

掌握化學未來的關鍵 工具：Reaxys 全方位 版助您突破研究

Customer Success

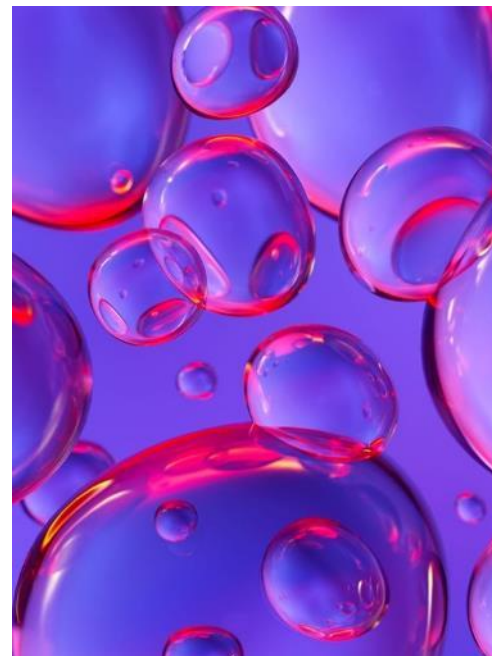
2025



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
索？

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

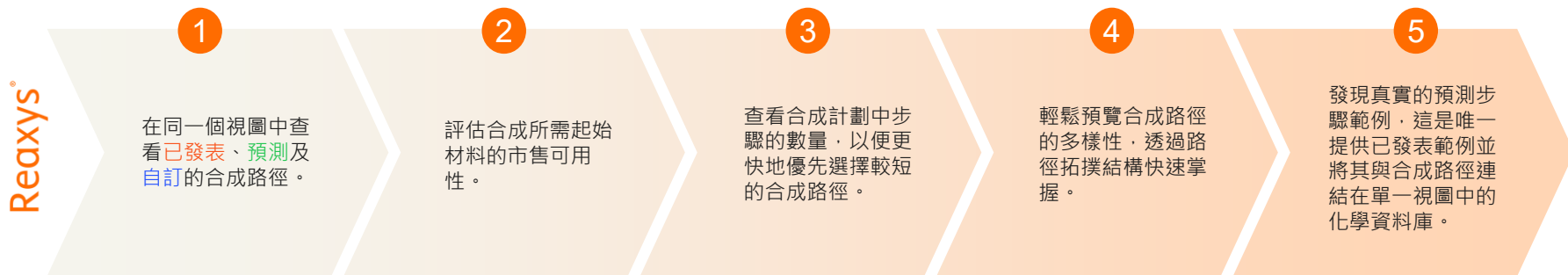
研究人員相信自己已經具備相關工具，但每一個「簡單」的搜尋背後都藏著一段繁雜、多工具交織的流程。在進行搜尋之前，他們其實已經在其他地方完成了一部分準備工作：



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® + 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

ELSEVIER

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
- 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 X

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?

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。

Reaxys RAE

檢索介面導覽

ELSEVIER

檢索介面介紹

The image shows the Reaxys search interface with the following components and annotations:

- Navigation Bar:** Includes the Reaxys logo, a search bar, and tabs for Quick search (1), Query builder (2), Results (3), Retrosynthesis (4), History (5), Alerts (6), and Reaxys AI Search (7). A "Beta" badge is next to the AI Search tab. A user profile icon with a question mark and "SS" is in the top right, with a callout for "使用者偏好設置與登出" (User preference settings and logout).
- Main Banner:** A blue banner with the text "Discover a more intuitive way to search — with Reaxys AI Search Beta." A callout points to a link for "常見問題、技術訓練影片、支援中心" (FAQ, technical training videos, support center).
- Search Scope:** A grey banner with the text "Search substances, reactions, documents and bioactivity data in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances." An "Import" button with a download icon is on the right, with a callout for "批次導入結構" (Batch import structure).
- Search Interface:** A white box with the title "Search Reaxys" containing a search input field and a "Find" button. The input field contains the text "Substance Molecular Formula, e.g. Pt(PPh3)3". A callout for "關鍵字檢索" (Keyword search) points to the input field.
- Chemical Structure Search:** Below the search bar is a section for "AND" with a "Draw" button (chemical structure icon). A callout for "化學結構檢索 (反應式、結構式)" (Chemical structure search (reaction, structure)) points to this section.
- Numbered Callouts:**
 - 1 Quick search: 關鍵字搜尋、結構搜尋
 - 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 History: 搜尋歷史。
 - 6 Alert: 瀏覽提示的搜尋內容
 - 7 Reaxys AI Search: AI 搜尋功能

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

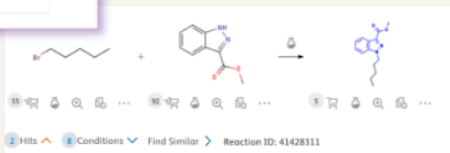
Reaxys serves a varying profile of chemist



I am a chemist where I mainly search using **structures**

Structure search:

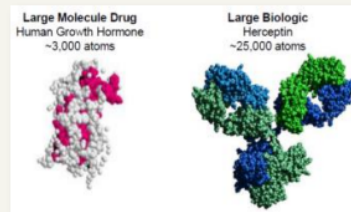
- Search for substances, reaction, properties that have been extracted by structure through structure or text search queries



I am a chemist where I search using **structures and text**

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



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

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:

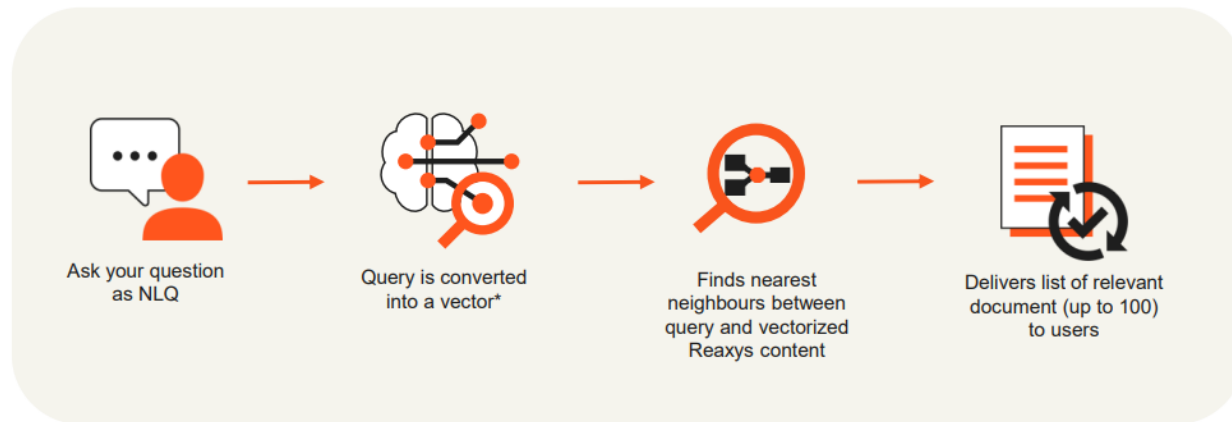
- ✓ 支援化學與其他學科結合的跨領域領域，例如聚合物、化學工程、材料科學等。
- ✓ 具有彈性的查詢功能，能夠處理拼寫錯誤、單數與複數、縮寫以及同義詞。

詳情請參閱 [Release Notes](#)

The screenshot displays the Reaxys AI Search interface. At the top, a navigation bar includes links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', 'Alerts', and a highlighted '+ Reaxys AI Search' button with a 'Beta' badge. Below the navigation bar, a blue banner reads 'Discover a more intuitive way to search — with Reaxys AI Search Beta'. The main search area contains a text input field with the query 'Benefits of using Single-Crystal Cathode Particles in lithium-ion batteries'. Below the input field, it states '100+ Documents found'. There are two search results listed. The first result is titled 'Single-crystal high-nickel layered cathodes for lithium-ion batteries: advantages, mechanism, challenges and approaches' and includes an abstract discussing the benefits of single-crystal materials over polycrystalline ones. The second result is titled 'Pulse High Temperature Sintering to Prepare Single-Crystal High Nickel Oxide Cathodes with Enhanced Electrochemical Performance' and includes an abstract discussing the optimization of sintering parameters for single-crystal cathodes. A red box highlights the 'View in Reaxys.com' link next to the first result, with an arrow pointing to it from the text 'To apply filters and explore structured data'.

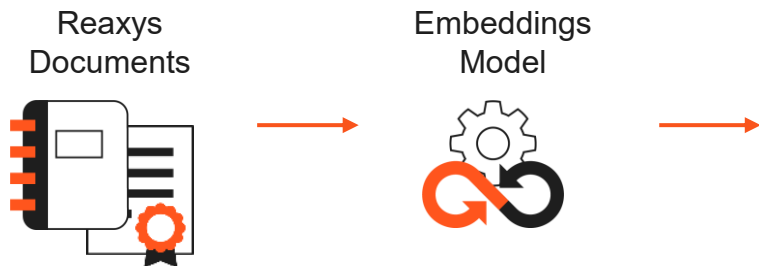
How does Reaxys AI search work?

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.

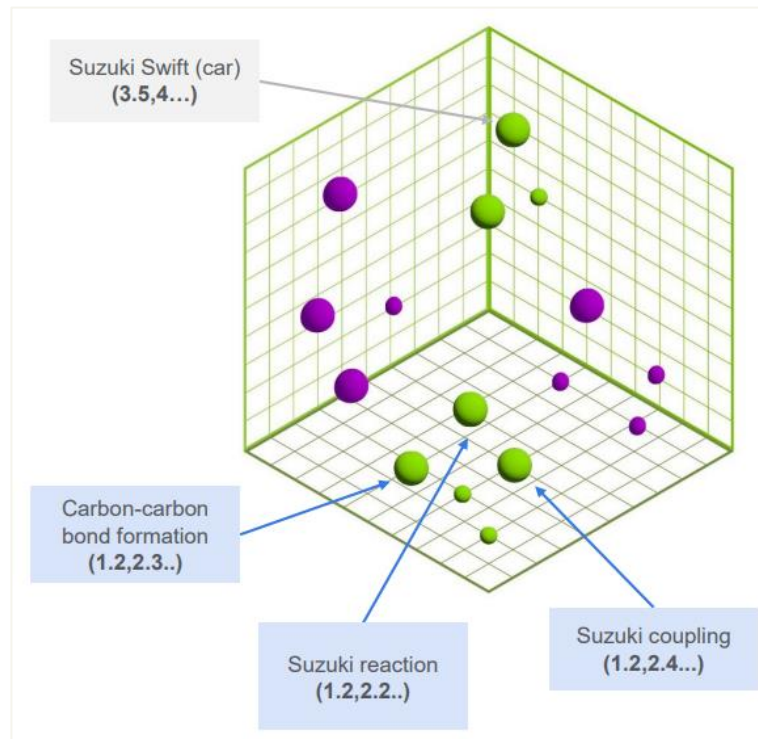


- ✓ BERT model is trained to answer chemistry-related questions with full Reaxys data (Title and Abstracts)
- ✓ Reviews more relevant results for natural language query
- ✓ Leverages strength of both vector & keyword-based search

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?

