新版 Reaxys 化學資料庫

收錄內容更多、操作更直覺

www.reaxys.com
new.reaxys.com

Elsevier 生命科學解決方案經理 梁成芝

2017

Reaxys 化學資料庫使用權限

- **Reaxys 化學資料庫**
  - IP 開放，免帳號密碼，無同時上線人數限制
  - www.reaxys.com
  - 新介面 https://new.reaxys.com

  - 可使用 proxy 或 VPN 遠端連線，詳情請洽各校圖書館

Reaxys 中文線上學習資源

Reaxys 中文學習平台

taiwan.elsevier.com/reaxyshelp

學習影片
Learning Video

利用學習影片自我學習如何有效使用Reaxys，一步一步教學，讓資訊檢索變得更簡單。

文件下載
Document Download

快速上手Reaxys，並用實例介紹如何使用Reaxys功能，您可快速找到答案，讓學習變得更有趣。

線上研討會
Webinar

邀請專家分享使用Reaxys技巧和實例演練操作，讓您從學習中了解如何與資訊互動。

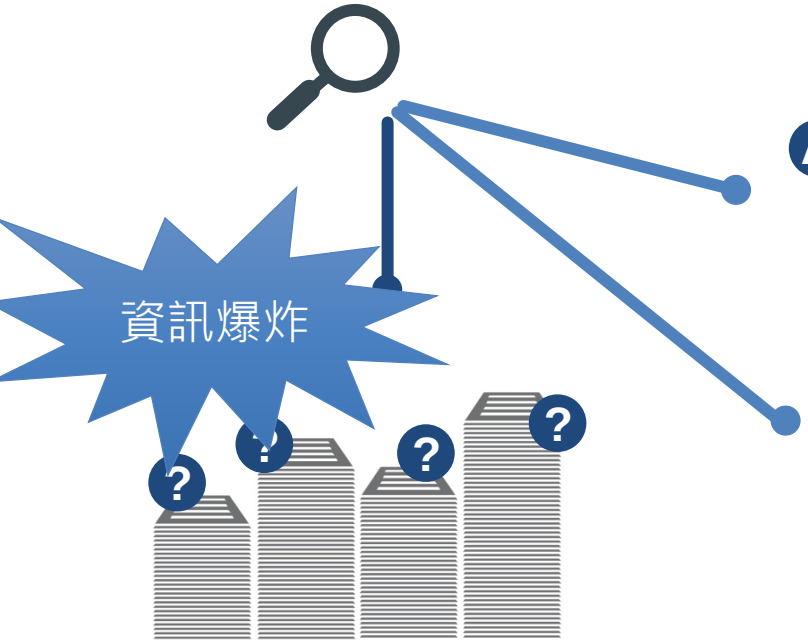
連線問題
Connection Issues

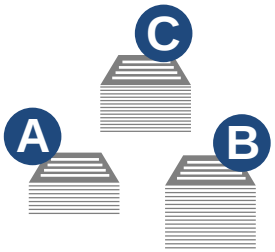
了解常見連線問題，並提供解決之道與聯絡方式。

本平台支援手機及平板使用

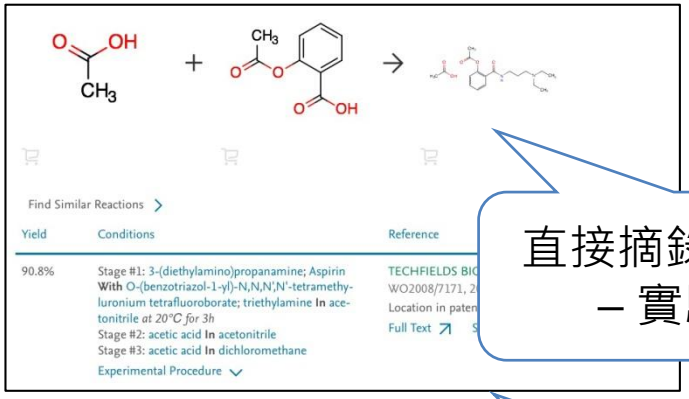
Elsevier R&D Solution 致力於更快找到答案

提供多種搜尋邏輯，除了關鍵字，可整合結構、分子式、數據等資料逆向搜尋





更系統性的
分類篩選文獻

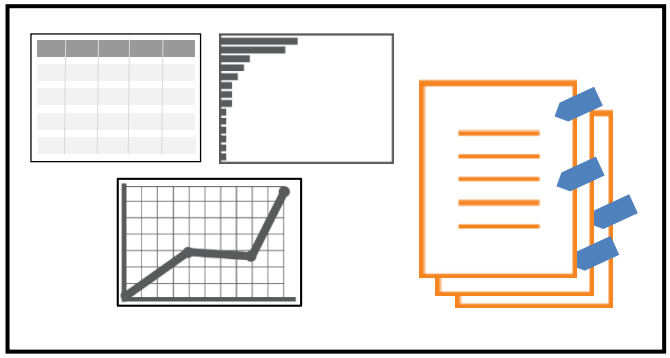


直接摘錄重要資訊
– 實驗數據

排序、分類篩選
實驗數據

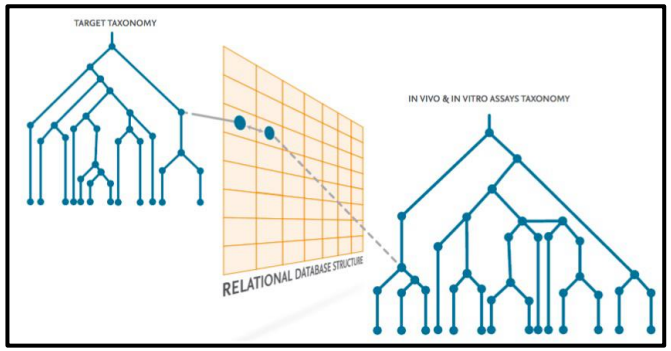
當其他資料庫的目標是提供更多
與關鍵字相關的**文獻列表**

新版 Reaxys 三大變化



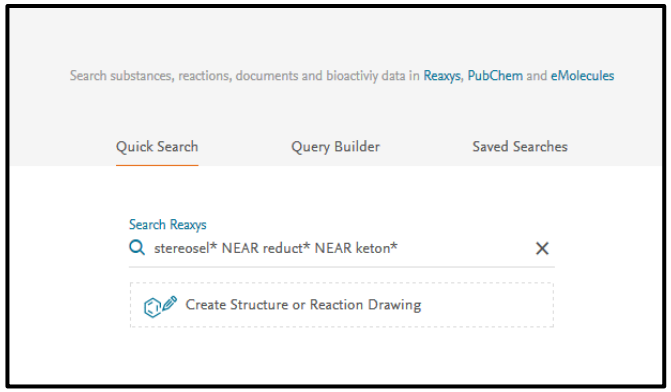
擴充收錄內容

- 16,000種期刊與主要專利局
- 5億筆實驗數據摘錄
- 281本期刊及專利**化學反應**全文材料方法摘錄



自動索引技術與資料庫架構

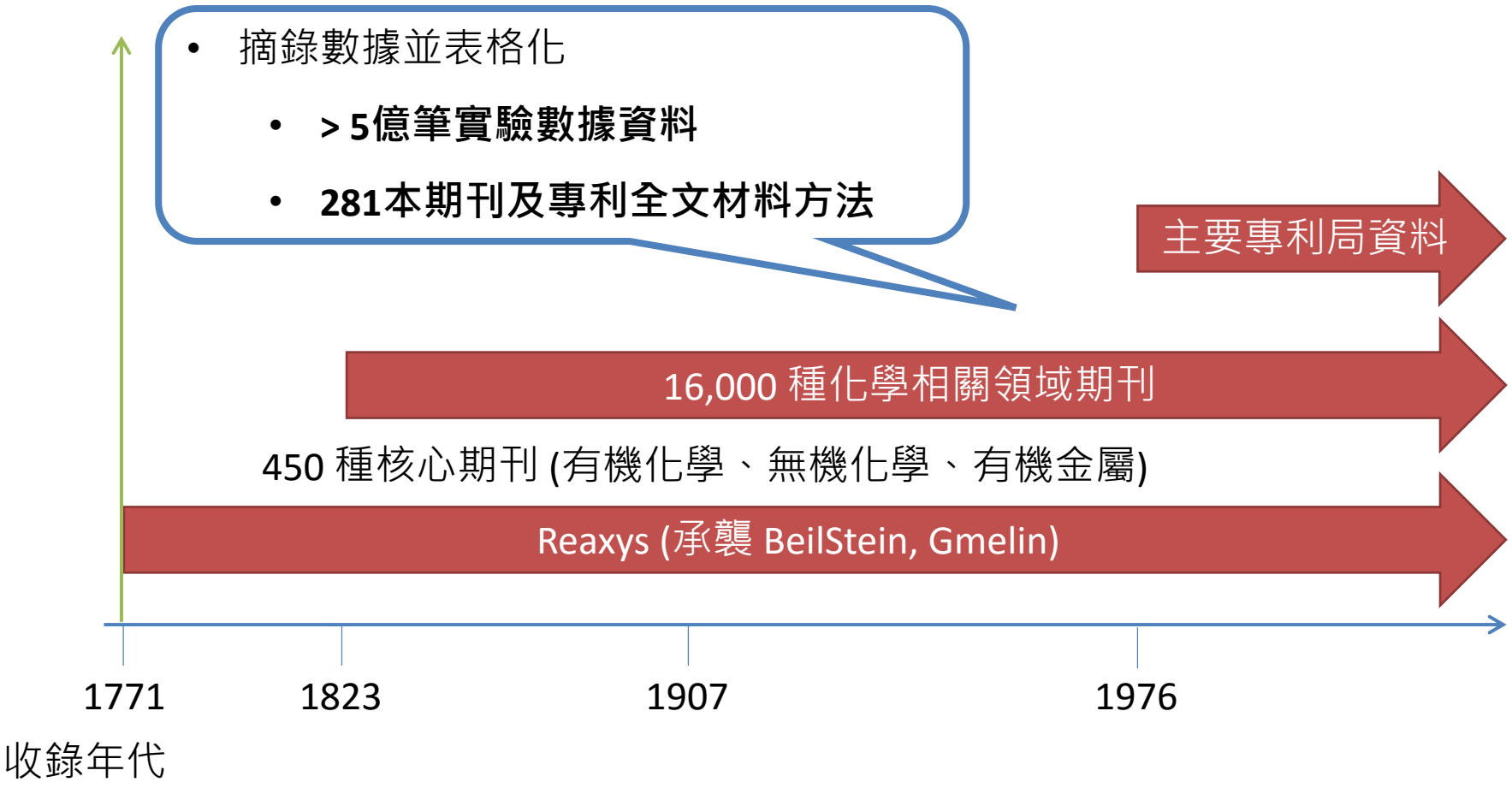
- 先進的全文自動索引技術
- 多元搜尋工具，如結構、實驗數值....更多
- 表格化整理與超連結串連



使用者介面

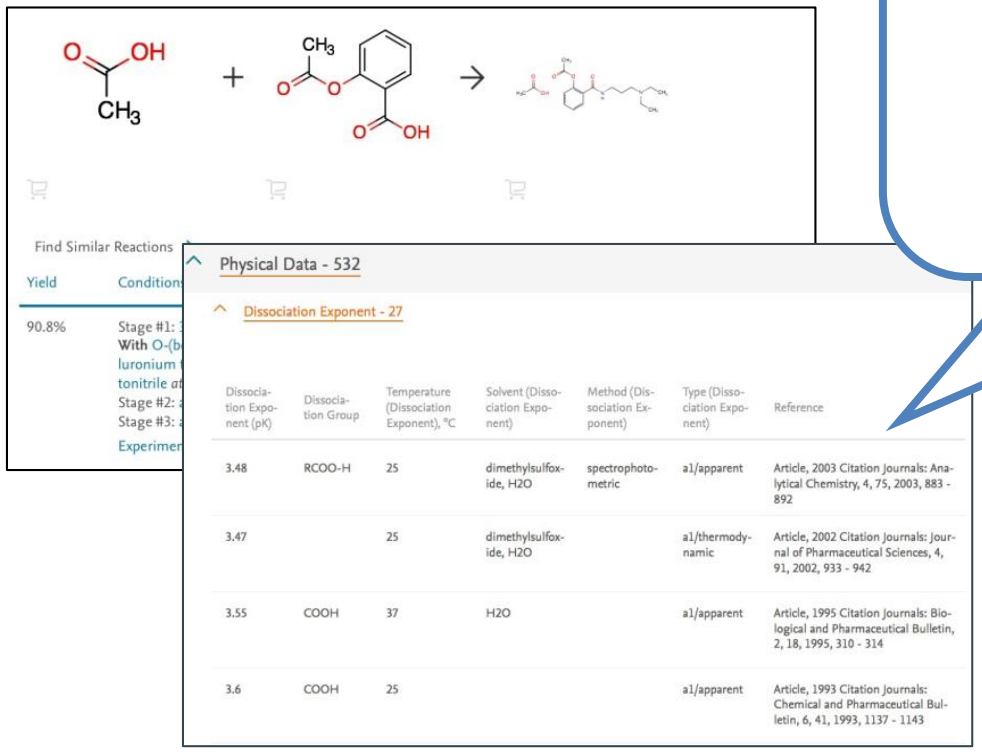
依據實際使用頻率設計
常用功能一目了然

Reaxys 收錄內容


• 摘錄數據並表格化
• > 5億筆實驗數據資料
• 281本期刊及專利全文材料方法
主要專利局資料
16,000 種化學相關領域期刊
450 種核心期刊 (有機化學、無機化學、有機金屬)
Reaxys (承襲 BeilStein, Gmelin)
1771
1823
1907
1976
收錄年代

