Reaxys化學資料庫介紹

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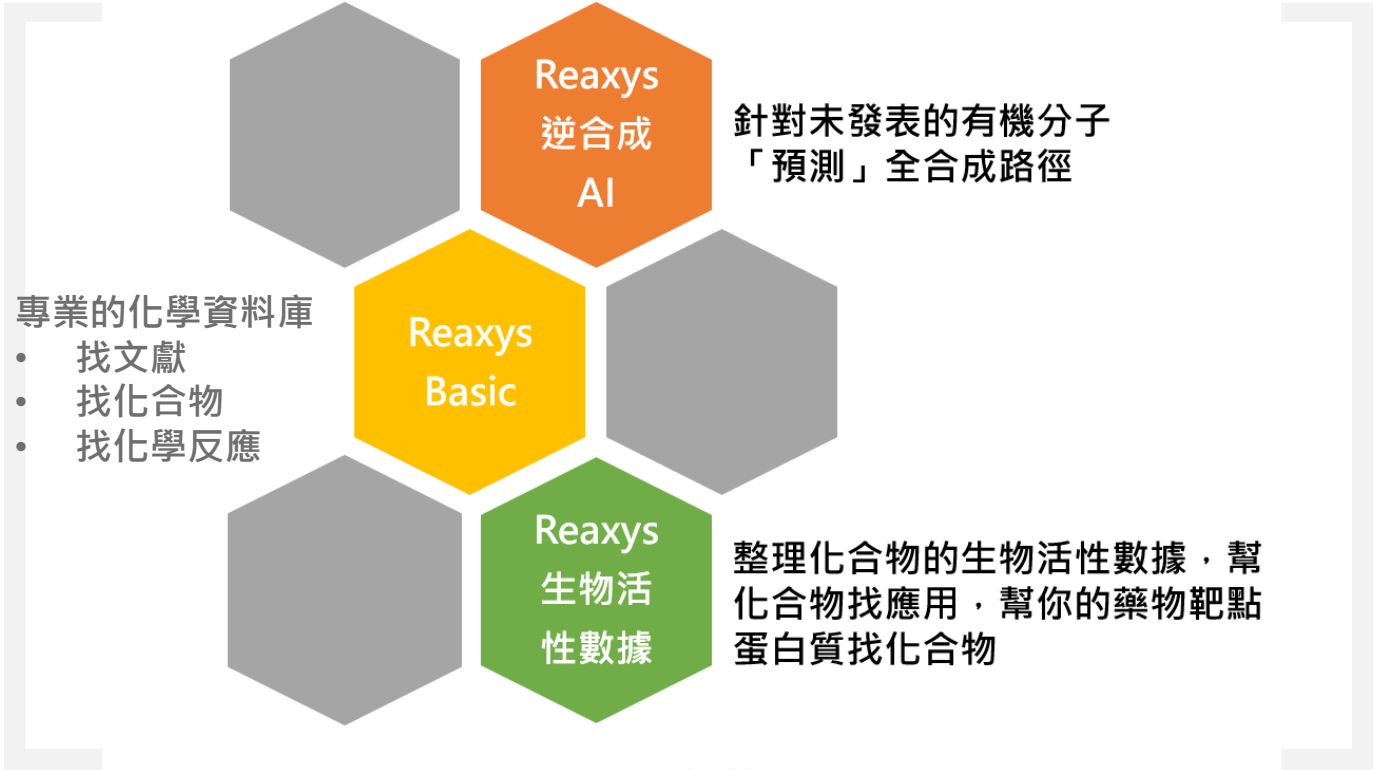
Agenda

- Reaxys 資料庫介紹
- Reaxys 介面介紹
- 快速搜尋 Quick Search
- 結構檢索 Draw
- 進階搜尋 Query Builder - 無機材料、實驗數據檢索
- 進階搜尋 Query Builder -天然萃取物的生物活性應用
- 逆合成工具 Retrosynthesis
- 反應式 Reactions 搜尋
- 線上自我學習資源

- Reaxys 資料庫介紹

Reaxys 全方位版 – 你值得更完整的研究體驗



Reaxys提供文章更著重於實驗數據

從化學相關的論文和專利中透過人工提取和整理關鍵的「實驗數據」

除了能搜尋文獻，更注重提供多元的檢索形式，讓您**更快的整理資料**，進行以資料驅動的決策(Data driven decisions)

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

Relevant answers to key research questions:

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

Reaxys涵蓋的範圍

學術論文

專家從大約460個期刊標題中手動提取實驗數據

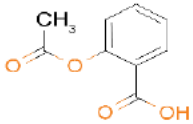
- 有機化学　1771年～
- 無機化学･有機金屬錯合物　1772年～

此外，從16,000個期刊標題中機器提取結構和其他資訊

專利

目前七個專利局手動提取，主要為有機化合物(WO,US,EP,JP,CN,KR,TW)

2021年起，覆盖範圍將擴大到105個專利局和所有化學品分類



>257 M
Substances

>500 M
Experimental data

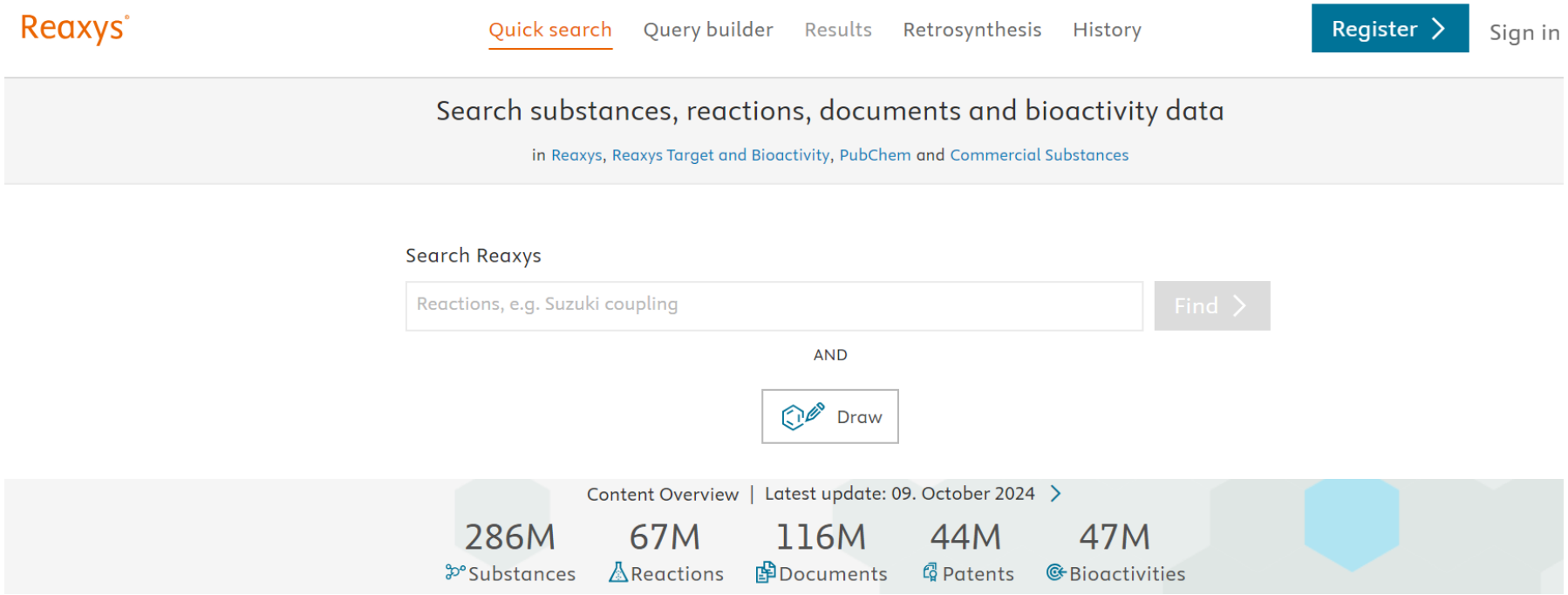
>60 M
Reactions

>101 M
Journal articles & Patents

ELSEVIER

Reaxys提供最即時的服務

在授權IP範圍內，打開瀏覽器鍵入 http://www.reaxys.com



Beginner

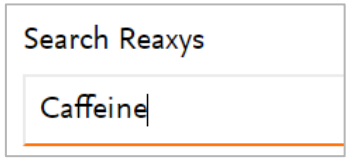
Reaxys檢索介面導覽

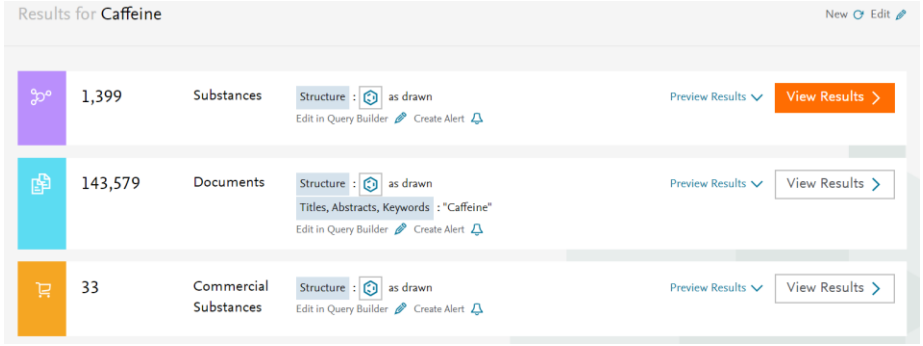
Beginner

Reaxys檢索介面導覽

ELSEVIER

可透過各種方式檢索

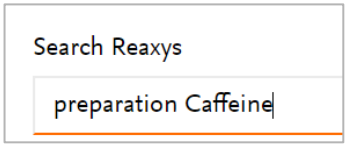




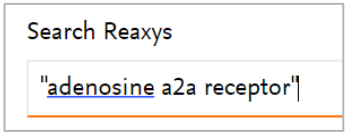
實驗數值與參考出處

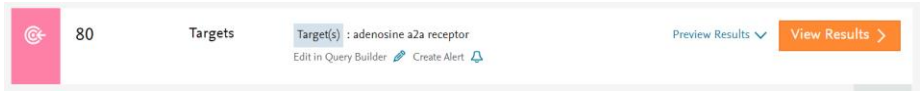
文獻、專利

供應商資訊



合成方法

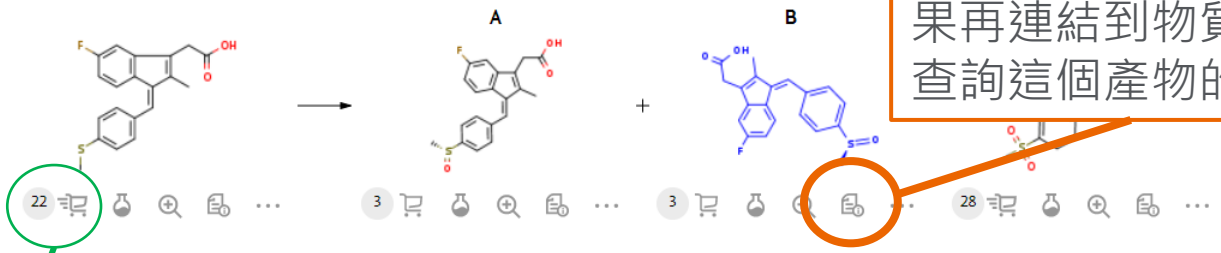




蛋白、可用藥靶點與化合物交互作用的數據

Reaxys資料庫中的資料互相串連①

Reaxys資料庫中的資料互相串連②



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。

從購物車連結到商用資料庫去評估實驗的成本

1 Conditions Find Similar Reaction ID: 35329138

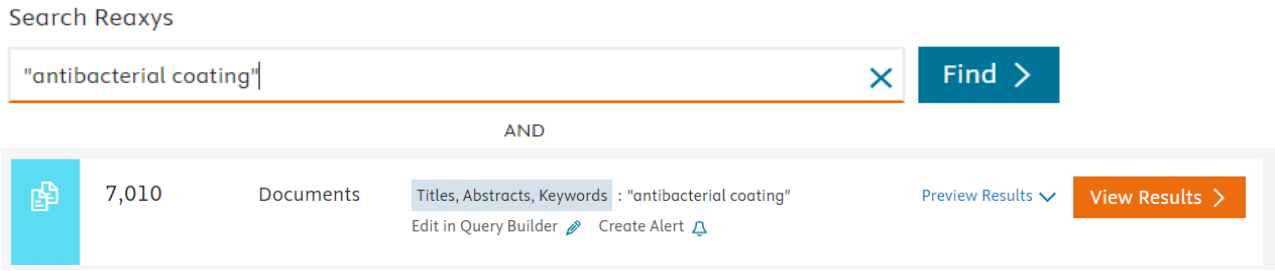
	Yield	Reference
idazole; $C_{84}H_{72}ClFeN_4O_{12}S_4^{(4-)}*4Na^{(1+)}$; dihydrogen peroxide **In** methanol; aq. phosphate buffer at rt atmosphere; Overall yield = 100 %Spectr.; enantioselective reaction; cedure	A n/a B n/a C n/a	Srour, Hassan; Jalkh, Joanna; Le Maux, Paul; Chevance, Soizic; Kobeissi, Marwan; Simonneaux, Gérard **[Journal of Molecular Catalysis A: Chemical, 2013**, vol. 370, p. 75 - 79] Full Text Cited 37 times Details Abstract

