



Reaxys Academic Edition

快速參考指南

May 2025



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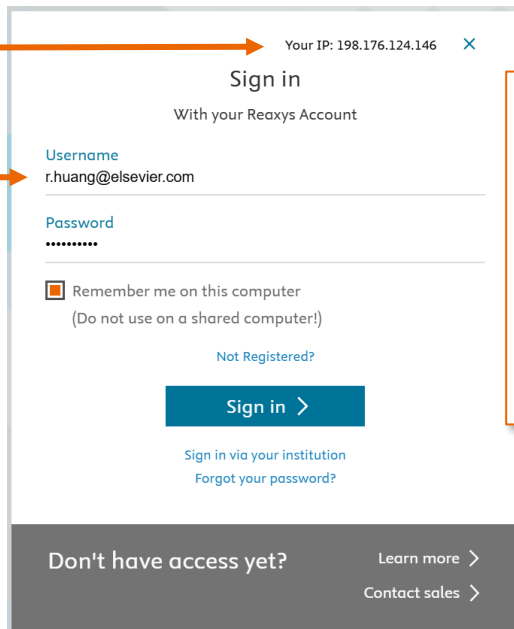
操作環境

Reaxys全國授權本連線說明

- 版本 Reaxys Academic Edition
- 連線網址：www.reaxys.com
- 登入帳號：自2025年七月起，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。

請確認位於校內網路範圍

請使用學校Email、目前
不支援免費信箱帳號。



The image shows the Reaxys sign-in page. At the top, it displays 'Your IP: 198.176.124.146' with a close button. Below this is the 'Sign in' heading, followed by 'With your Reaxys Account'. The form includes fields for 'Username' (with the example 'r.huang@elsevier.com') and 'Password' (masked with dots). There is a checkbox for 'Remember me on this computer' with a note '(Do not use on a shared computer!)'. Below the password field is a link for 'Not Registered?'. A large blue 'Sign in >' button is centered. At the bottom of the form, there are links for 'Sign in via your institution' and 'Forgot your password?'. A footer section 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首頁畫面

使用者偏好設置
與登出

常見問題、
技術訓練影片
、支援中心



- 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。

結構編輯器介面

可以從化合物的名稱中調出結構。

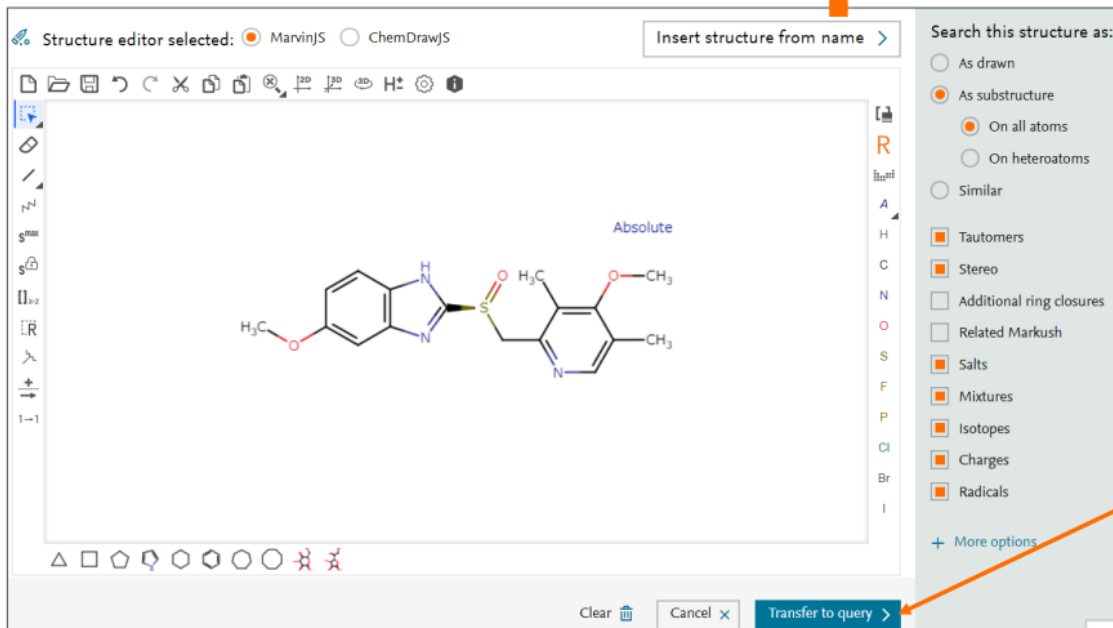
可以用“ctrl+alt+C”複製ChemDraw中繪製的結構黏貼到Marvin JS上。

Create structure template from name

is

Enter a chemical name, CAS-RN, InChIkey or SMILES





點擊「Transfer to query」，
進入搜索介面。

結構編輯器的搜尋選項

搜索選項

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

① 結構搜索選項

- 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 : 只在雜原子上進行結構搜索
- Similar : 類似的化合物與反應

② 其他搜索選項

- 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

Quick Search 搜尋預覽介面

Search for Preparation of Vitamin D3

Search Reaxys

Preparation of Vitamin D3 ✕ Find >

AND

 Draw



重新或編輯目前的搜索



快速搜尋會分析輸入的關鍵
字，提供物質、反應式、文
件或商業物質的選項。

Results for Preparation of Vitamin D3					New 	Edit 
	179	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results >	
	66,068	Documents	Structure :  as drawn Titles, Abstracts, Keywords : "Preparation", "Vitamin D3" Edit in Query Builder  Create Alert 	Preview Results 	View Results >	
	236,949	Documents	Structure :  as drawn Titles, Abstracts, Keywords : "Vitamin D3" Edit in Query Builder  Create Alert 	Preview Results 	View Results >	

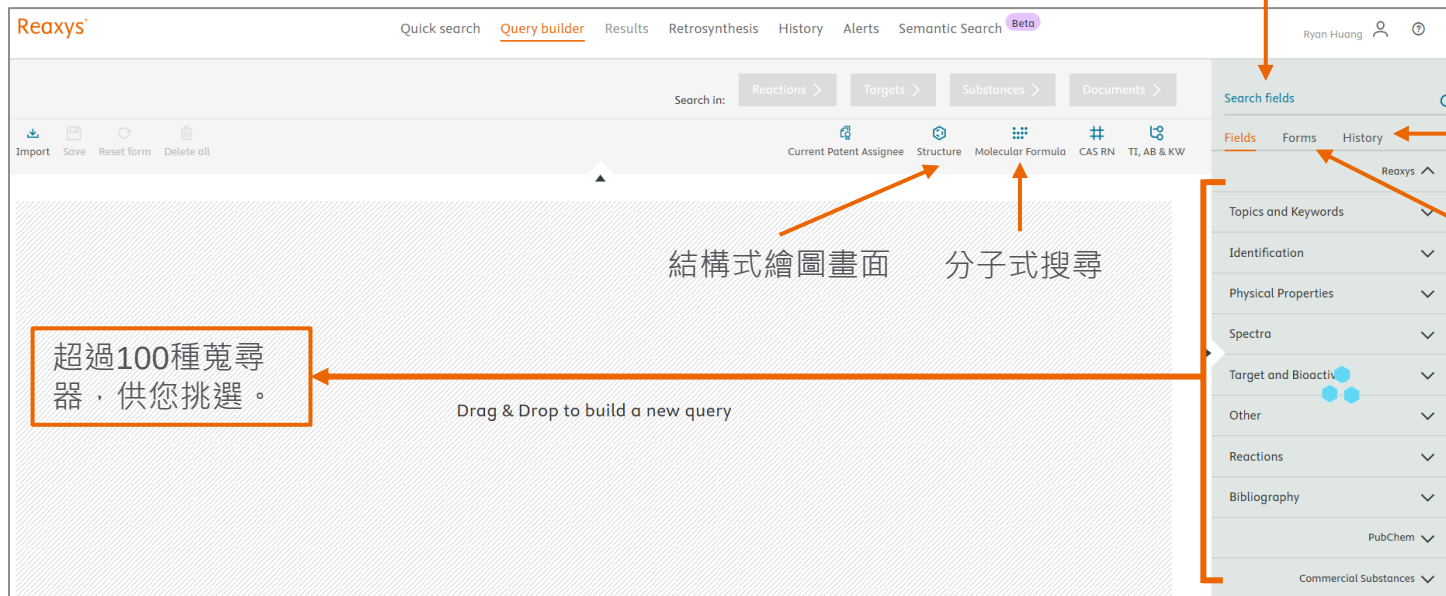
View Result
進入搜尋結
果介面



Query Builder①

靈活組合>100種蒐尋器組成檢索公式以減少雜訊

輸入關鍵字以查找特定搜索器。
例如：輸入“*Boil*”來尋找“*boiling point*”搜索器。



Reaxys® Quick search Query builder Results Retrosynthesis History Alerts Semantic Search Beta Ryan Huang