自動索引技術 -- 資料表格化

直接比較數據資料，節省全文閱讀的時間與經費

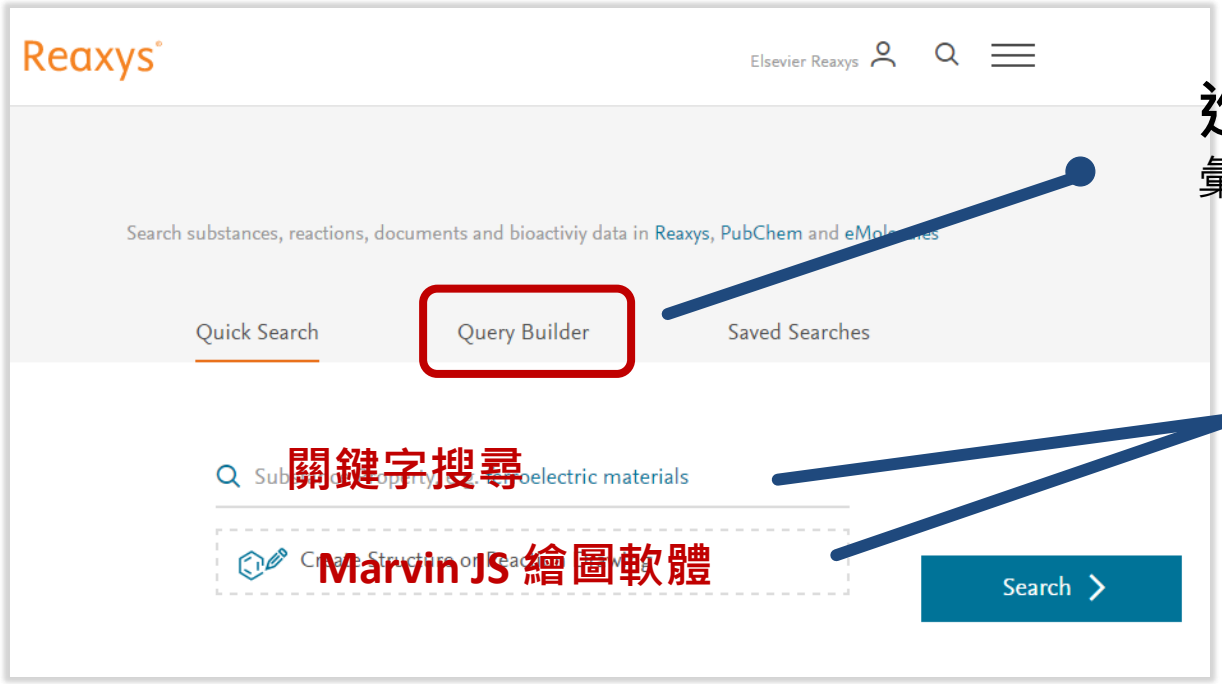


- 表格中的文字皆可篩選
- 沒有購買全文也可以獲得
  - 5 億筆實驗數據資料
  - 281 種期刊及專利的合成材料方法

450 → 12,000 本期刊

使用者介面

依據實際使用頻率設計，常用功能一目了然



進階搜尋

彙整 > 400 種搜尋欄位

> 95% 使用者

最常使用

關鍵字 + 結構搜尋

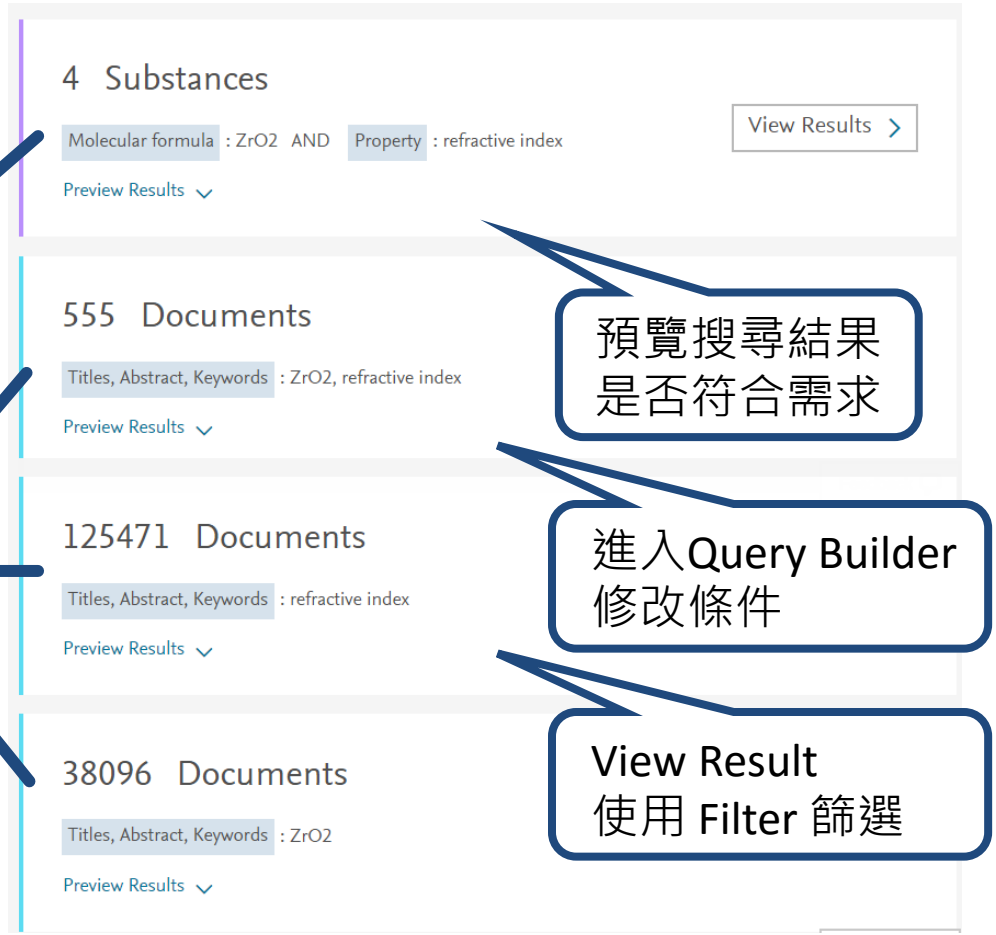
智慧辨識與預覽功能

自動辨識關鍵字，推薦相關結果，供您預覽及挑選

關鍵字搜尋
支援 AND OR NOT * 等指令

自動辨識提供
化合物及物化特性搜尋結果

自動推薦其他相關結果



預覽搜尋結果
是否符合需求

進入Query Builder
修改條件

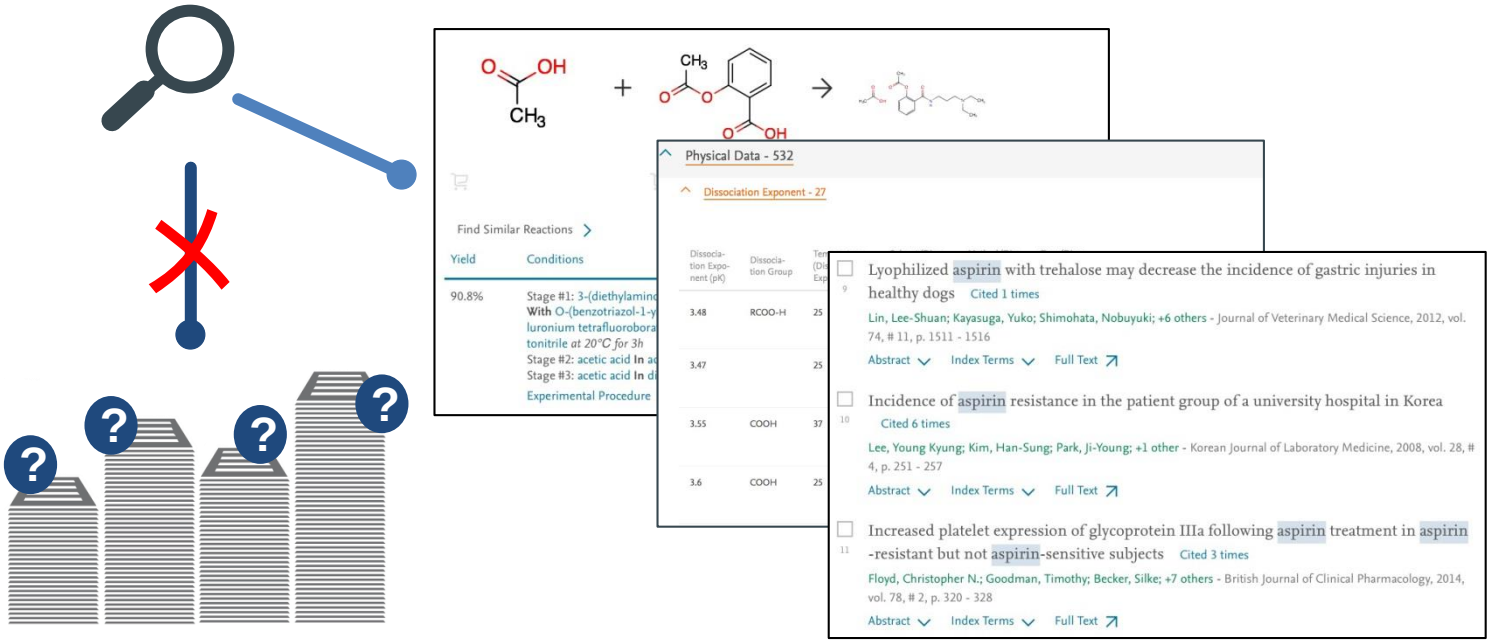
View Result
使用 Filter 篩選

多元搜尋工具 – Query Builder

自由結合超過 400種欄位、歷史搜尋紀錄、搜尋指定數值的實驗數據

開始使用 Reaxys

- ✓ 找到**答案**而非堆積如山的待唸文獻
- ✓ 摘錄更多數據資料、合成方法
- ✓ 搜尋方法更多元彈性



Reaxys 搜尋實例與技巧

不同領域適用不同搜尋範例：

有機化學、分析方法、複合材料 (合金、陶瓷)與特性、高分子、藥物生物活性數據

Presented By

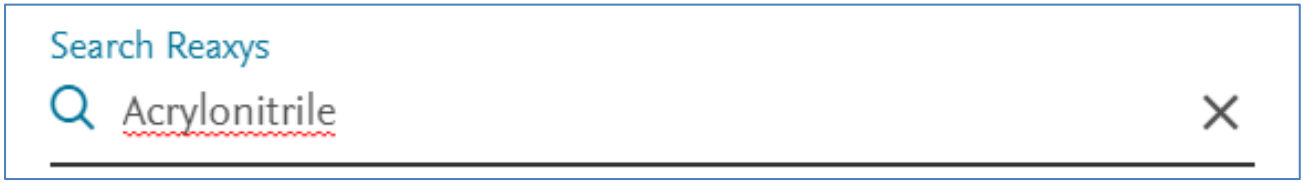
Date

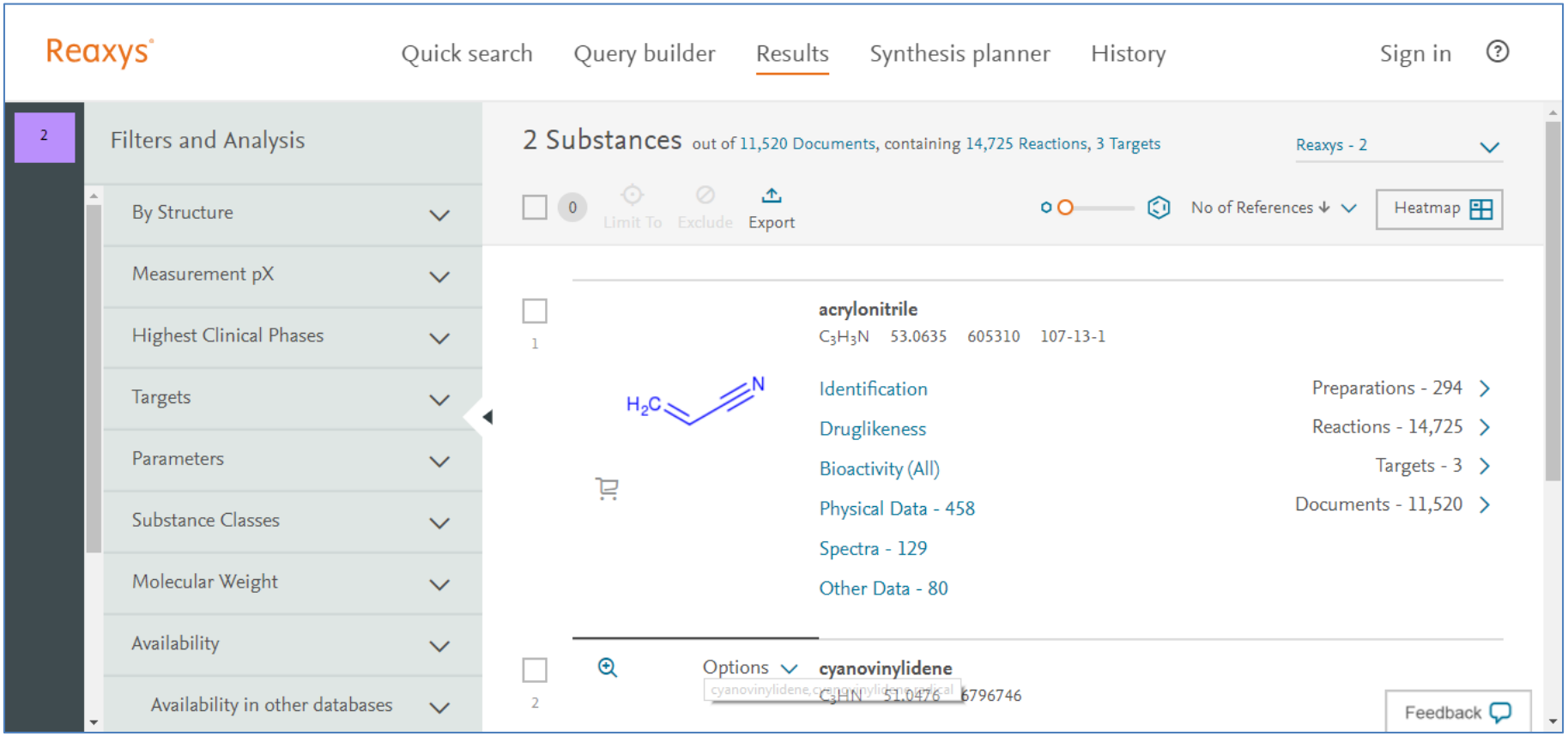
大綱

- **Quick Search 關鍵字自動辨識**
  - 自動辨識 – 化合物、數據名稱
  - 自動辨識 – 關鍵字
  - 自動辨識 – 反應類型
- **搜尋結果**
  - 合成路徑規劃 (進階)
  - 包裝價格查詢
  - 查詢合成與分析材料方法「全文」(進階)
  - 文獻匯出到 EndNote
- **Marvin JS 繪圖軟體**
  - 基本操作
  - 反應搜尋功能 (進階)
  - 衍生物相關功能 (進階)
- **Query Builder 進階搜尋**
  - 數據數值範圍搜尋
  - 搜尋結果關鍵字限縮 (進階)
  - 分子式衍生物搜尋功能 (進階)

