecular Formula

CAS RN

TI, AB & KW

Structure

As drawn



AND ▼

Reaction Data & Conditions

is ▼

microbiolog\*

Search in: Reactions > Targets > Substances > Documents >

Close Panel >>

reaction

Reaxys

Reaction Data & Conditions

Solvent (Reaction Details)

Time (Reaction Details)

Temperature (Reaction Details)

Product XRN (Reaction)

Product XRN (Reaction Details)

Product (Reaction Details)

Pressure (Reaction Details)

Feedback

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跨學科搜尋具體化合物或反應提及的文獻（包括同行評審文章和專利），而非僅限關鍵字。

### 搜尋流程

1. 進行結構、物質、關鍵字或自然語言查詢
2. 查看文件結果，並閱讀若有提供的 AI 摘要及相關參考連結
3. 依期刊類型、專利局等進行篩選

注意：文獻包含期刊論文與專利。

The screenshot displays the Reaxys search results page. At the top, the Reaxys logo and navigation tabs (Quick search, Query builder, Results, Retrosynthesis) are visible. A search bar at the top left shows the results count: 171,133 Documents. On the left side, a 'Filters' panel allows refining results by criteria such as Publication Year, Document Type, Authors of Scientific Documents, Current Affiliation, Inventors of Patents, Current Patent Assignee, Patent Office, Journal Title, Substance Classes, Reaction Classes, and Index Terms (List). The main search results area shows two entries. The first entry, 'Application of catechin in pharmacy', includes a summary, patent information (CN101474314, 2009, A), and an abstract hit: '...application of catechin in the pharmaceutical field. The catechin of the invention is...'. The second entry, 'Synthesis of [2-C, 4-C]-(2R,3S)-catechin and [2-C, 4-C]-(2R,3R)-epicatechin', shows 12 citations, a journal reference (Sharma, Pradeep K.; He, Min; Romanczyk, Leo J.; Schroeter, Hagen; Journal of labelled compounds and radiopharmaceuticals, 2010, vol. 53, # 10, p. 605 - 612, 10.1002/jlcr.1791), and an abstract hit: '...[2-C, 4-C]-(2R,3S)-catechin 15 and [2-C, 4-C]-(2R,3R)-epicatechin 18 starting from labeled 2-hydroxy-4,...'. The interface also includes options to save searches, create alerts, and edit the query builder.

化合物

反應式

文獻

專利

生物活性

### 搜尋流程

4. 存取全文、摘要、權利要求及索引詞中的重點化學內容
5. 追溯提取的物質、反應及生物活性資訊



**進階用戶技巧：**用簡單明瞭的語言提問，先閱讀摘要以了解大意，然後透過參考預覽打開引用的文件及查看摘要或全文來驗證關鍵主張。



1

#### Application of catechin in pharmacy

[In summary](#)

CN101474314, 2009, A

Current Patent Assignee: PUER GOVERNMENT TEA INDUSTRY D

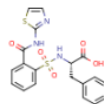
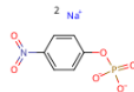
Office: CN [View full patent family](#)

4

[Abstract](#) [Index Terms](#) [Claims](#) [Bibliographic Info](#) [Substances \(2\)](#) [Full Text](#)**Abstract hit:** {...application of catechin in the pharmaceutical field. The catechin of the invention is...}**Claims Hit:** {...1. Catechin in preparation of the treatment or prevention of diabetes type...}

5

#### Substances



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專利結果將專利文件與映射的化學資料連結，讓您能夠追蹤新穎性和所有權。可依專利局篩選，並匯出精選資料集以供審查或報告使用。

## 搜尋流程

1. 輸入化合物或關鍵字。
2. 按專利局篩選（例如，EPO、USPTO）。
3. 查看對應的反應或藥物靶點。
4. 匯出為專利報告。



進階用戶技巧：挖掘專利資料庫以揭示化合物和反應，識別治療宣稱，並比較不同司法管轄區內的受保護合成路徑。

Reaxys

1 Quick search Query builder Results Retrosynthesis

Search > Preview results 171.13 K Documents, 215.32 K Reactions

171,133 Documents with 402,751 Substances, 215,324 Reactions, 3,079 Targets

2

Publication Year  
Document Type  
Authors of Scientific Documents  
Current Affiliation  
Inventors of Patents  
Current Patent Assignee  
Patent Office

3

Application of catechin in pharmacy

1

In summary

CN101474314, 2009, A  
Current Patent Assignee: PUER GOVERNMENT TEA INDUSTRY D  
Office: CN View full patent family

