Reaxys 化學資料庫介紹
如何聰明的搜尋化學資料節省時間

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ELSEVIER LIFE SCIENCES

OUR SHARED PURPOSE

TO ACCELERATE SCIENCE TO IMPROVE HEALTH

A Knowledge & Information Analytics Company

OUR PROMISE

Partners in propelling research and innovation forward to transform the way you bring new medicines to the world

OUR KEY DIFFERENTIATORS

- Customer First Commitment
- Our Roots As A Knowledge Company
- Open Integrated Systems
- Accelerating Data-Driven Decisions
- Market-Leading Talent

140+

years of scientific knowledge curated as semantically rich content to enable tomorrow's medical breakthroughs

RELX

$1.4bn
on technology annually

~30,000
employees

Serving customers in
180+ countries

Partnering with
90%
of top Pharma companies

Reaxys 全國學術授權版本

- 科技部科政中心贊助，授權設有化學、應化、藥學等大專院校限研究、教學使用
- 免費教育推廣、技術支援、網路自學資源
- Webinars網路會議分享化學研究新知
- 4/6 亞太區使用者大會

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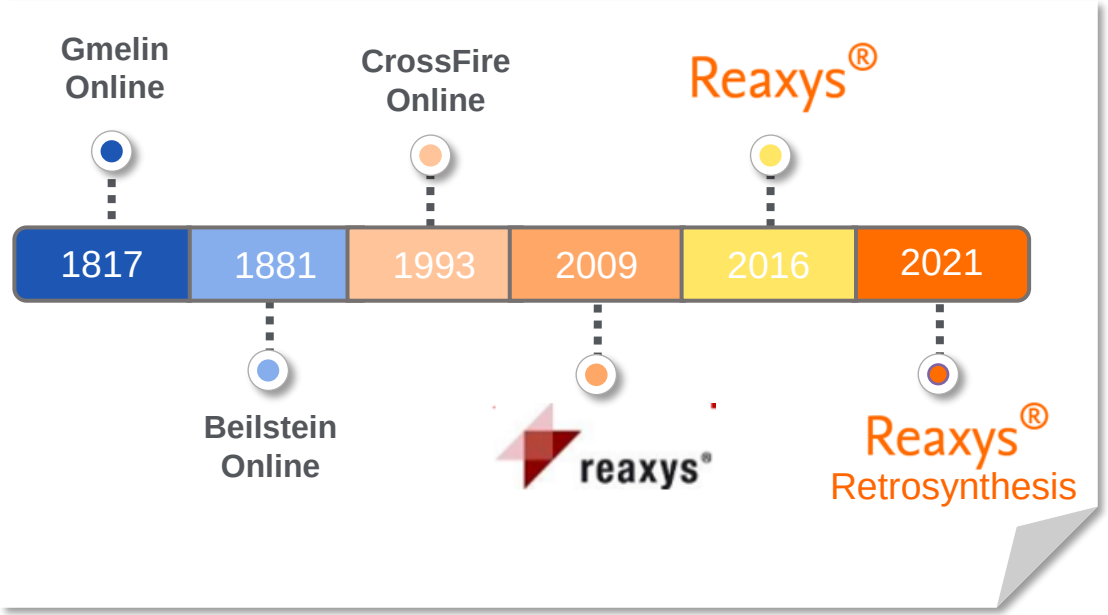
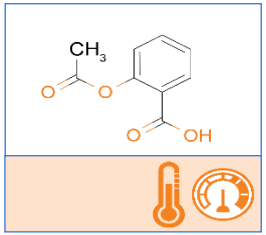
Agenda

1. Reaxys是甚麼?
2. Reaxys如何取得?
3. 基本介面導覽
4. 如何學習結構搜尋? 
5. 如何學習搜尋物質的化學性質? Video by Professor Damon Ridley
6. 命名反應的手機APP  
7. 甚麼是逆合成?AI工具的演進
8. 網路自我學習資源 Youtube
9. 化學供應商資料庫

Reaxys是充滿歷史與先進的化學資料庫





>118 Million
有機、無機及有機金屬物質

>500 Million
公開實驗數據(物性、光譜、生物活性等)