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

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

Drag & Drop to build a new query

Search fields

Fields Forms History

Topics and Keywords

Identification

Physical Properties

Spectra

Target and Bioactive

Other

Reactions

Bibliography

PubChem

Commercial Substances

超過100種蒐尋器，供您挑選。

結構式繪圖畫面

分子式搜尋

搜索歷史也可用於建構檢索公式。

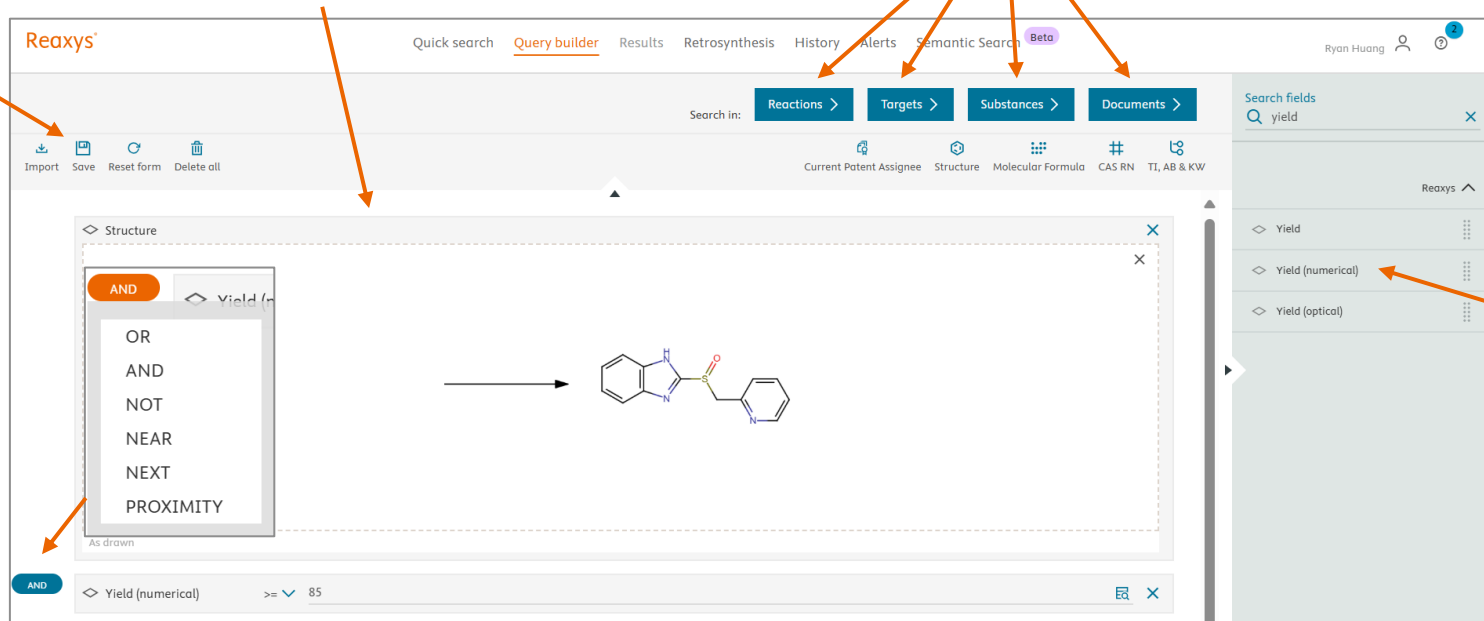
調用你自己創造的檢索公式或嘗試我們為您建立的公式範本。

Query Builder②

選擇反應式、蛋白靶點、物質或文獻搜索。

你所選擇的搜索器會被顯示出來。

你可以保存你所創建的檢索公式。



Reaxys

Quick search Query builder Results Retrosynthesis History Alerts Semantic Search Beta

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

Import Save Reset form Delete all

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

Structure

AND

OR

AND

NOT

NEAR

NEXT

PROXIMITY

As drawn

AND

Yield (numerical) >= 85

Search fields

Q yield

Reaxys

Yield

Yield (numerical)

Yield (optical)

點擊來調用一個項目。

- OR : 或
- AND : 和
- NOT : 不包括
- NEAR : 雙方必須靠近對方
- NEXT : 雙方必須靠近並保留前後順序
- PROXIMITY : 兩個靠近的資料格

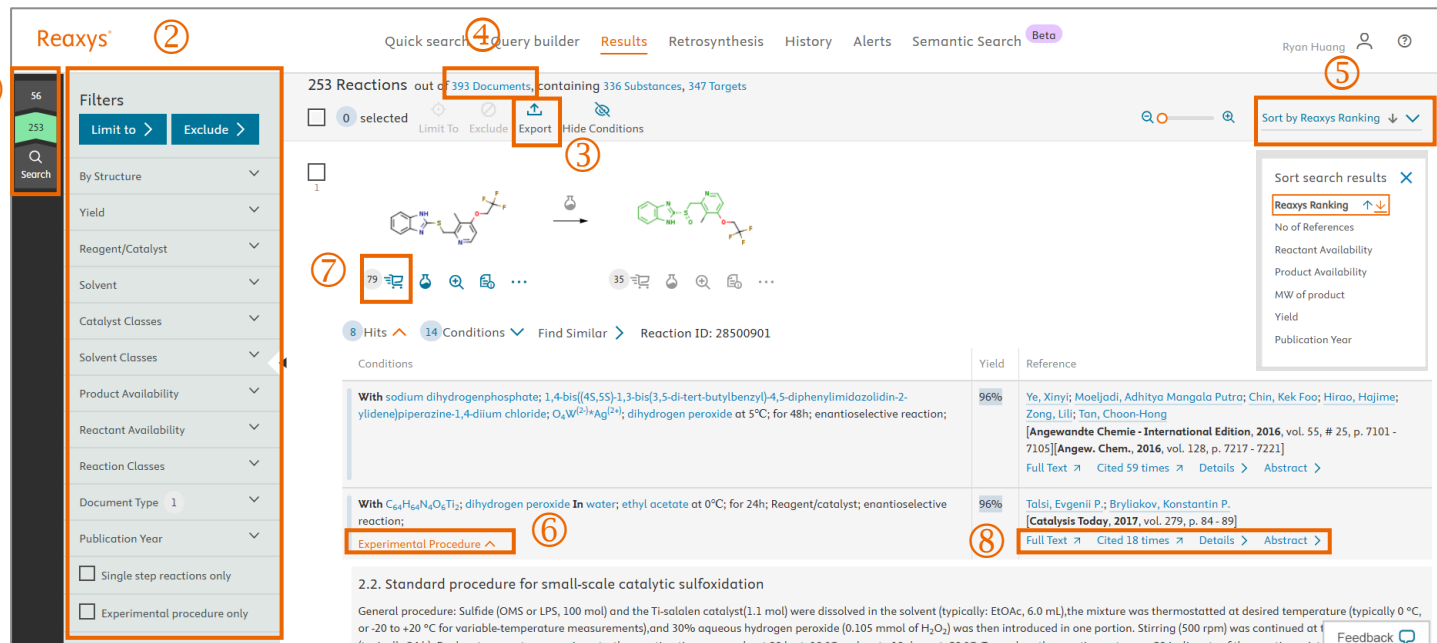
反應式搜尋結果介面

Reaxys Ranking:

預設依實用性順序推薦，可調整依年份或產量排序。

< 項目 >

- ① 瀏覽搜索結果的軌跡
- ② 過濾功能
- ③ 匯出按鈕 (參考 P.22)
- ④ 反應數據的來源文獻
- ⑤ 搜索結果的排序推薦
- ⑥ 詳細實驗步驟
- ⑦ 商業試劑資訊
- ⑧ 文獻出處、引用強度、原文連結



The screenshot displays the Reaxys search results page. The interface includes a sidebar with filters (1), a top navigation bar with search and query builder options (2), and a main results area. The results area shows a chemical reaction scheme (3) and a table of search results. The table columns are Conditions, Yield, and Reference. The first result is for a reaction with sodium dihydrogenphosphate and 1,4-bis((4S,5S)-1,3-bis(3,5-di-tert-butylbenzyl)-4,5-diphenylimidazolidin-2-ylidene)piperazine-1,4-dilium chloride, yielding 96% (4). The second result is for a reaction with C₆₄H₆₄N₄O₆Ti₂ and dihydrogen peroxide in water, yielding 96% (5). The table also includes links for Full Text, Cited, Details, and Abstract (6). A sidebar on the right allows sorting search results by Reaxys Ranking, No of References, Reactant Availability, Product Availability, MW of product, Yield, and Publication Year (7). The bottom section provides a detailed experimental procedure for small-scale catalytic sulfoxidation (8).

Conditions	Yield	Reference
With sodium dihydrogenphosphate; 1,4-bis((4S,5S)-1,3-bis(3,5-di-tert-butylbenzyl)-4,5-diphenylimidazolidin-2-ylidene)piperazine-1,4-dilium chloride; O ₄ W ⁽²⁺⁾ Ag ⁽²⁺⁾ ; dihydrogen peroxide at 5°C; for 48h; enantioselective reaction;	96%	Ye, Xinyi; Moeljadi, Adhitya Mangala Putra; Chin, Kek Foo; Hirao, Hajime; Zong, Lili; Tan, Choon-Hang [Angewandte Chemie - International Edition, 2016, vol. 55, # 25, p. 7101 - 7105][Angew. Chem., 2016, vol. 128, p. 7217 - 7221] Full Text ↗ Cited 59 times ↗ Details > Abstract >
With C ₆₄ H ₆₄ N ₄ O ₆ Ti ₂ ; dihydrogen peroxide In water; ethyl acetate at 0°C; for 24h; Reagent/catalyst; enantioselective reaction;	96%	Talsi, Evgenii P.; Bryliakov, Konstantin P. [Catalysis Today, 2017, vol. 279, p. 84 - 89] Full Text ↗ Cited 18 times ↗ Details > Abstract >

2.2. Standard procedure for small-scale catalytic sulfoxidation
General procedure: Sulfide (OMS or LPS, 100 mol) and the Ti-salalen catalyst (1.1 mol) were dissolved in the solvent (typically: EtOAc, 6.0 mL), the mixture was thermostatted at desired temperature (typically 0 °C, or -20 to +20 °C for variable-temperature measurements), and 30% aqueous hydrogen peroxide (0.105 mmol of H₂O₂) was then introduced in one portion. Stirring (500 rpm) was continued at

反應式搜尋結果篩選工具

Filters

Limit to >
Exclude >

By Structure ▾
Yield ▾
Reagent/Catalyst ▾
Solvent ▾
Catalyst Classes ▾
Solvent Classes ▾
Product Availability ▾
Reactant Availability ▾
Reaction Classes ▾
Document Type ▾
Publication Year ▾
☐ Single step reactions only
☐ Experimental procedure only

例如：溶劑的過濾

Solvent

☐ water 131
☐ dichloromethane 61
☐ ethanol 59
☐ methanol 54
☐ toluene 43
☐ isopropyl alcohol 34
☐ acetonitrile 28

Filter by value ▾
[View more](#)