自動辨識 – 化合物 Acrylonitrile

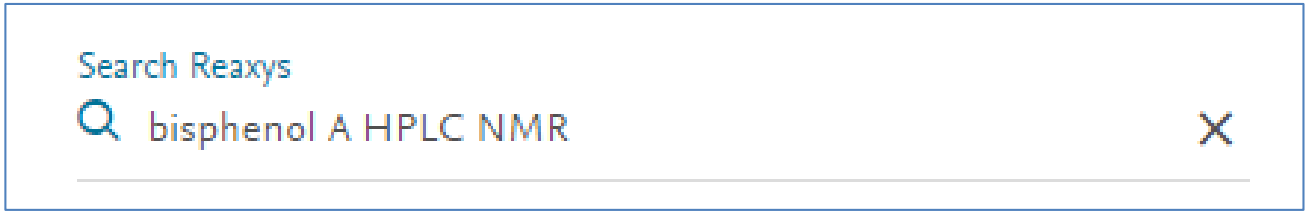
Acrylonitrile Mechanical Property

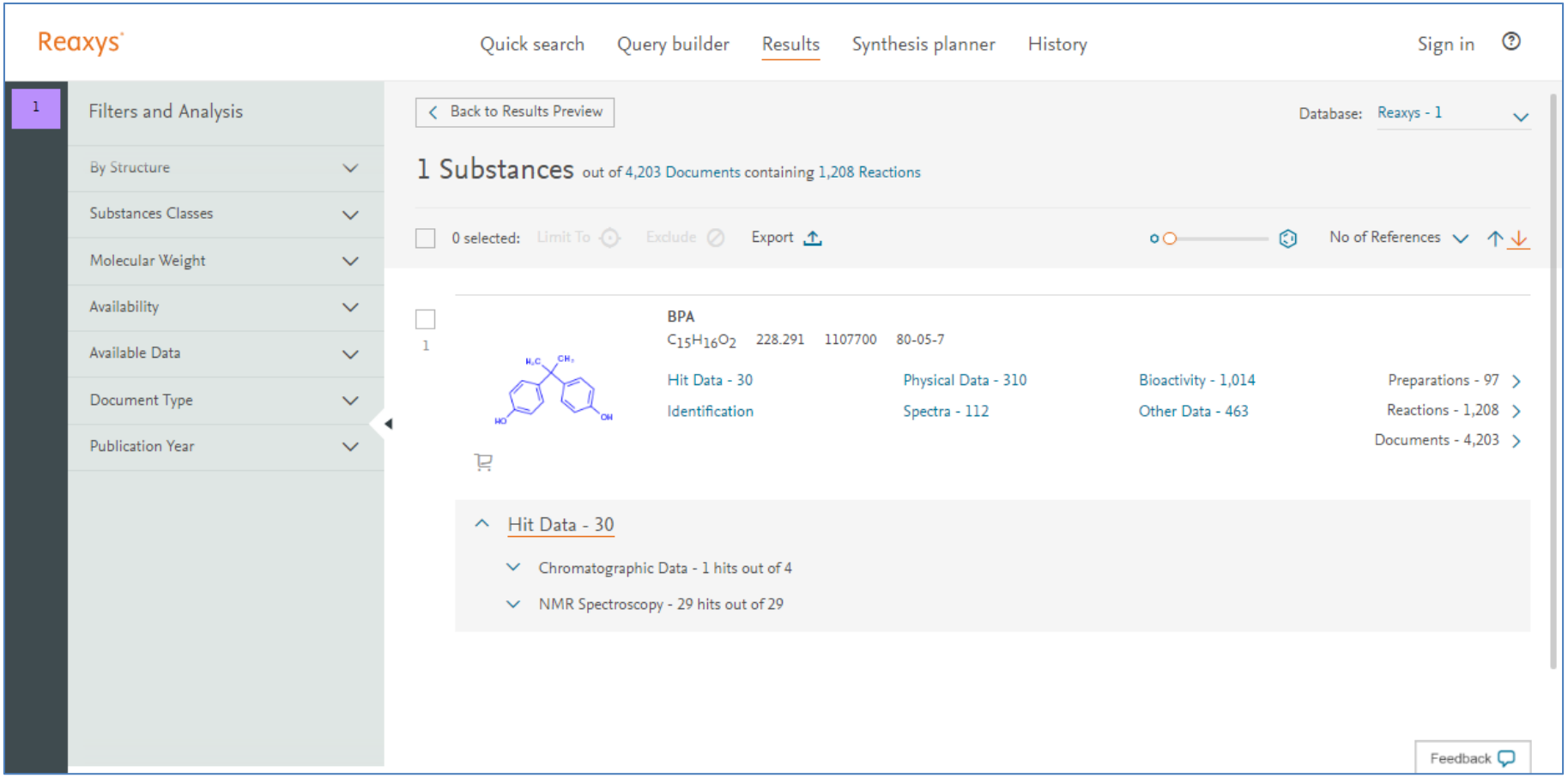




自動辨識 – 化合物 Bisphenol A

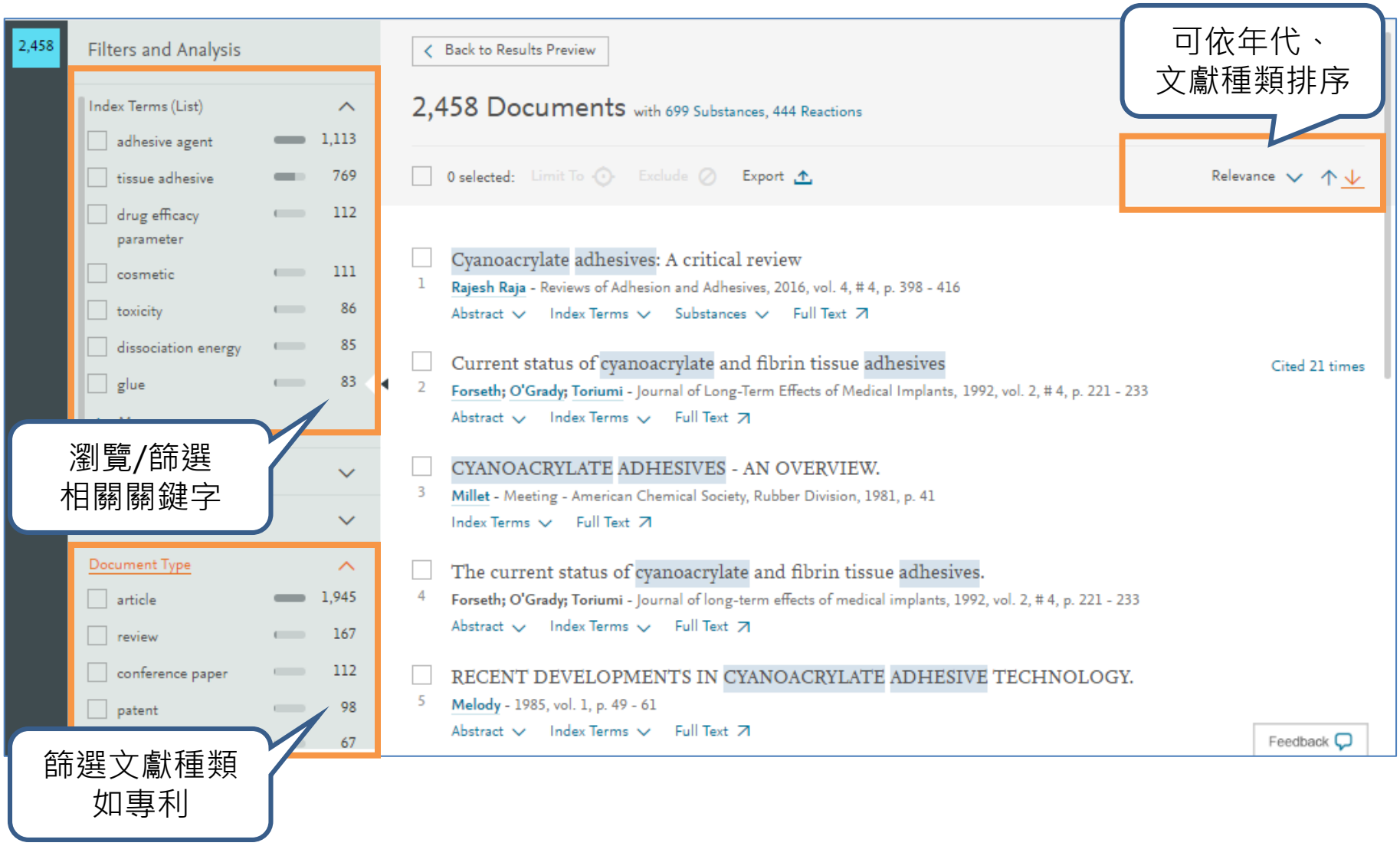
EPICHLOROHYDRIN



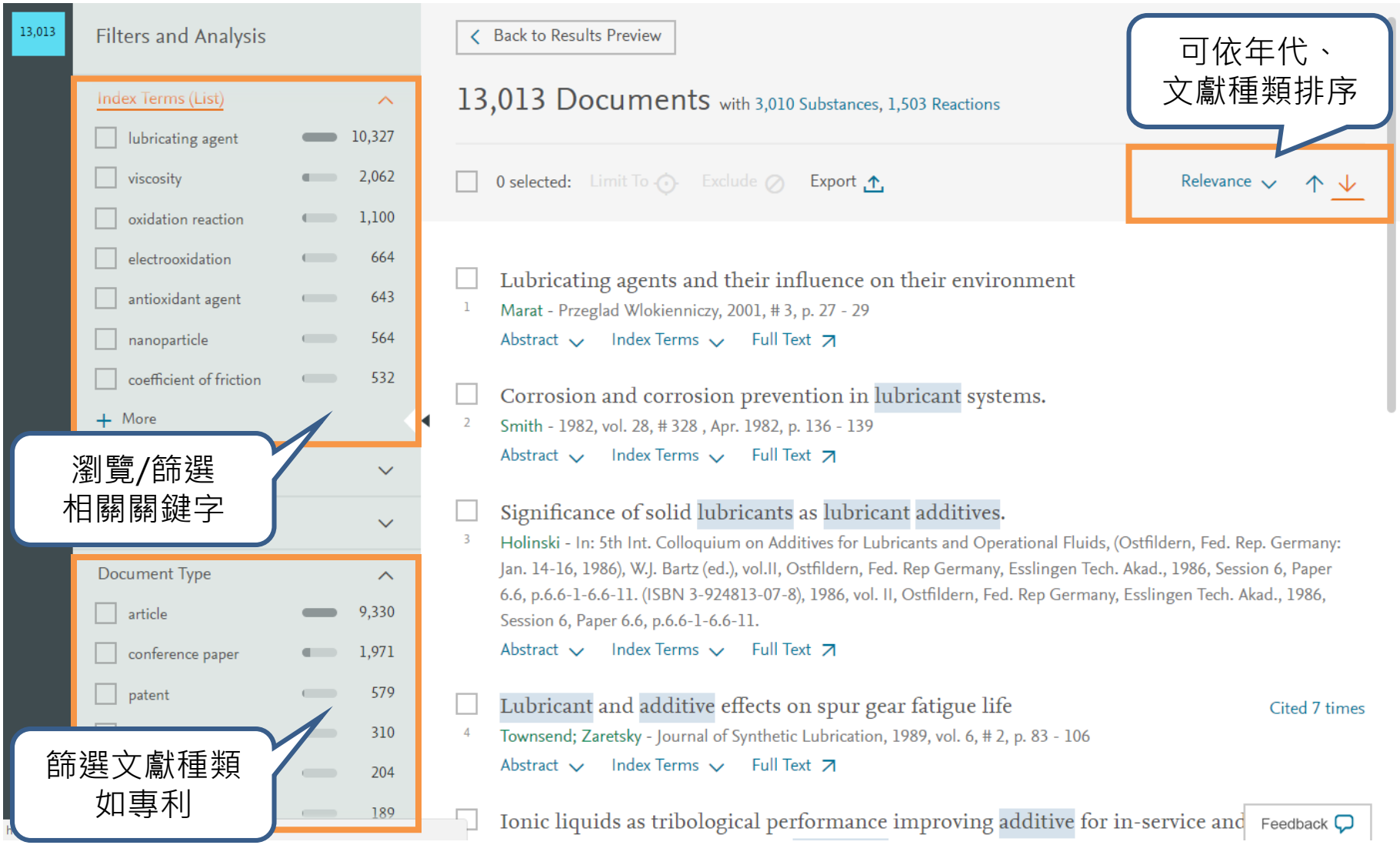


自動辨識 – 關鍵字 Cyanoacrylate Adhesive, UV curing,

文獻列表

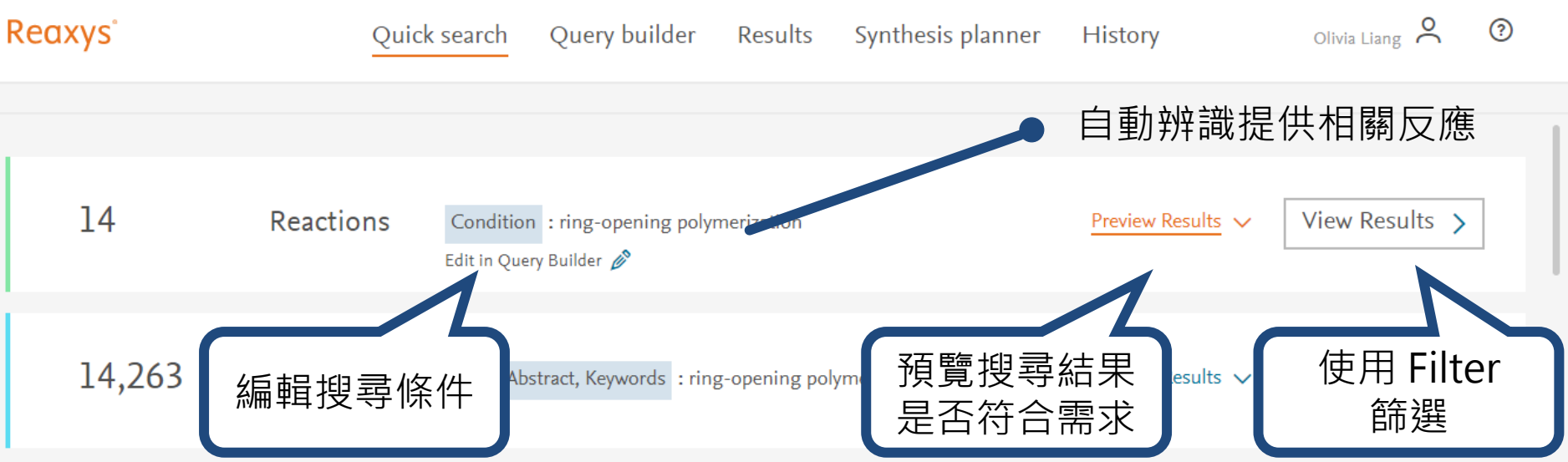


自動辨識 – 關鍵字 Lubricant Additives



關鍵字自動辨識 -- 反應類型

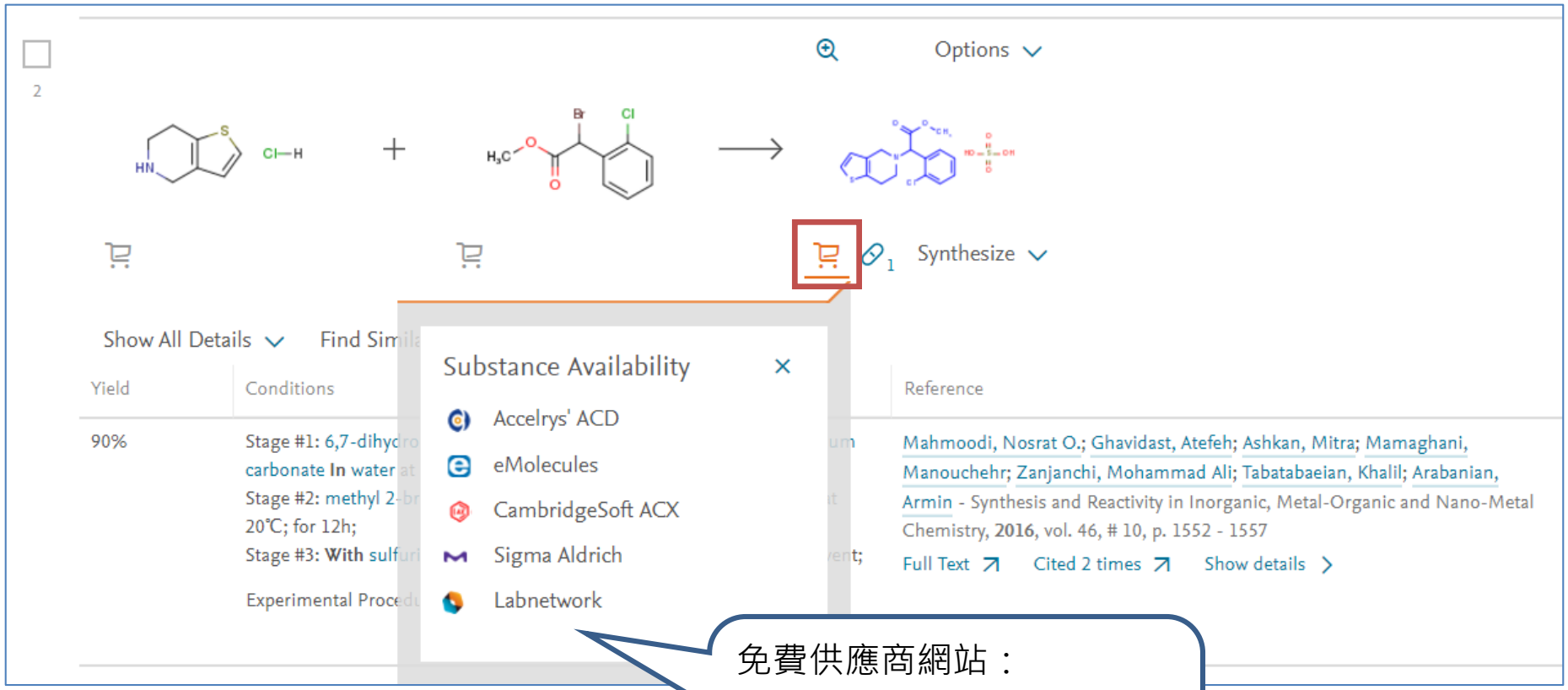
RING-OPENING POLYMERIZATION



關鍵字自動辨識 -- 反應類型

EPOXIDATION

搜尋結果 – 包裝價格查詢

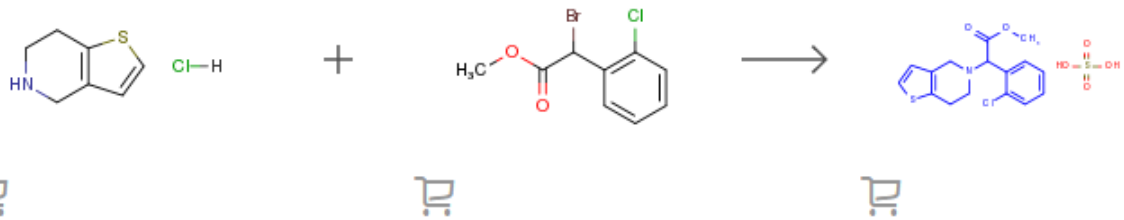


免費供應商網站：

- eMolecures
- Sigma Aldrich
- Labnetwork

搜尋結果 – 合成方法全文內容 Experimental Procedure

Clopidogrel Synthesis



Show All Details Find Similar Reactions

Yield	Conditions	Reference
90%	Stage #1: 6,7-dihydro-4H-thie… **With** sodium carbonate **In** wat… Stage #2: methyl 2-bromo-2-(… water; toluene at 20℃ for 12… Stage #3: **With** sulfuric ac… **In** ;Reagent/catalystSolve… Experimental Procedure	

Experimental Procedure

One-Pot Procedure for the Synthesis of Racemic ClopidogrelBisulfate (2)

To a vessel equipped with Dean-Stark assembly, 2-(thiophen-2-yl)ethanamine 5 (0.48 g, 4 mmol), PFA (0.13 g,4.3 mmol), and toluene (6 mL) were added and the reaction mixture was refluxed for 2 h to obtain a yellow solution contain imine. After cooling to 20C, a solution of6N HCl (0.7 mL) in DMF was added into the reactionmixture and continued to heat at 50C for 1 h to produce 4as a white precipitate. The reaction was cooled to 25Cand aqueous solution of 10percent Na2CO3 was added andstirred for 30 min. Then a solution of methyl-2-bromo-2-(2-chlorophenyl)acetate 3 (1.04 g, 4 mmol) in toluene (7mL) was added to the reaction mixture. The reaction mixture stirred at room temperature for 12 h. The aqueouslayerisdiscardedandtheorganiclayerwaswashedwithwater. The organic phase was evaporated, to afford viscose oil. To this oil, conc. H2SO4 (0.42 mL) and EtOAc(8 mL) was added. The mixture was stirred for 1 h. Theprecipitated crystalsfiltered off and washed with cool acetone. The pure racemic clopidogrel bisulfate 2was driedin oven at 50C (1.35 g, 90percent yield). White powder; mp220–222C; IR:v (KBr, cm–1) 3434 (OH stretch), 3100,2989, 2953, 1755 (C DO stretch), 1239, 1222 (C-Ostretch), 1063.