>49 Million
化學反應(反應條件、溶劑、催化劑及產率等)

>54 M 文獻記錄
>16,000 期刊，專利
涉及有機化學，材料化學，生物醫藥，地球科學，工程等多種領域

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Reaxys提供關鍵的實驗數據，讓研究人員回答重要的研究問題

Journals, patents, conference proceedings

人工閱讀、擷取重要的"實驗數據

結構、物理特性、光譜、製備反應、生物活性(藥物毒性、藥物靶點蛋白、藥物活性、細胞、動物試驗)

回答關鍵的研究問題:

- 具有美白功能的天然萃取物質有哪些?證據在哪裡?實驗室萃取的X物質是有人報導過的嗎?
- 能夠有抗病毒活性的化合物長甚麼樣子? 我們實驗室的化合物值得拿來發展藥物嗎?
- 我的研究所題目有人做過類似的實驗嗎?有其他的應用被發表嗎?
- 我要合成一個目標分子才能繼續做實驗?怎麼辦?該怎麼找參考文獻?

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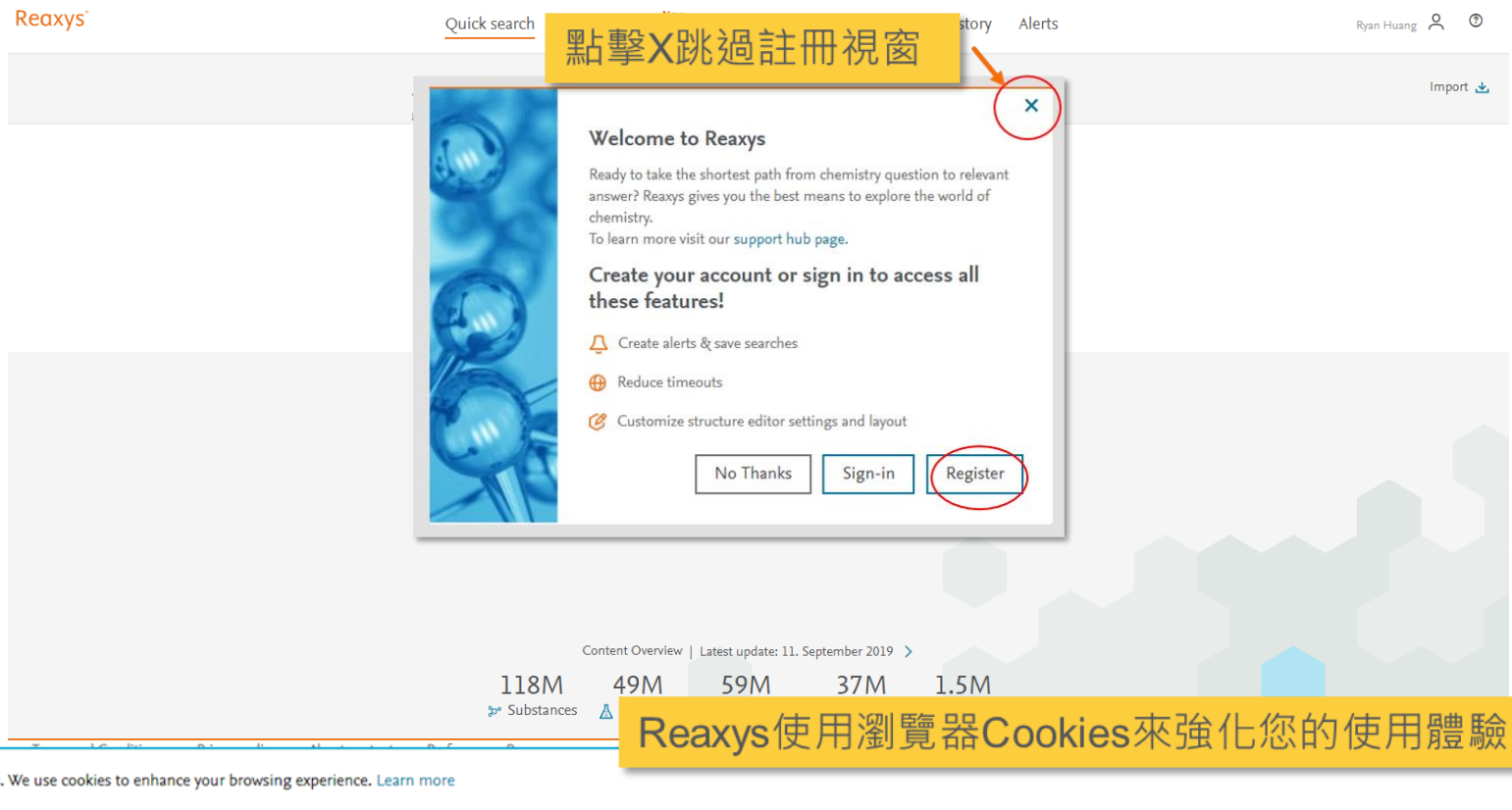
如何連上Reaxys