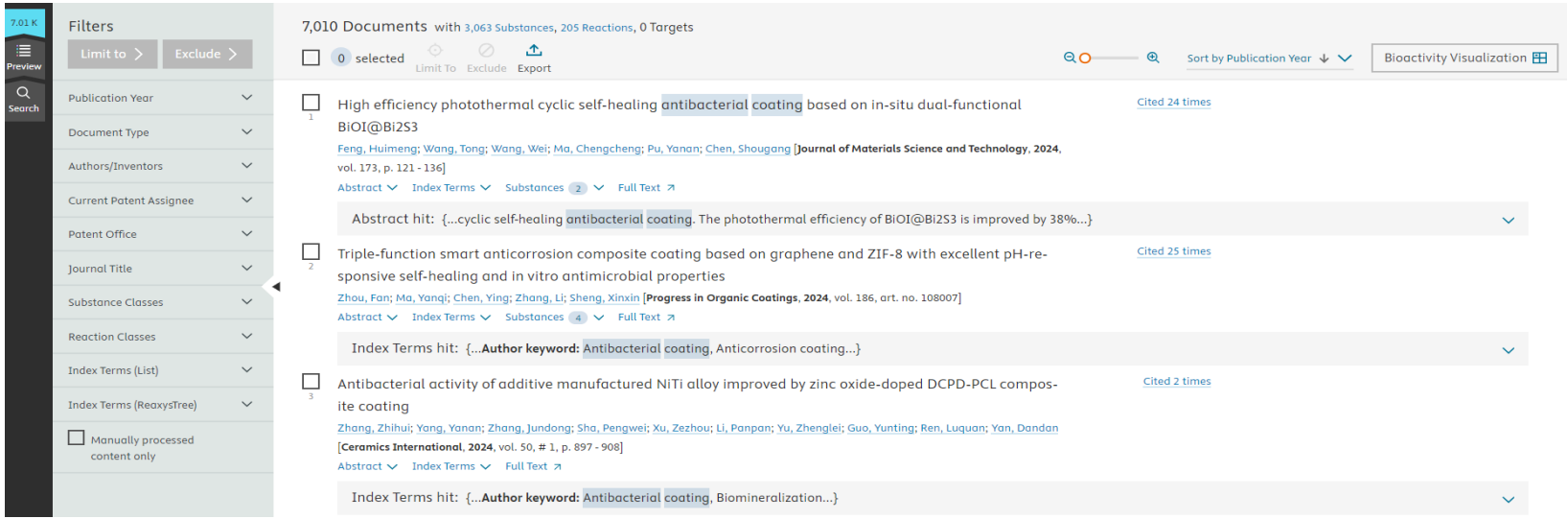
rocedure for asymmetric sulfoxidation

General procedure: Methyl phenyl sulfoxide. Manganese porphyrin complex 1 (1.6 mg, 1 μmol) and imidazole (1.7 mg, 25 μmol) were placed in a test tube under argon. The solvent (375 μL MeOH + 125 μL PBS, pH 7) was then added via syringe, followed by the sulfide (5 μL, 42.3 μmol). Finally, hydrogen peroxide (1.8 μL, 21.2 μmol) was added in one portion to the solution. The reaction was followed by gas chromatography (GC). From GC we knew that the reaction was over after 2 h with a 100% yield containing 1% sulfone. The solution was extracted with dichloromethane three times and then dried over $MgSO_4$. The ee was then determined by HPLC to be 33%.

- 快速搜尋 Quick Search

快速搜尋 -藉由關鍵字搜尋文獻 Text Search





快速搜尋 – Material science 藉由機械性質搜尋

Search Reaxys

"bend strength" of Aluminium

Find

Substance Properties, e.g. melting point of xylitol

Hit Data - 8

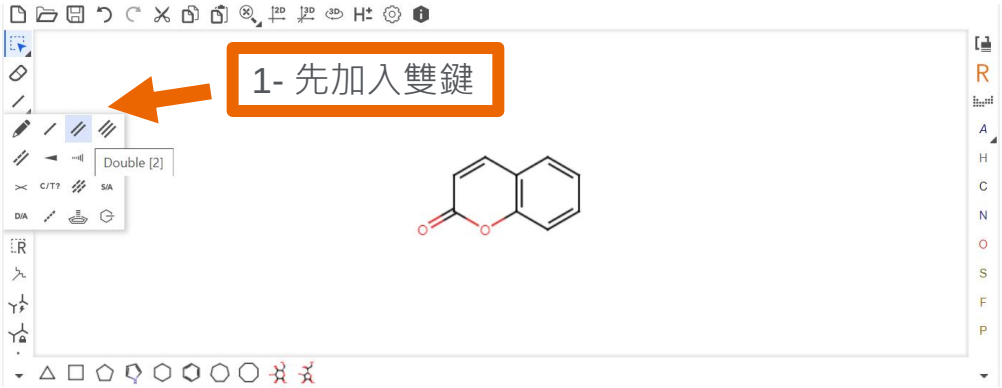
Mechanical Properties - 8 hits out of 362

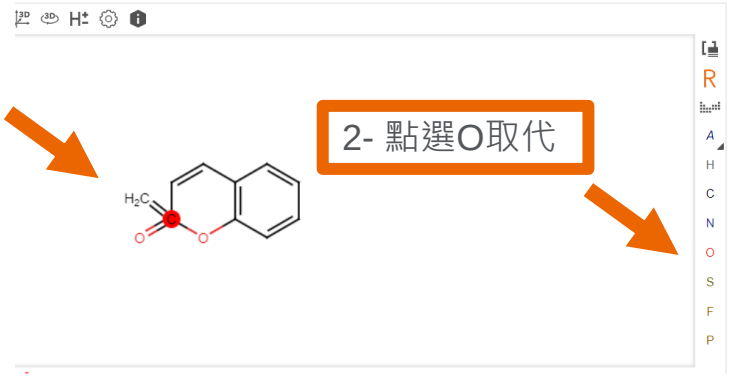
Show/Hide columns

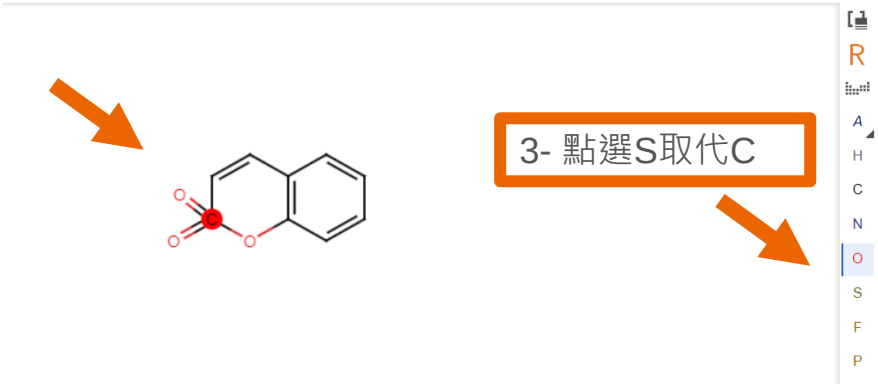
Description (Mechanical Properties)	Comment (Mechanical Properties)	Reference
Bend strength	value of strength = 188 N/mm**2 - 190 N/mm**2	Abenojar; Martinez; Velasco[**Journal of Alloys and Compounds**, **2006**, vol. 422, # 1-2, p. 67 - 72] Full Text ↗ Cited 31 times ↗ Details > Abstract >
Bend strength	value of strength = 29 N/mm**2	Linicus, W.; Scheuer, E.[**Metallwirtschaft, Metallwissenschaft, Metalltechnik**, **1934**, vol. 13, p. 850 - 850] Full Text ↗ Details > No author[**Gmelin Handbuch der Anorganischen Chemie**, Gmelin Handbook: Al: MVol.A4, 17, page 579 - 582] Full Text ↗ Details >

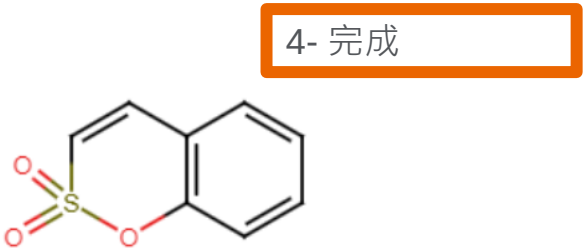
- 結構檢索 Draw

畫圖示範 Carbonyl Group to Sulfonyl Group





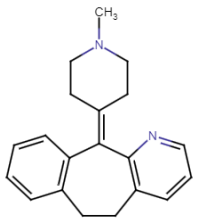




Beginner

Reaxys三種結構搜尋與怎麼用

我感興趣的結構



Azatadine
CAS# 3964-81-6

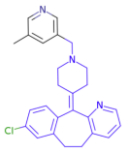
As drawn

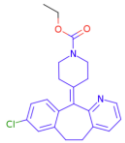
尋找跟我畫的「一模一樣」結構

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

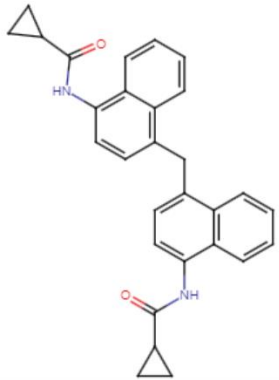
「結構類似」的化合物
提供不同程度的結構變化

線上示範

Beginner

示範- 結構探索

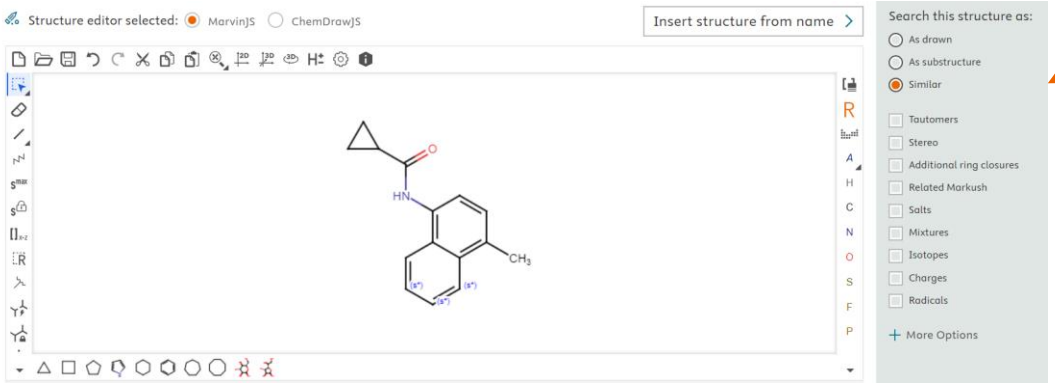
我有一個實驗室感興趣的結構，是沒有人發表過的，如何從有**相似化學結構**的文獻中，找尋可以參考應用、關鍵的實驗數據。