- ← 結構
- ← 產率
- ← 試劑、催化劑
- ← 溶劑
- ← 催化劑類別
- ← 溶劑類別
- ← 產物的可能性
- ← 反應物的可能性
- ← 反應類別
- ← 來源的種類(文獻、專利)
- ← 出版年份
- ← 縮小到只有一步反應
- ← 縮小到只包含實驗性術語的名單

- 每個專案的細目可以通過點擊打開。
- 這些專案按照案件數量的順序進行排序。
- 可以通過輸入數位或單詞來過濾專案。

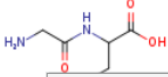
Solvent 2
Clear selected ✕
Sort by Occurrence ▾
✕

☐ water 131
☐ dichloromethane 61
☒ ethanol 59
☒ methanol 54
☐ toluene 43
☐ isopropyl alcohol 34
☐ acetonitrile 28
☐ ethyl acetate 24
☐ acetone 24
☐ tetrahydrofuran 22
☐ tert-butyl methyl ether 11

1 2 >

Limit to >
Exclude >

商業試劑目錄資訊



DL-glycylnorvaline
 $C_7H_{14}N_2O_3$ 174.2 17255

Shipping time: **Up to 5 days**
Best price: **14 USD/g**
Largest available package size: **Greater than 10 kg**

65    

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。

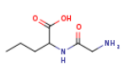
Reaxys - 1 **Commercial Substances - 1** PubChem - 1

1 Substances

☐ 0 selected Limit To Exclude Export

Sort by Commercial Substance ID  

  Grid 



2-(2-aminoacetamido)pentanoic acid
 $C_7H_{14}N_2O_3$ 174.2 66983 2189-27-7

Identification

Commercial Suppliers - 65

Shipping time: Up to 5 days
Best price: 14 USD/g
Largest available package size: Greater than 10 kg

2-(2-aminoacetamido)pentanoic acid 

 Identification

 **Commercial Suppliers - 65**

Commercial Suppliers	Product	Purity	Package size & price	Availability
Envigen Pharmaceuticals Inc.  USA	GLYCYL-DL-NORVALINE 2189-27-7 ENV56889	97%	1 g 87 USD	Stock availability: In stock Last updated: 2025-03-10

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

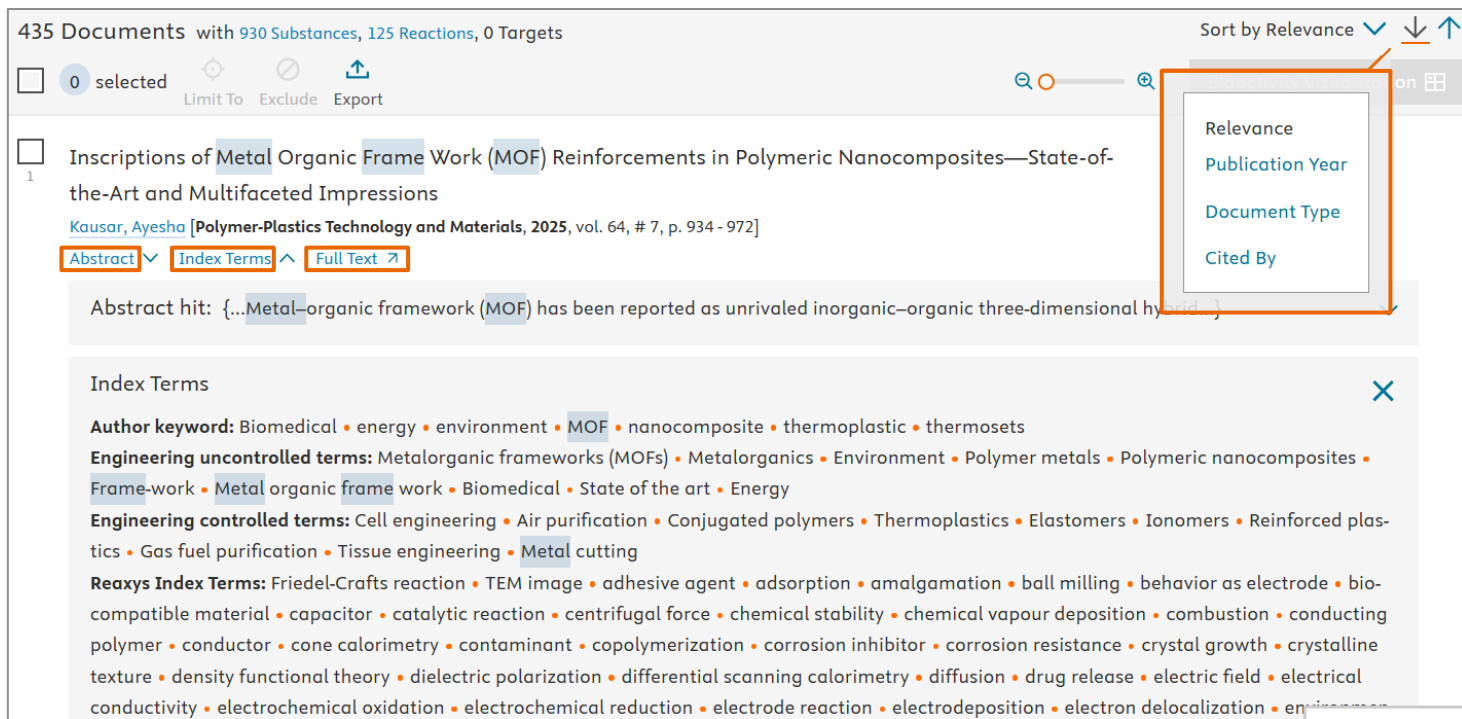
文獻搜尋結果介面

Full Text：移動到期刊的文章頁面。

Cited X times：來自 Scopus 的引用數量(點擊查看 引用該文章的參考文獻列表)。

Index Term：文章的索引詞。

Abstract：查看文章的摘要。



435 Documents with 930 Substances, 125 Reactions, 0 Targets

Sort by Relevance

0 selected Limit To Exclude Export

1 Inscriptions of Metal Organic Frame Work (MOF) Reinforcements in Polymeric Nanocomposites—State-of-the-Art and Multifaceted Impressions

Kausar, Ayesha [Polymer-Plastics Technology and Materials, 2025, vol. 64, # 7, p. 934 - 972]

Abstract Index Terms Full Text

Abstract hit: {...Metal-organic framework (MOF) has been reported as unrivaled inorganic-organic three-dimensional hybrid }

Index Terms

Author keyword: Biomedical • energy • environment • MOF • nanocomposite • thermoplastic • thermosets

Engineering uncontrolled terms: Metalorganic frameworks (MOFs) • Metalorganics • Environment • Polymer metals • Polymeric nanocomposites • Frame-work • Metal organic frame work • Biomedical • State of the art • Energy

Engineering controlled terms: Cell engineering • Air purification • Conjugated polymers • Thermoplastics • Elastomers • Ionomers • Reinforced plastics • Gas fuel purification • Tissue engineering • Metal cutting

Reaxys Index Terms: Friedel-Crafts reaction • TEM image • adhesive agent • adsorption • amalgamation • ball milling • behavior as electrode • bio-compatible material • capacitor • catalytic reaction • centrifugal force • chemical stability • chemical vapour deposition • combustion • conducting polymer • conductor • cone calorimetry • contaminant • copolymerization • corrosion inhibitor • corrosion resistance • crystal growth • crystalline texture • density functional theory • dielectric polarization • differential scanning calorimetry • diffusion • drug release • electric field • electrical conductivity • electrochemical oxidation • electrochemical reduction • electrode reaction • electrodeposition • electron delocalization • en

文獻搜尋結果篩選工具

Publication Year	✓	← 出版年份
Document Type	✓	← 文獻類型
Authors of Scientific Documents	✓	← 文獻作者
Current Affiliation	✓	← 目前隸屬機構
Inventors of Patents	✓	← 專利發明者
Current Patent Assignee	✓	← 目前專利授予者
Patent Office	✓	← 專利辦公室
Journal Title	✓	← 期刊名稱
Substance Classes	✓	← 化合物種類
Reaction Classes	✓	← 反應式種類

Index Terms (List)	✓	← 文獻索引詞統計清單
Index Terms (ReaxysTree)	✓	← 索引詞化學分類

↓

Index Terms (ReaxysTree)

- ☐ physico chemical properties 330
- ☐ physico chemical analysis methods 307
- ☐ chemical transformations 284
- ☐ quantum chemical calculation methods 42

[View more](#)

Index Terms (ReaxysTree) 23

- Index Terms (ReaxysTree) 392
 - physico chemical properties 330
 - physico chemical analysis methods 307**
 - spectroscopic analysis 232
 - separation method 204
 - sample preparation method 97
 - substance clean up 87
 - crystallization 60
 - chromatography 35
 - liquid chromatography 23**
 - column chromatography 4
 - electrophoresis 4
 - gas chromatography 11

Selected search items:

liquid chromatogr...