Abstract Index Terms Claims Bibliographic Info Substances (2) Full Text

Abstract hit: {...application of catechin in the pharmaceutical field. The catechin of the invention is...}

Claims Hit: {...1. Catechin in preparation of the treatment or prevention of diabetes type...}

Synthesis of [2-C, 4-C]-{2R,3S}-catechin and [2-C, 4-C]-{2R,3R}-epicatechin

2

12 citations

Sharma, Pradeep K.; He, Min; Romanczyk, Leo J.; Schroeter, Hagen  
Journal of labelled compounds and radiopharmaceuticals. 2010, vol. 53, # 10, p. 605-612, 10.1002/jlcr.1791

Abstract Index Terms Substances (27) Reactions (148) Full Text

Hit Substances (1)

Abstract hit: {...[2-C, 4-C]-{2R,3S}-catechin 15 and [2-C, 4-C]-{2R,3R}-epicatechin 18 starting from labeled 2-hydroxy-4-...}

Index Terms Hit: {...EMTREE drug term: epicatechin, benzaldehyde derivative...}

Catechins in cancer therapy: integrating traditional and complementary approaches

3

In summary

Feedback

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## 文獻專利搜尋結果篩選工具

出版年份  
文獻類型  
論文作者  
目前隸屬機構  
專利發明者  
目前專利授予者  
專利局  
期刊名稱  
化合物種類  
反應式種類  
文獻索引詞統計清單  
索引詞化學分類

Filters ←

Search within results

Type a keyword to refine the results

☒ 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)

☒ Index Terms (ReaxysTree)

☐ Manually curated content only

Limit to Exclude Clear

Index Terms (ReaxysTree) 6141 ×

☒ Index Terms (ReaxysTree) 137,810

- ☐ physico chemical properties 88,647
- ☒ chemical transformations 82,110
  - ☐ chemical reaction class 70,457
  - ☒ reaction kinetic 37,300
    - ☐ kinetic type 27,385
    - ☒ surface area 6,141
      - ☒ catalyst surface area 10
    - ☐ reaction reactivity 2,978
    - ☐ reaction activation energy 1,136

Selected search items:  
surface area ×

Clear selected ×

Limit to > Exclude >

Index Terms (ReaxysTree)

☐ physico chemical properties 88,647

☐ chemical transformations 82,110

☐ physico chemical analysis methods 73,630

☐ quantum chemical calculation methods 4,342

View more >

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

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生物活性結果將化合物與目標以及測試結果聯繫起來，以支持結構活性關係（SAR）和作用機制（MoA）研究。可根據端點和目標屬性進行篩選，然後導出表格以便分析或提交。

## 搜尋流程

1. 輸入結構或化合物名稱。
2. 依生物活性結果篩選（例如 IC<sub>50</sub>、K<sub>i</sub>、EC<sub>50</sub>）。
3. 切換靶點類型、靶點分類或物種的篩選條件。



[Watch Target & Bioactivity expert tips](#) playlist

Reaxys

1 Quick search Query builder Results Retrosynthesis

Search > Preview results > 171.13 K Documents > 3.08 K Targets

3,079 Targets out of 137,810 Documents, 402,751 Substances, 215,324 Reactions

Save search Create alert Edit in Query Builder

Sort by Sort alphabetically A-Z Zoom structures Bioactivity Visualization

Filters

- Targets
- Target Species
- Target Type
- Measurement pX
- Parameters
  - ic<sub>50</sub> 3,705
  - Inhibition percentage 2,010
  - qualitative 1,855
  - K<sub>i</sub> (inhibition constant) 1,348
  - Inhibition rate 590
  - K<sub>m</sub> (Michaelis constant) 474
  - activity 402
- Substance action on target

Filter by value View more

Limit to Exclude Clear

2

3

selected Limit To Exclude Export

1 Single protein  
(+)-harreaticin hydroxylase, chloroplastic (Wild)  
Synonyms: (+)-harreaticin hydroxylase, chloroplastic, polyphenol oxidase  
Mutant/chimera Details: Wild  
Show target details

2 Single protein  
1,4-beta-D-glucan glucohydrolase (Wild)  
Synonyms: 1,4-beta-D-glucan glucohydrolase, beta-D-glucoside glucohydrolase, beta-glucosidase, bgla, ggla, glucan 1,4-beta-glucosidase, glucan glucohydrolase  
Mutant/chimera Details: Wild  
Show target details

3 Single protein  
1,8-cineole 2-endo-monooxygenase (rat, Wild)

Substances - 1 > Documents - 1 >

Substances - 19 > Documents - 2 >

Substances - 1 >

Example structure

mixture (composition partially given)