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

線上示範

修改結構, 點選 Similar



結果顯示

2	Substances	Structure : tight similarity	Edit in Query Builder	Create Alert	Preview Results / View Results
2	Substances	Structure : near similarity	Edit in Query Builder	Create Alert	Preview Results / View Results
18	Substances	Structure : average similarity	Edit in Query Builder	Create Alert	Preview Results / View Results

Reaxys 線上學習資源 – 結構編輯器

- Reaxys 結構編輯器 - 基本介紹
- Reaxys 結構編輯器 - 不定位鍵
- Reaxys 結構編輯器 - 縮寫官能基團
- Reaxys 結構編輯器 - 原子列表與原子列表非
- Reaxys 結構編輯器 - R 基團與末端定義工具
- Reaxys 結構編輯器 - 自訂反應中心
- Reaxys 結構編輯器 - 相似結構搜尋 原子鎖工具
- Reaxys 結構編輯器 - G 任意官能基工具定義
- Reaxys 結構編輯器 - 原子屬性列表
- Reaxys 結構編輯器 - 鹽類與同位素

- 進階搜尋 Query Builder
  -無機材料, 實驗數據檢索

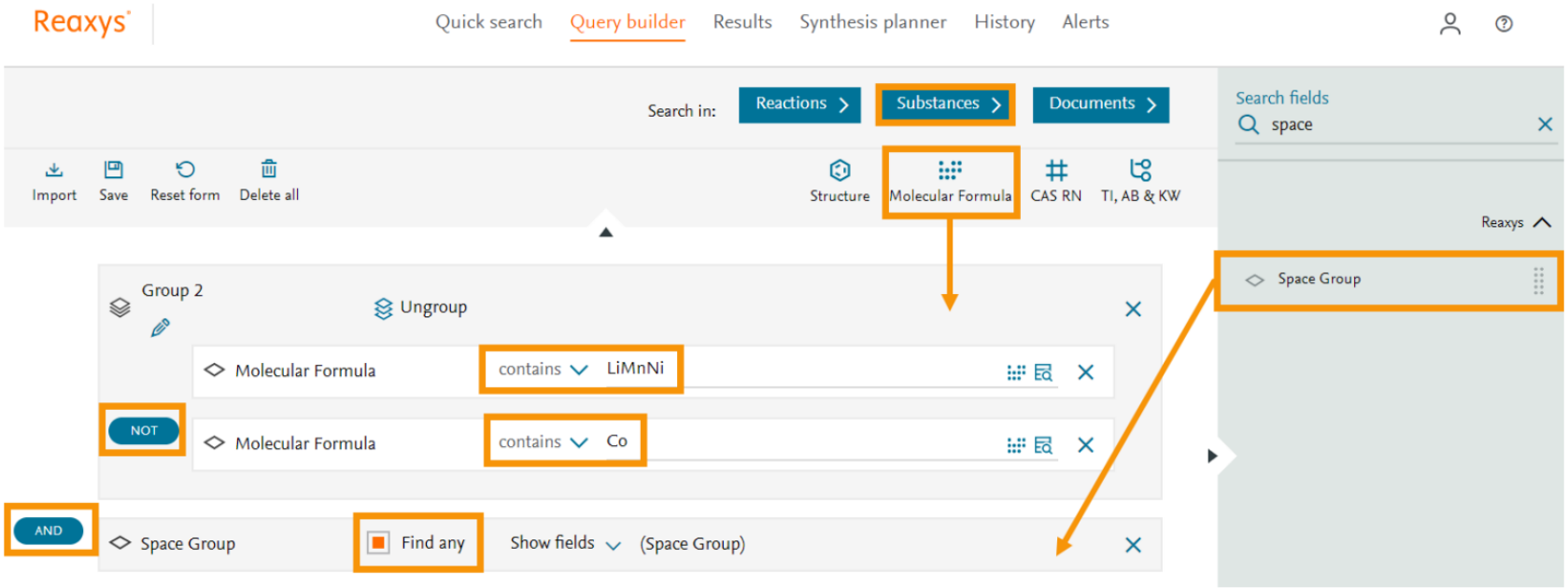
Beginner

分子式檢索

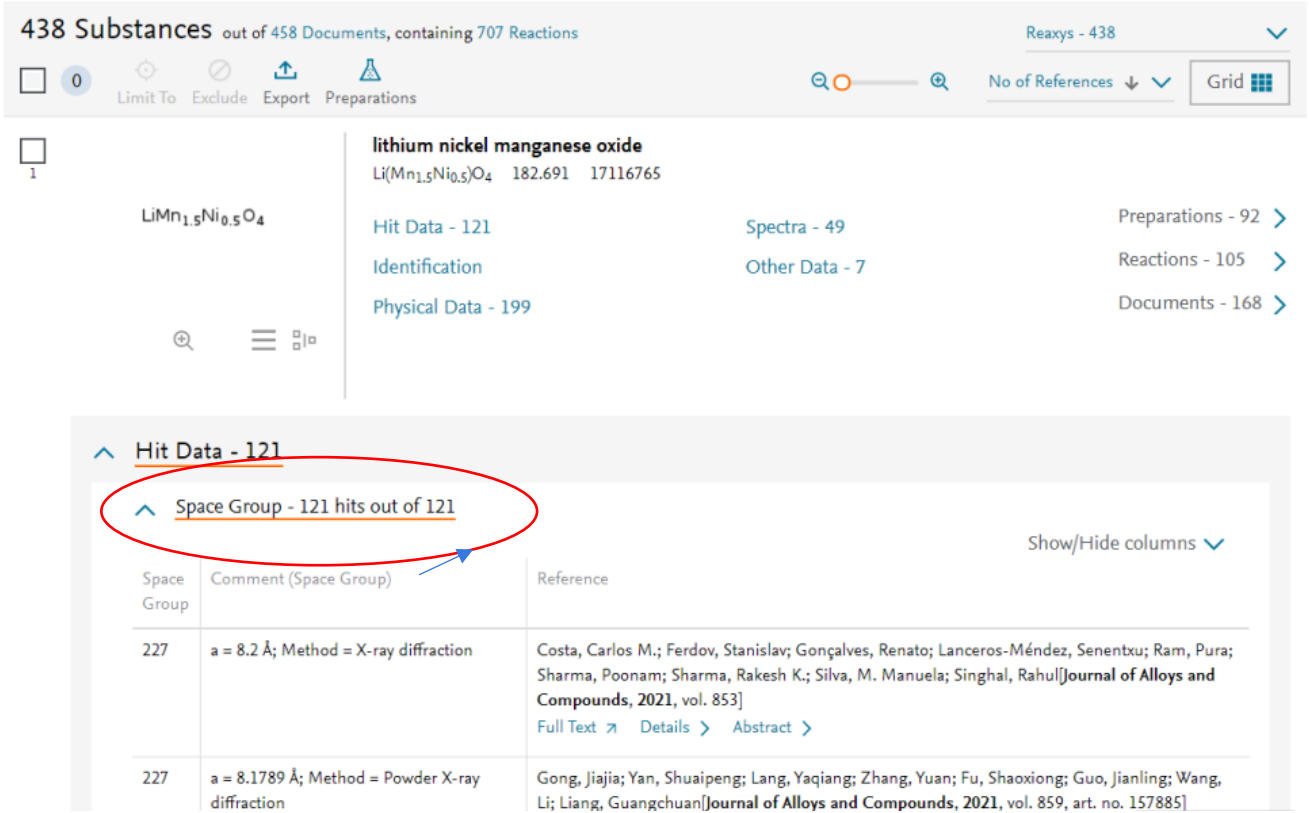
Question: “鈷是很常見的電極材料，然而因為社會經濟、環境與安全性的考量，實驗室希望設計不含鈷的鋰電池電極材料。”

利用進階搜尋工具「Molecular Formula」

分子式検索①


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Search in:
Reactions
Substances
Documents
Import
Save
Reset form
Delete all
Structure
Molecular Formula
CAS RN
TI, AB & KW
Search fields
space
Reaxys
Space Group
Group 2
Ungroup
Molecular Formula
contains
LiMnNi
NOT
Molecular Formula
contains
Co
AND
Space Group
Find any
Show fields
(Space Group)

分子式検索②


438 Substances out of 458 Documents, containing 707 Reactions
Reaxys - 438
0
Limit To
Exclude
Export
Preparations
No of References
Grid
1
LiMn1.5Ni0.5O4
lithium nickel manganese oxide
Li(Mn1.5Ni0.5)O4 182.691 17116765
Hit Data - 121
Spectra - 49
Preparations - 92
Identification
Other Data - 7
Reactions - 105
Physical Data - 199
Documents - 168
Hit Data - 121
Space Group - 121 hits out of 121
Show/Hide columns
Space Group
Comment (Space Group)
Reference
227
a = 8.2 Å; Method = X-ray diffraction
Costa, Carlos M.; Ferdov, Stanislav; Gonçalves, Renato; Lanceros-Méndez, Senentxu; Ram, Pura; Sharma, Poonam; Sharma, Rakesh K.; Silva, M. Manuela; Singhal, Rahul[Journal of Alloys and Compounds, 2021, vol. 853]
Full Text
Details
Abstract
227
a = 8.1789 Å; Method = Powder X-ray diffraction
Gong, Jiajia; Yan, Shuaipeng; Lang, Yaqiang; Zhang, Yuan; Fu, Shaoxiong; Guo, Jianling; Wang, Li; Liang, Guangchuan[Journal of Alloys and Compounds, 2021, vol. 859, art. no. 157885]