ELSEVIER

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](#)

☒ [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.

Reaxys

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

100 Filters

Limit to > Exclude >

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) >

100 Documents with 366 Substances, 39 Reactions, 0 Targets

0 selected Limit To Exclude Export

Sort by Relevance > < < >

Bioactivity Visualization

1 Coordination polymer particles as potential drug delivery systems [Cited 240 times](#)
Imaz, Inhar; Rubio-Martinez, Marta; Garcia-Fernandez, Lorena; Garcia, Francisco; Ruiz-Molina, Daniel; Hernandez, Jordi; Puentes, Victor; MasPOCH, Daniel
Chemical Communications, 2010, vol. 46, # 26, p. 4737 - 4739, 10.1039/c003084h
Abstract > Index Terms > Substances (3) > Full Text >

2 Unusual microporous polycatenane-like metal-organic frameworks for the luminescent sensing of Ln³⁺ cations and rapid adsorption of iodine [Cited 98 times](#)
Chen, Lei; Tan, Ke; Lan, Ya-Qian; Li, Shun-Li; Shao, Kui-Zhan; Su, Zhong-Min
Chemical Communications, 2012, vol. 48, # 47, p. 5919 - 5921, 10.1039/c2cc31257c
Abstract > Index Terms > Substances (7) > Reactions (3) > Full Text >

3 Peptide targeted lipid nanoparticles for anticancer drug delivery [Cited 177 times](#)
Shroff, Kamlesh; Pearce, Timothy R.; Kakkoli, Efrasin
Advanced Materials, 2012, vol. 24, # 28, p. 3803 - 3822, 10.1002/adma.201200832
Abstract > Index Terms > Full Text >

4 Lipid nanocapsules: A new platform for nanomedicine [Cited 533 times](#)
Huynh; Passirani; Saulnier; Benoit
International Journal of Pharmaceutics, 2009, vol. 379, # 2, p. 201 - 209, 10.1016/j.ijpharm.2009.04.026
Abstract > Index Terms > Full Text >

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](#)

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

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? [👍](#) [👎](#)

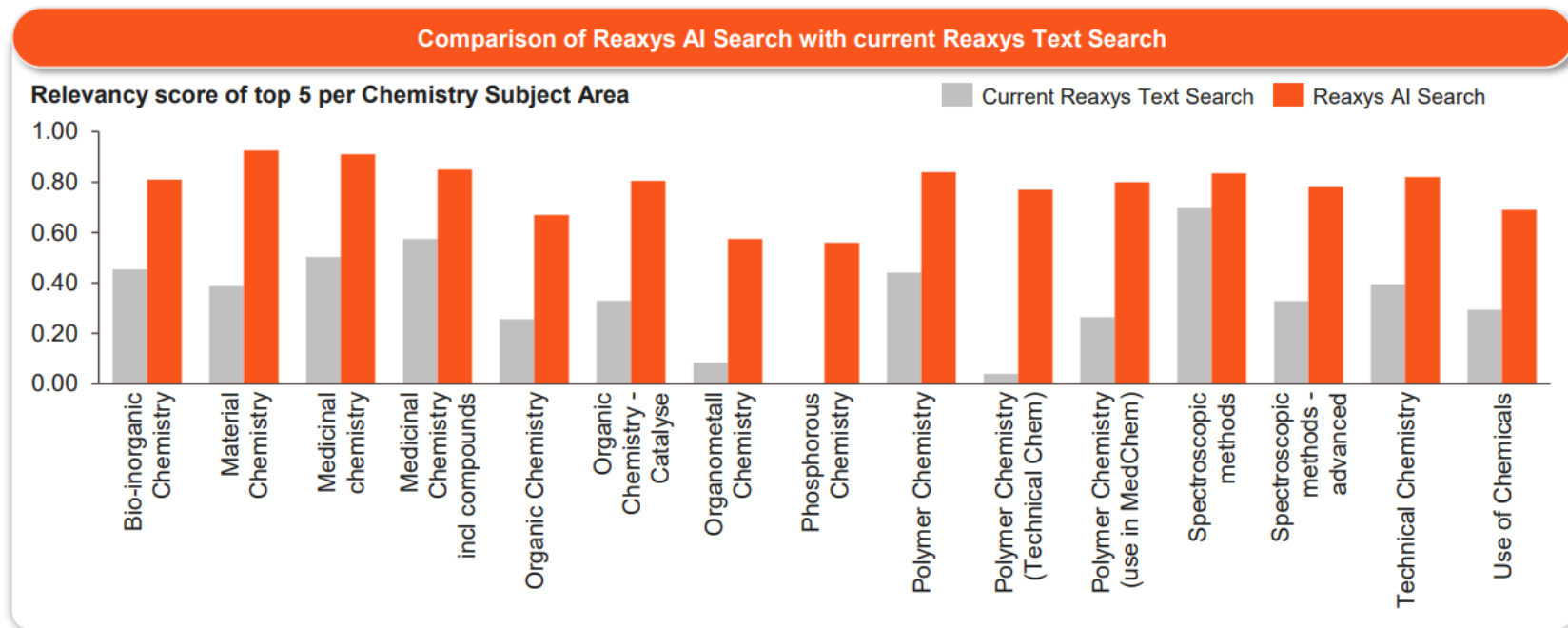
☐ 2 [Effects of high hydrostatic pressure and thermal processing on anthocyanin content, polyphenol oxidase and \$\beta\$ -glucosidase activities, color, and antioxidant activities of blueberry \(*Vaccinium* Spp.\) puree](#)

[2021]

Score: 0.995587

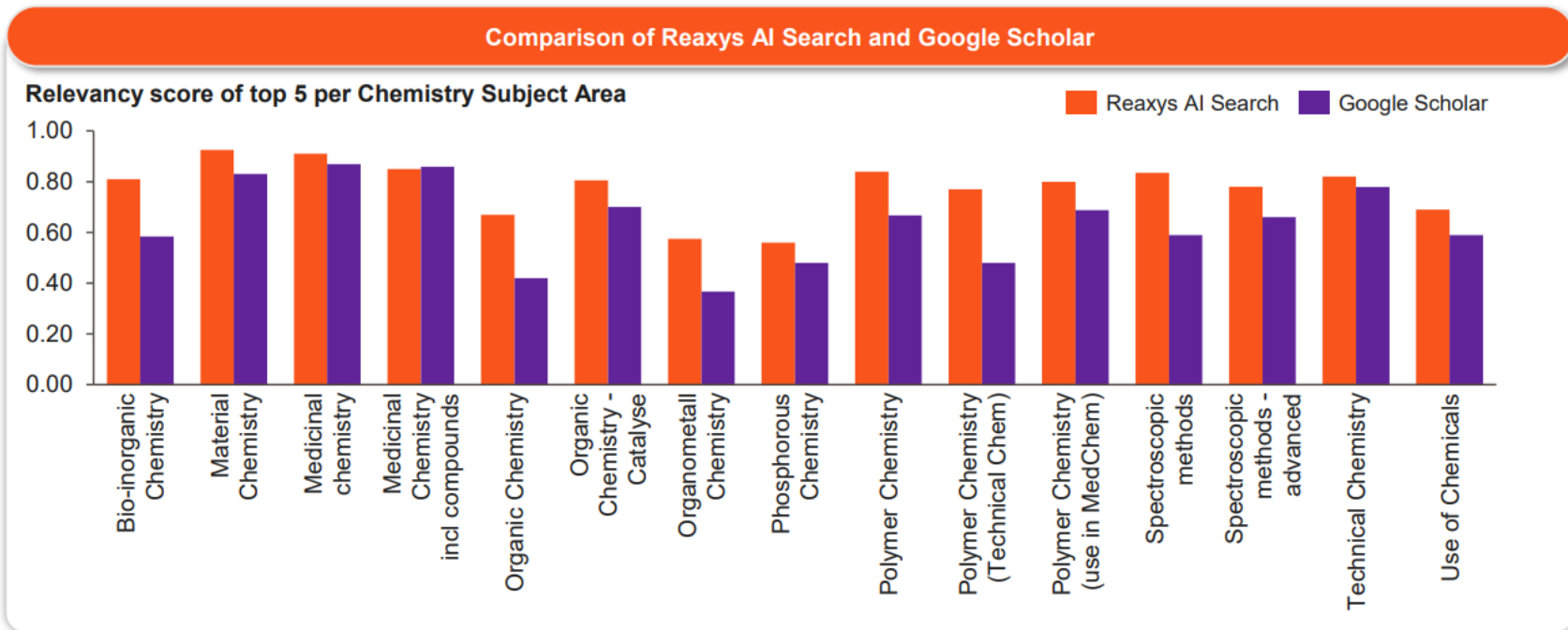
Did the results answer your question? [Yes](#) [No](#)