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



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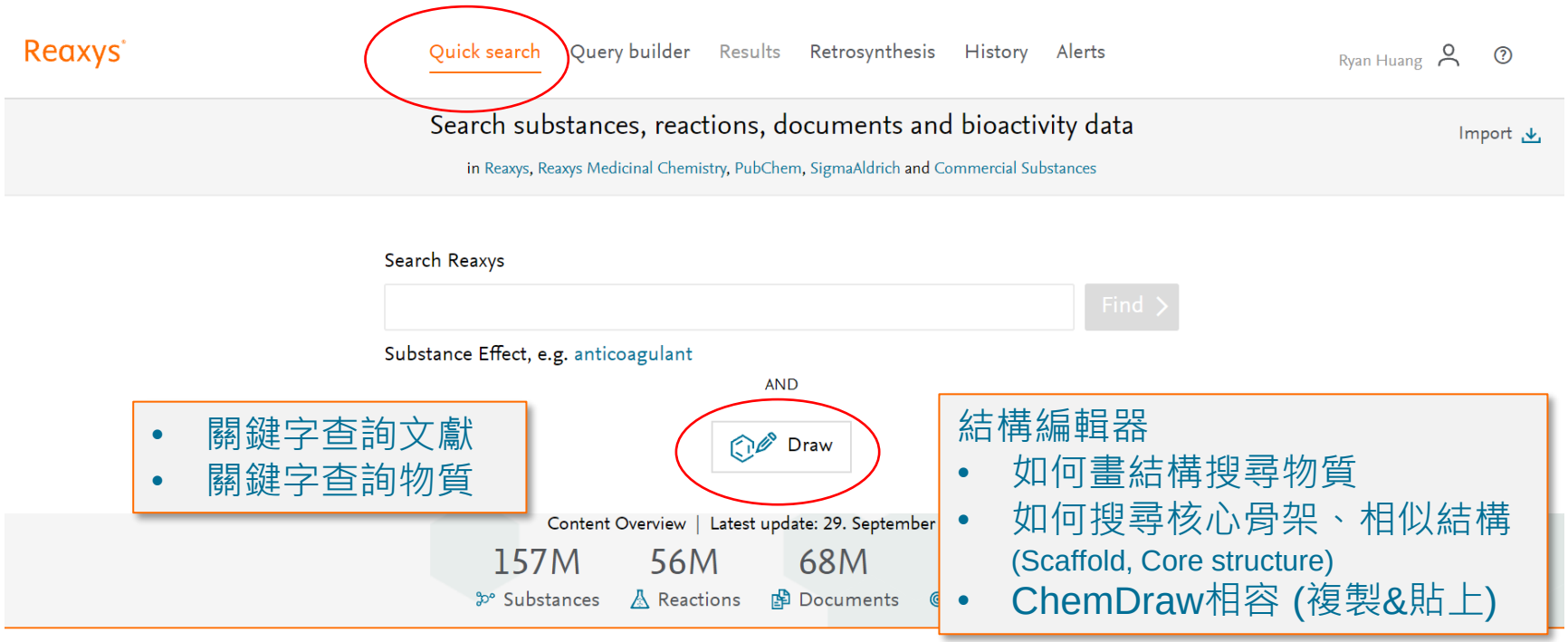
Reaxys介面導覽