搜尋結果 – 分析方法全文內容 Supporting information

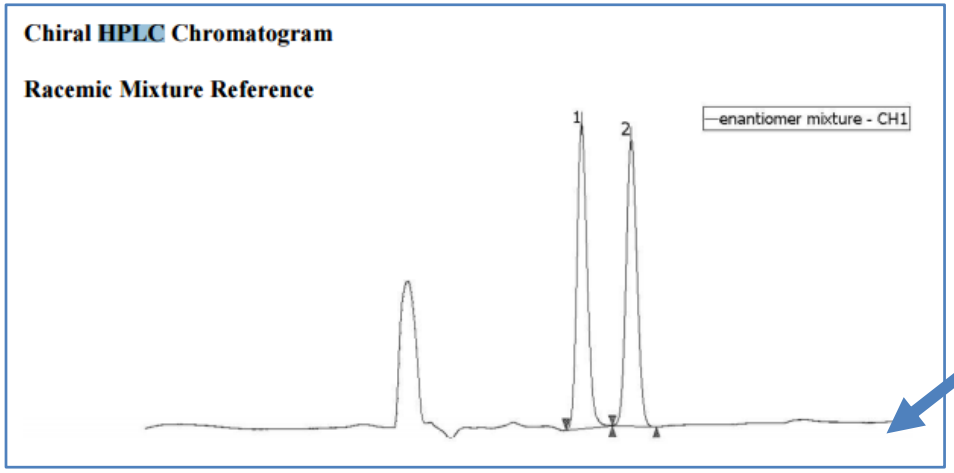
分析材料方法若放在 Supporting Information 中，可以直接下載

HPLC (High performance liquid chromatography)

supporting information

Zhu, Yaoqiu; Zhou, Jiang; Jiao, Bo - ACS Medicinal Chemistry Letters, 2013, vol. 4, # 3, p. 349 - 352

Full Text ↗ Cited 6 times ↗ Show details >



點選Full Text
打開 supporting information

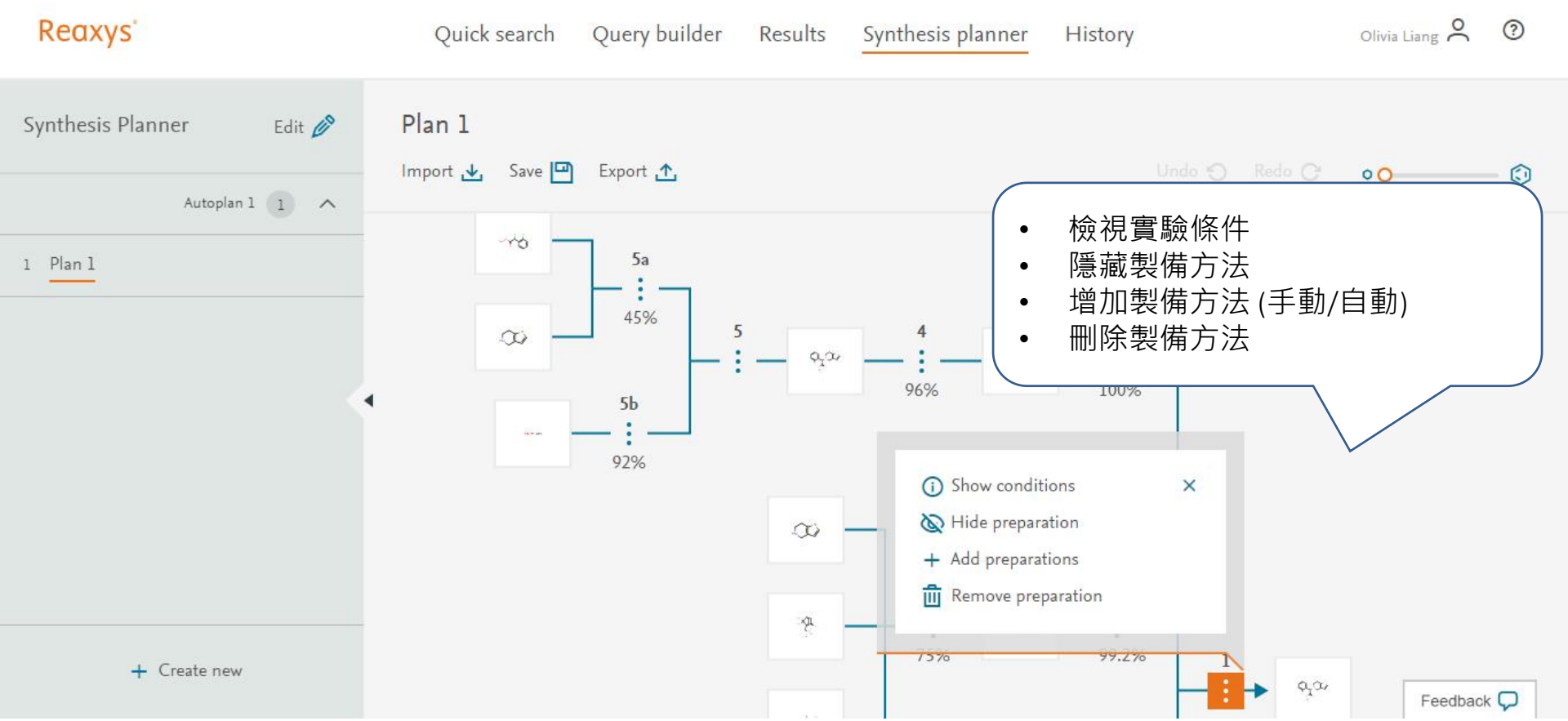
Supporting information link
http://pubs.acs.org/doi/suppl/10.1021/ml300460t/suppl_file/ml300460t_si_001.pdf

獲得重要資訊

Chiral Analysis.
The synthesized clopidogrel (CPG) hydrochloride salts were subjected to chiral analysis on an LC-2000Plus HPLC system (Jasco, Tokyo, Japan) with a Chiralpak AD-H column (Daicel, Osaka, Japan) using a standard isocratic program for CPG analysis (10-15% i-propanol in n-hexane, 10 min, 1.0 mL/min).1 Racemic CPG (with 50% of each enantiomer) was used as reference.

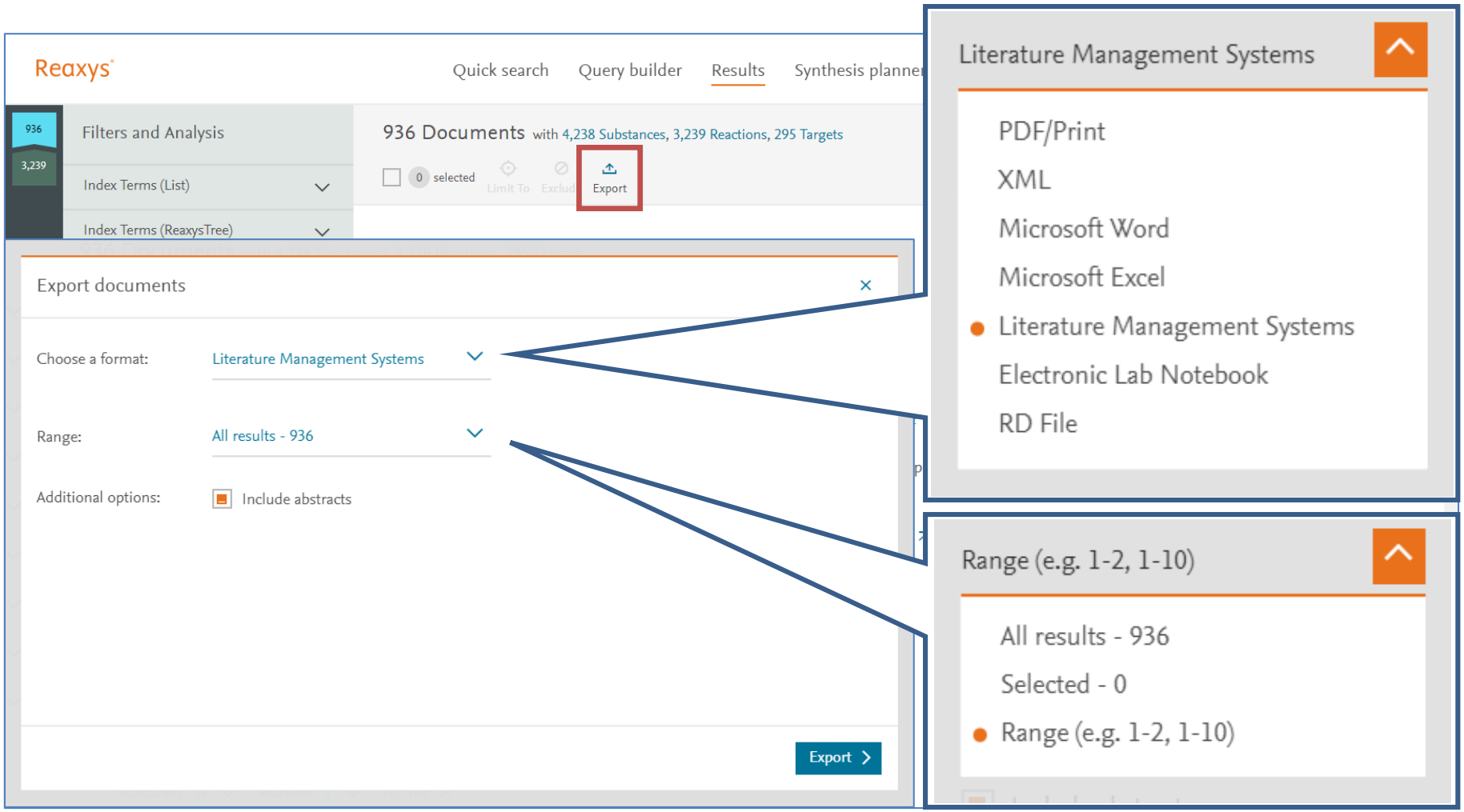
搜尋結果 -- 合成路徑規劃

Clopidogrel Synthesis

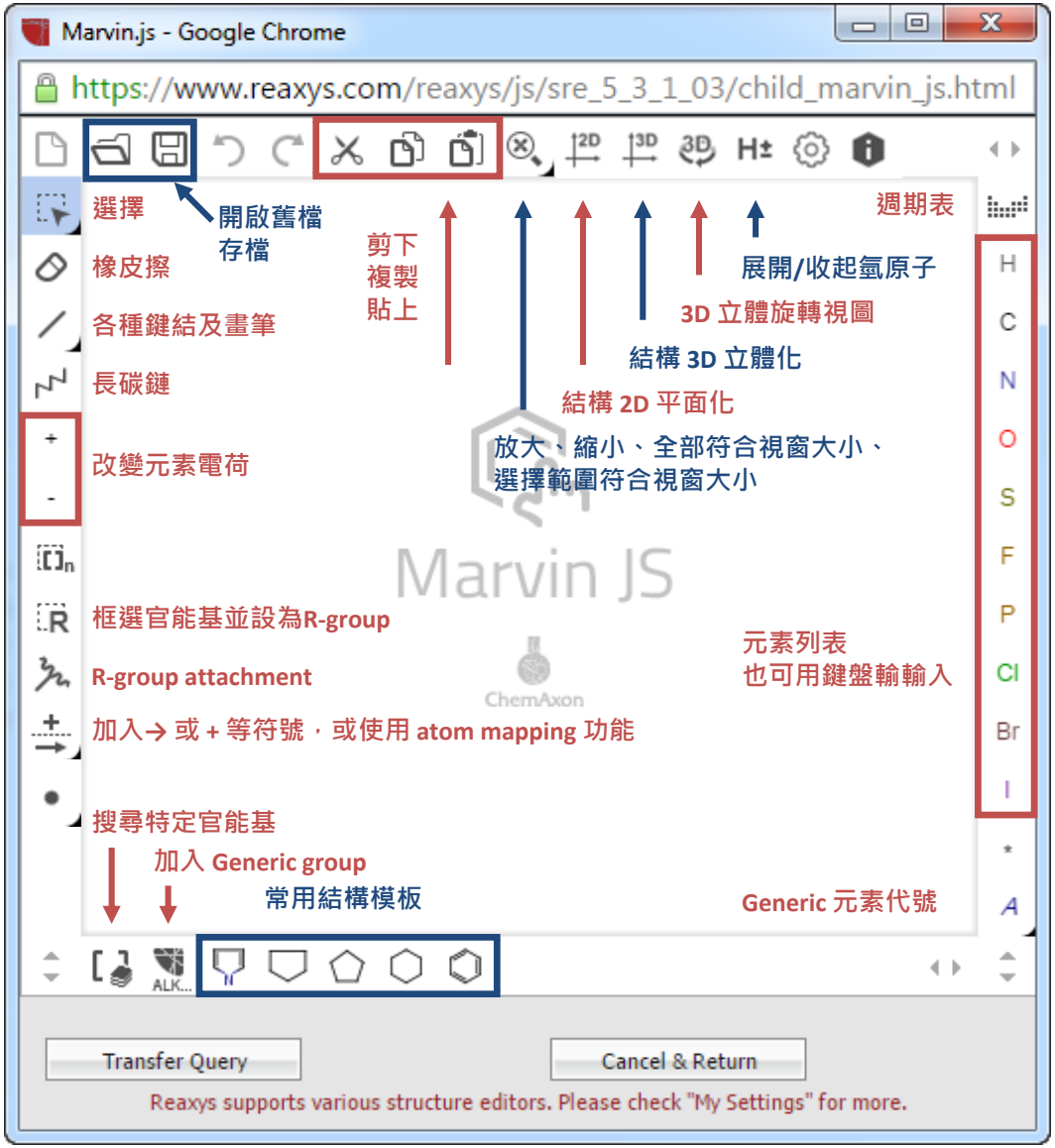


搜尋結果 – 文獻匯出到EndNote

由文獻列表點選 Export，設定檔案格式與輸出範圍



Marvin JS 繪圖軟體 – 基本功能



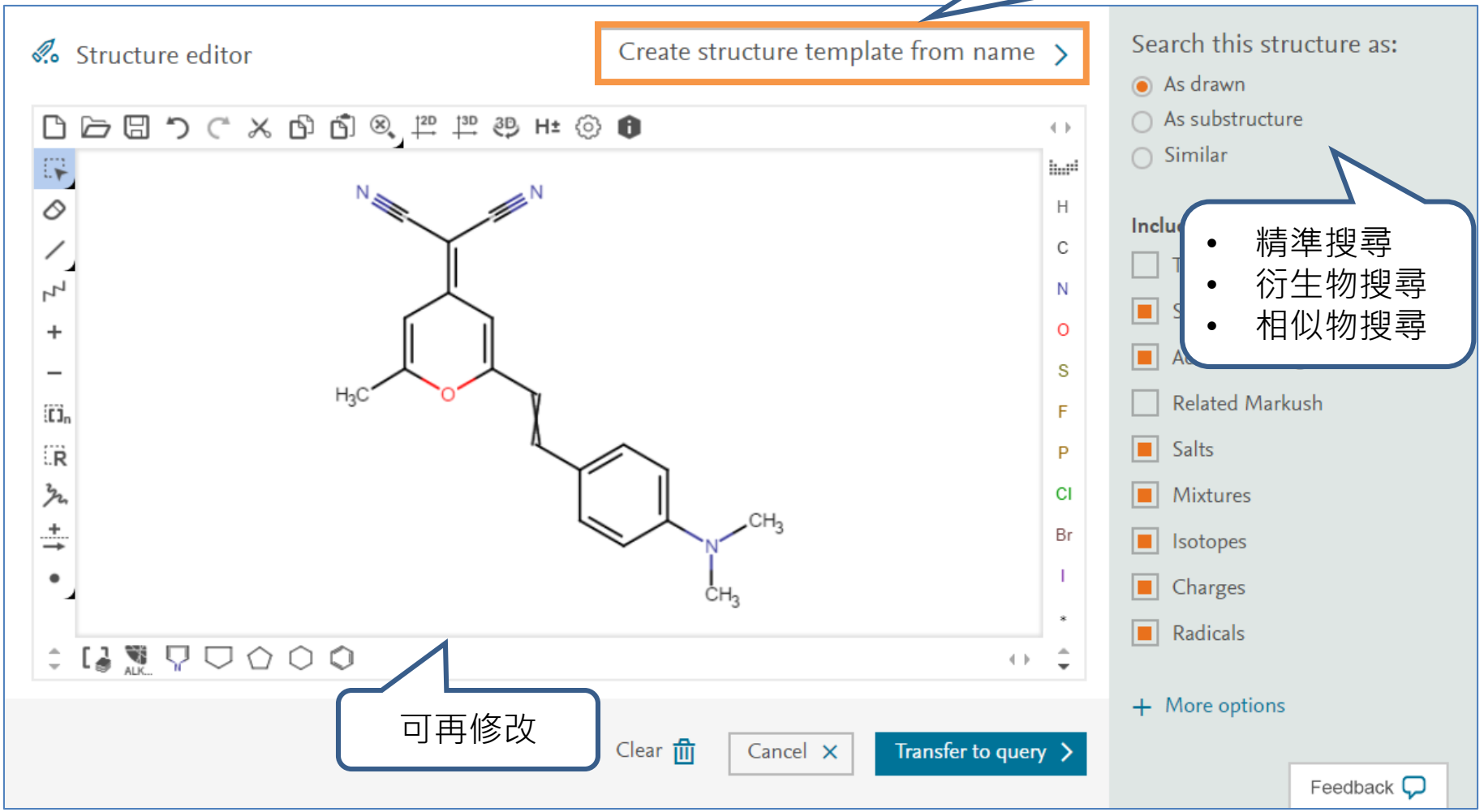
- 無須 JAVA
- 可從 ChemDraw 複製貼上
- 輸出成透明背景高解析圖檔