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



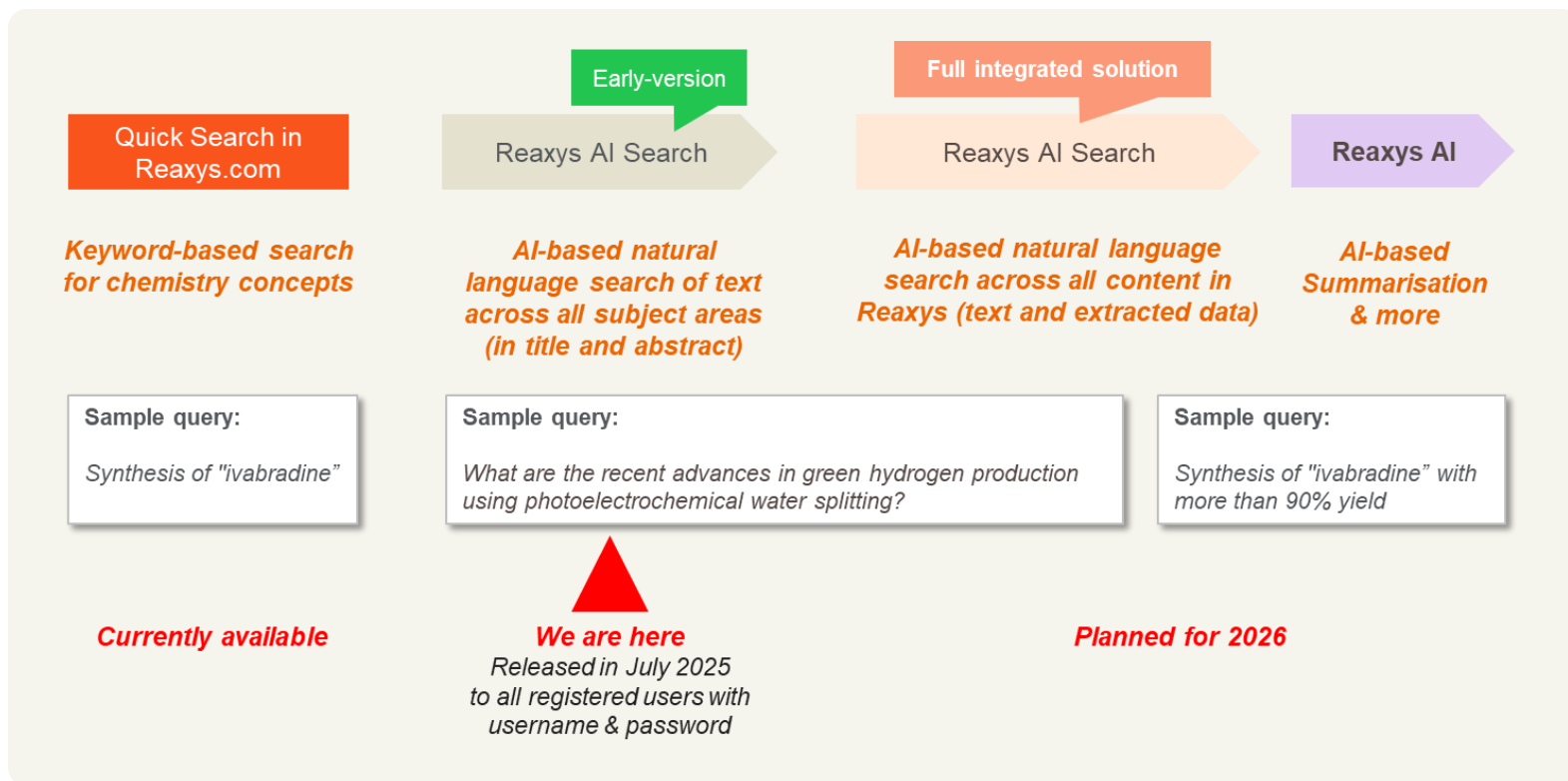
Disclaimer: Reaxys text search wasn't built for natural languages queries

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



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

× Find >

Substance Properties, e.g. [solubility of vitamin D3](#)

化學性質搜尋

Search Reaxys

× Find >

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

逆合成搜尋

Search Reaxys

× Find >

Substance CAS Registry Number, e.g. [102625-70-7](#)

化學作用搜尋

Search Reaxys

× Find >

Reactions, e.g. [phosphorylation](#)

文獻搜尋

Search Reaxys

× Find >

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](#)

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

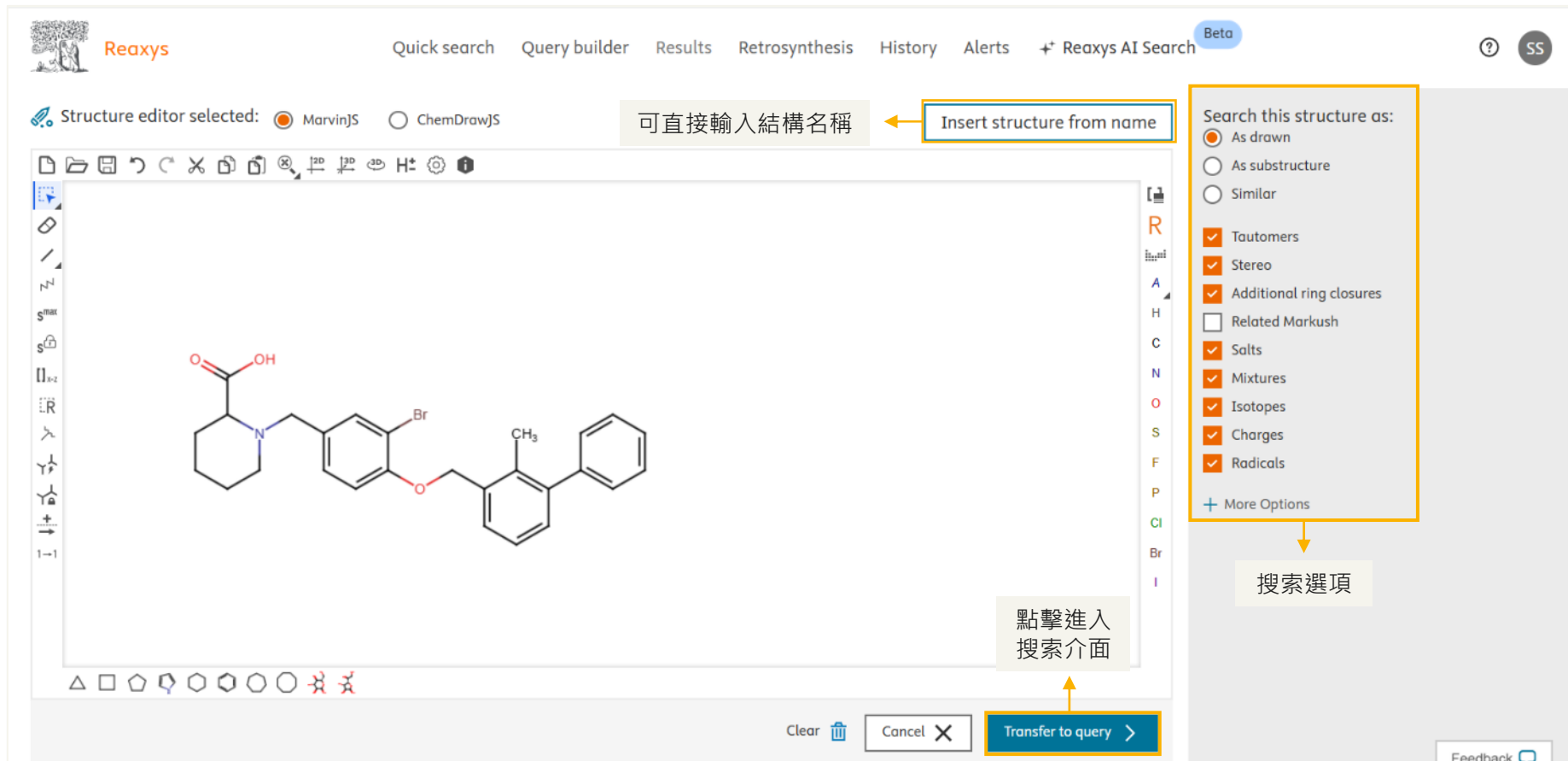
- ☒ Tautomers
- ☒ Stereo
- ☒ Additional ring closures
- ☐ Related Markush
- ☒ Salts
- ☒ Mixtures
- ☒ Isotopes
- ☒ Charges
- ☒ Radicals

+ More Options

搜索選項

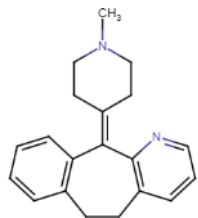
點擊進入搜索介面

Transfer to query >

O=C1CCCCCN1Cc2ccc(OCc3ccccc3C)c(Br)c2

Reaxys 三種結構搜尋與怎麼用

我感興趣的結構



Azatadine
CAS# 3964-81-6

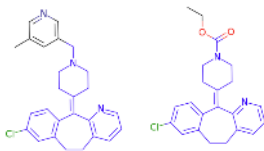
As drawn

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

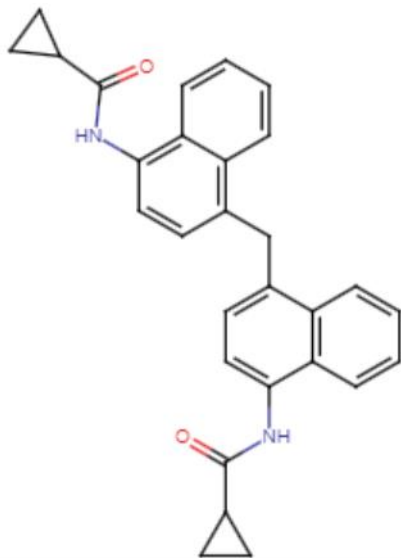
+ [More Options](#)

- 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。



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

Query builder 檢索介面

 **Reaxys**

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

?