Clear selected X

Limit to > Exclude >

用常見的化學概念來整理索引詞
 以「層析」chromatography的文獻為例：點擊View more >physical chemical analysis methods >separation method >substance clean up >chromatography >liquid chromatography

Retrosynthesis探索合成途徑①

~如何繪製目標化合物的結構並進行合成分析~

需登入個人帳號以開啟
AI Predicted選項

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。

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



Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

Insert structure from name >

Parameters

Predicted

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

Published

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

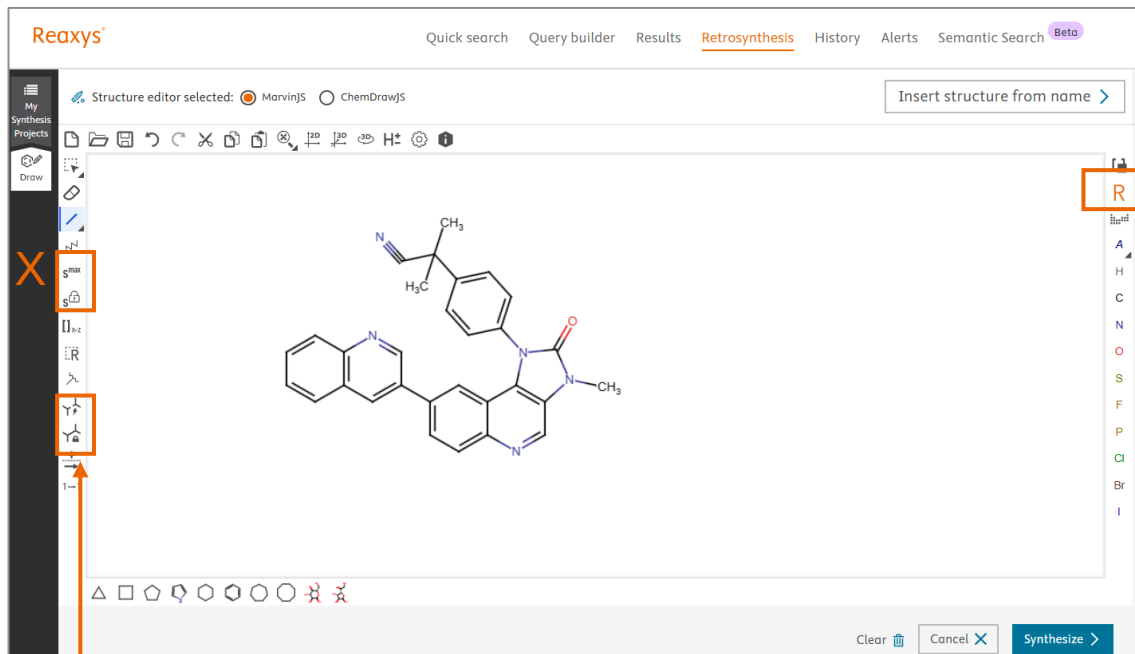
Clear Cancel Synthesize >

繪製Retrosynthesis的目標化合物「無須」添加反應式箭頭

進行分析

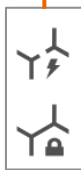
Retrosynthesis探索合成途徑②

~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A kyl 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探索合成途徑③

~如何調整逆合成分析參數Published~

☒ Published ⓘ ⬆

Length & depth of synthesis plans ⓘ

☒ Full routes: 10 ▼

☐ Last step only

Branches per step: 5 ▼

Max. number of steps: 10 ▼

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

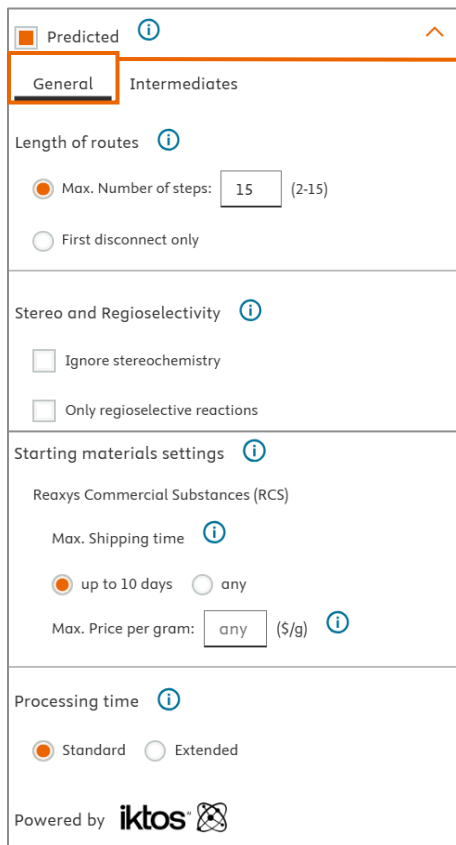
Assumed yield for reactions without a given yield

0%100%

- 生成的路線的最大數目
- 線上的最大分支數量
- 最大的步驟數
- 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)
- 設定各反應的允許產量

Retrosynthesis探索合成途徑④

~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) ⓘ

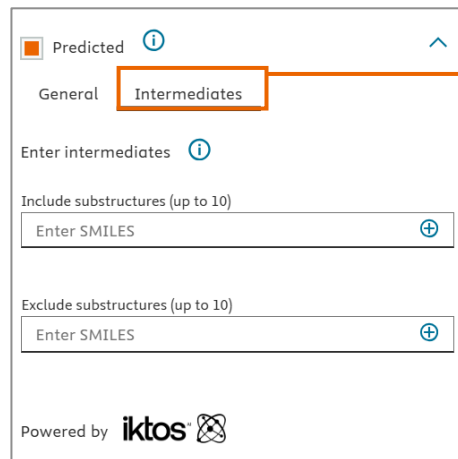
Processing time ⓘ

☒ Standard ☐ Extended

Powered by **iktos** 

基本設定

- 生成的路最大的步驟數
- 忽視立體化學選擇性
- 考慮立體化學選擇性
- 合成材料僅使用有庫存材料
- 合成材料價格上限
- 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 **iktos** 

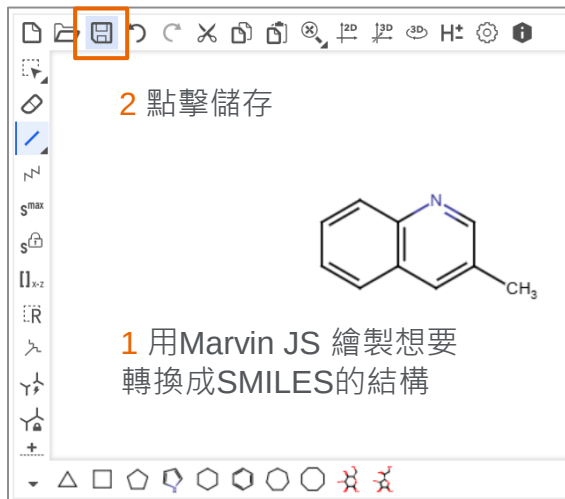
中間產物

- 可要求AI一定要採用某個化合物作為中間產物
- 可要求AI避免某個化合物作為中間產物

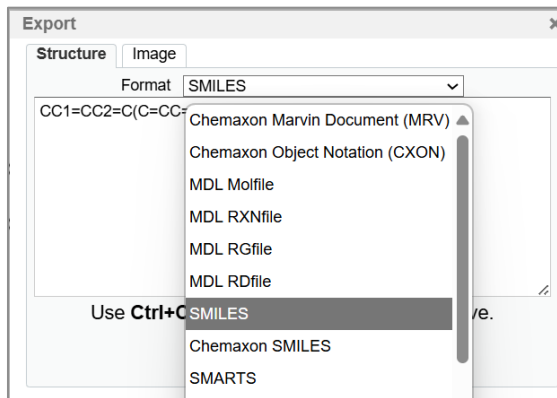
本功能需將結構預先轉換成SMILES格式，操作方法見下頁。

Retrosynthesis探索合成途徑⑤

~將中間產物結構轉為SMILES格式~



3 選擇SMILES格式



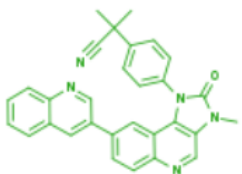
4 呈現的字串為SMILES格式，可反白複製



| | |
|--------|--------|
| 😊 表情圖示 | Win+句號 |
| 🗣 語音輸入 | Win+H |
| ✂ 剪下 | Ctrl+X |
| 📄 複製 | Ctrl+C |
| 📄 貼上 | Ctrl+V |