- 基本功能
  - 模板、鍵結、元素與週期表
  - 選擇、旋轉、移動、縮放
  - 2D/3D 轉換、氫原子展開

Marvin JS 繪圖軟體 – 基本功能

DCM, OLED 材質由名稱匯入結構

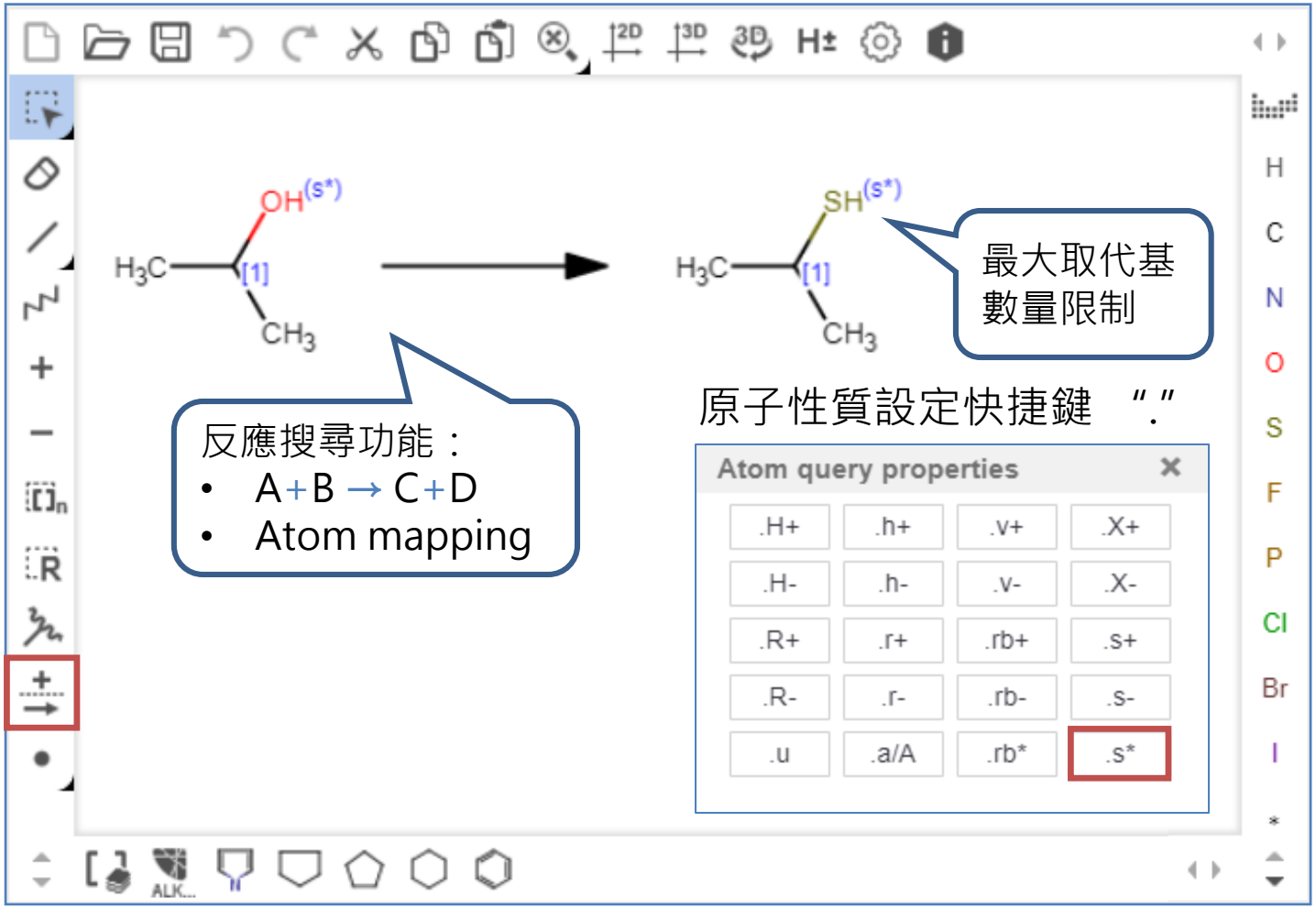
由名稱、CAS編號匯入結構

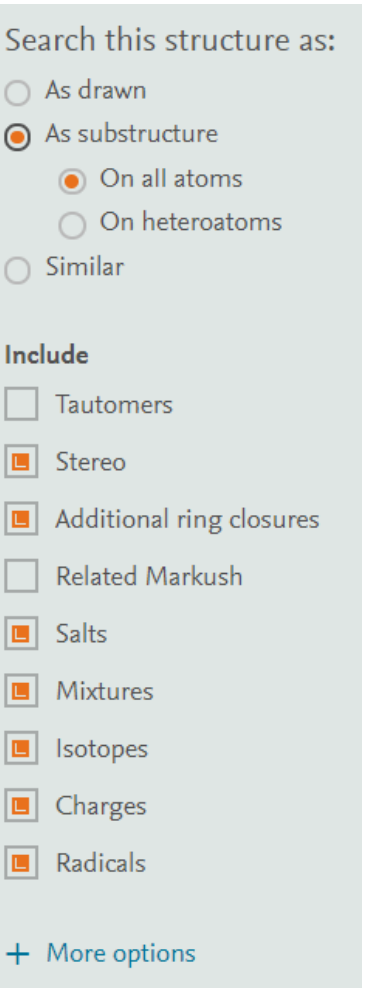


- 精準搜尋
- 衍生物搜尋
- 相似物搜尋

可再修改

Marvin JS 繪圖軟體 – 反應搜尋功能





Reaction 搜尋結果

找到 1,235 筆反應

1,235 Reactions 495 Documents 1,970 Substances, 64 Targets

0 Limit To Exclude Export Reaxys Ranking

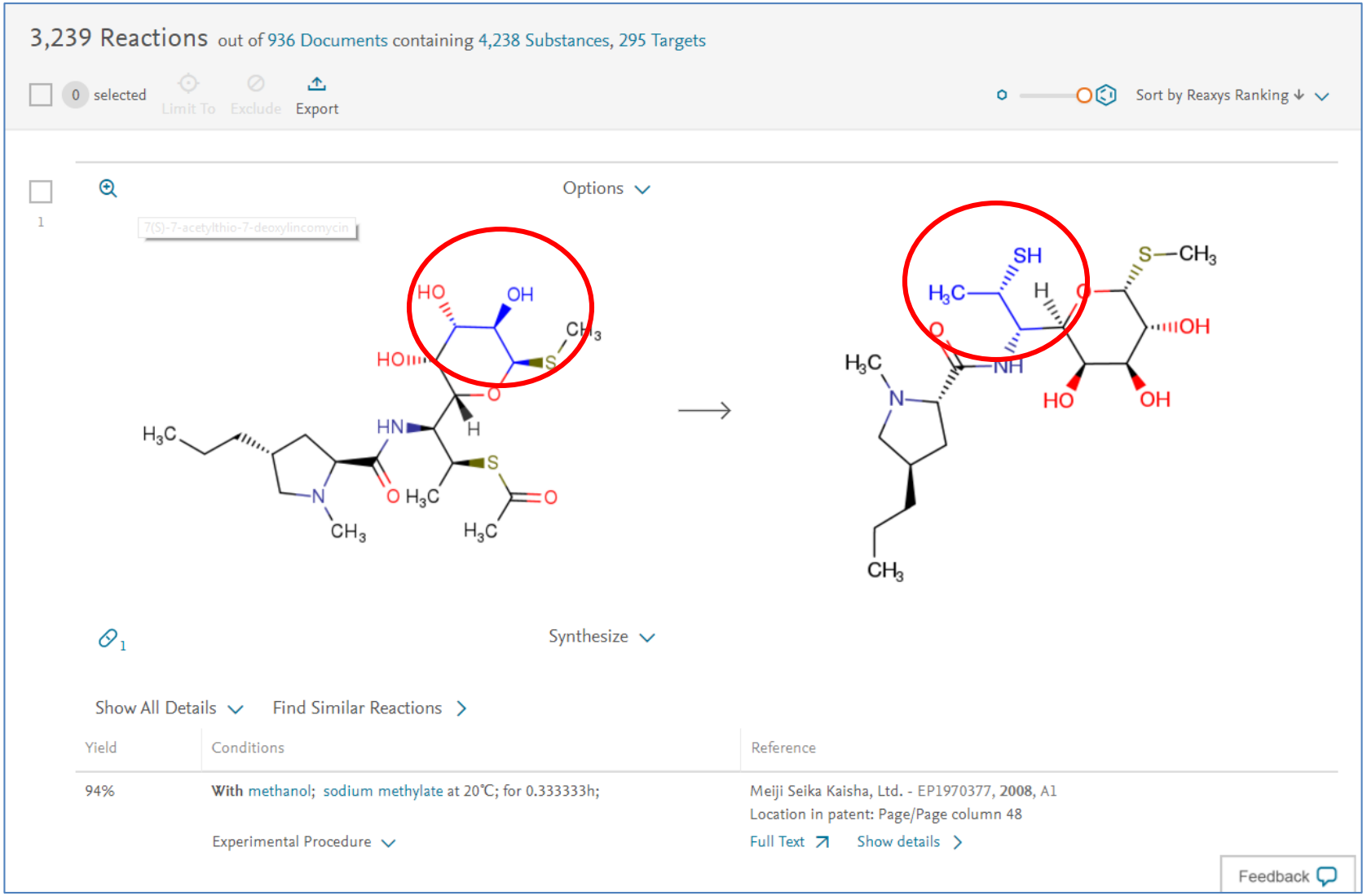
1

Show All Details Find Similar Reactions

Yield	Conditions	Reference
94%	**With** Lawessons reagent **In** toluene for 0.5h; Heating;	Nishio, Takehiko - Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), **1993**, # 10, p. 1113 - 1118 Full Text Cited 24 times Show details

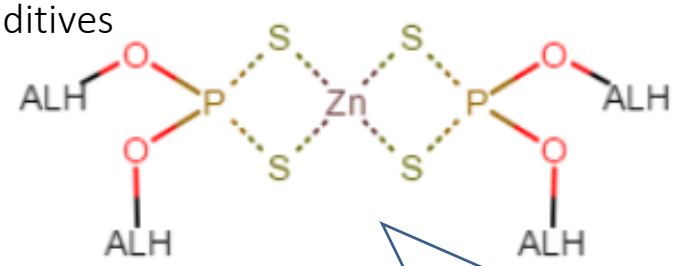
若不使用 atom mapping

找到 3,239 個反應，但官能基的位置可能不同



Marvin JS 繪圖軟體 – 結構衍生物搜尋

ZDDP Zinc Dithiophosphate 潤滑油抗磨添加劑 Anti Wear Additives



完備的衍生物搜尋設定

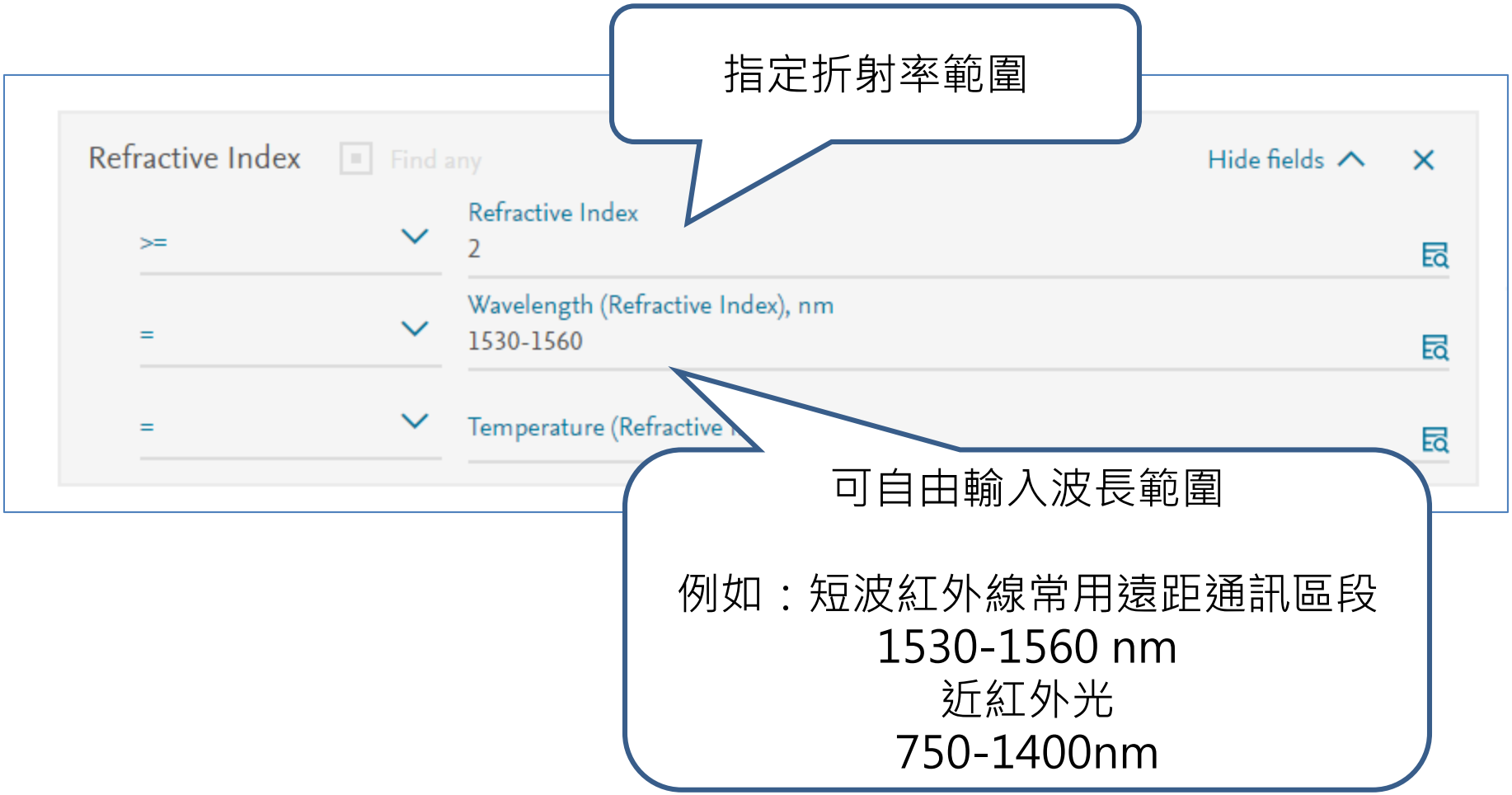
24	Substances	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results	View Results
1	Substances	Structure : average similarity; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results	View Results
8	Reactions	Product(s) : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results	View Results