No quantitative value reported

Most active substance:

K<sub>i</sub> (inhibition constant)=66μM

Example structure

Feedback

化合物

反應式

文獻

專利

生物活性

## 搜尋流程

- 瀏覽相關的靶點、化合物及文件連結。
- 匯出生物活性表格，用於結構活性關係 ( SAR )、驗證或提交。



進階用戶技巧：挖掘專利資料庫以揭示化合物和反應，識別治療宣稱，並比較不同司法管轄區內的受保護合成路徑。

Reaxys

Quick search Query builder **Results** Retrosynthesis

Search > Preview results > 171.13 K Documents > 3.08 K Targets

3,079 Targets out of 137,810 Documents, 402,751 Substances, 215,324 Reactions

Save search Create alert Edit in Query Builder

Sort by Sort alphabetically A-Z Zoom structures Bioactivity Visualization

Filters

- Targets
- Target Species
- Target Type
- Measurement pX
- Parameters
  - ic50 3,705
  - Inhibition percentage 2,010
  - qualitative 1,855
  - Ki (inhibition constant) 1,348
  - Inhibition rate 590
  - Km (michaelis constant) 474
  - activity 402
- Substance action on target

Filter by value View more

Limit to Exclude Clear

4

5

1 Single protein  
(+)-Harreatricin hydroxylase, chloroplastic (Wild)  
Synonyms: (+)-harreatricin hydroxylase, chloroplastic, polyphenol oxidase  
Mutant/chimera Details: Wild  
Show target details

2 Single protein  
1,4-beta-D-glucan glucohydrolase (Wild)  
Synonyms: 1,4-beta-d-glucan glucohydrolase, beta-d-glucoside glucohydrolase, beta-glucosidase, bgla, ggla, glucan 1,4-beta-glucosidase, glucan glucohydrolase  
Mutant/chimera Details: Wild  
Show target details

3 Single protein  
1,8-cineole 2-endo-monooxygenase (rat, Wild)

Example structure

mixture (composition partially given)

No quantitative value reported

Most active substance:

Ki (inhibition constant)=66µM

Example structure

Feedback

# 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。

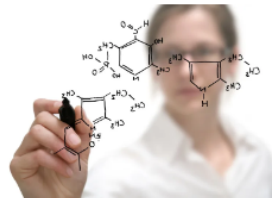


開始測驗

### Reaxys 化學 101

預估完成時間: 45-60 分鐘

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

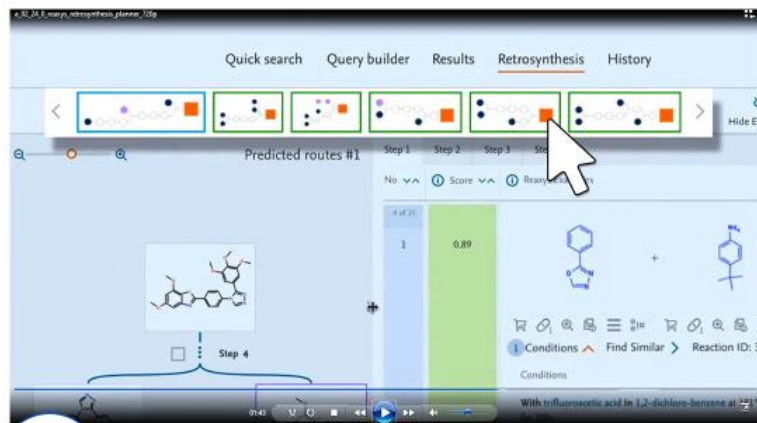


開始測驗

# 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



### 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](#)



### [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

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

個人帳號：

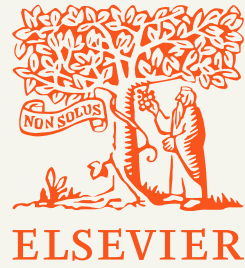
- 第一次使用者，請於單位IP範圍內，前往 [www.reaxys.com](http://www.reaxys.com)，點選 Register，以學校機構的 email 申請。
- 若過往已於 Reaxys Basic Edition 或其他 Elsevier 資料庫 (ScienceDirect, Scopus, Embase, Engineering Village 等) 申請過帳號，但非以學校機構的 email 申請，則請循第一次使用者方式重新申請；若現有帳號已經是以學校機構的 email 申請，即可直接使用。



## 課程滿意度調查

Elsevier 教育訓練問卷調查 2026  
Post-training Feedback Survey  
2026





Advancing human progress together