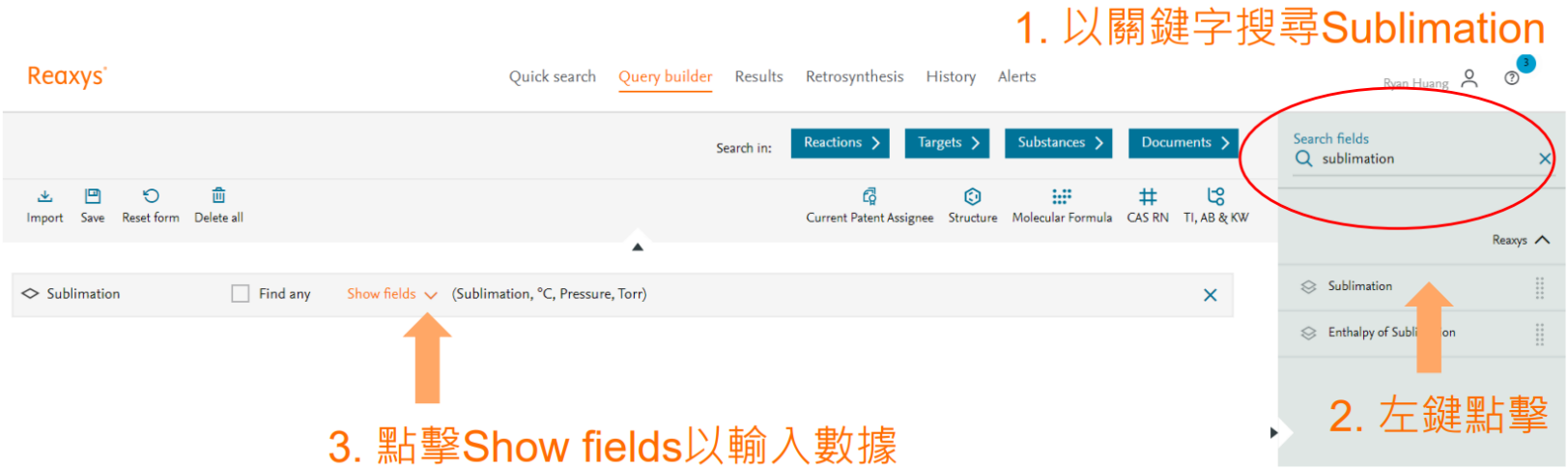
Beginner

實驗數據檢索

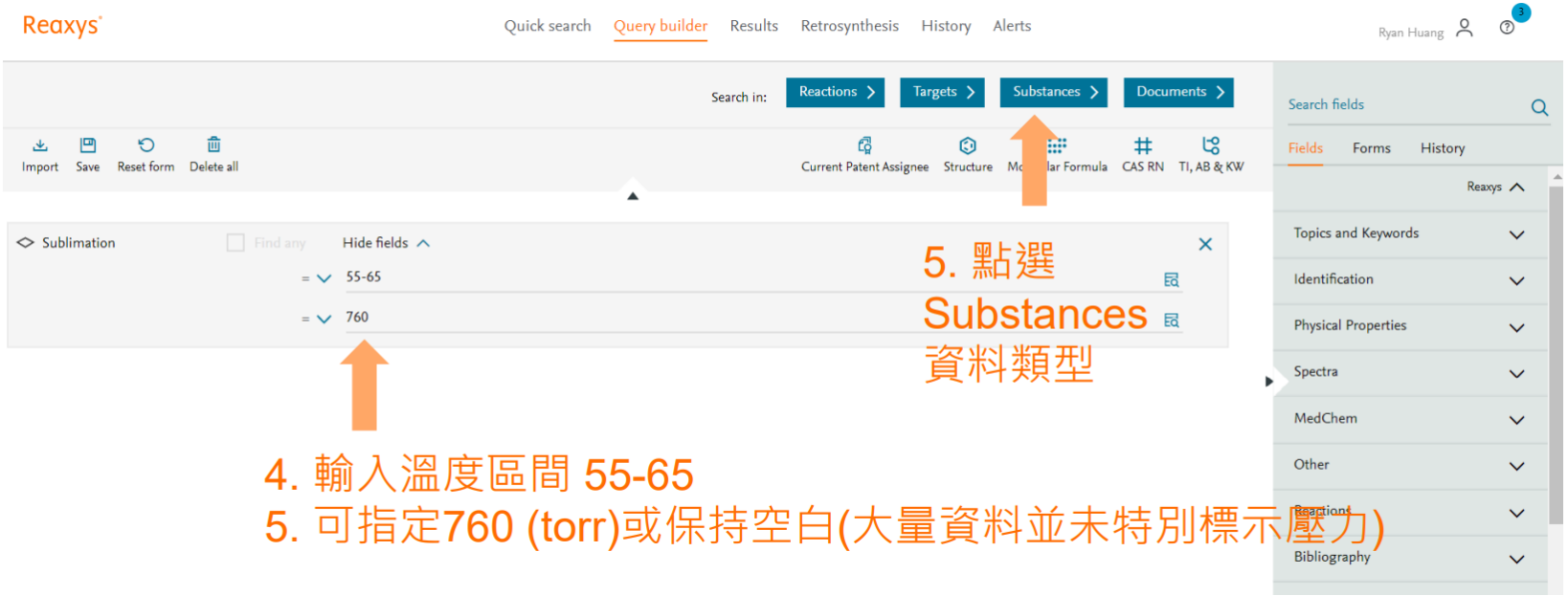
Question: 實驗室需尋找加熱至約60度可昇華的材料，然而利用Google取得的資訊雜訊太多，如何從實驗數據搜尋符合的材料再連結至相關文獻”

利用進階搜尋工具「Sublimation」

實驗數據檢索①


1. 以關鍵字搜尋Sublimation
Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Current Patent Assignee
Structure
Molecular Formula
CAS RN
TI, AB & KW
Search fields
sublimation
Reaxys
Sublimation
Enthalpy of Sublimation
Sublimation
Find any
Show fields
(Sublimation, °C, Pressure, Torr)
2. 左鍵點擊
3. 點擊Show fields以輸入數據

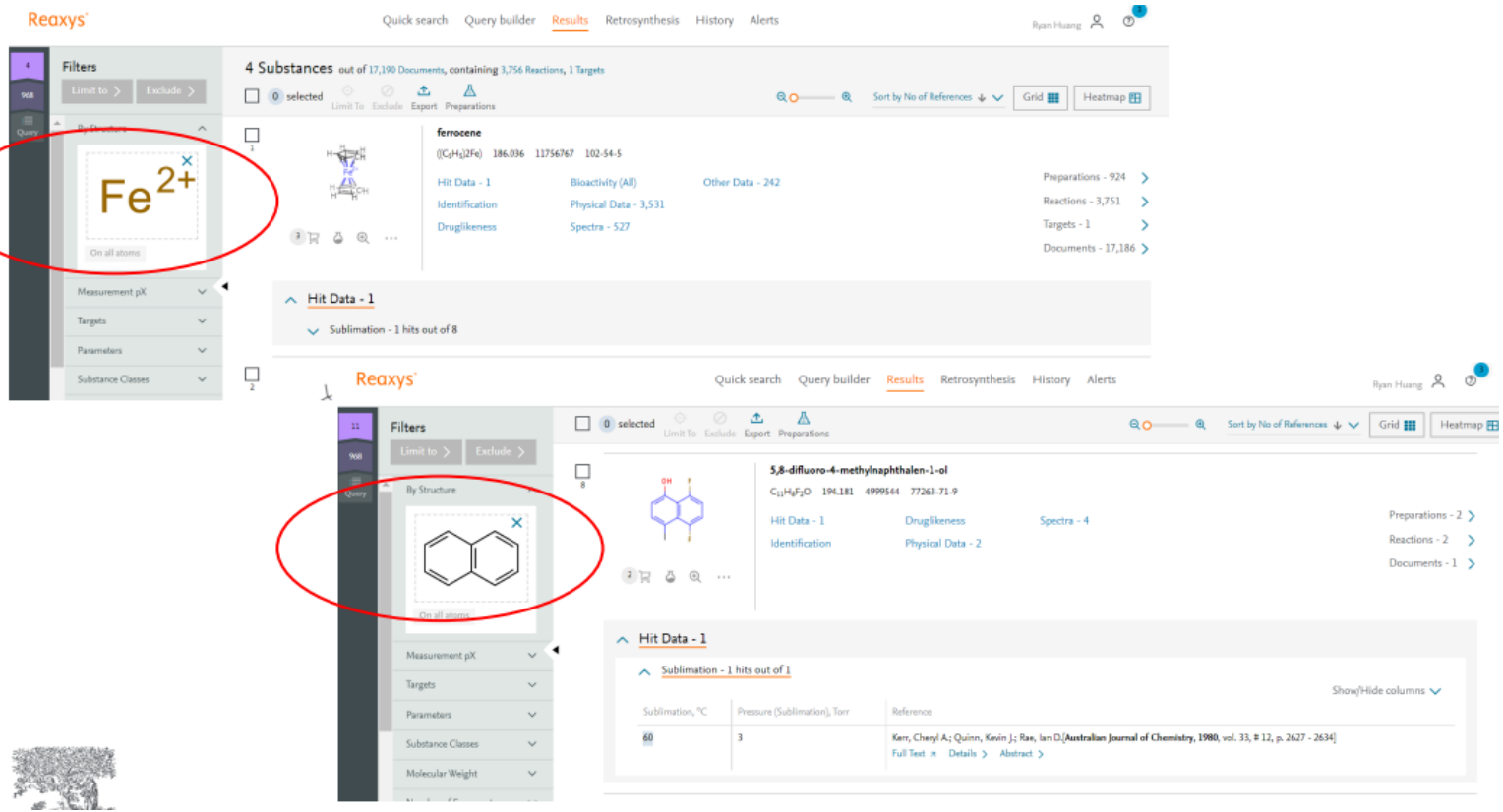
實驗數據檢索②


Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Ryan Huang
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Current Patent Assignee
Structure
CAS RN
TI, AB & KW
Search fields
Fields
Forms
History
Reaxys
Topics and Keywords
Identification
Physical Properties
Spectra
MedChem
Other
Bibliography
Sublimation
Find any
Hide fields
55-65
760
5. 點選
Substances
資料類型
4. 輸入溫度區間 55-65
5. 可指定760 (torr)或保持空白(大量資料並未特別標示壓力)

實驗數據檢索③

系統會將Sublimation資料標示於Hit Data方便比較並列出文獻出處

實驗數據檢索④


Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Ryan Huang
Filters
Limit to
Exclude
4 Substances out of 17,190 Documents, containing 3,756 Reactions, 1 Targets
0 selected
Limit To
Exclude
Export
Preparations
Sort by No of References
Grid
Heatmap
Fe2+
On all atoms
Measurement pX
Targets
Parameters
Substance Classes
ferrocene
((C5H5)2Fe) 186.036 11756767 102-54-5
Hit Data - 1
Bioactivity (All)
Other Data - 242
Identification
Physical Data - 3,531
Druglikeness
Spectra - 527
Preparations - 924
Reactions - 3,751
Targets - 1
Documents - 17,186
Hit Data - 1
Sublimation - 1 hits out of 8
Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Ryan Huang
Filters
Limit to
Exclude
0 selected
Limit To
Exclude
Export
Preparations
Sort by No of References
Grid
Heatmap
By Structure
On all atoms
Measurement pX
Targets
Parameters
Substance Classes
Molecular Weight
5,8-difluoro-4-methylnaphthalen-1-ol
C11H8F2O 194.181 4999544 77263-71-9
Hit Data - 1
Druglikeness
Spectra - 4
Identification
Physical Data - 2
Preparations - 2
Reactions - 2
Documents - 1
Hit Data - 1
Sublimation - 1 hits out of 1
Show/Hide columns
Sublimation, °C
Pressure (Sublimation), Torr
Reference
60
3
Kerr, Cheryl A.; Quinn, Kevin J.; Rae, Ian D.[Australian Journal of Chemistry, 1980, vol. 33, # 12, p. 2627 - 2634]
Full Text
Details
Abstract