自動辨識提供不同相似程度化合物搜尋結果

自動推薦其他相關結果

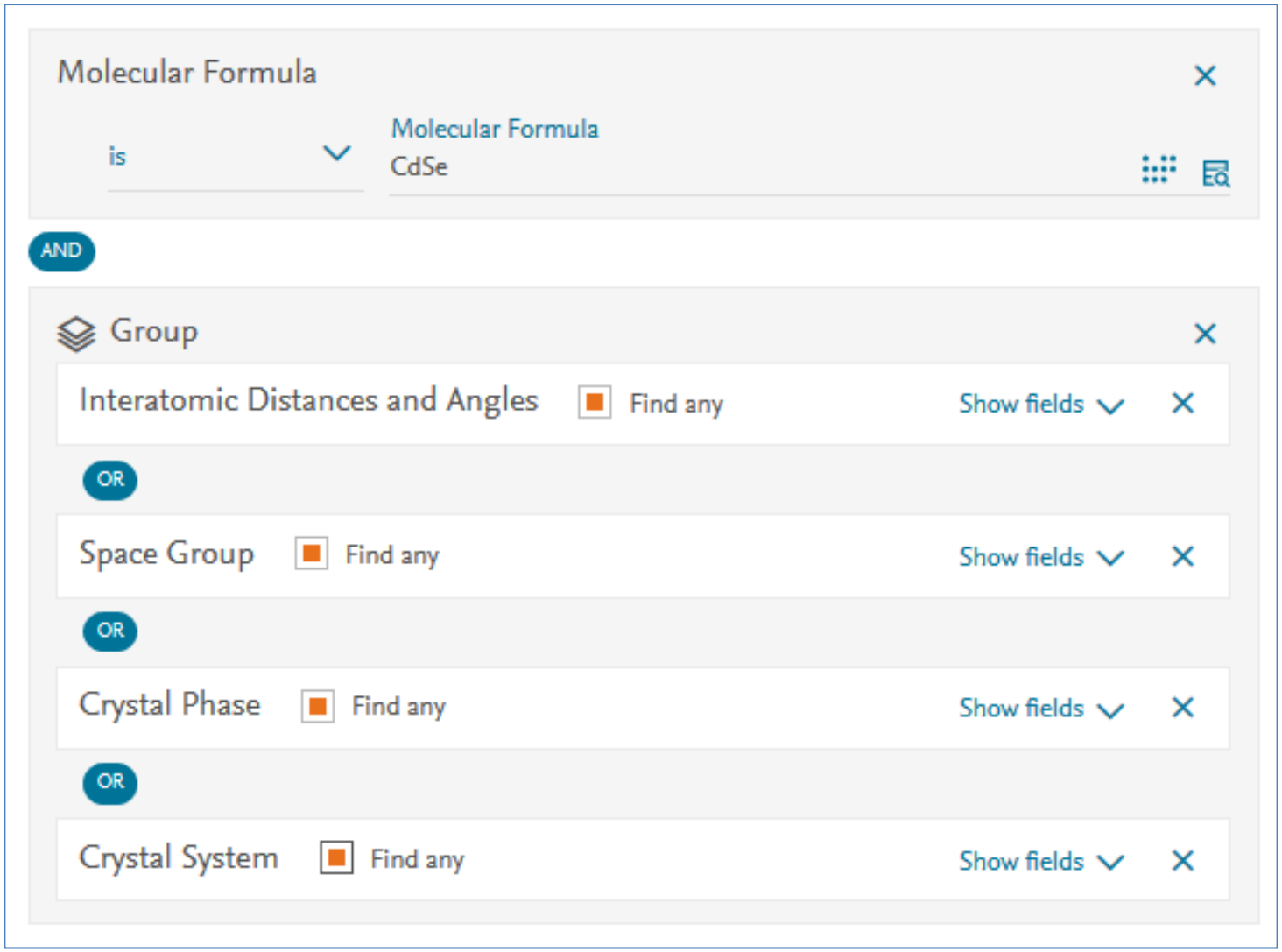
Query Builder 搜尋指定波長範圍高折射率材料

REFRACTIVE INDEX



QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據 -- 原子間距離與角度、空間群、結晶相、晶體體系



QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據-搜尋結果

1

cadmium(II) selenide
CdSe 191.37 11323271

CdSe

Hit Data - 91
Spectra - 226
Preparations - 174
Identification
Bioactivity - 72
Reactions - 468
Physical Data - 605
Other Data - 140
Documents - 1371

Hit Data - 91

- Crystal Phase - 27 hits out of 27
- Crystal System - 4 hits out of 4
- Interatomic Distances and Angles - 2 hits out of 2
- Space Group - 58 hits out of 58

QueryBuilder -- 實驗數據搜尋

CdSe 的 XRD 數據-搜尋結果

Space Group - 58 hits out of 58

Location	Comment (Space Group)	Reference
	Method = Powder X-ray diffraction	Han, Guoping; Wang, Lin; Pei, Cuijin; +5 others - Journal of Alloys and Compounds, 2014, vol. 610, p. 62 - 68 Full Text ↗ Cited 4 times ↗ Show details › Jin, Feng; Zheng, Mei-Ling; Zhang, Mei-Lin; +2 others - RSC Advances, 2014, vol. 4, # 63, p. 33206 - 33214 Full Text ↗ Cited 5 times ↗ Show details › Oyetunde, Temidayo; Afzaal, Mohammad; Vincent, Mark A.; +1 other - Dalton Transactions, 2016, vol. 45, # 46, p. 18603 - 18609 Full Text ↗ Show details ›

Crystal Phase - 6 hits out of 27

Description (Crystal Phase)	Reference
Zinc blende (ZnS), Powder X-ray Diffraction	Mastai; Polsky; Koltypin; +2 others - Journal of the American Chemical Society, 1999, vol. 121, # 43, p. 10047 - 10052 Full Text ↗ Cited 69 times ↗ Show details › Manna; Scher; Alivisatos - Journal of the American Chemical Society, 2000, vol. 122, # 51, p. 12700 - 12706 Full Text ↗ Cited 1,440 times ↗ Show details › Kumar; Sharma - Journal of Physics and Chemistry of Solids, 1998, vol. 59, # 8, p. 1321 - 1325 Full Text ↗ Cited 18 times ↗ Show details ›

搜尋單重態與三重態電子轉移數據

磷光與螢光光譜資料

Phosphorescence Spectroscopy Find any Hide fields

is Description (Phosphorescence Spectroscopy) energy transfer from triplet state

is Solvent (Phosphorescence Spectroscopy)

= Temperature (Phosphorescence Spectroscopy), °C

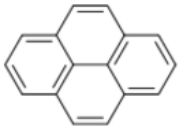
AND

Fluorescence Spectroscopy Find any Hide fields

is Description (Fluorescence Spectroscopy) energy transfer from singlet state

is Solvent (Fluorescence Spectroscopy)

= Temperature (Fluorescence Spectroscopy), °C



pyrene

$C_{16}H_{10}$ 202.255 1307225 129-00-0

Hit Data - 2

Identification

Hit Data - 2

Fluorescence Spectroscopy - 1 hits out of 537

Description (Fluorescence Spectroscopy)	Reference
Energy transfer from singlet state	Ehli, Christian; Aminur Rahman; Jux, Norbert; +9 others - Journal of the American Chemical Society, 2006, vol. 128, # 34, p. 11222 - 11231 Full Text Cited 212 times Show details

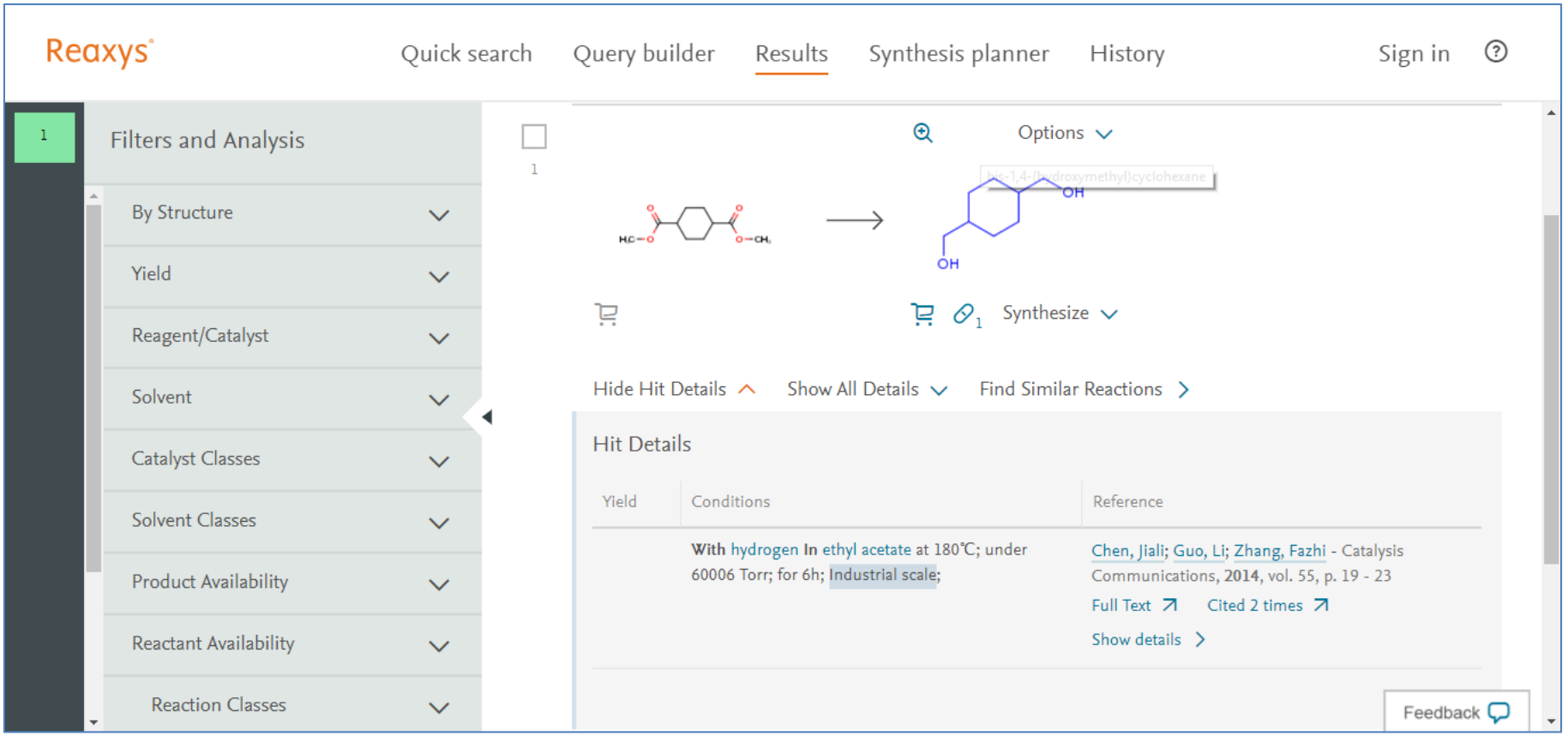
也可搜尋 delayed fluorescence

Phosphorescence Spectroscopy - 1 hits out of 43

Description (Phosphorescence Spectroscopy)	Reference
Energy transfer from triplet state	Borisevich, N. A.; Kazakov, S. M.; Kolesnik, E. E.; +4 others - Journal of Applied Spectroscopy, 2001, vol. 68, # 3, p. 447 - 454, Zhurnal Prikladnoi Spektroskopii, 2001, vol. 68, # 3, p. 343 - 348 Full Text Show details

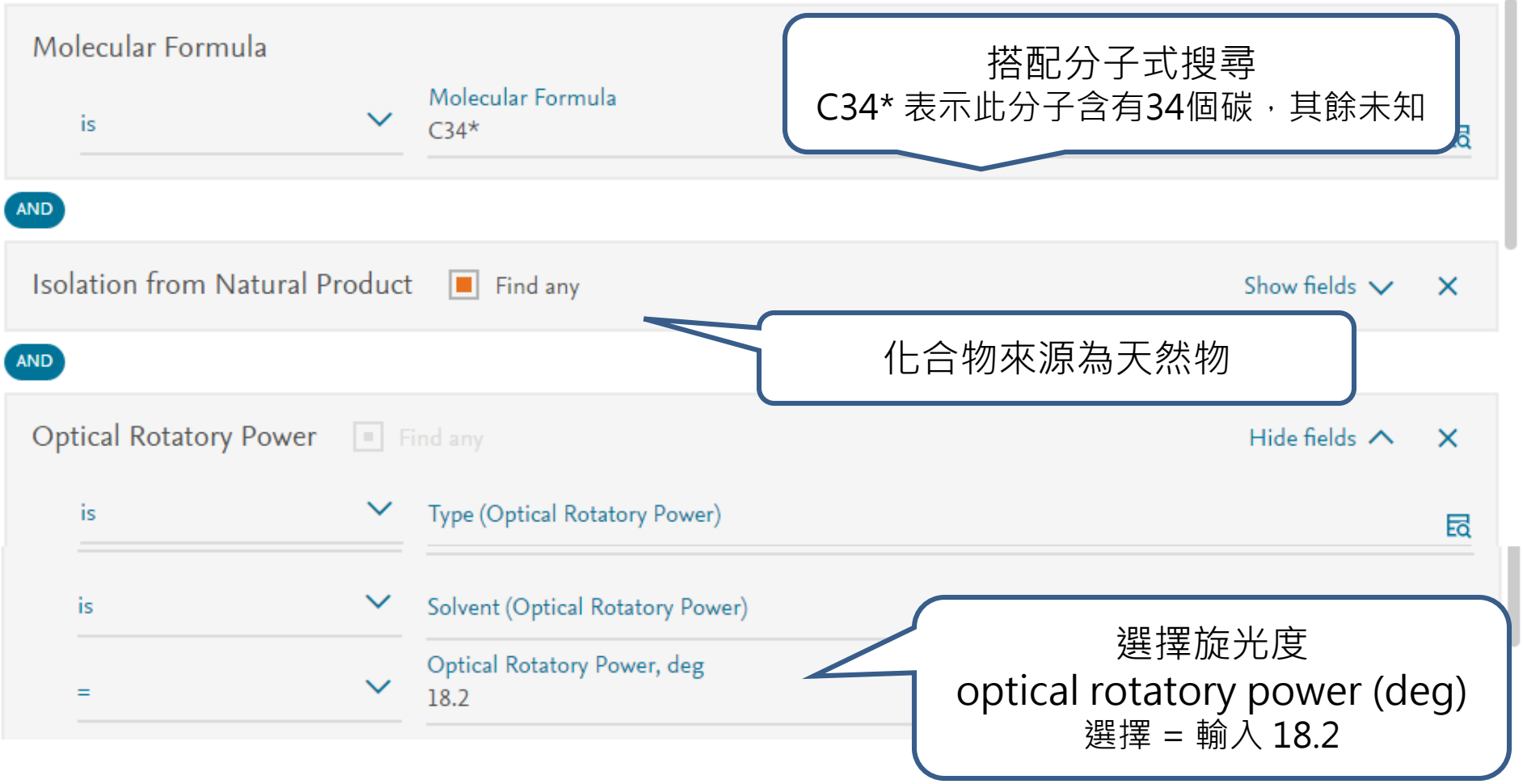
Query Builder – 反應搜尋結果關鍵字限縮 Reaction Basic Index