Retrosynthesis探索合成途徑⑥

~如何分析化合物搜尋結果中感興趣化合物的合成途徑~



2-methyl-2-[4-(3-me
C₃₀H₂₃N₅O 469.546

Identification
Druglikeness

Create synthesis Plan

81 

Synthesize

> Find preparations

> Create retrosynthesis plans

自動將您查到的化合物代入Retrosynthesis面板

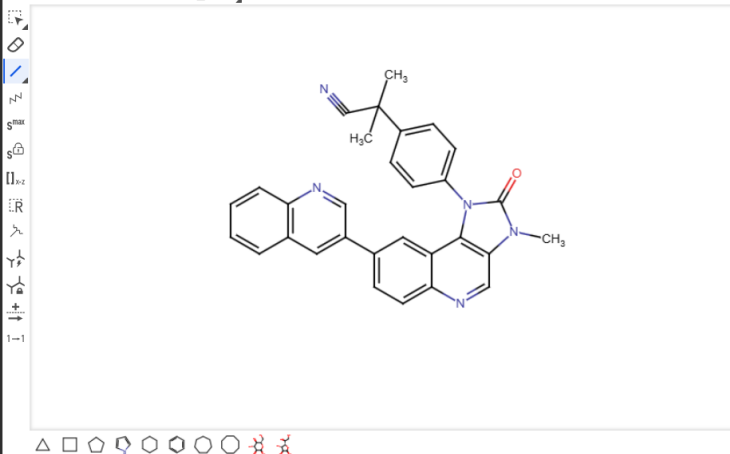
Reaxys®

Quick search Query builder Results Retrosynthesis

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

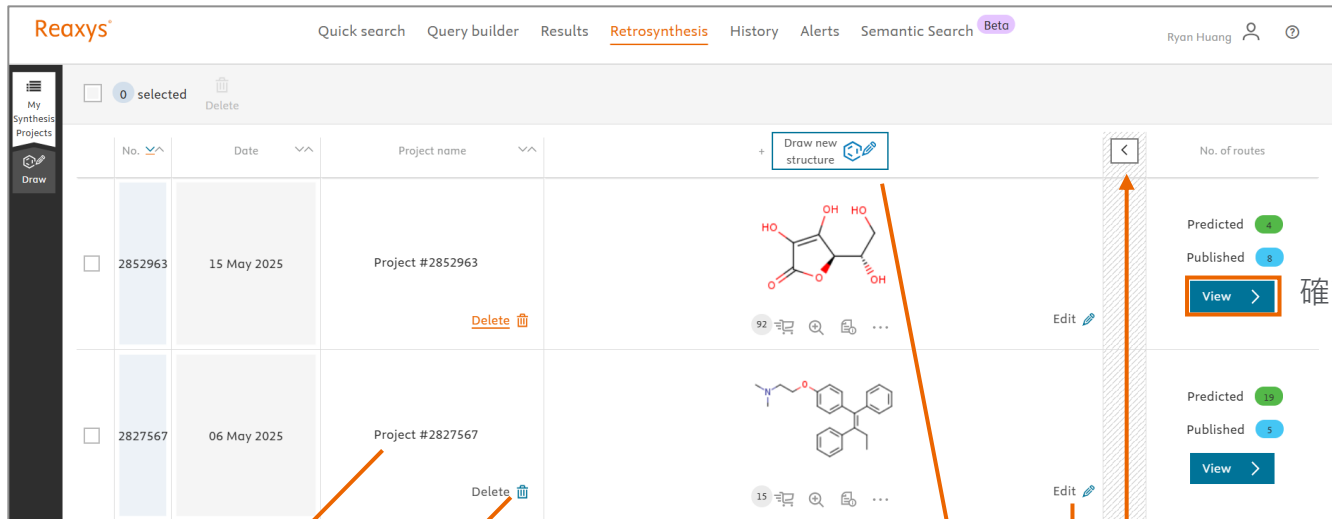
My Synthesis Projects

Draw



Retrosynthesis探索合成途徑⑦

~ 合成途徑開發的專案管理介面 ~



The screenshot shows the Reaxys Retrosynthesis interface. At the top, there's a navigation bar with 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted), 'History', 'Alerts', and 'Semantic Search Beta'. The user 'Ryan Huang' is logged in. On the left, a sidebar shows 'My Synthesis Projects' and a 'Draw' button. The main area displays a table of projects:

| No. | Date | Project name | No. of routes |
|---------|-------------|------------------|--|
| 2852963 | 15 May 2025 | Project #2852963 | Predicted 4
Published 8
View > |
| 2827567 | 06 May 2025 | Project #2827567 | Predicted 19
Published 5
View > |

Each project row includes a checkbox, a 'Delete' button, and a chemical structure. The first structure is a complex molecule with multiple hydroxyl groups. The second structure is a substituted benzene ring. Arrows point from the project names to the text '點擊重新命名' (Click to rename), from the 'Delete' buttons to '刪除' (Delete), and from the chemical structures to '創建並分析一個新的結構' (Create and analyze a new structure). A 'View >' button is highlighted with a red box and labeled '確認路徑' (Confirm path).

點擊重新命名

刪除

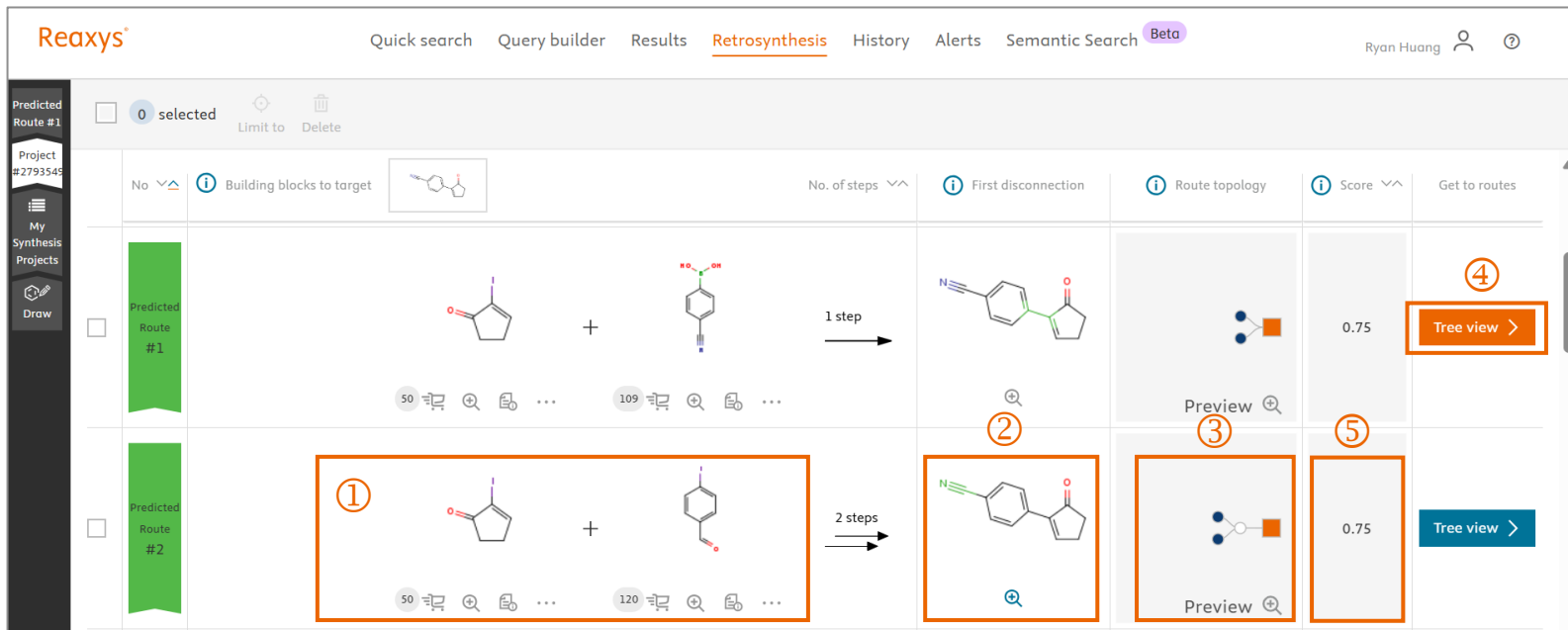
創建並分析一個新的結構

調整參數並重新分析
或適度修改目標分子

| Predicted parameters | | Published parameters | |
|---|--|---|--|
| <div>Close parameters</div> | | | |
| 15 steps per route (up to) | | 10 full routes (up to) | |
| Stereochemistry supported | | 10 steps per route (up to) | |
| Regioselectivity ignored | | 5 branches per step (up to) | |
| RCS: delivery time up to 10 days | | Stop at commercial building blocks | |
| RCS: no price limit | | 20% yield per step (assumed, if not published) | |
| Standard processing time | | | |
| No intermediates defined | | | |

Retrosynthesis探索合成途徑⑧

~ 生成的合成路線的清單界面 ~

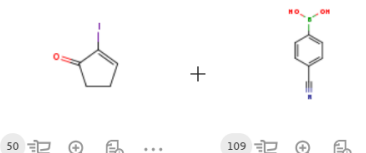
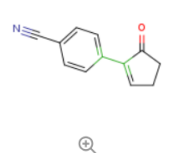
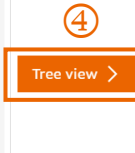
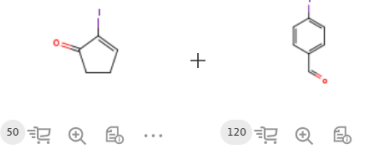
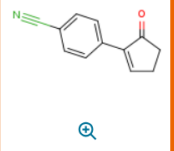
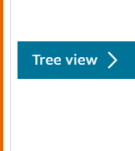


Reaxys[®] Quick search Query builder Results Retrosynthesis History Alerts Semantic Search Beta Ryan Huang

Predicted Route #1 0 selected Limit to Delete

Project #2793549

My Synthesis Projects Draw

| No | Building blocks to target | No. of steps | First disconnection | Route topology | Score | Get to routes |
|--------------------|---|--------------|---|---|-------|---|
| Predicted Route #1 |  | 1 step |  |  | 0.75 |  |
| Predicted Route #2 |  | 2 steps |  |  | 0.75 |  |

① 該合成路徑需要的起始原料與材料金額

② 第一個斷鍵位置

③ 路徑長度與分支呈現，方便比較。

④ 詳細路徑以樹狀路徑呈現

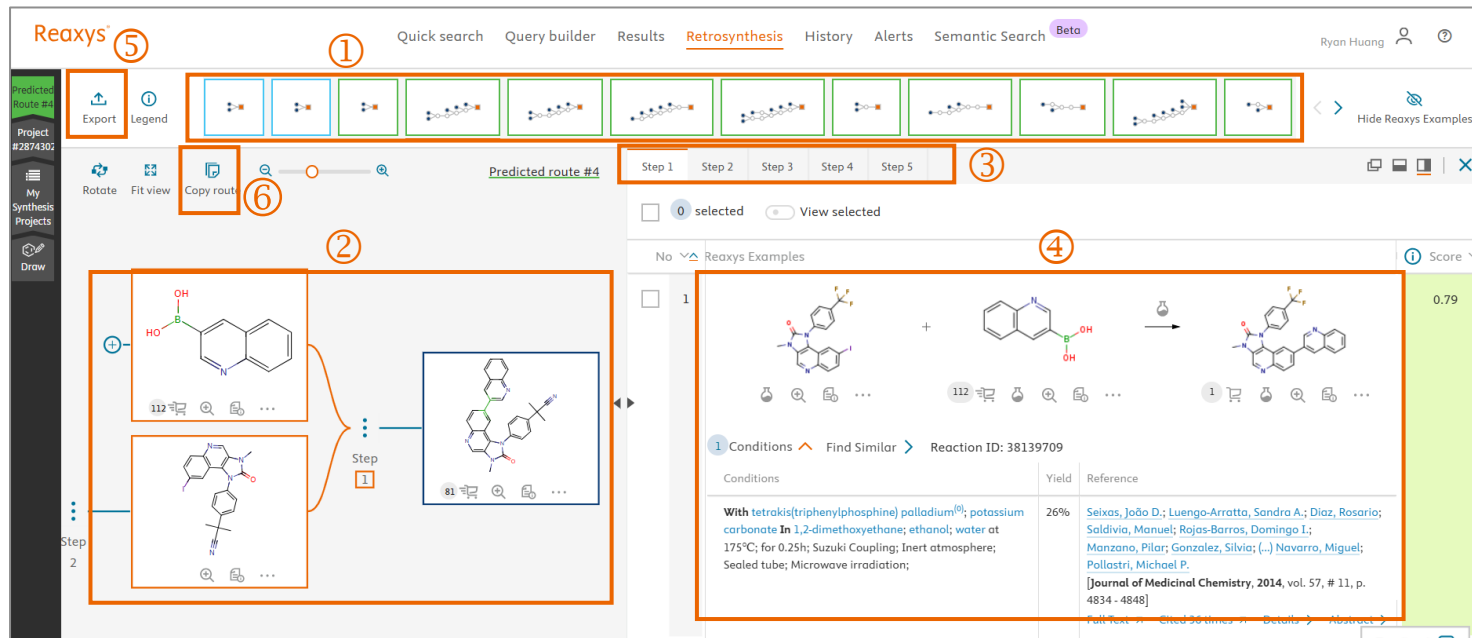
⑤ Confidence Score：評估該預測路徑的信賴度，從1分至0分。(1分很有可能，0分非常不可能)