- 進階搜尋 Query Builder
- 天然萃取物的生物活性應用

Beginner

天然萃取物檢索

Question: 探索藥用植物萃取物的生物活性應用, 已發表文獻中有那些 Substances 紀錄

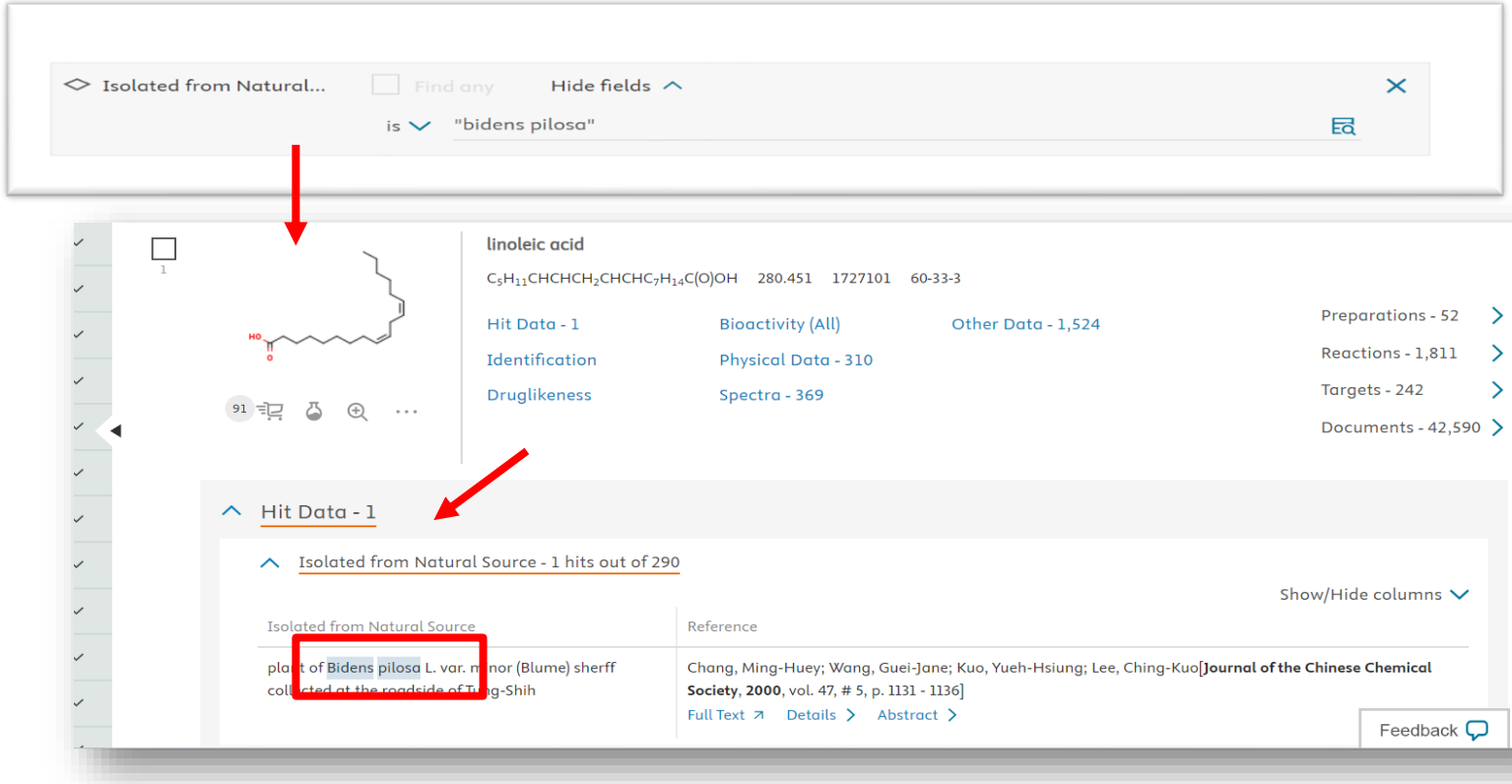
方法一

- 檢索Bidens Pilosa的文獻
- 取得文獻中人工提取的Substances清單

方法二

- 利用進階工具- Isolated from natural sources

天然萃取物檢索


Isolated from Natural...
Find any
Hide fields
is
"bidens pilosa"
linoleic acid
C5H11CHCHCH2CHCHC7H14C(O)OH 280.451 1727101 60-33-3
Hit Data - 1
Bioactivity (All)
Other Data - 1,524
Identification
Physical Data - 310
Druglikeness
Spectra - 369
Preparations - 52
Reactions - 1,811
Targets - 242
Documents - 42,590
Hit Data - 1
Isolated from Natural Source - 1 hits out of 290
Show/Hide columns
Isolated from Natural Source
Reference
Chang, Ming-Huey; Wang, Guei-Jane; Kuo, Yueh-Hsiung; Lee, Ching-Kuo[Journal of the Chinese Chemical Society, 2000, vol. 47, # 5, p. 1131 - 1136]
Full Text
Details
Abstract
Feedback

Reaxys 線上學習資源 – 進階檢索

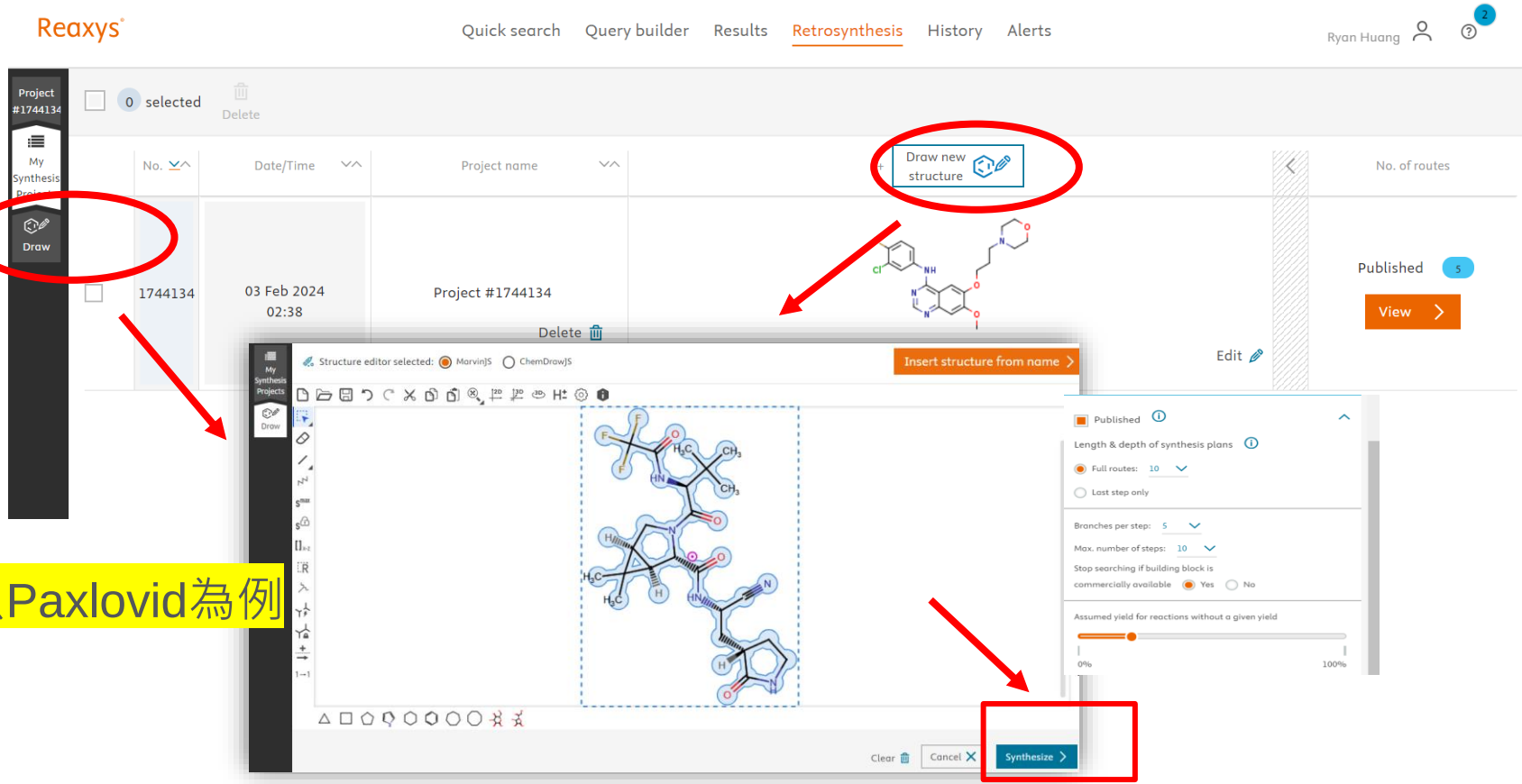
- Reaxys - 進階搜尋
- Reaxys 進階檢索 - 化合物檢索與理化性質
- Reaxys 進階檢索 - 天然產物檢索
- Reaxys 進階檢索 - 電化學理化性質案例
- Reaxys 進階檢索 - 化合物文獻定位
- Reaxys 進階檢索 - 鈣鈦礦類化合物搜尋