SS

Search in: Reactions > Targets > Substances > Documents > 6

Import Save Options Reset Query Delete Query

1

2

3

4

5

Current Patent Assignee

Structure

Molecular Formula

CAS RN

TI, AB & KW

7

8

9

Fields

Forms

History

Reaxys

Topics and Keywords

Identification

Physical Properties

Spectra

Target and Bioactivity

Other

Reactions

Bibliography

PubChem

Commercial Substances

Structure

Feedback

Search fields and forms

Find Any

Hide fields

Melting Point

=

Melting Point, °C

is

Solvent (Melting Point)

AND

Measurement pX

=

Measurement pX

AND

Reagent/Catalyst

is

Reagent/Catalyst

1

2

3

4

5

7

8

9

Current Patent Assignee

Structure: 結構式繪圖畫面

Molecular formula: 分子式搜尋

CAS RN: CAS 代號

TI, AB & KW: 標題 · 摘要 · 關鍵字


Search: 化學條件項目搜尋欄位

Fields: 化學條件項目

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

History: 搜索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 ? SS

可以保存創建的檢索公式

Import **Save Options** Reset Query Delete Query

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

選擇反應式、蛋白靶點、物質或文獻搜索

☰ Melting Point

Find Any

Hide fields ^

= ▾

50 - 50.1

🔍

is ▾

acetic acid

🔍

AND ^

OR
AND
NOT
NEAR
NEXT
PROXIMITY

Reagent/Catalyst

= ▾

Measurement pX

🔍

is ▾

Reagent/Catalyst

🔍

Identification ▾

Physical Properties ^

Melting Point

Boiling Point

Sublimation

Refractive 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, the Reaxys logo is on the left, and navigation tabs include 'Quick search', 'Query builder' (highlighted), 'Results', 'Retrosynthesis', 'History', 'Alerts', and 'Reaxys AI Search' (marked as Beta). A search bar at the top right contains 'sublimation'. Below the navigation, a 'Search in:' section has buttons for 'Reactions', 'Targets', 'Substances' (highlighted with a red box and labeled 6), and 'Documents'. A toolbar below this includes 'Import', 'Save Options', 'Reset Query', and 'Delete Query'. On the right, a 'Close Panel' button is visible. The main query area on the left shows a table with columns for 'Sublimation'. Two rows are visible: one with '55-56' (labeled 4) and another with '760' (labeled 5). A 'Show fields' button (labeled 3) is located above the table. On the right side of the interface, a sidebar shows a list of search results: 'Sublimation' (labeled 2) and '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

☐ 0 selected

Limit To

Exclude

Export

Preparations

Sort by No of References

Grid

Bioactivity Visualization

☐ 1

2

(E)-2,2,6,6-tetramethylhept-4-en-3-one

(CH3)3CCHCHCOC(CH3)3 168.279 1904245 20859-13-6

Hit Data - 1

Identification

Druglikeness

Physical Data - 12

Spectra - 25

Preparations - 14 >

Reactions - 62 >

Documents - 44 >

^ Hit Data - 1

^ Sublimation - 1 hits out of 1

系統會將 Sublimation 資料標示於 Hit Data >> 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] Full Text Cited 69 times Details

ELSEVIER

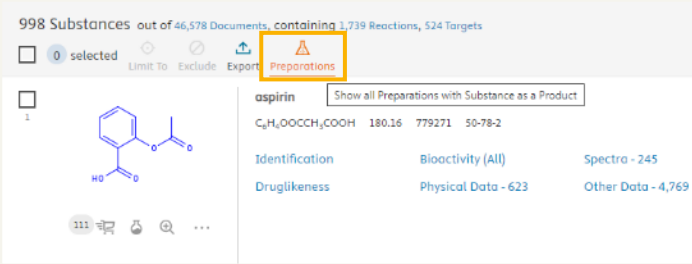
反應式搜尋

How to search chemical reactions

ELSEVIER

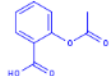
尋找反應式 (Chemical equation) 的方法

1. 已知物質的製備方式
(從 substance 介面連結 preparations)



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

0 selected Limit To Exclude Export Preparations

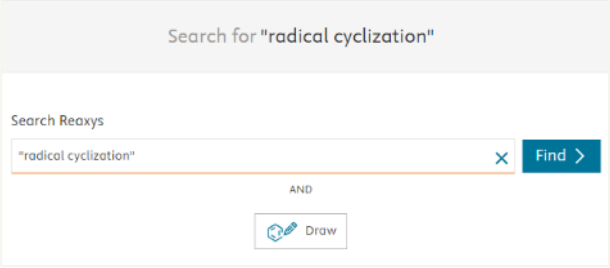
1 

aspirin Show all Preparations with Substance as a Product

C6H4(OOCCH3)COOH 180.16 779271 50-78-2

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

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



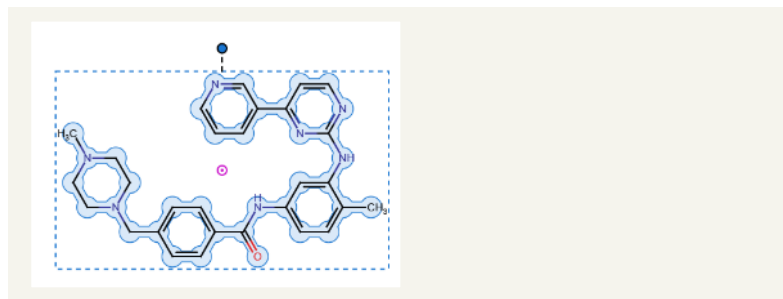
Search for "radical cyclization"

Search Reaxys

"radical cyclization"

AND

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

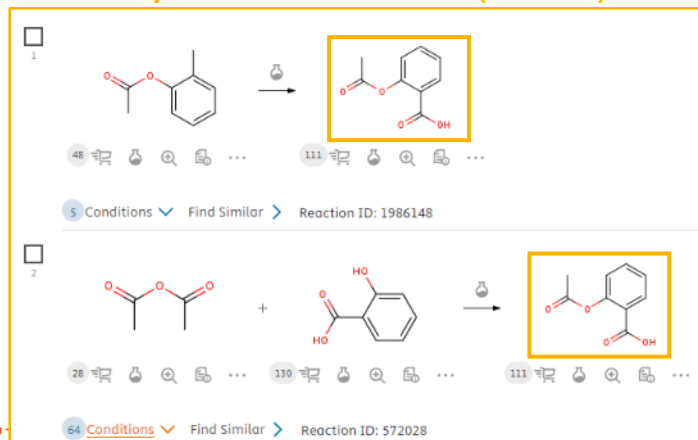
0 Limit To Exclude Export Preparations No of References Grid Bioactivity Visualization

aspirin
CC(=O)Oc1ccccc1C(=O)O 180.16 779271 50-78-2

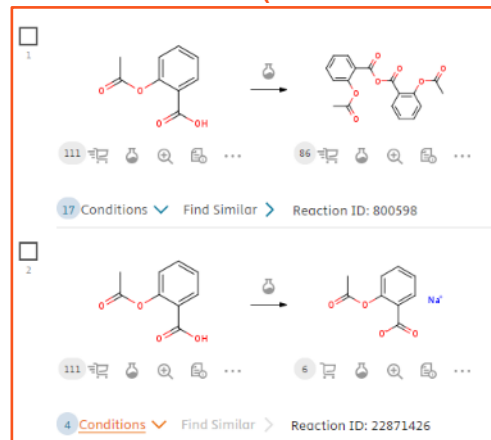
Identification Physical Data - 623
Druglikeness Spectra - 245
Bioactivity (All) Other Data - 4,769

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" × Find >

AND

 Draw

Results for "radical cyclization"					New 	Edit 
	75	Reactions	Condition : radical cyclization	Preview Results 	View Results 	
			Edit in Query Builder 	Create Alert 		
	9,499	Documents	Titles, Abstracts, Keywords : "radical cyclization"	Preview Results 	View Results 	
			Edit in Query Builder 	Create Alert 		

尋找反應式的方法：關鍵字檢索

Reaxys®

Quick searchQuery builder**Results**RetrosynthesisHistoryAlerts

Stephanie Su

75

Preview

Search

Filters

Limit to >Exclude >

By Structure >

Yield >

Reagent/Catalyst >

Solvent >

Catalyst Classes >

Solvent Classes >

Product Availability >

Reactant Availability >

Reaction Classes >

Document Type >

Publication Year >

☐ Single step reactions only

☐ Experimental procedure only

75 Reactions out of 86 Documents, containing 232 Substances, 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, Shiho; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao [Organic Letters, 2000, vol. 2, # 3, p. 307 - 310] Full Text Cited 77 times Details Abstract

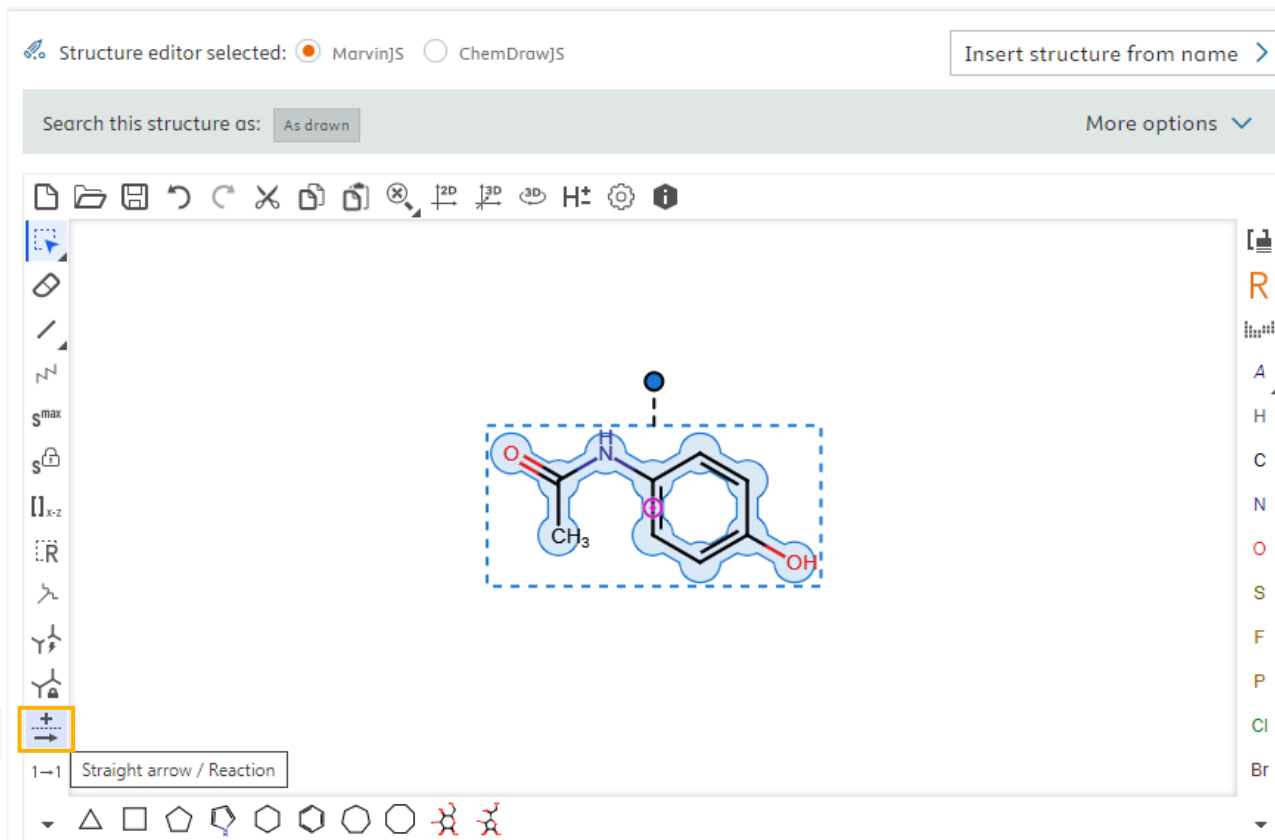
2



40 racemate

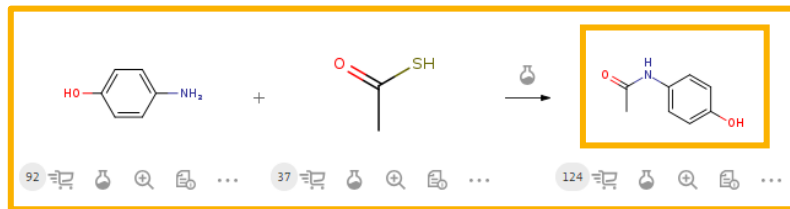
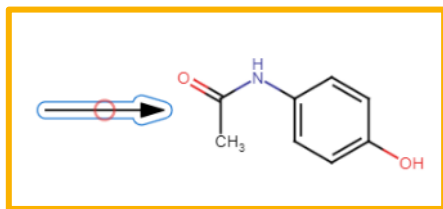
Feedback