Retrosynthesis探索合成途徑⑨

~ 合成途徑的樹狀圖畫面 ~

< 項目 >

- 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



The screenshot displays the Reaxys Retrosynthesis interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted), 'History', 'Alerts', 'Semantic Search', and 'Beta'. The user 'Ryan Huang' is logged in. The interface is divided into several sections:

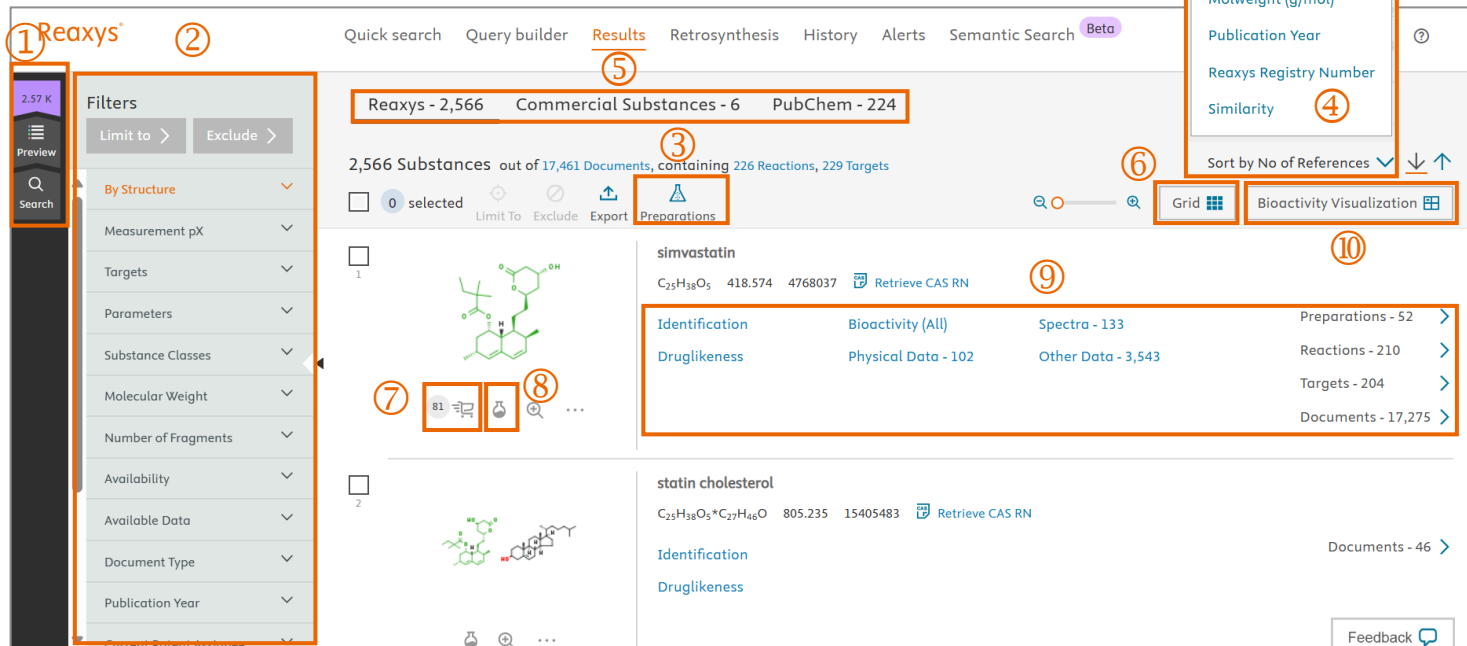
- Left Sidebar:** Contains 'Predicted Route #4', 'Project #2874302', 'My Synthesis Projects', and 'Draw'.
- Top Bar:** Includes 'Export' (⑤), 'Legend', and a series of icons for navigating between different predicted routes (①).
- Central Panel:** Shows 'Predicted route #4' with a tree diagram of synthesis steps. Step 1 is highlighted with an orange box (②). A 'Copy route' button (⑥) is located above the diagram.
- Right Panel:** Displays 'Step 1' details, including a chemical reaction scheme (④) and a table of conditions, yield, and references.

| Conditions | Yield | Reference |
|---|-------|---|
| With tetrakis(triphenylphosphine) palladium ⁰ ; potassium carbonate in 1,2-dimethoxyethane; ethanol; water at 175°C; for 0.25h; Suzuki Coupling; Inert atmosphere; Sealed tube; Microwave irradiation; | 26% | Seixas, João D.; Luengo-Arratta, Sandra A.; Diaz, Rosario; Saldivia, Manuel; Rojas-Barros, Domingo I.; Manzano, Pilar; Gonzalez, Silvia; (-) Navarro, Miguel; Pollostri, Michael P. [Journal of Medicinal Chemistry, 2014, vol. 57, # 11, p. 4834 - 4848] |

化合物檢索結果畫面

< 項目 >

- ① 瀏覽搜索結果的軌跡
- ② 過濾功能
- ③ 顯示化合物製備方法
- ④ 搜索結果的排序功能
- ⑤ 切換數據庫
- ⑥ 切換到網格顯示
- ⑦ 商業試劑資訊
- ⑧ 化合物的合成規劃
- ⑨ 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
- ⑩ 生物活性熱圖分析



The screenshot displays the Reaxys search results page. The interface includes a top navigation bar with tabs for Quick search, Query builder, Results (selected), Retrosynthesis, History, Alerts, and Semantic Search. A search bar at the top shows results for Reaxys (2,566), Commercial Substances (6), and PubChem (224). The main content area lists 2,566 substances, with a summary of 226 reactions and 229 targets. A left sidebar contains a 'Filters' section with various criteria like Structure, Measurement pX, Targets, Parameters, Substance Classes, Molecular Weight, Number of Fragments, Availability, Available Data, Document Type, and Publication Year. A right sidebar shows a 'Sort by' dropdown set to 'No of References' and a 'Grid' button. The main results list shows two entries: simvastatin and statin cholesterol, each with a chemical structure, molecular formula, and various data links. A 'Preparations' tab is highlighted for simvastatin, showing a table of data including Identification, Bioactivity (All), Spectra (133), Preparations (52), Reactions (210), Targets (204), and Documents (17,275). A 'Feedback' button is located at the bottom right.

① Reaxys

② Filters

③ Results

④ Sort by No of References

⑤ Reaxys - 2,566 Commercial Substances - 6 PubChem - 224

⑥ Grid

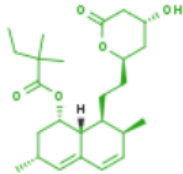
⑦ 81

⑧

⑨

⑩

詳細的化合物數據



81    ...

simvastatin

C₂₅H₃₈O₅ 418.574 4768037  79902-63-9

Identification Bioactivity (All) Spectra - 133

Druglikeness Physical Data - 102 Other Data - 3,543

④ Preparations - 52 >

⑤ Reactions - 210 >

⑥ Targets - 204 >

⑦ Documents - 17,275 >

^ Bioactivity (All)

- ✓ In vitro: Efficacy - 3692
- ✓ In vivo: Animal Model - 2145
- ✓ Metabolism - 547
- ✓ Pharmacokinetic - 2767
- ✓ Toxicity/Safety Pharmacology - 1305

^ Physical Data - 102

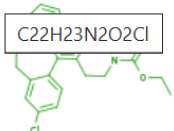
- ✓ Melting Point - 15
- ✓ Density - 5
- ✓ Association (MCS) - 10
- ✓ Chromatographic Data - 12
- ✓ Circular Dichroism - 1

^ Spectra - 133

- ✓ NMR Spectroscopy - 61
- ✓ IR Spectroscopy - 18
- ✓ Mass Spectrometry - 28
- ✓ UV/VIS Spectroscopy - 21
- ✓ Raman Spectroscopy - 3

- ④ 製備反應(作為產物)
- ⑤ 包含此化合物的所有反應
- ⑥ 與此化合物有活性證據的靶點蛋白
- ⑦ 參考文獻

生物活性數據介面



C22H23N2O2Cl

loratadine

C22H23N2O2Cl 382.89 4273483 79794-75-5

Identification
Bioactivity (All)

Druglikeness
Physical Data - 66

更多的參數預設隱藏，手動開啟。

Bioactivity (All)

In vitro: Efficacy - 619

Quantitative Results

| pX | Parameter | Value (qual) | Value (quant) | Unit | Biological Species | Action on target | Target | Tissue/Organ | Cell | Dose | Effect | Concomitants | 1. |
|------|-----------|--------------|---------------|------|--------------------|------------------|------------------------------------|--------------|----------------|-----------------|----------------------|------------------------------|----|
| 8.52 | IC50 | | 3 - 1 | nM | | Inhibitor | Aldehyde oxidase:Wild | | | | | | |
| 8.27 | IC50 | | 5.4 | nM | | Antagonist | Histamine H1 receptor [human]:Wild | | HeLa cell line | 0.01 - 10000 nM | antihistaminic agent | Stimulating agent: histamine | |