- 逆合成工具 Retrosynthesis

Retrosynthesis 逆合成工具

- 為已知和新穎化合物創建合成計劃。

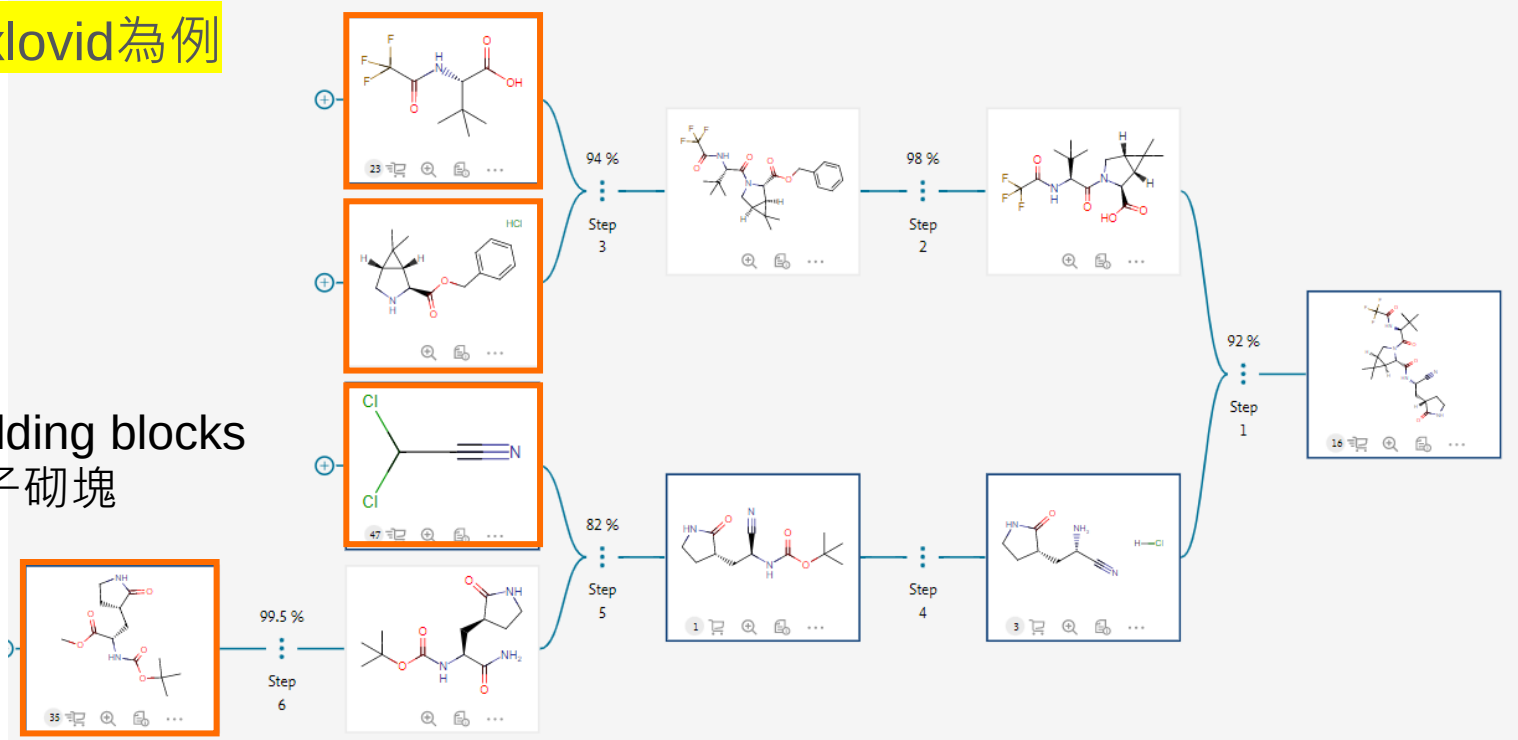
畫出分子架構, 選擇條件, 並點選 Synthesize 合成



以Paxlovid為例

Retrosynthesis 逆合成計畫

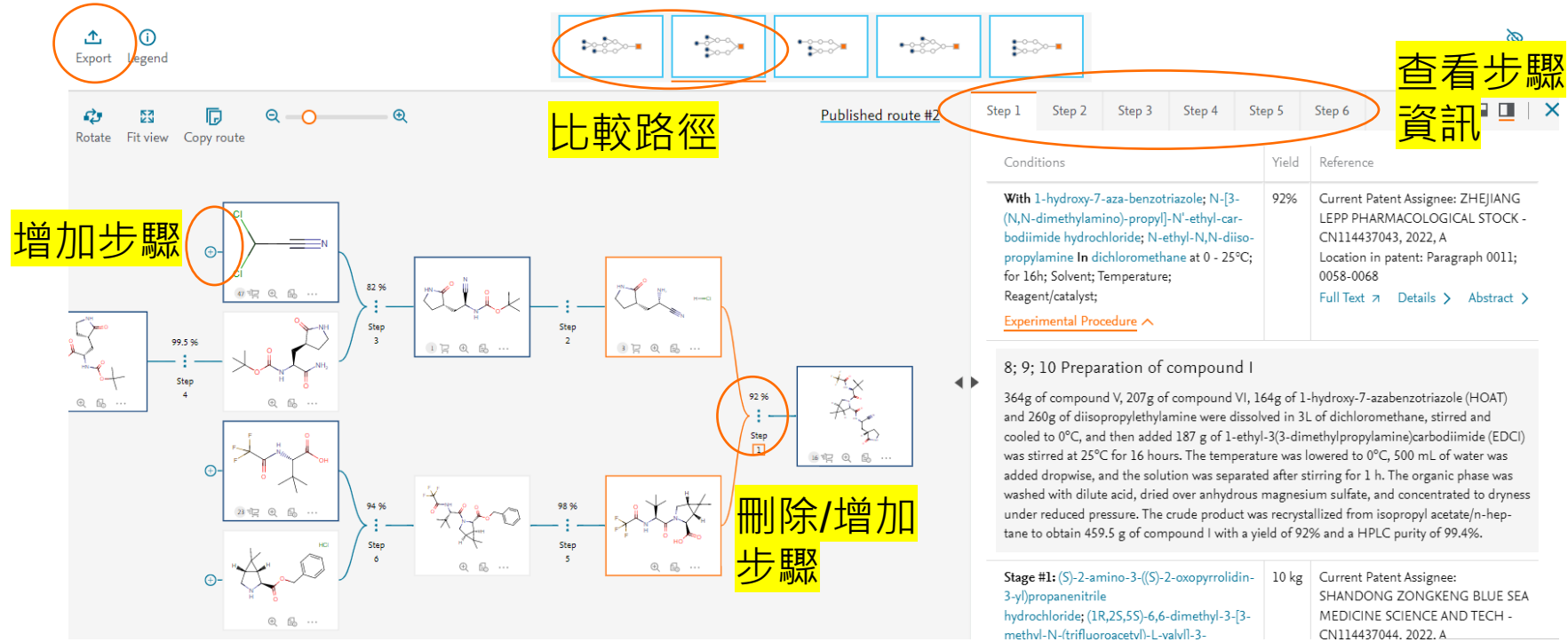
以Paxlovid為例



Building blocks
分子砌塊

Retrosynthesis 逆合成計畫

匯出資料



- 反應式 Reactions 搜尋

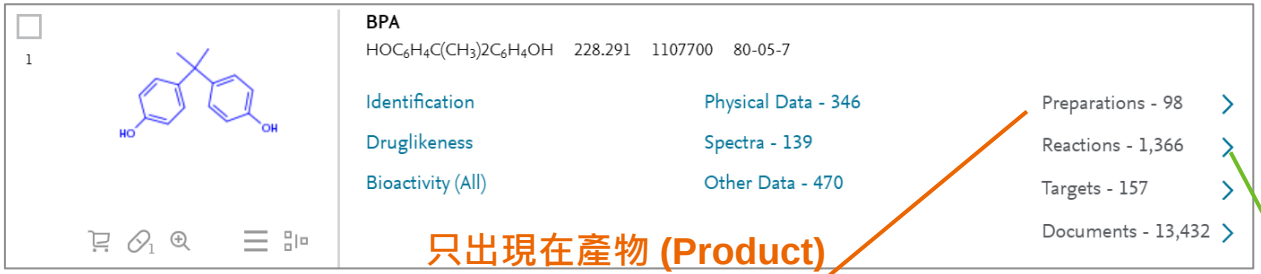
Reaxys尋找反應式的方法

1. 已知物質的製備方式 (從substance介面連結preparations)
2. 關鍵字檢索 (例：radical cyclization)、命名反應式(例：Suzuki coupling)
3. 直接畫出反應式 (完整、半個反應式)

Beginner

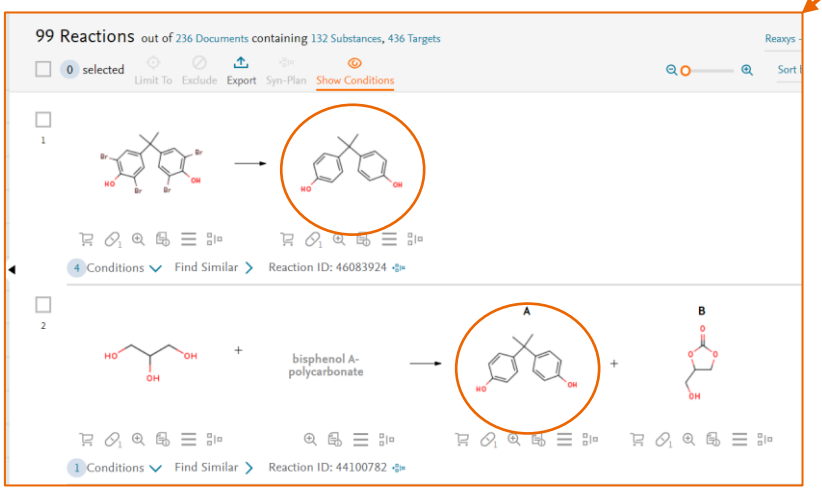
Reaxys尋找反應式的方法

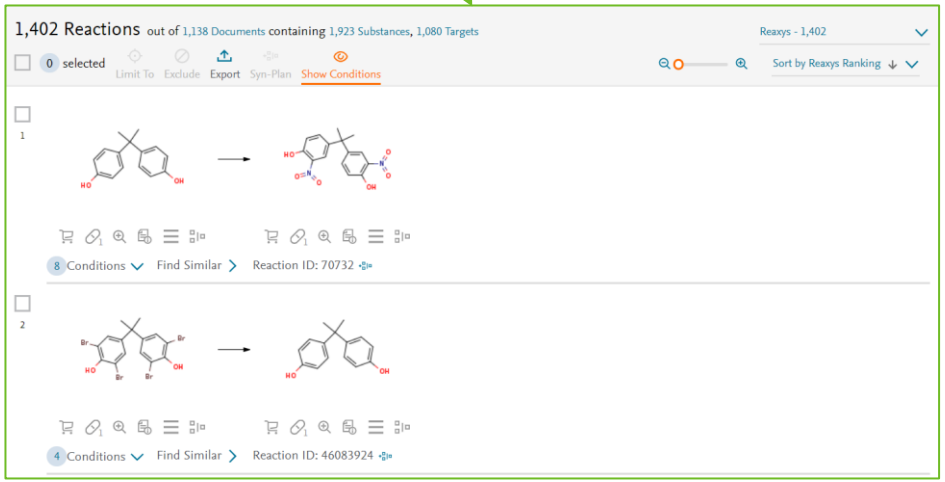
~已知物質的製備方式~



只出現在產物 (Product)

產物或起始物 (Reactants or Products)