尋找反應式的方法：繪製反應式

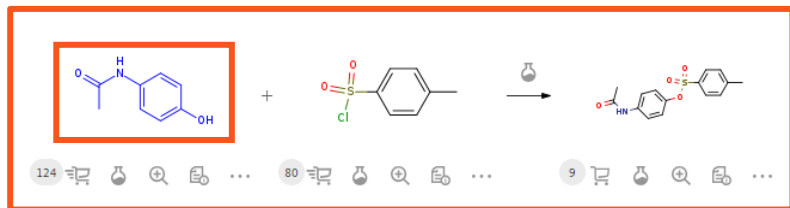
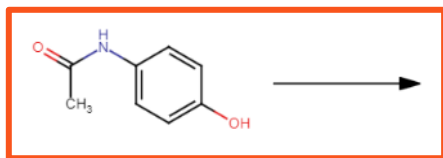


尋找反應式的方法：繪製反應式

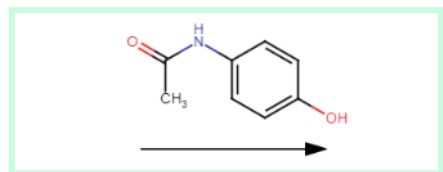
產物：箭頭在左



起始物：箭頭在右



催化劑或溶劑：箭頭在下















Conditions

With 4-acetaminophen; 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 [▼](#)

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 Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	9,368	Reactions	Reaction Query :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	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 ? SS

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

microbiolog*

Reaction Data & Conditions is microbiolog*

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

Feedback

Chemical structure diagram showing the reaction of N-(4-hydroxyphenyl)acetamide (paracetamol) to form a product, indicated by an arrow.






























小提示: 利用 contains 與結合萬用字元「*」來進行自首搜尋。

搜尋結果種類

Types of search results

ELSEVIER

搜尋預覽介面

<div>Search Reaxys</div> <div>Caffeine</div>	<div> 1,554 Substances</div> <div>Structure :  as drawn Edit in Query Builder  Create Alert </div> <div>Preview Results  View Results </div>	實驗數值與 參考出處
<div>Search Reaxys</div> <div>Caffeine</div>	<div> 161,183 Documents</div> <div>Structure :  as drawn Titles, Abstracts, Keywords : "caffeine" Edit in Query Builder  Create Alert </div> <div>Preview Results  View Results </div>	文獻、專利
<div>Search Reaxys</div> <div>Caffeine</div>	<div> 174 Commercial Substances</div> <div>Structure :  as drawn Edit in Query Builder  Create Alert </div> <div>Preview Results  View Results </div>	供應商資訊
<div>Search Reaxys</div> <div>Caffeine preparation</div>	<div> 431 Reactions</div> <div>Reaction Query :  as drawn Edit in Query Builder  Create Alert </div> <div>Preview Results  View Results </div>	合成方法
<div>Search Reaxys</div> <div>"adenosine a2a receptor"</div>	<div> 83 Targets</div> <div>Target(s) : adenosine a2a receptor Edit in Query Builder  Create Alert </div> <div>Preview Results  View Results </div>	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

48.01 K

Filters

Limit to > Exclude >

By Structure Measurement pX Targets Parameters Substance Classes Molecular Weight Number of Fragments Availability Available Data Document Type Publication Year Current Patent Assignee LogP H Bond Donors H Bond Acceptors Rotatable Bonds TPSA

1

2

3

4

5

6

7

8

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

0 selected Limit To Exclude Export Preparations

Sort by No of References

Grid Bioactivity Visualization

quercetol

(HO)2C6H3C9H2O(O)(OH)3 302.24 317313 117-39-5

Identification Bioactivity (All) Other Data - 5,272

Druglikeness Physical Data - 1,297

Bioactivity (Hit Data) Spectra - 1,993

Preparations - 208

Reactions - 1,646

Targets - 1,616

Documents - 69,689

3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione

C5H(CH3)3O2N4 194.193 17705 58-08-2

Identification Bioactivity (All) Other Data - 1,701

Druglikeness Physical Data - 804

Bioactivity (Hit Data) Spectra - 297

Preparations - 139

Reactions - 1,454

Targets - 361

Documents - 60,555

dc

C2

Id

Di

Bi

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

Preparations - 94

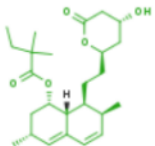
Reactions - 535

Targets - 788


Documents - 60,364

Feedback

詳細的化合物數據



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

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
 Apply

Show/Hide columns

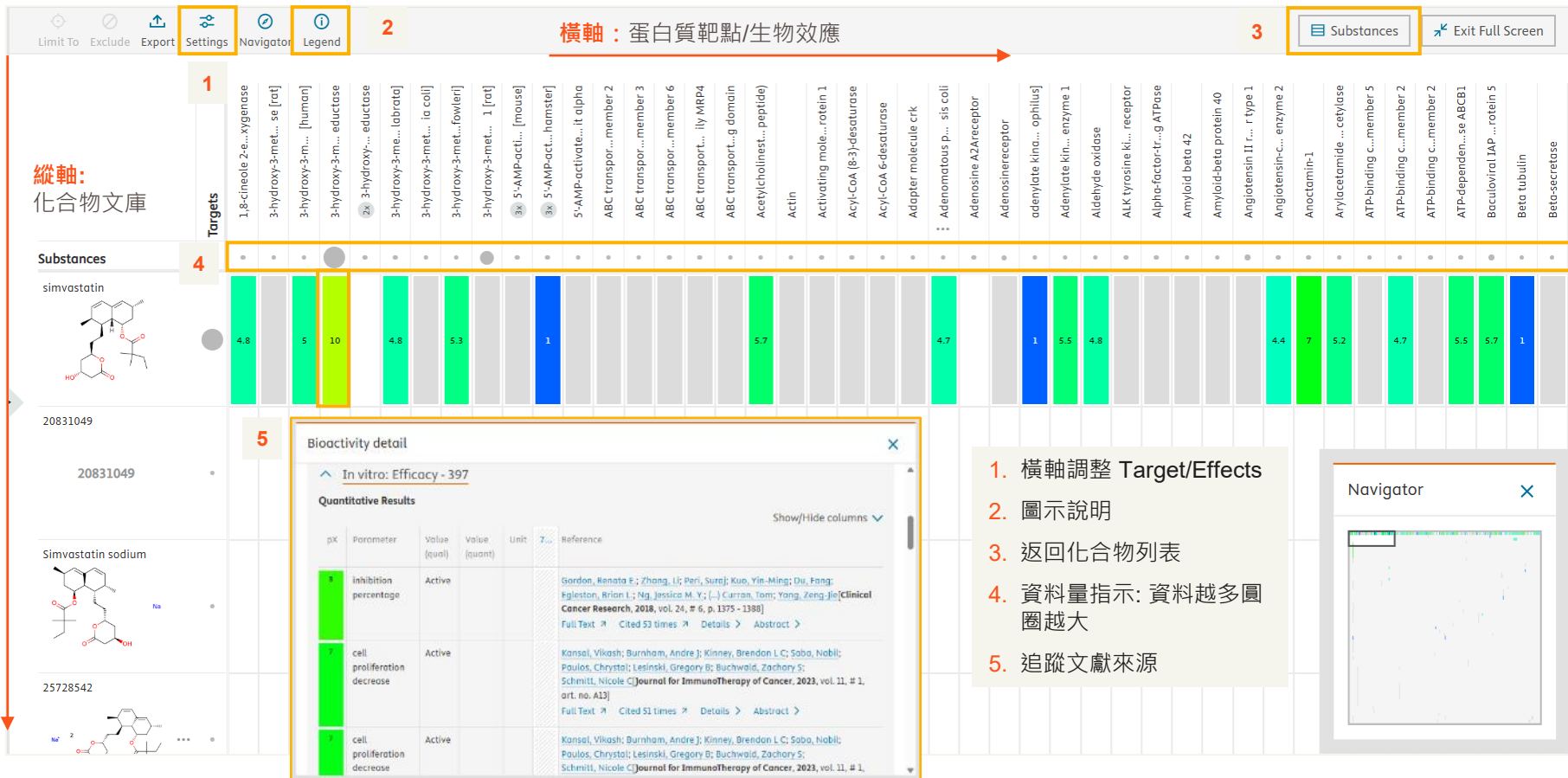
- ☒ pX
- ☒ Parameter
- ☒ Value (qual)
- ☒ Value (quant)
- ☒ Unit
- ☒ Biological Species
- ☒ Action on target
- ☒ Target
- ☐ (Clinical) findings / disease
- ☒ Tissue/Organ
- ☒ Cell
- ☐ Bioassay
- ☒ Dose
- ☒ Effect
- ☒ Concomitants
- ☐ Metabolites
- ☒ Reference

更多的參數
預設隱藏

Reset to default >

Apply >

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 > 以次結構篩選

Measurement pX > pX值篩選

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

Targets > 蛋白靶點

Target Species > 蛋白靶點物種

Target Type > 蛋白靶點類型 (野生型 ; 突變型)