66 個反應中，工業級大量生產的方法，只有 1 種



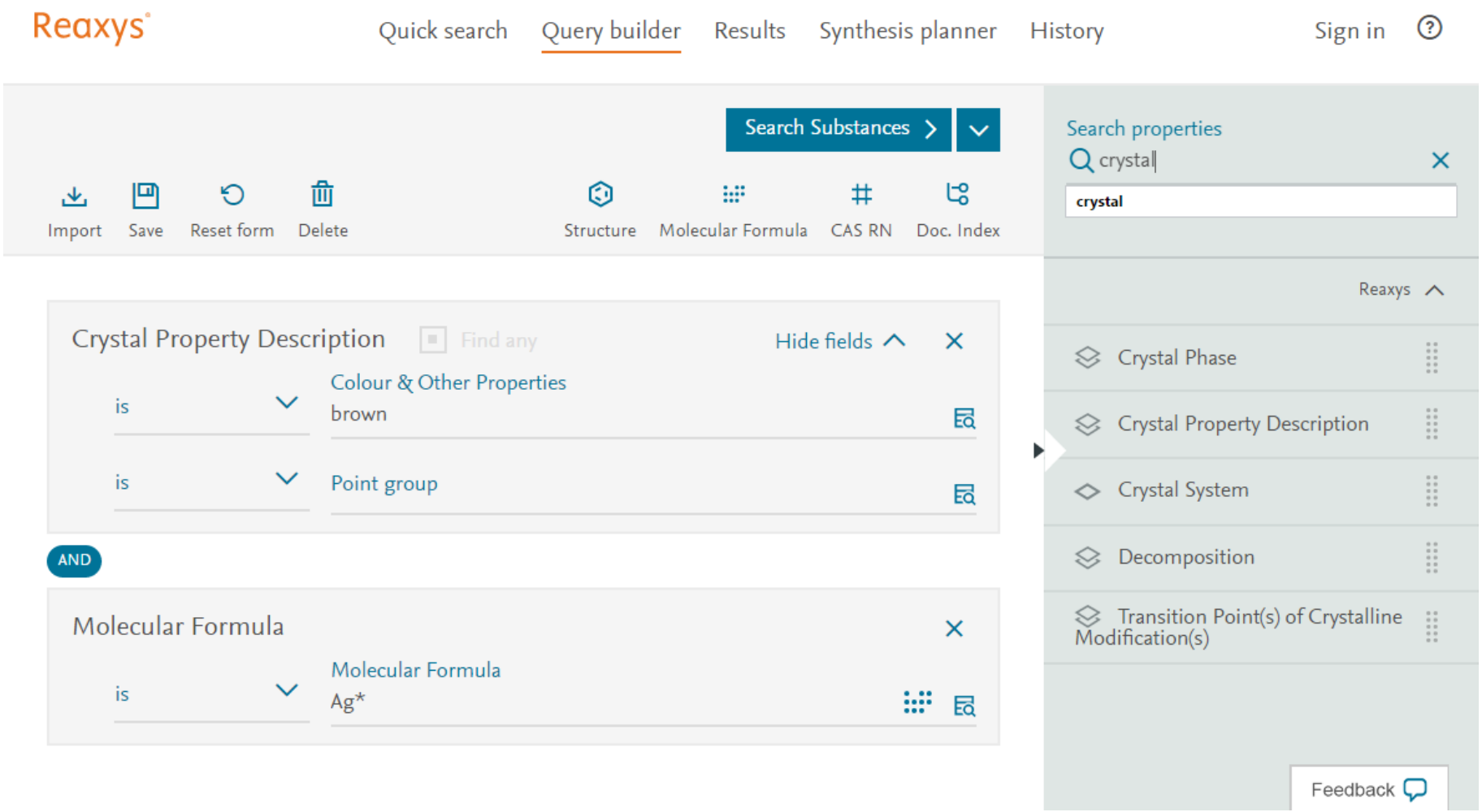
QueryBuilder – 分子式衍生物搜尋

未知物鑑定 -- 由天然物純化出、包含34個碳，旋光度=18.2的所有化合物



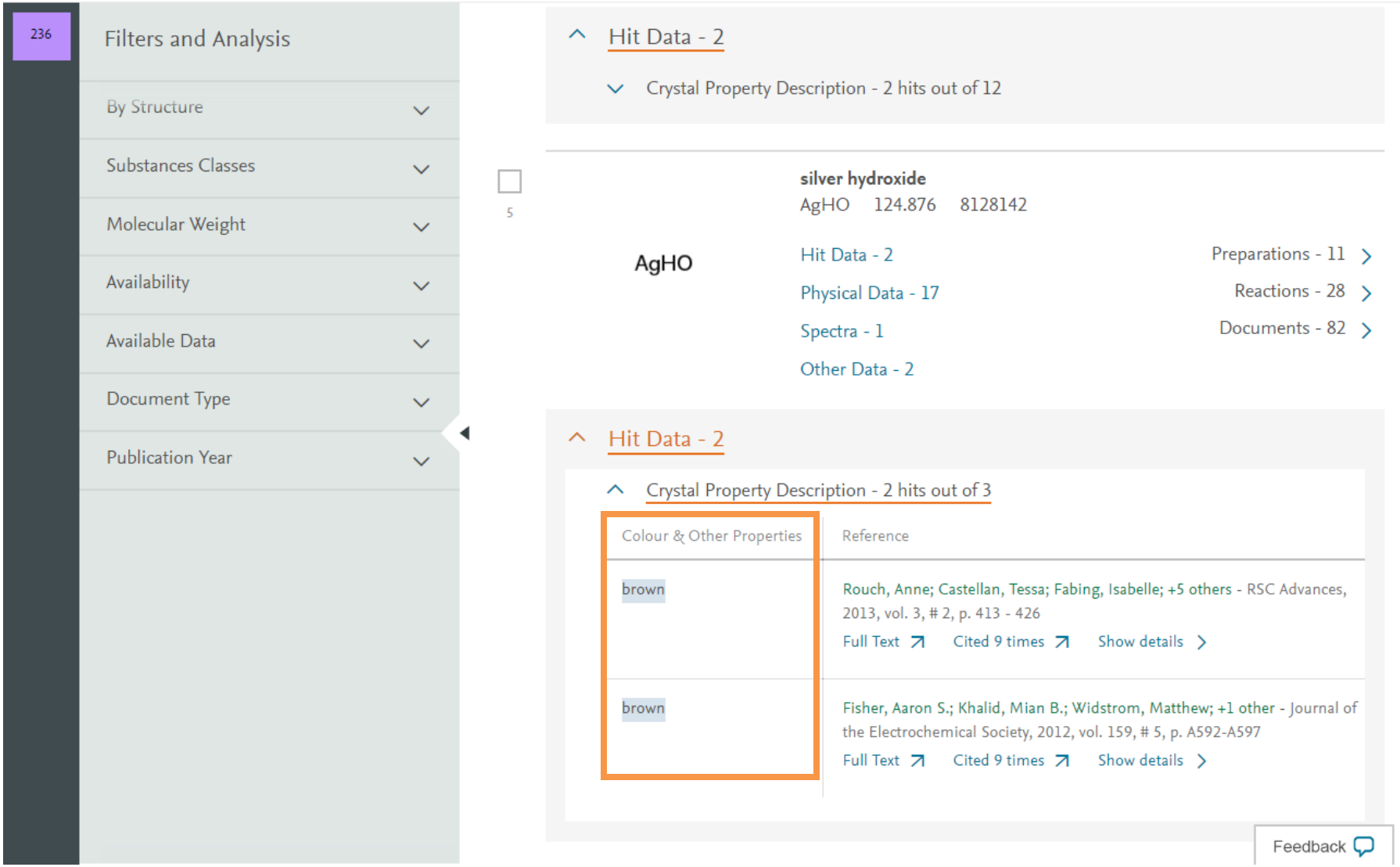
QueryBuilder --分子式衍生物搜尋

搜尋結晶外觀/顏色



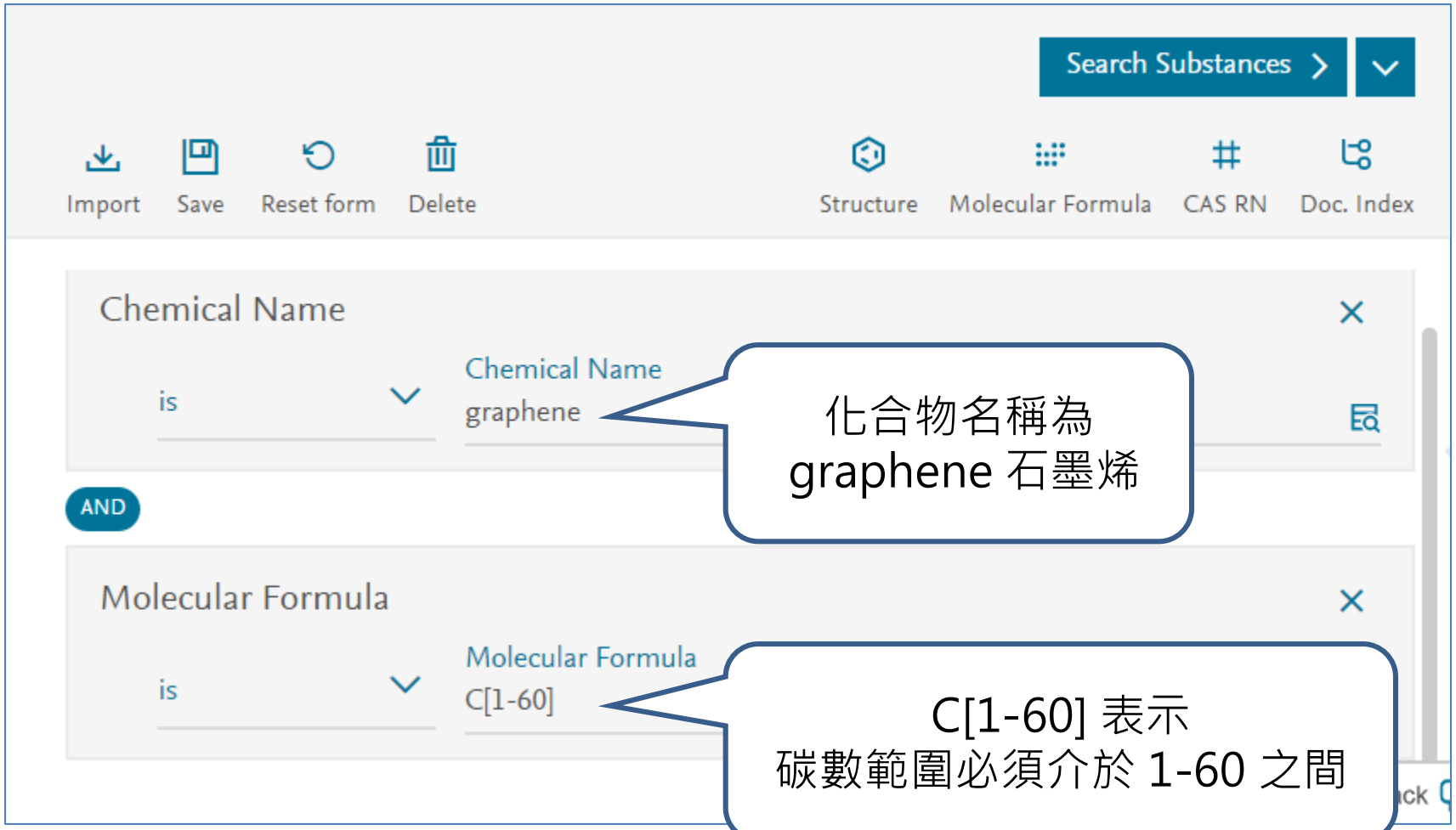
QueryBuilder --分子式衍生物搜尋

未知物鑑定 -- 搜尋含銀的咖啡色結晶，找到 236 種可能化合物



活用分子式搜尋與分子量排序

搜尋指定碳數區間的石墨烯 (135種 → 14 種)



Query Builder 搜尋未知比例合金

Ti?Al?V?* 表示此分子含有
未知數量的鈦Ti, 鋁 Al, 釩 V，
並含有其他未知成份

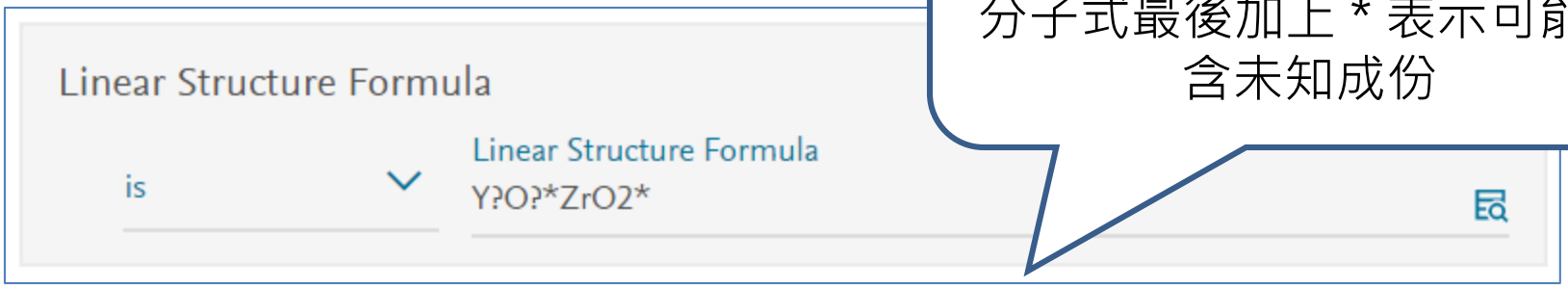
必須含有 Mechanical Properties 數據

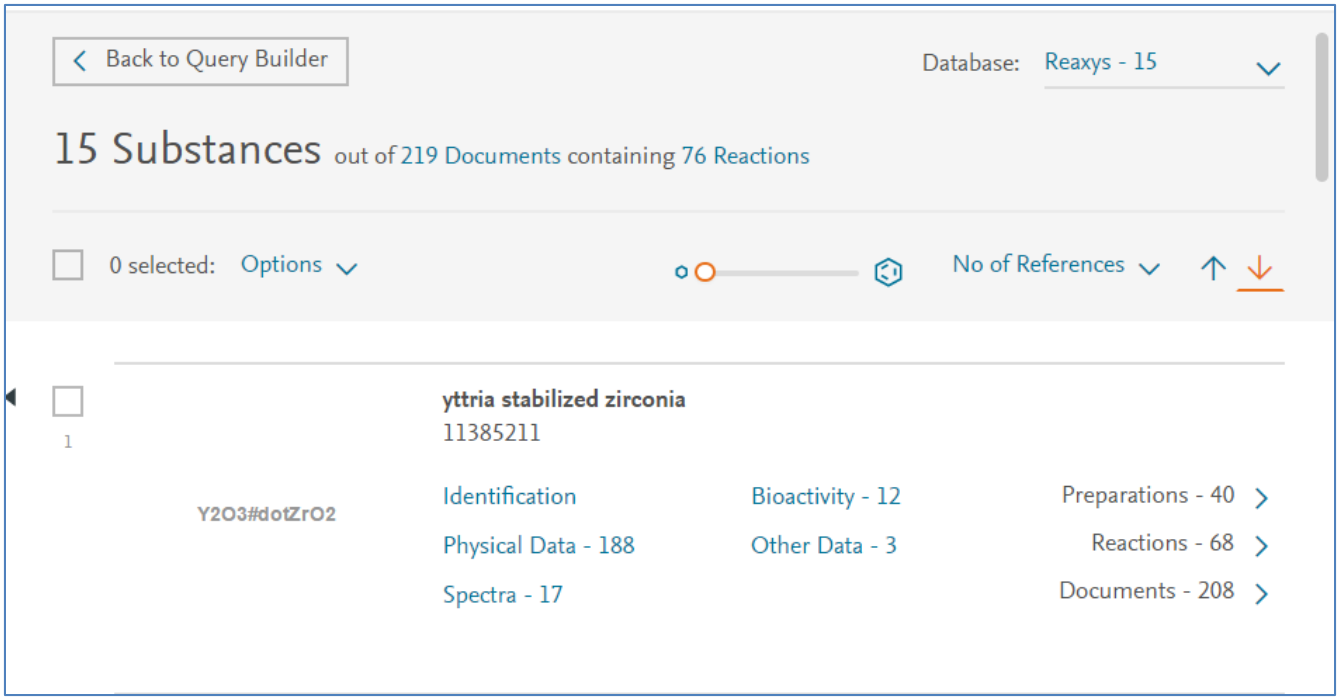
例如：拉伸強度 Tensile strength、降伏點 (彈性極限) yield point

搜尋陶瓷複合材料

活用 LINEAR STRUCTURE FORMULA 欄位

Y?O? 表示氧化釔種類未限定
*表示混合物比例未知
分子式最後加上 * 表示可能包含未知成份





Reaxys 中文線上學習資源

Reaxys 中文學習平台

taiwan.elsevier.com/reaxyshelp

學習影片
Learning Video

利用學習影片自我學習如何有效使用Reaxys，一步一步教學，讓資訊檢索變得更簡單。

文件下載
Document Download

快速上手Reaxys，並用實例介紹如何使用Reaxys功能，您可快速找到答案，讓學習變得更有趣。

線上研討會
Webinar

邀請專家分享使用Reaxys技巧和實例演練操作，讓您從學習中了解如何與資訊互動。

連線問題
Connection Issues

了解常見連線問題，並提供解決之道與聯絡方式。

本平台支援手機及平板使用

ELSEVIER

Thank You!