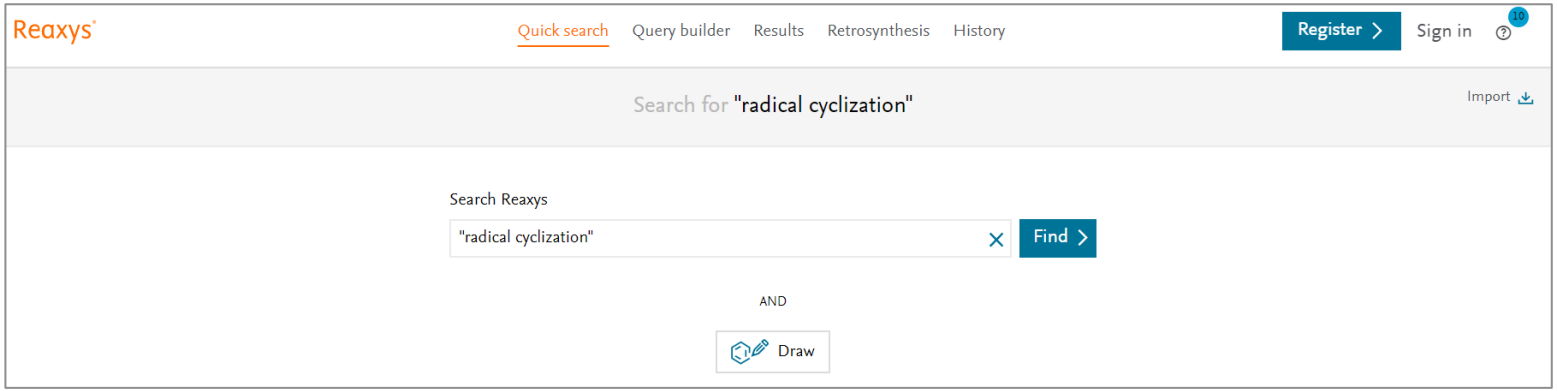


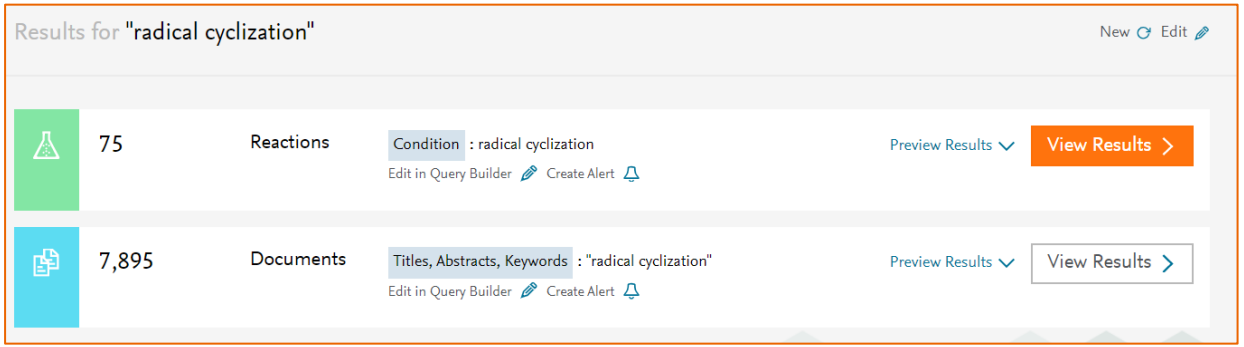


beginner

Reaxys尋找反應式的方法

~關鍵字檢索①~

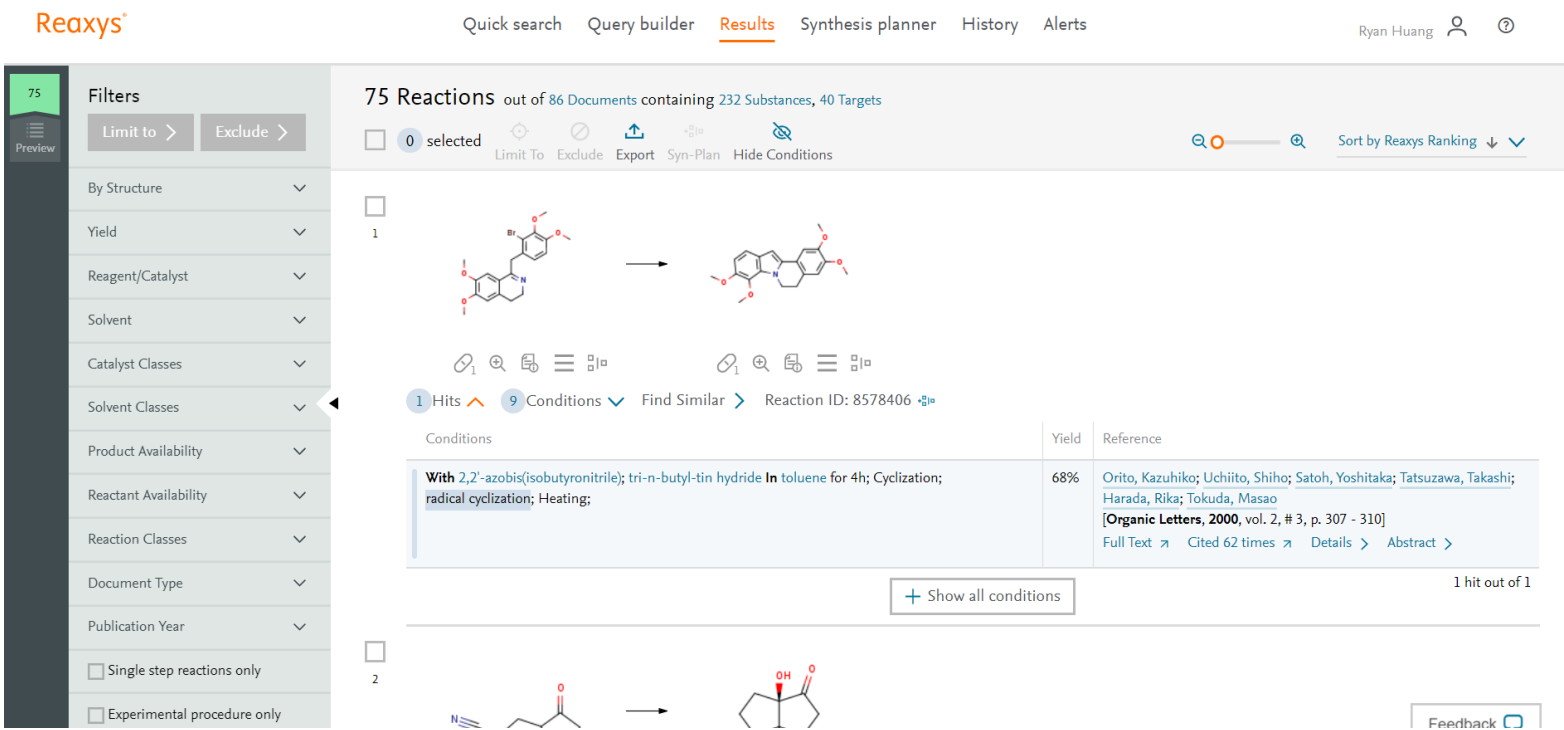




beginner

Reaxys尋找反應式的方法

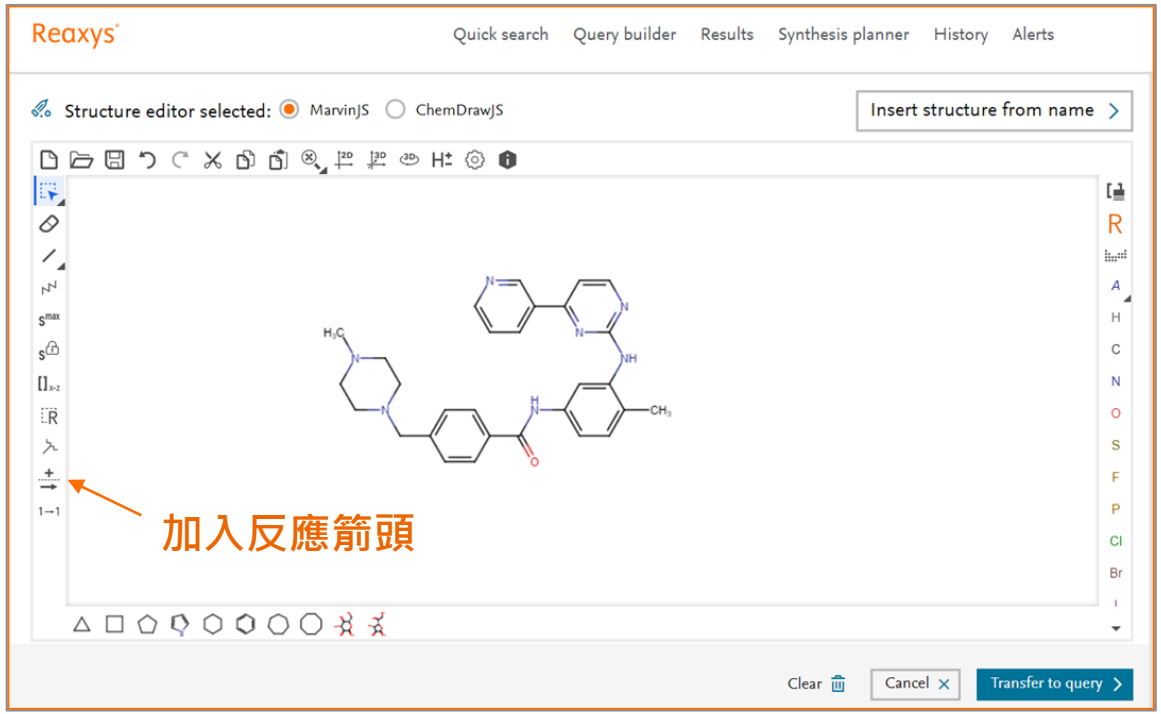
~關鍵字檢索②~



beginner

Reaxys尋找反應式的方法

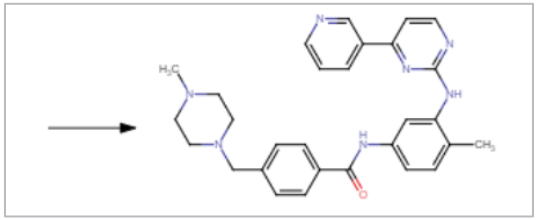
~繪製反應式①~



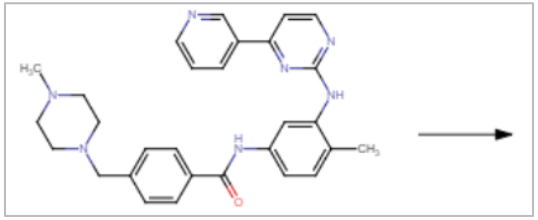
beginner

Reaxys尋找反應式的方法

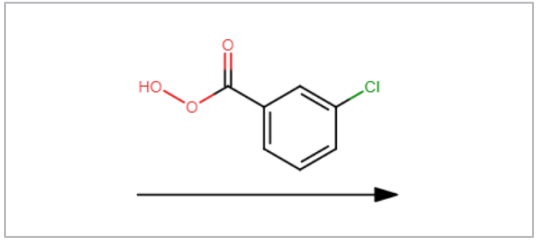
~繪製反應式②~



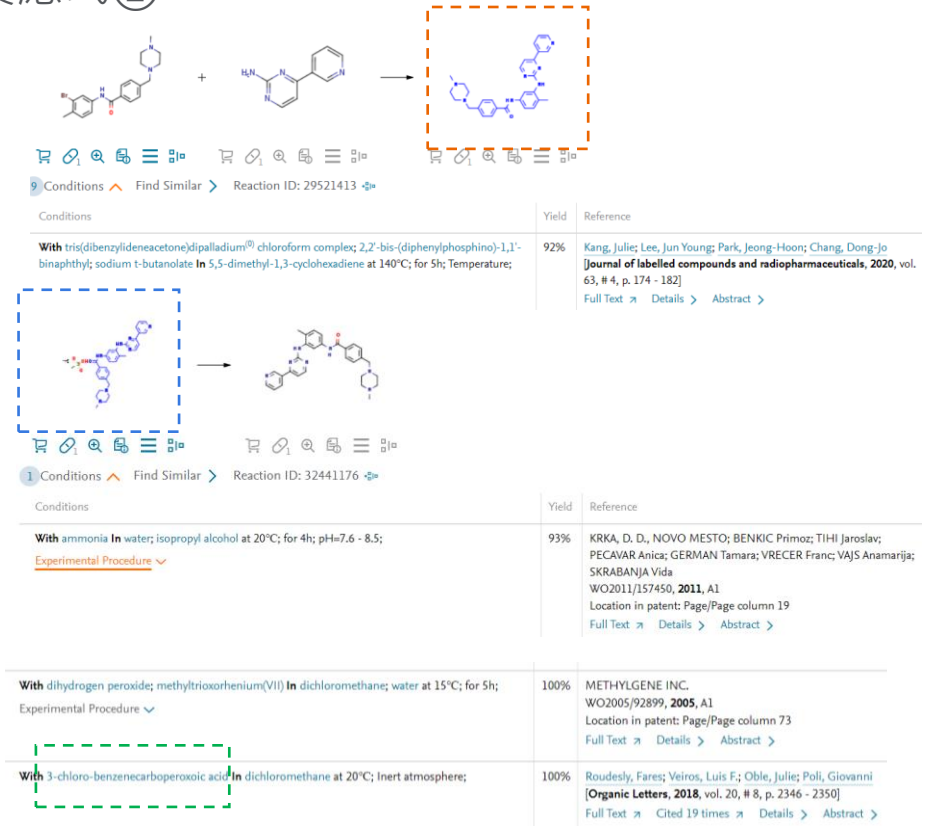
箭頭在左
產物



箭頭在右
起始物



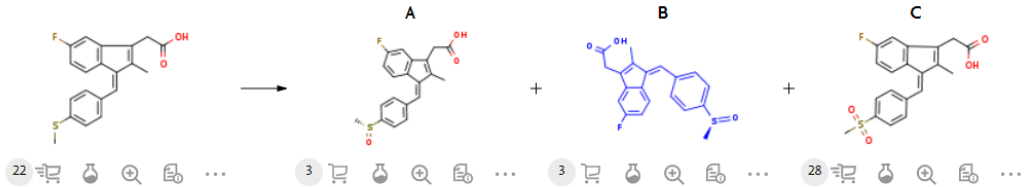
箭頭在下
催化劑或溶劑



Advance

Reaxys進階反應式檢索

~Reaxys 反應式介面提供的資訊~



人工索引欄位名稱:
Reaction Data & Condition

溶劑、催化劑
也包含反應資訊
Enzymatic reaction;
Enantioselective reaction;
Green chemistry;
Flow reactor;
Irradiation….等

1 Conditions Find Similar Reaction ID: 35329138

Conditions	Yield	Reference
With 2-methylimidazole; $C_{84}H_{72}ClFeN_4O_{12}S_4^{(4-)}*4Na^{(1+)}$; dihydrogen peroxide In methanol; aq. phosphate buffer at -20°C; for 1h; Inert atmosphere; Overall yield = 100 %Spectr.; enantioselective reaction;	A n/a B n/a C n/a	Srour, Hassan; Jalkh, Joanna; Le Maux, Paul; Chevance, Soizic; Kobeissi, Marwan; Simonneaux, Gérard [Journal of Molecular Catalysis A: Chemical, 2013, vol. 370, p. 75 - 79] Full Text Cited 37 times Details Abstract

Experimental Procedure

2.3 General procedure for asymmetric sulfoxidation

General procedure: Methyl phenyl sulfoxide. Manganese porphyrin complex 1 (1.6 mg, 1 μmol) and imidazole (1.7 mg, 25 μmol) were placed in a test tube under argon. The solvent (375 μL MeOH + 125 μL PBS, pH 7) was then added via syringe, followed by the sulfide (5 μL, 42.3 μmol). Finally, hydrogen peroxide (1.8 μL, 21.2 μmol) was added in one portion to the solution. The reaction was followed by gas chromatography (GC). From GC we knew that the reaction was over after 2 h with a 100% yield containing 1% sulfone. The solution was extracted with dichloromethane three times and then dried over $MgSO_4$. The ee was then determined by HPLC to be 33%.