Substance action on target > 化合物作用機轉

Molecular Weight > 分子量篩選

Effect > 生物活性效益

Document Type > 文獻類型

Publication Year > 發表年份

Current Patent Assignee > 目前專利授予者

Limit To Exclude Export Settings Navigator Legend

3-hydroxy-3-met... fowleri]	3-hydroxy-3-met... 1 [rat]	3x 5'-AMP-acti... [mouse]	3x 5'-AMP-act... 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

反應式搜尋結果篩選工具

Filters

Limit to > Exclude >

By Structure > 結構

Yield > 產率

Reagent/Catalyst > 試劑，催化劑

Solvent > 溶劑

Catalyst Classes > 催化劑類別

Solvent Classes > 溶劑類別

Product Availability > 產物的可能性

Reactant Availability > 反應物的可能性

Reaction Classes > 反應類別

Document Type > 來源種類 (文獻，專利)

Publication Year > 出版年份

☐ Single step reactions only 縮小到只有一步反應

☐ Experimental procedure only 縮小到只包含實驗性術語的名單

可展開查看篩選細項

- 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)

> Inorganic

> Protic

> Green

> Aprotic apolar

> Aprotic dipolar

> Red

21

17

9

8

8

1

1

1

Selected search items:

Inorganic

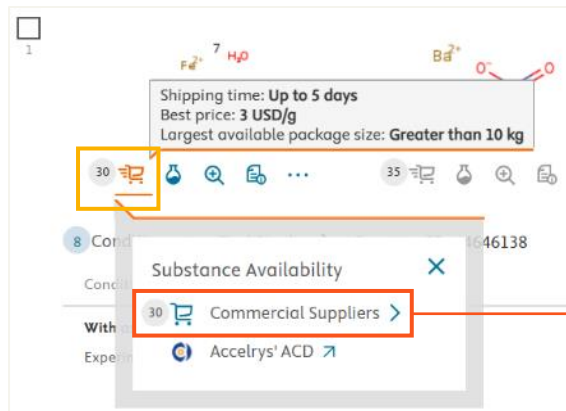
Low boiling (<100°C)

Clear selected

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。



- 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

ELSEVIER

Reaxys - 21 Commercial Substances - 1 PubChem - 3

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 >

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 SDS		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 SDS		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 SDS		5 kg 459 USD	Shipment country: North America Last updated: 2025-04-03
AK Scientific Inc.	Iron(II) sulfate heptahydrate, ACS 7782-63-0 8648AF	>99percent	5 g 18 USD	Stock availability: in stock Last updated: 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 Cited 21 times

van Weert; Shang [Hydrometallurgy, 1993, vol. 33, # 3, p. 255 - 271]





Abstract  Index Terms  Full Text 

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 Cited 9 times

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 

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 Cited 73 times

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 

Abstract hit: {...electron acceptors ferric iron and nitrate, and biochar, acting as an electron shuttle,...}

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

出版年份
文獻類型
文獻作者
目前隸屬機構
專利發明者
目前專利授予者
專利辦公室
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

Limit to > Exclude >

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

Index Terms (ReaxysTree) 3195

Index Terms (ReaxysTree)

physico chemical properties

chemical transformations

chemical reaction class

reaction kinetic

surface area

catalyst surface area

kinetic type

reaction reactivity

reaction activation energy

reaction order

catalytic kinetic

reaction constant

34,389

21,174

16,126

14,614

6,141

3,127

33

2,336

1,095

485

68

28

78

Selected search items:

surface area

reaction order

Clear selected

Limit to >

Exclude >

Index Terms (ReaxysTree)

☐ physico chemical properties

21,174

☐ chemical transformations

16,126

☐ physico chemical analysis methods

14,742

☐ quantum chemical calculation methods

458

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

ELSEVIER

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

Search 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 [Cited 2 times](#)
[Semy, Khikeya; Singh, Maibam Romeo](#) [Tropical Ecology, 2024, vol. 65, # 1, p. 16 - 25]
[Abstract](#) [Index Terms](#) [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 [Cited 3 times](#)
[Shah, Vijendra; Dani, Pooja; Davey, Achlesh](#) [Applied Biochemistry and Biotechnology, 2024, vol. 196, # 5, p. 2399 - 2413]
[Abstract](#) [Index Terms](#) [Substances](#) [1](#) [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 [Cited 3 times](#)
[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](#)

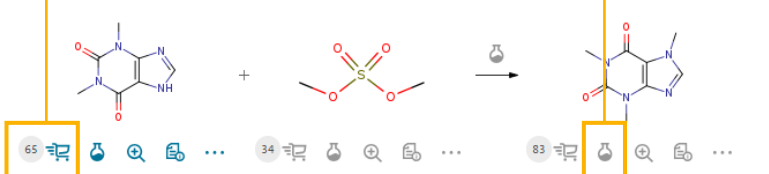
Index Terms hit: {...wheat germ agglutinin, **Bidens pilosa** extract, unclassified drug...}

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 Find Similar > 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 Full Text Details Abstract
potassium fluoride on basic alumina In acetonitrile for 24h; Ambient temperature;	88%	Yamawaki, Junko; Ando, Takashi; Hanafusa, Terukiyo [Chemistry Letters, 1981, p. 1143 - 1146] Full Text Details Abstract
With sodium hydroxide		Biltz; Beck [Journal fur praktische Chemie (Leipzig 1954), 1928, vol. <2>118, p. 161] Full Text Details
With sodium hydroxide		Chmelewskii; Abramowa [Zhurnal Obshchei Khimii, 1958, vol. 28, p. 1970,1972;engl.Ausg.S.2012,2014] Full Text Details
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] Full Text Cited 41 times Details Abstract

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		
6.11	IC50	7.8	nM		
8	IC50	10	nM	Inhibitor	Bcr-ABL p210 (T315A):Wild

Substructure	Target 1	Target 2	Target 3	Target 4	Target 5	Target 6
						
						
						
						
						

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？高活性的有那些？

藥物靶點檢索

Reaxys

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

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

Search Reaxys

tyrosine-protein Kinase JAK3

Find

Target Names
tyrosine-protein kinase jak3

47	Targets	Target(s) : tyrosine-protein kinase jak3 Edit in Query Builder Create Alert	Preview Results View Results
67,068	Substances	Target(s) : tyrosine-protein kinase jak3 Edit in Query Builder Create Alert	Preview Results View Results
17,186	Documents	Titles, Abstracts, Keywords : "tyrosine-protein kinase jak3" Edit in Query Builder Create Alert	Preview Results View Results

藥物靶點檢索

利用生物活性專屬的過濾工具

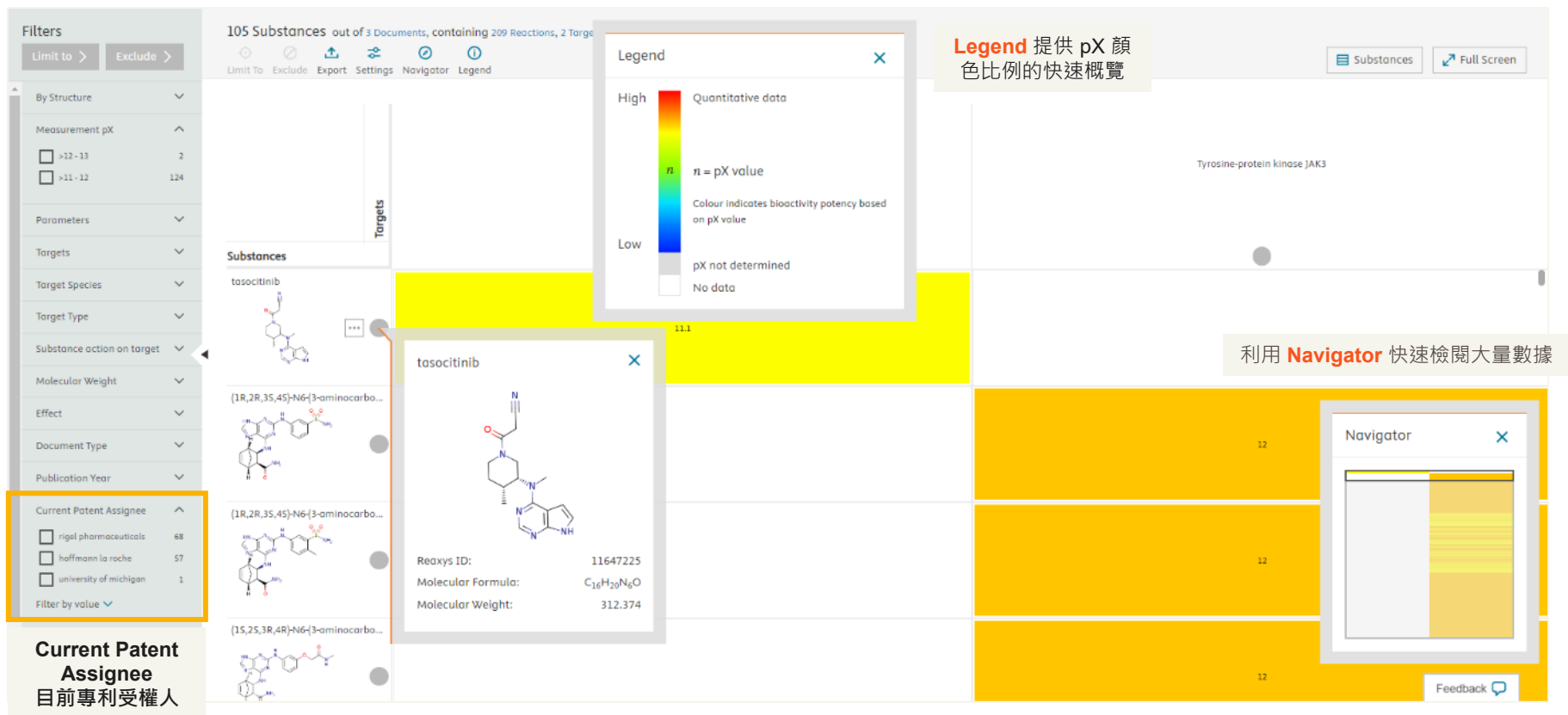
The screenshot displays a chemical database interface with the following components:

- Filters Panel (Left):** Includes a 'Limit to' button (highlighted with an orange box) and various filter categories like 'By Structure', 'Measurement pK', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', 'Number of Fragments', 'Availability', 'Available Data', 'Document Type', 'Publication Year', 'Current Patent Assignee', 'LogP', and 'H Bond Donors'.
- Substance Details (Center):** Shows details for 'tasocitinib' (C₁₈H₂₀N₆O, 312.374, 11647225). It includes tabs for 'Identification', 'Bioactivity (All)', 'Other Data - 1,104', 'Druglikeness', 'Physical Data - 33', and 'Spectra - 39'. The 'Bioactivity (Hit Data)' tab is highlighted with an orange box.
- Bioactivity (Hit Data) Table:** Displays quantitative results for 'In vitro: Efficacy - 1'. The table has columns: pX, Parameter, Value (quant), Unit, and Target. A row is highlighted in yellow.