Show/Hide columns

pX值。
數字越大
活性越高

實驗數值

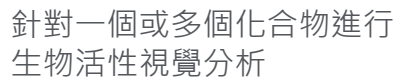
作用
機制

活性
蛋白
靶點

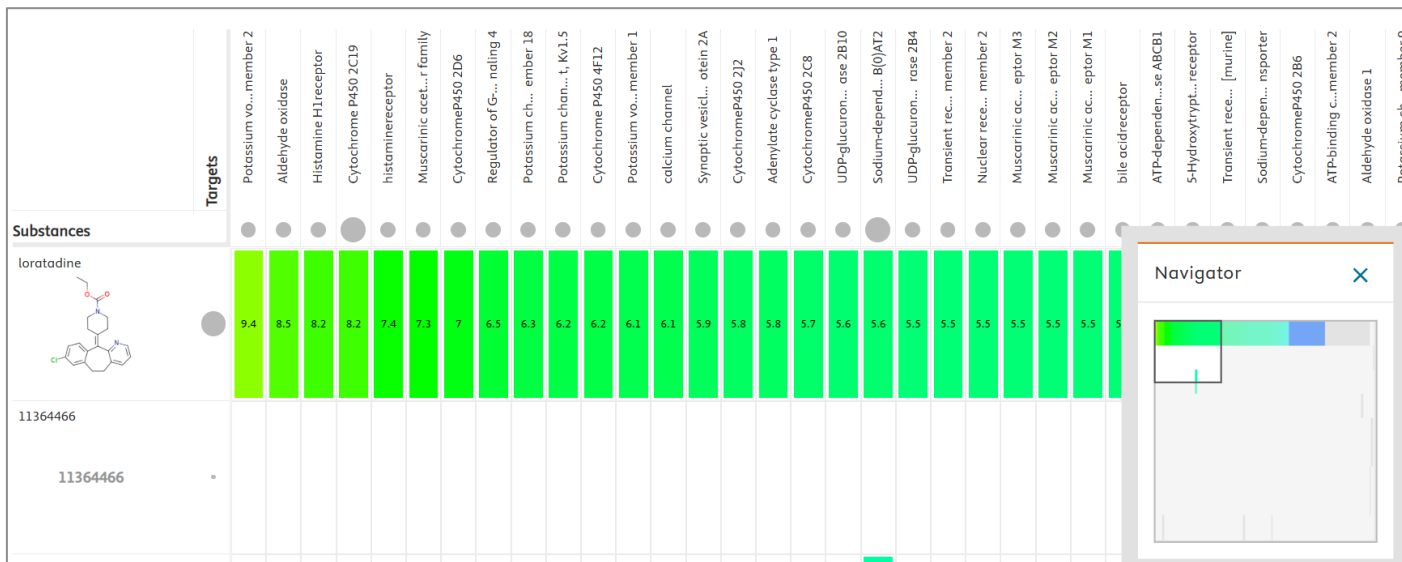
- Show/Hide columns
- ☒ pX
 - ☒ Parameter
 - ☒ Value (qual)
 - ☒ Value (quant)
 - ☒ Unit
 - ☒ Biological Species
 - ☒ Action on target
 - ☒ Target
 - ☐ (Clinical) findings / disease
 - ☒ Tissue/Organ
 - ☒ Cell
 - ☐ Bioassay
 - ☒ Dose
 - ☒ Effect
 - ☒ Concomitants
 - ☐ Metabolites
 - ☒ Reference

Reset to default >

Apply >



橫軸：蛋白質靶點/生物效應



生物活性視覺化分析②

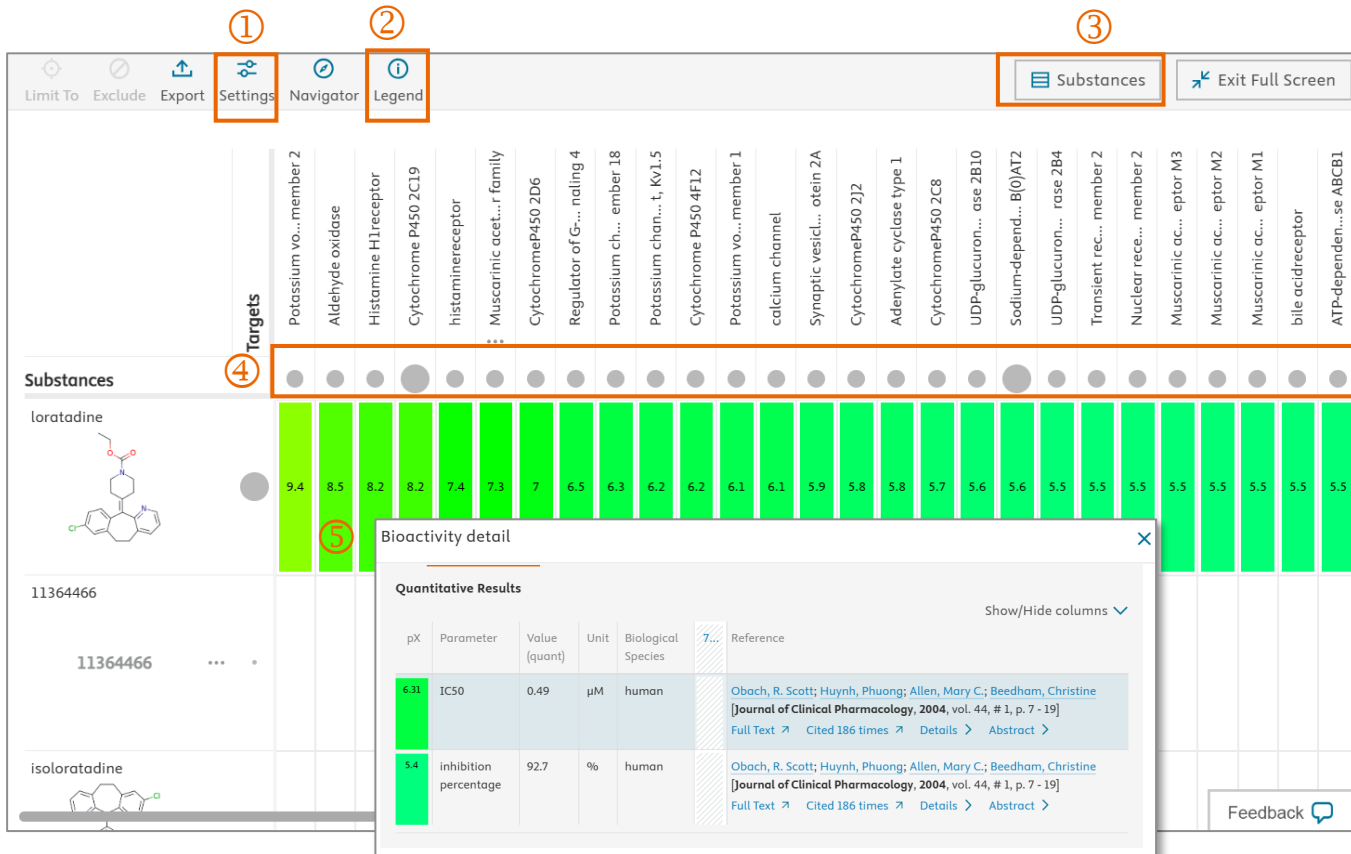
① 橫軸調整Target/Effects

② 圖示說明

③ 返回化合物列表

④ 資料量指示，資料越多
圓圈越大

⑤ 追蹤文獻出處



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 |

複合搜尋結果的篩選工具

| Filters | |
|---------------------------------|-----------|
| Limit to > | Exclude > |
| By Structure | ▼ |
| Substances Classes | ▼ |
| Molecular Weight | ▼ |
| Number of Fragments | ▼ |
| Availability | ▼ |
| Availability in other databases | ▼ |
| Available Data | ▼ |
| Document Type | ▼ |
| Publication Year | ▼ |

- ← 構造
- ← 化合物分類
- ← 分子量
- ← 分支數
- ← 取得的可能性
- ← 包括在其他資料庫中
- ← 可供查看的資料（如反應、物理特性等）
- ← 文獻的種類（文獻、專利等）
- ← 出版年份

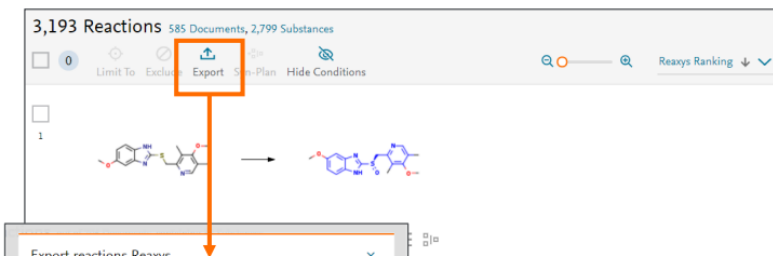
例如：分子量的過濾

| Molecular Weight | | |
|--------------------------|------------|---------------------------|
| ☐ | >348 - 360 | 1 |
| ☐ | >360 - 372 | 3 |
| ☐ | >372 - 384 | 6 |
| ☐ | >384 - 396 | 31 |
| ☐ | >396 - 408 | 85 |
| ☐ | >408 - 420 | 144 |
| ☐ | >420 - 432 | 43 |
| Filter by value ▼ | | View more |