附錄

Marvin JS 搜尋小技巧

由 ChemDraw 複製結構到 MarvinJS

Reaxys 結構搜尋 – 匯入與匯出 – 1

Edit → Copy as → SMILES

Ctrl + V 貼上

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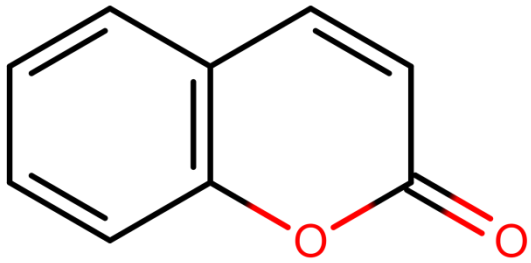
由化合物名稱產生結構

Reaxys 結構搜尋 – 匯入與匯出 – 2

化合物名稱
Coumarin

Create structure template from name >



https://youtu.be/Y2sBPaQpt4o

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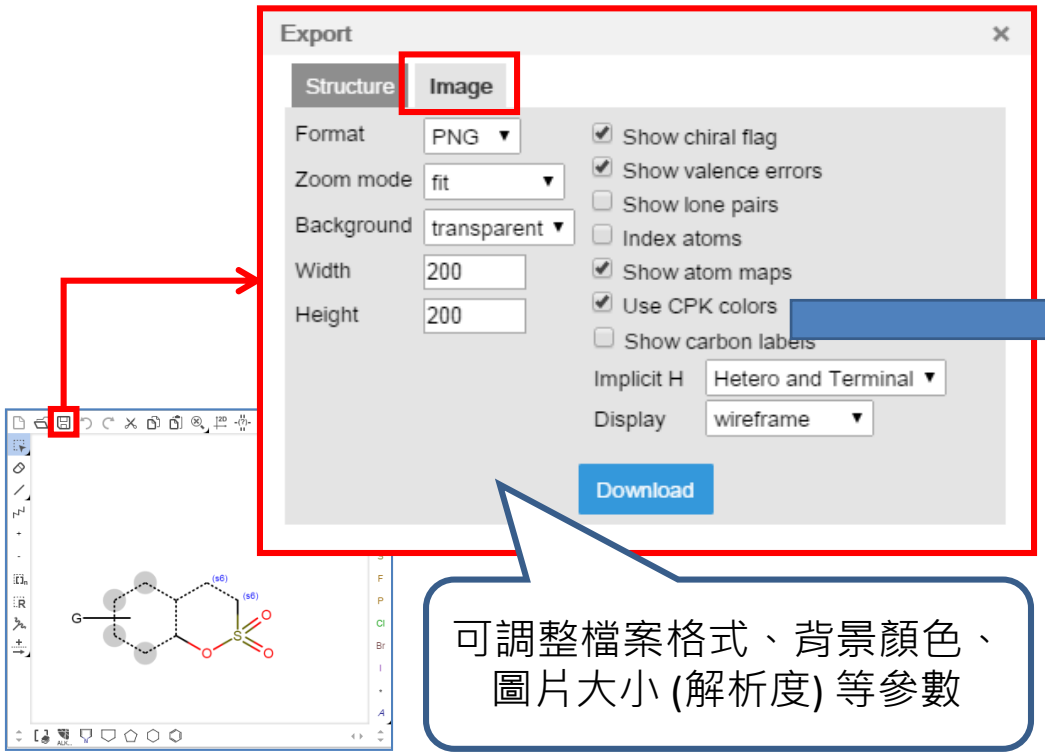
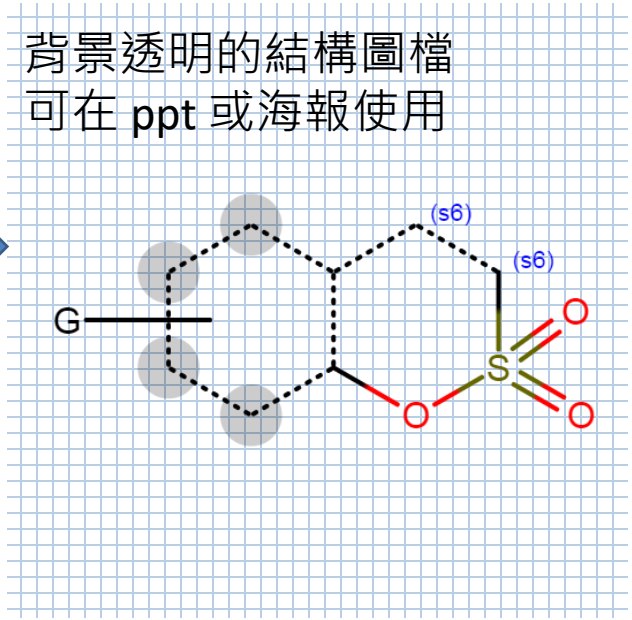
將化學結構存成透明背景的圖檔

Reaxys 結構搜尋 – 匯入與匯出 – 3



可調整檔案格式、背景顏色、圖片大小 (解析度) 等參數



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儲存可編輯的結構檔 .mrv

Reaxys 結構搜尋 – 匯入與匯出 – 4

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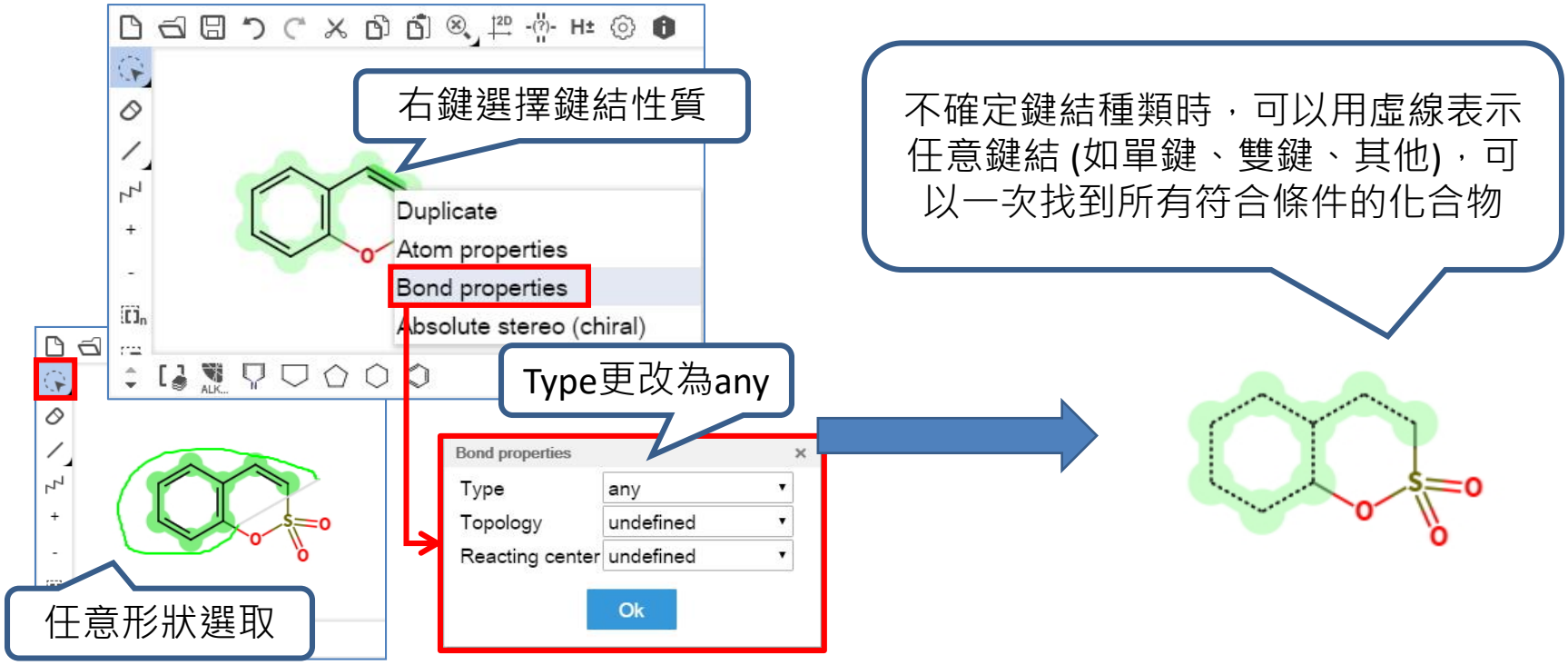
不確定鍵結種類，該如何搜尋?

Reaxys 結構搜尋 – 衍生物搜尋 – bond property



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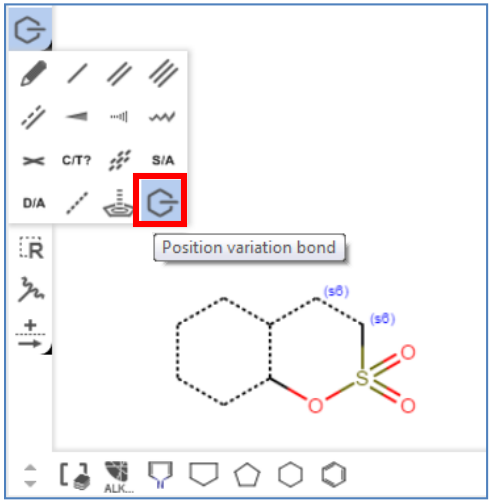
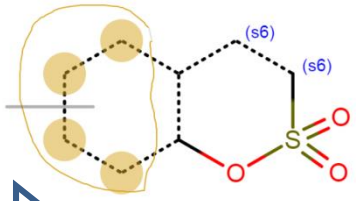
不確定鍵結位置，該如何搜尋?

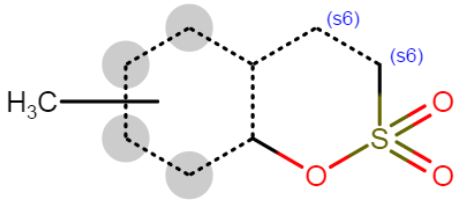
Reaxys 結構搜尋 – 衍生物搜尋 – position variation bond



圈選可能接上
取代基的原子



鍵結與官能基種類
可以再調整



4 個灰色標記的原子
任 1 個接上甲基
就會被搜尋到

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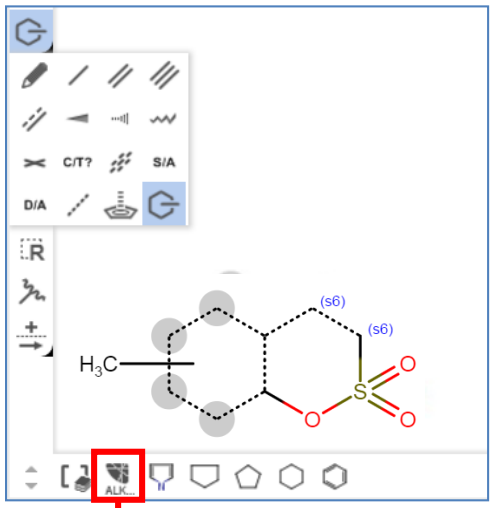
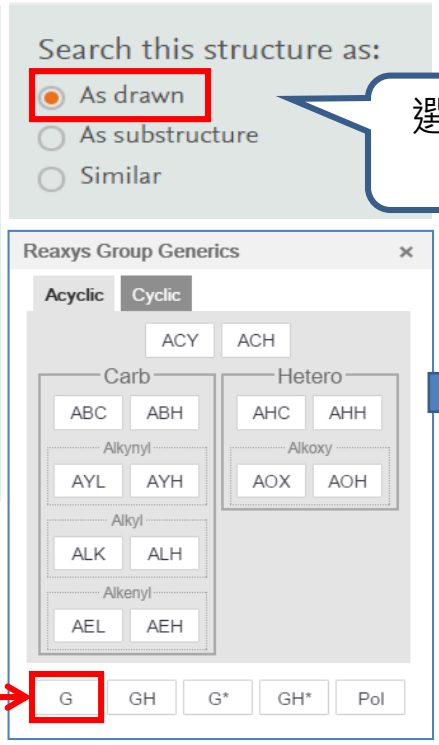
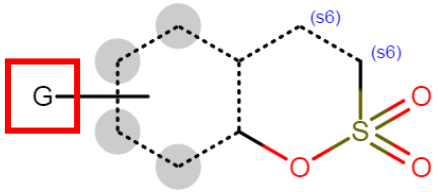
在指定位置，搜尋任意官能基

Reaxys 結構搜尋 – 衍生物搜尋 – G 代表 any functional group





選擇精準搜尋
As drawn



搜尋結果中 G 的位置
可能接上任意官能基

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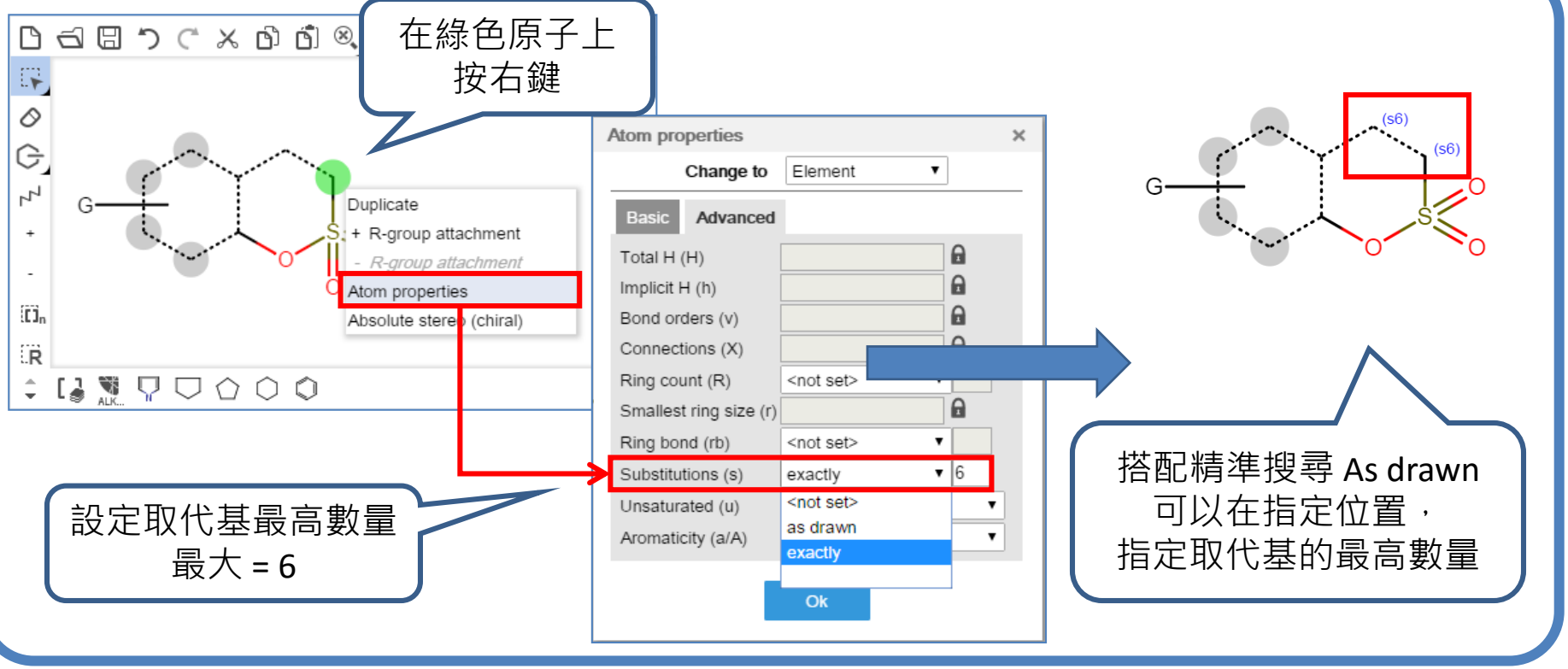
允許取代基

Reaxys 結構搜尋 – 衍生物搜尋 – Substitution 最高數量



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