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 Visualization Settings (Right):** A dialog box with a 'Targets' dropdown and a 'Substances' dropdown. The 'Substances' dropdown is open, showing options like 'Bioassays', 'Targets', 'Target Species', 'Biological Species', 'Effects', 'Parameter', 'Cell Lines', and 'Substances' (highlighted with an orange box).
- Top Right:** A 'Bioactivity Visualization' button (highlighted with an orange box) and a 'Grid' button.
- Right Sidebar:** Lists various data categories with counts: Preparations - 105, Reactions - 314, Targets - 668, Documents - 1,863, etc.

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

The screenshot displays the Reaxys web interface. At the top, navigation tabs include 'Quick search', 'Query builder', 'Results' (active), 'Retrosynthesis', 'History', and 'Alerts'. The user is logged in as 'Stephen Xu'. On the left, a 'Filters' sidebar is visible. The main area shows '105 Substances' out of 4 documents, containing 208 bioactivities. A modal window titled 'Export substances and bioactivities' is open, showing options to 'Choose a format' (Microsoft Excel New Layout, Microsoft Excel, Tab-delimited text, XML, SD/Molfile), 'Range', 'Export', and 'Additional options' (Include structures). A disclaimer states: 'Disclaimer: please refer to our Terms and Conditions before downloading data.' An 'Export' button is at the bottom right of the modal. In the background, a table of results is visible, with columns for 'Substances' and 'Targets'. The 'Targets' column lists 'Tyrosine-protein kinase JAK3'. A 'Navigator' window is also open in the bottom right corner, showing a list of results.

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Stephen Xu

Filters

105 Substances out of 4 documents, containing 208 bioactivities

Export substances and bioactivities

Choose a format: Microsoft Excel New Layout

Range:

Export:

Additional options: ☒ Include structures

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

Export

Substances

Targets

Tyrosine-protein kinase JAK3


Navigator

逆合成 AI 工具

Retrosynthesis AI

ELSEVIER

Retrosynthesis AI: 探索合成途徑

 **Reaxys**

[Quick search](#) [Query builder](#) [Results](#) **Retrosynthesis** [History](#) [Alerts](#) [+ Reaxys AI Search](#) Beta ? SS

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

Discover a molecule 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

 **ELSEVIER**

[Remote access](#) [Terms and Conditions](#) [Privacy policy](#) [About content](#) [Accessibility](#) [Contact support](#)

We use cookies to help provide and enhance our service and tailor content. [Cookie Settings](#)

All content on this site: Copyright © 2025 Elsevier B.V., its licensors, and contributors. All rights are reserved, including those for text and data mining, AI training, and similar technologies. For all open access content, the relevant licensing terms apply.

 **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 searchQuery builderResultsRetrosynthesisHistoryAlerts+ Reaxys AI SearchBeta

My Synthesis ProjectsDraw

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Parameters

Structure editor toolbar

O=C(O)N1CCCCC1Cc2ccc(Br)cc2CCc3ccccc3C

Retrosynthesis icons

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

Retrosynthesis analysis results

✓ 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

Edit

✓ 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)

Edit


ClearCancelSynthesize


進行分析


如何更精準地控制 AI 的合成規劃策略

The screenshot displays the Reaxys Retrosynthesis interface. At the top, the Reaxys logo is on the left, and navigation links for Quick search, Query builder, Results, Retrosynthesis, History, Alerts, and Reaxys AI Search are on the right. Below the navigation bar, a status bar indicates the selected structure editor (MarvinJS or ChemDrawJS) and a search input field labeled 'Insert structure from name'. The main workspace contains a chemical structure of a complex molecule with a cyclohexane ring, a carboxylic acid group, a brominated benzene ring, and a biphenyl system. On the left sidebar, the 'Draw' section is active, showing icons for 'smax' (highlighted with a yellow box), 'slock' (highlighted with a yellow box), and 'make/break' (highlighted with a yellow box). On the right sidebar, the 'Retrosynthesis' section is active, showing icons for 'R' (highlighted with a yellow box), 'A' (highlighted with a yellow box), and 'make/break' (highlighted with a yellow box). The bottom of the interface features a 'Clear' button, a 'Cancel' button, and a 'Synthesize' button.

 **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 ⓘ

General

Intermediates

Length of routes ⓘ

☒ Max. Number of steps: (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: (\$/g) ⓘ

Processing time ⓘ

☒ Standard

☐ Extended

Powered by

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 ⓘ

General

Intermediates

Enter intermediates ⓘ

Include substructures (up to 10)

+

Exclude substructures (up to 10)

+

Powered by

中間產物

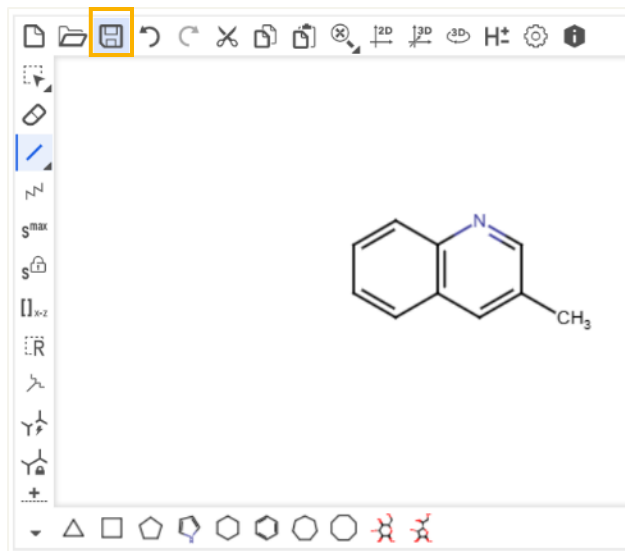
- Include substructures:** 可要求AI一定要採用某個化合物作為中間產物
- Exclude substructures*:** 可要求AI避免某個化合物作為中間產物
*(本功能需將結構預先轉換成 SMILES 格式，操作方法見下頁)

ELSEVIER

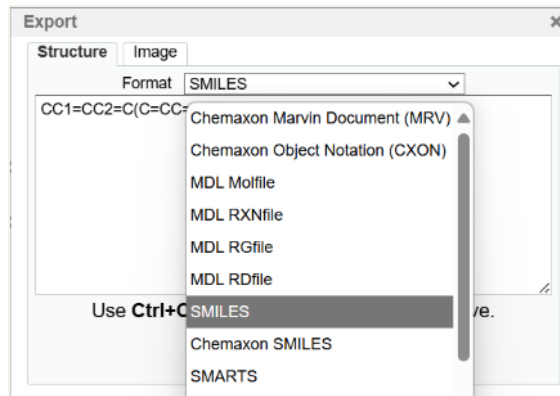
將中間產物結構轉為 SMILES 格式

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**  [Edit](#) 


☒ Published  

Length & depth of synthesis plans 

☒ Full routes: 


☐ Last step only

Branches per step: 

Max. number of steps: 

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

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

Cc1ccc2c(c1)c3c(c2)c4c(c3)c5c6c7c8c9c10c11c12c13c14c15c16c17c18c19c20c21c22c23c24c25c26c27c28c29c30c31c32c33c34c35c36c37c38c39c40c41c42c43c44c45c46c47c48c49c50c51c52c53c54c55c56c57c58c59c60c61c62c63c64c65c66c67c68c69c70c71c72c73c74c75c76c77c78c79c80c81c82c83c84c85c86c87c88c89c90c91c92c93c94c95c96c97c98c99c100c101c102c103c104c105c106c107c108c109c110c111c112c113c114c115c116c117c118c119c120c121c122c123c124c125c126c127c128c129c130c131c132c133c134c135c136c137c138c139c140c141c142c143c144c145c146c147c148c149c150c151c152c153c154c155c156c157c158c159c160c161c162c163c164c165c166c167c168c169c170c171c172c173c174c175c176c177c178c179c180c181c182c183c184c185c186c187c188c189c190c191c192c193c194c195c196c197c198c199c200c201c202c203c204c205c206c207c208c209c210c211c212c213c214c215c216c217c218c219c220c221c222c223c224c225c226c227c228c229c230c231c232c233c234c235c236c237c238c239c240c241c242c243c244c245c246c247c248c249c250c251c252c253c254c255c256c257c258c259c260c261c262c263c264c265c266c267c268c269c270c271c272c273c274c275c276c277c278c279c280c281c282c283c284c285c286c287c288c289c290c291c292c293c294c295c296c297c298c299c300c301c302c303c304c305c306c307c308c309c310c311c312c313c314c315c316c317c318c319c320c321c322c323c324c325c326c327c328c329c330c331c332c333c334c335c336c337c338c339c340c341c342c343c344c345c346c347c348c349c350c351c352c353c354c355c356c357c358c359c360c361c362c363c364c365c366c367c368c369c370c371c372c373c374c375c376c377c378c379c380c381c382c383c384c385c386c387c388c389c390c391c392c393c394c395c396c397c398c399c400c401c402c403c404c405c406c407c408c409c410c411c412c413c414c415c416c417c418c419c420c421c422c423c424c425c426c427c428c429c430c431c432c433c434c435c436c437c438c439c440c441c442c443c444c445c446c447c448c449c450c451c452c453c454c455c456c457c458c459c460c461c462c463c464c465c466c467c468c469c470c471c472c473c474c475c476c477c478c479c480c481c482c483c484c485c486c487c488c489c490c491c492c493c494c495c496c497c498c499c500c501c502c503c504c505c506c507c508c509c510c511c512c513c514c515c516c517c518c519c520c521c522c523c524c525c526c527c528c529c530c531c532c533c534c535c536c537c538c539c540c541c542c543c544c545c546c547c548c549c550c551c552c553c554c555c556c557c558c559c560c561c562c563c564c565c566c567c568c569c570c571c572c573c574c575c576c577c578c579c580c581c582c583c584c585c586c587c588c589c590c591c592c593c594c595c596c597c598c599c600c601c602c603c604c605c606c607c608c609c610c611c612c613c614c615c616c617c618c619c620c621c622c623c624c625c626c627c628c629c630c631c632c633c634c635c636c637c638c639c640c641c642c643c644c645c646c647c648c649c650c651c652c653c654c655c656c657c658c659c660c661c662c663c664c665c666c667c668c669c670c671c672c673c674c675c676c677c678c679c680c681c682c683c684c685c686c687c688c689c690c691c692c693c694c695c696c697c698c699c700c701c702c703c704c705c706c707c708c709c710c711c712c713c714c715c716c717c718c719c720c721c722c723c724c725c726c727c728c729c730c731c732c733c734c735c736c737c738c739c740c741c742c743c744c745c746c747c748c749c750c751c752c753c754c755c756c757c758c759c760c761c762c763c764c765c766c767c768c769c770c771c772c773c774c775c776c777c778c779c780c781c782c783c784c785c786c787c788c789c790c791c792c793c794c795c796c797c798c799c800c801c802c803c804c805c806c807c808c809c810c811c812c813c814c815c816c817c818c819c820c821c822c823c824c825c826c827c828c829c830c831c832c833c834c835c836c837c838c839c840c841c842c843c844c845c846c847c848c849c850c851c852c853c854c855c856c857c858c859c860c861c862c863c864c865c866c867c868c869c870c871c872c873c874c875c876c877c878c879c880c881c882c883c884c885c886c887c888c889c890c891c892c893c894c895c896c897c898c899c900c901c902c903c904c905c906c907c908c909c910c911c912c913c914c915c916c917c918c919c920c921c922c923c924c925c926c927c928c929c930c931c932c933c934c935c936c937c938c939c940c941c942c943c944c945c946c947c948c949c950c951c952c953c954c955c956c957c958c959c960c961c962c963c964c965c966c967c968c969c970c971c972c973c974c975c976c977c978c979c980c981c982c983c984c985c986c987c988c989c990c991c992c993c994c995c996c997c998c999 2-methyl-2-[4-(3-methy
C₃₀H₂₃N₅O 469.546 12