學習展示要點

快速搜尋 – 研究學習的第一步



- 關鍵字查詢文獻
- 關鍵字查詢物質

結構編輯器

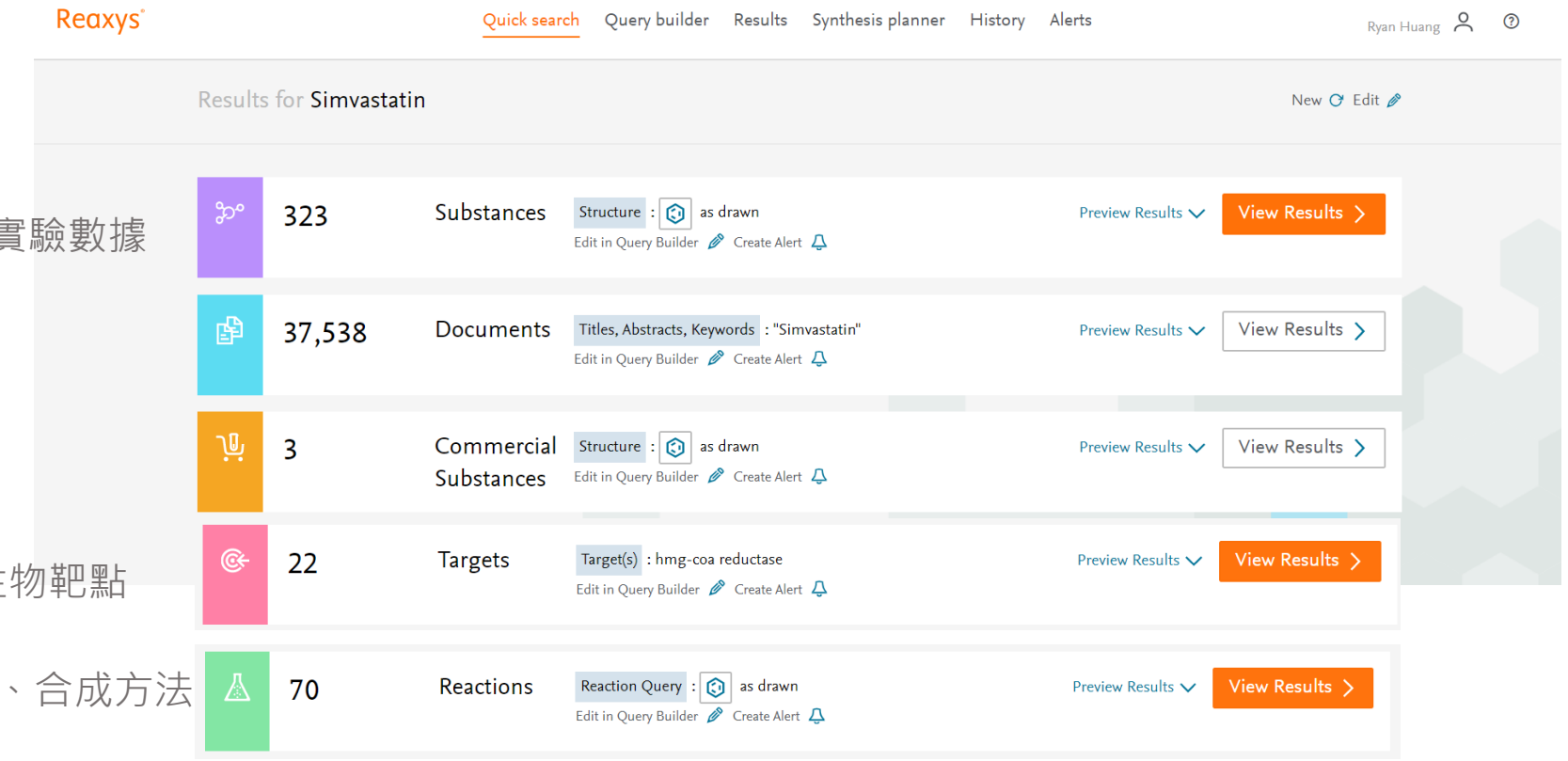
- 如何畫結構搜尋物質
- 如何搜尋核心骨架、相似結構 (Scaffold, Core structure)
- ChemDraw相容 (複製&貼上)