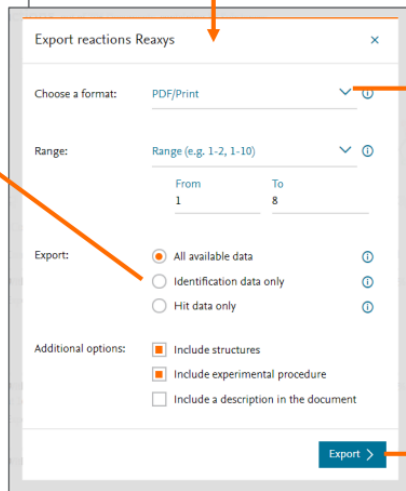
- 每個專案的細目可以通過點擊打開。
- 這些專案按照案件數量的順序進行排序。
- 可以通過輸入數位或單詞來過濾專案。

| Molecular Weight 2 | | Clear selected ✕ | ↓ | ↑ | Sort by Occurrence ▼ | ✕ |
|-------------------------------------|------------|----------------------|---|---|----------------------|---|
| ☐ | >408 - 420 | | | | 144 | |
| ☐ | >396 - 408 | | | | 85 | |
| ☒ | >432 - 444 | | | | 60 | |
| ☒ | >444 - 456 | | | | 48 | |
| ☐ | >456 - 468 | | | | 43 | |
| ☐ | >420 - 432 | | | | 43 | |
| ☐ | >384 - 396 | | | | 31 | |
| ☐ | >516 - 528 | | | | 27 | |
| ☐ | >492 - 504 | | | | 25 | |
| ☐ | >468 - 480 | | | | 22 | |
| ☐ | >480 - 492 | | | | 20 | |
| 1 2 3 > | | Limit to > Exclude > | | | | |

搜尋結果的輸出



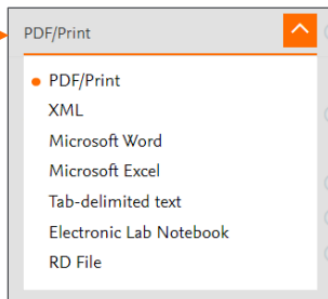
在搜索結果界面上，點擊「Export」



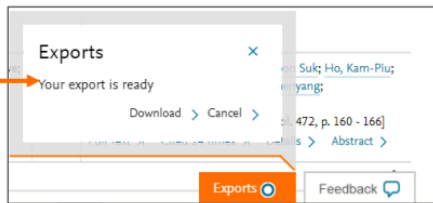
任何記錄或欄位都可以從
搜索結果中選擇並匯出

輸出設定界面：

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



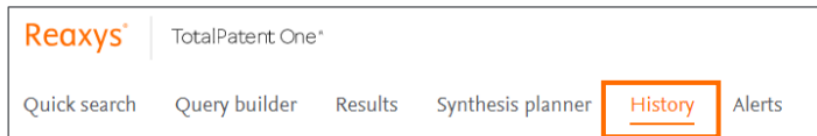
*如果您未登錄通過IP身份驗證，則無法導出。



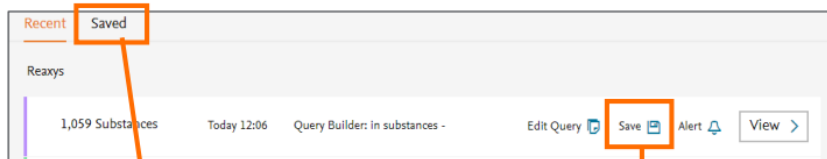
搜尋結果的保存

可以存儲搜索結果中的任意記錄

- 保存的記錄可以在“History”介面上查看(如果使用者登錄個人帳號，在關閉視窗後將不會被刪除。)



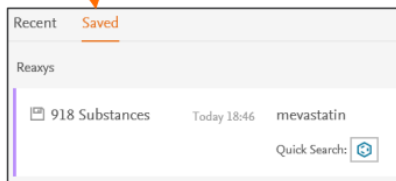
打開畫面最上面的“History”標籤



點擊你想保存的記錄的「Save」圖示

點擊 Save 

為結果輸入一個名稱，然後點擊「Save」



點擊“Saved”選項
出現存儲資料的管理介面
註冊數據以列表形式顯示

Alert的設定與管理①

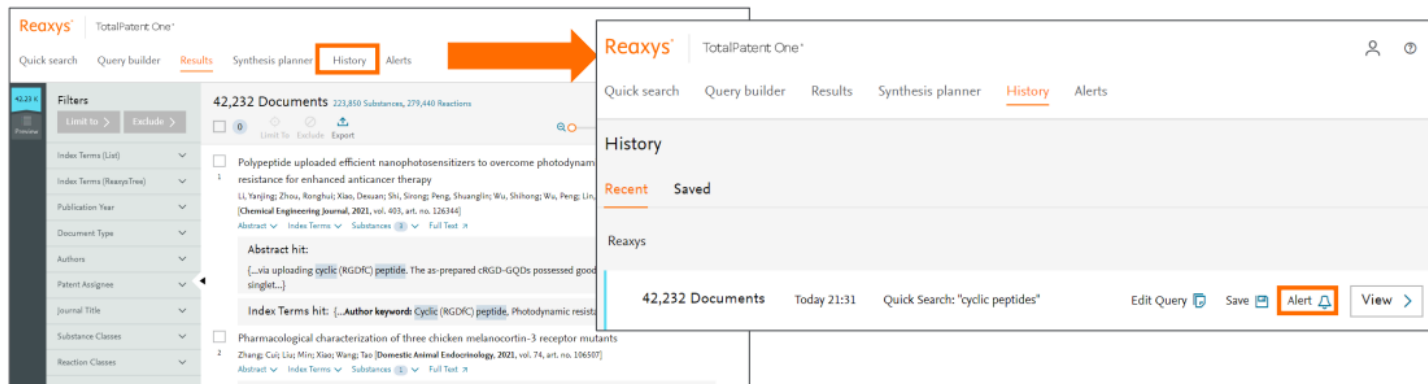
Alert會儲存你的搜索指令，資料庫會定期自動提供符合標準的搜索結果。

- 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結果將被發送到註冊的電子郵寄地址，同樣地Alert結果也可以發送給其他用戶並分享。
- * 使用Alert需要登入

Alert的設定：

- ① 在執行了您設置的Alert搜索後，打開歷史記錄。
- ② 在“History”介面上，選擇要設置Alert的搜索歷史記錄。

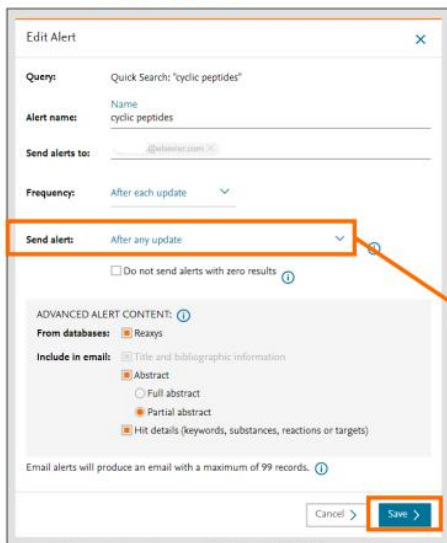
搜索歷史中會顯示各種選項，點擊”Alert”。



The screenshot displays the Reaxys web interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. The 'History' tab is selected, showing a list of search results. An orange arrow points from the 'Alerts' tab to the 'Alert' button in the bottom right corner of the interface. The 'Alert' button is highlighted with an orange border. The interface also shows a sidebar with filters and a main content area with search results.

Alert的設定與管理②

Alert的設定：



Edit Alert

Query: Quick Search: "cyclic peptides"

Alert name: Name: cyclic peptides

Send alerts to: @elsevier.com

Frequency: After each update

Send alert: After any update

☐ 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)

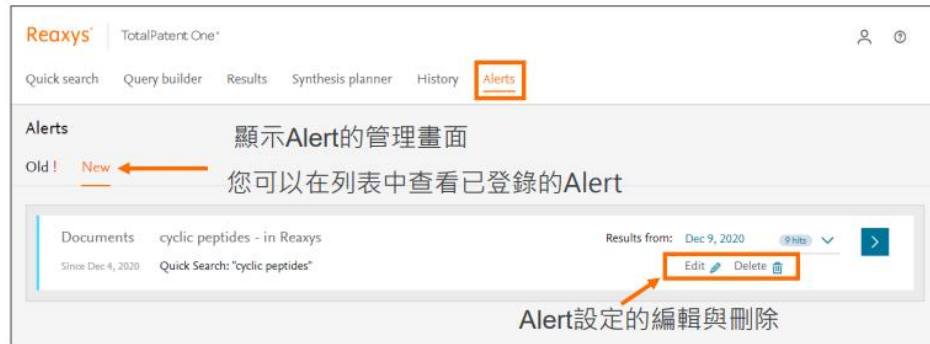
Email alerts will produce an email with a maximum of 99 records.

Cancel Save

- Alert name: Alert名稱
- Send alerts to: 設定送達的電子郵件地址(可複數輸入)
- Frequency: 通知頻率(可以指定星期和日期。)
- Alert Content: 所需的資訊內容

設置上述內容並點擊「Save」

Alert的管理：



Reaxys TotalPatent One

Quick search Query builder Results Synthesis planner History Alerts

Alerts

顯示Alert的管理畫面

您可以在列表中查看已登錄的Alert

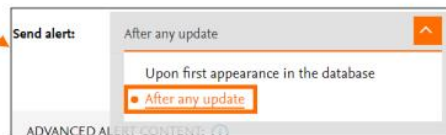
Old New

Documents cyclic peptides - in Reaxys Results from: Dec 9, 2020

Since Dec 4, 2020 Quick Search: "cyclic peptides"

Edit Delete

Alert設定的編輯與刪除



Send alert:

After any update

Upon first appearance in the database

After any update

ADVANCED ALERT CONTENT

※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」，僅在包括新化合物等情況下才會傳送資訊。

因此，不會傳遞持續更新資訊。

操作環境

操作環境：

- Firefox (版本49以上)
- Chrome (版本53以上)
- Edge (版本14以上)
- Safari (版本9)
- Internet Explorer (版本11)

-Reaxys可以在無Java的環境中使用
-可用於Windows和Macintosh



ELSEVIER

Thank you

如果您在使用Reaxys方面有任何問題，請聯繫Elsevier

- ◆ 聯絡資訊: r.huang@elsevier.com
- ◆ 電話號碼: +886-2-2522-5937

有關Reaxys的資訊可以在以下連結中找到

- ◆ <https://www.elsevier.com/zh-tw/solutions/reaxys>