Identification
Druglikeness

Create synthesis Plan

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
<input type="checkbox"/> 2891288	29 May 2025	Project #2891288	 Edit	<div>Predicted In queue</div> <div>Published 2</div> <div>View </div>
<input type="checkbox"/> 2891279	29 May 2025	Project #2891279	 Edit	<div>Predicted In progress</div> <div>Published Click here for options</div> <div>View </div>

合成途徑開發的專案管理介面

The screenshot displays a web application for managing synthesis projects. On the left is a sidebar with 'My Synthesis Projects' and a 'Draw' button. The main area contains a table of projects. The first project, 'Project #2891288', has a chemical structure of a complex organic molecule. The second project, 'Project #2891279', has a chemical structure of a molecule with a carboxylic acid group. To the right of the table are two panels: 'Predicted parameters' and 'Published parameters'. The 'Predicted parameters' panel lists various metrics like '15 steps per route', 'Stereochemistry supported', and 'RCS: delivery time up to 10 days'. The 'Published parameters' panel lists similar metrics, including '10 full routes', '10 steps per route', and '20% yield per step'. At the bottom right, there is a 'View' button.

No.	Date	Project name		Predicted parameters	Published parameters	No. of routes
2891288	29 May 2025	Project #2891288		<ul style="list-style-type: none">15 steps per route (up to)Stereochemistry supportedRegioselectivity ignoredRCS: delivery time up to 10 daysRCS: no price limitStandard processing timeNo intermediates defined	<ul style="list-style-type: none">10 full routes (up to)10 steps per route (up to)5 branches per step (up to)Stop at commercial building blocks20% yield per step (assumed, if not published)	Predicted 11 Published 2 View
2891279	29 May 2025	Project #2891279		<ul style="list-style-type: none">15 steps per route (up to)Stereochemistry supportedRegioselectivity ignoredRCS: delivery time up to 10 daysRCS: no price limitStandard processing timeNo intermediates defined	<ul style="list-style-type: none">10 full routes (up to)10 steps per route (up to)5 branches per step (up to)Stop at commercial building blocks20% yield per step (assumed, if not published)	Predicted 25 Published 1 View

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

Project #2891280
0 selected
Limit to Delete

My Synthesis Projects
Draw

No Building blocks to target

1

2

3

4

5

Predicted Route #3

114 34

1 step

Preview

Score 1

Tree view >

Predicted Route #4

29 114 41

2 steps

Preview

Score 0.73

Tree view >

- 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

The screenshot displays the Reaxys software interface for analyzing synthetic routes. The main window shows a 'Predicted route #4' with a tree view of synthesis steps. Callout 1 points to the 'Export' button in the top left. Callout 2 points to the 'Copy route' button. Callout 3 points to the 'Step 1' tab. Callout 4 points to the 'Reaxys Examples' section showing reaction details for Reaction ID: 43268572. Callout 5 points to the 'Export' button. Callout 6 points to the 'Copy route' button.

Reaction Details (Reaction ID: 43268572):

Conditions	Yield	Reference
With potassium <i>tert</i> -butoxide in dichloromethane at 20°C; for 4h; Experimental Procedure	50%	Current Patent Assignee: SICHUAN UNIVERSITY - CN103254203, 2016, B Location in patent: Paragraph 0330; 0331; 0332; 0333 Full Text Details Abstract

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, contain

0 selected Limit To Exclude Export Preparations

1

CC(C)(C)C(=O)O[C@H]1C[C@@H](C[C@H]2[C@@H](C[C@H](C2)O)C[C@H](C1)O

simvasta
C₂₅H₃₈O₅

Identific
Druglike

80

Export substances Reaxys

Choose a format: PDF/Print

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

From 1 To 9

Export:

- ☒ All available data
- ☐ Identification data only
- ☐ Hit data only
- ☐ Choose specific 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

儲存搜尋結果

The screenshot shows the Reaxys interface with the 'History' tab selected. Under the 'Recent' sub-tab, two search results are listed:

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

An orange box highlights the 'Save' button (floppy disk icon) for the second search result, with an orange arrow pointing down to the 'Save substances' dialog box shown in the next block.

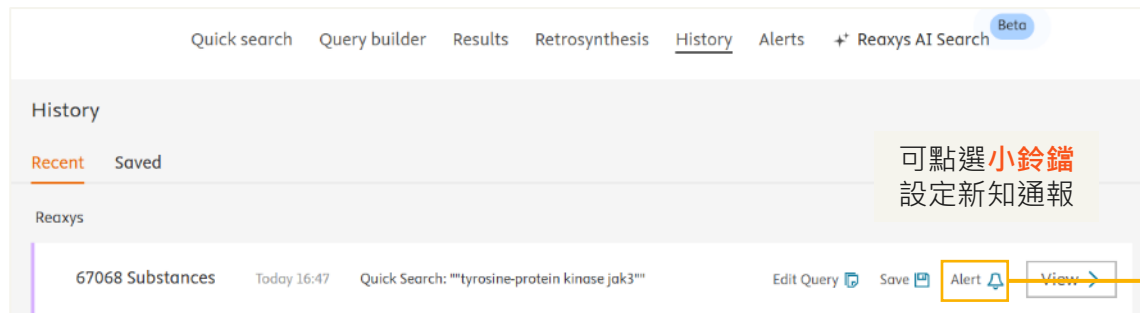
可於 **History** 頁面查看
搜尋紀錄並設定儲存

The 'Save substances' dialog box is shown, which is used to save search results. It contains a text input field for the 'Name of result set:' with a placeholder 'Enter a name'. At the bottom right, there are 'Cancel' and 'Save' buttons.

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



- 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信件，因此，不會傳遞更新的消息

Create Alert

Query: Quick Search: "simvastatin" AND

Alert name: Name alert1

Send alerts to: ssu1@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"

Results from:

No alert results

← Edit Delete

Query: Quick Search: ""simvastatin"" AND

Alert 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

編輯新知
通報設定

ELSEVIER

線上自我學習及 用戶資源

ELSEVIER

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。

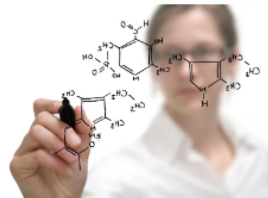


開始測驗

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。

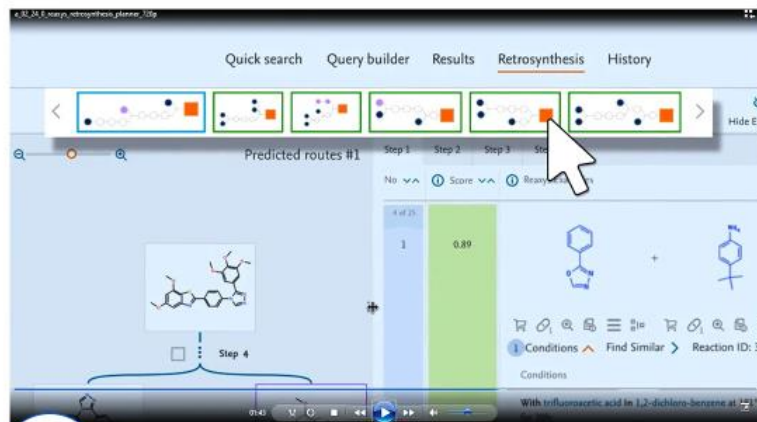


開始測驗

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

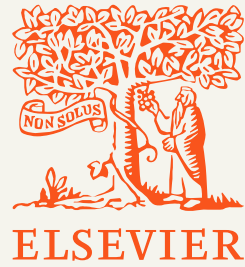
由於 RAE 允許使用者將自己的分子(目標分子)上傳進行 AI 預測，所得之 AI 預測結果(相應的合成計畫)會加密保存在使用者的 Reaxys 個人帳號內。是故能有更好的保護，同時避免非法授權者違法行為影響資料庫系統的穩定性，使用方式將採雙認證機制：

IP + 個人帳號登入 www.reaxys.com

個人帳號：

- 第一次使用者，請於單位IP範圍內，前往 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