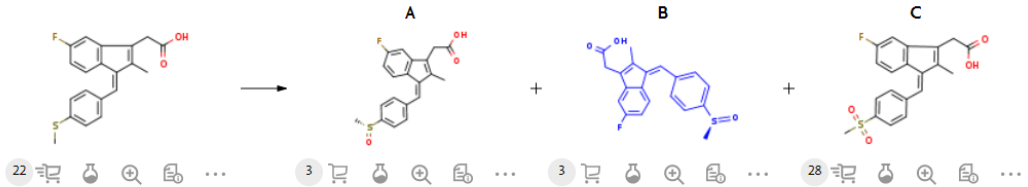
欄位名稱: fulltext of reaction

詳細實驗步驟(文獻原文移植)
資訊量最豐富，包含詳細步驟、分析方法、數值

Advance

Reaxys進階反應式檢索

~Reaxys 反應式介面提供的資訊~



人工索引欄位名稱:
Reaction Data & Condition

溶劑、催化劑
也包含反應資訊
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Enantioselective reaction;
Green chemistry;
Flow reactor;
Irradiation….等

1 Conditions Find Similar Reaction ID: 35329138

Conditions	Yield	Reference
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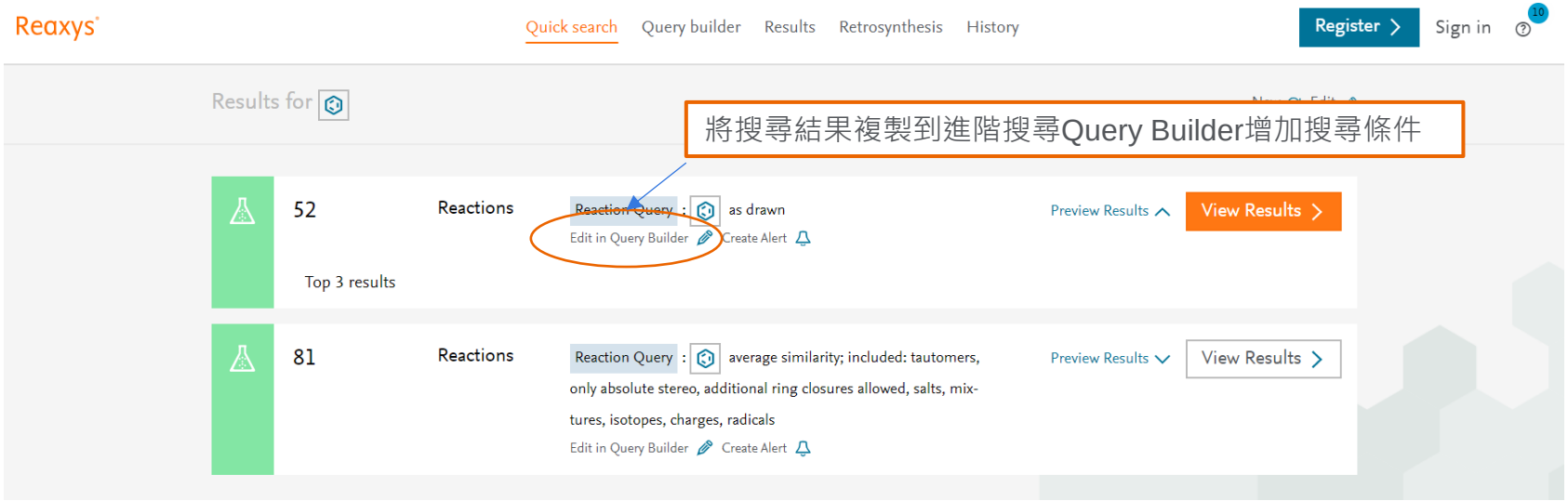
欄位名稱: fulltext of reaction

詳細實驗步驟(文獻原文移植)
資訊量最豐富，包含詳細步驟、分析方法(HPLC)、數值

Advance

Reaxys進階反應式檢索

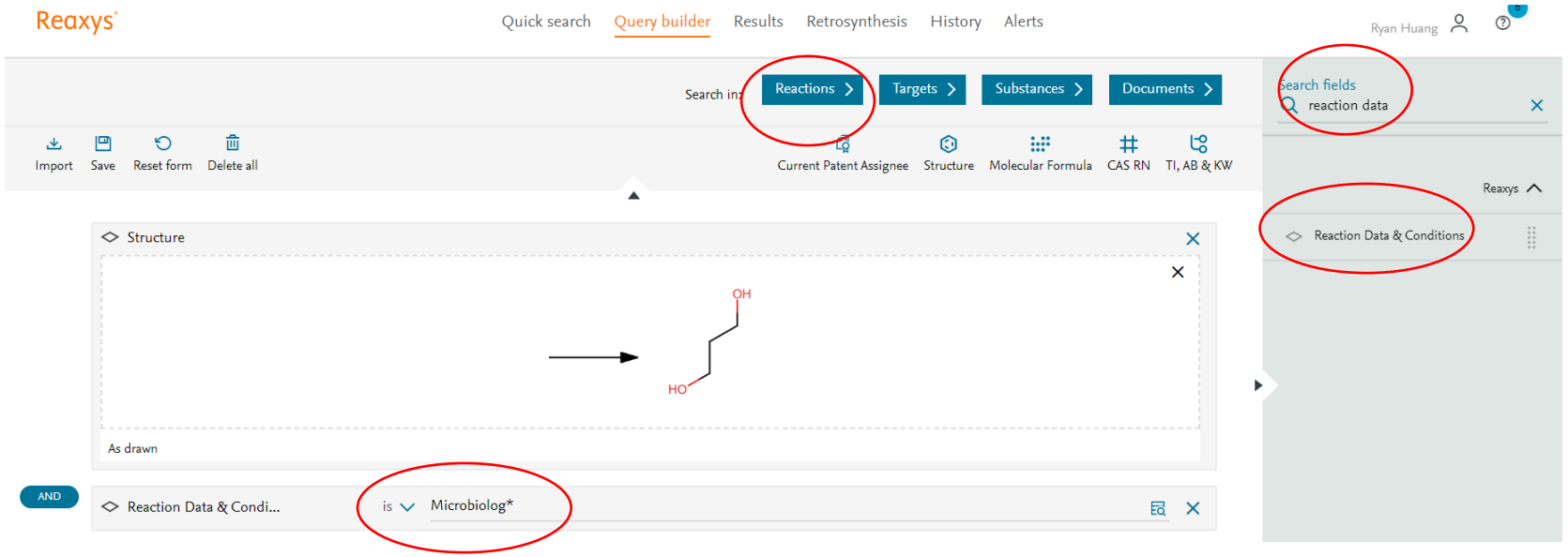
~利用Query builder進一步「加工」搜尋條件~



Advance

Reaxys進階反應式檢索

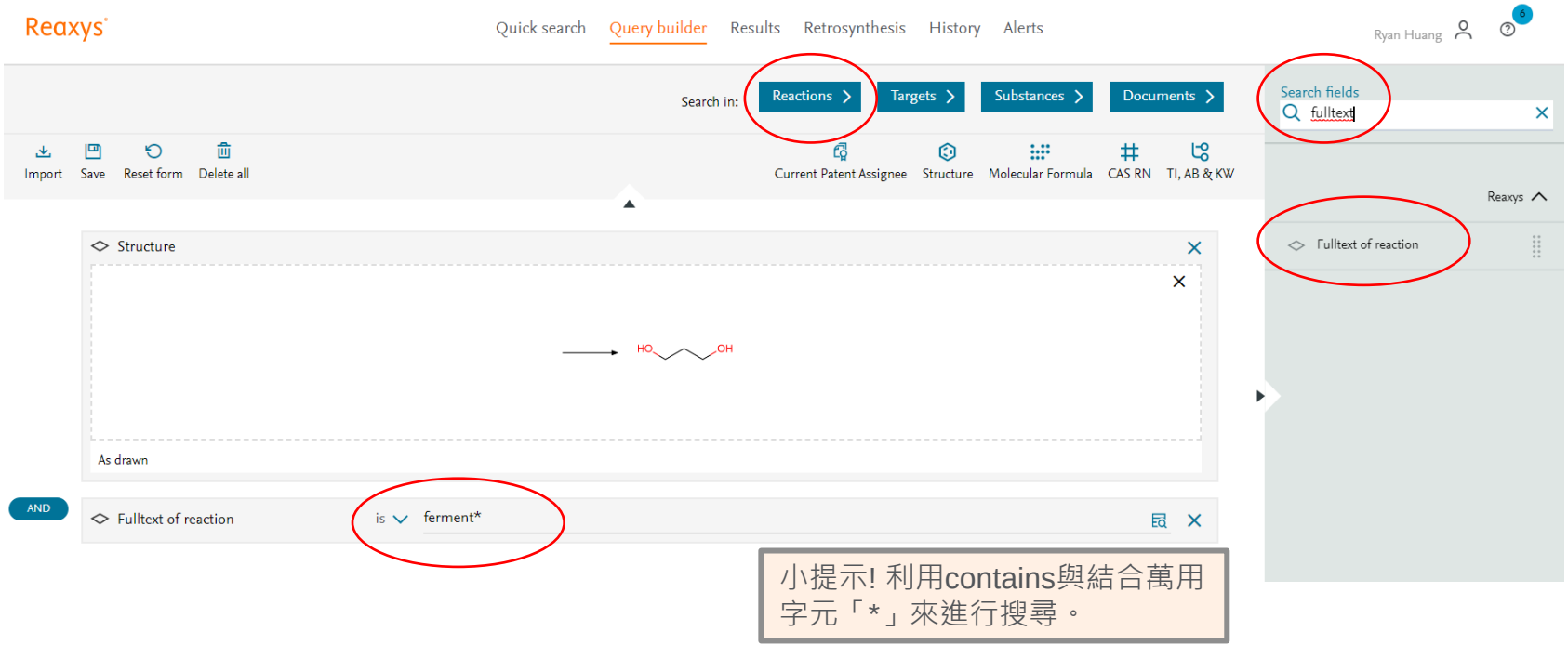
~利用Query builder進一步「加工」搜尋條件~



Advance

Reaxys進階反應式檢索

~利用Query builder進一步「加工」搜尋條件~



小提示! 利用contains與結合萬用字元「*」來進行搜尋。

Reaxys 線上學習資源 – 反應式搜尋

- Reaxys 反應式搜尋 - 基本過濾工具
- Reaxys 反應式搜尋 - 如何定義反應條件
- Reaxys 反應式搜尋 - 反應機構參考文獻的查詢
- Reaxys 反應式搜尋 - 選擇性氧化、還原、脫保護基反應
- Reaxys 反應式搜尋 - 關於環的定義
- Reaxys 反應式搜尋 - 結構中有特殊要求的反應定義
- Reaxys 反應式搜尋 - 篩選邏輯

自我學習: 透過Reaxys學習化學

https://www.elsevier.com/research-platforms/academies/reaxys

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- Complete a short quiz at the end of each module, and
- If you score 100%, download your certificate of completion and badges to share on LinkedIn and email

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Self-paced cours

Th

ased, chemical

earch for chemical

ical structures and substance

imate time to complete – 30-45

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ELSEVIER

Thank you