預覽頁面

實驗數據

生物靶點

反應、合成方法



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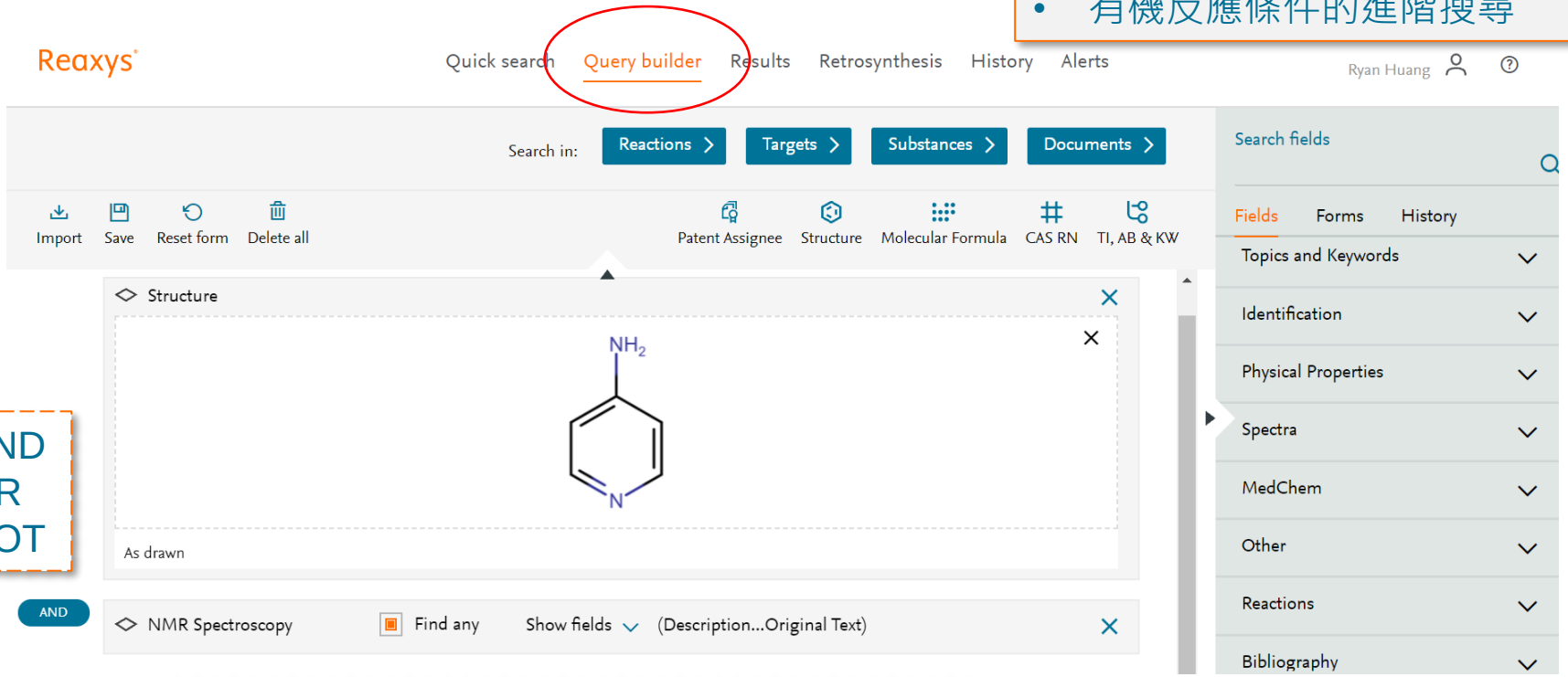
進階搜尋 Query Builder

- 天然萃取物搜尋
- NMR圖譜的搜尋
- 有機反應條件的進階搜尋



AND
OR
NOT

自行組合搜尋條件 (例如結合結構+NMR圖譜)

超過百種搜尋條件

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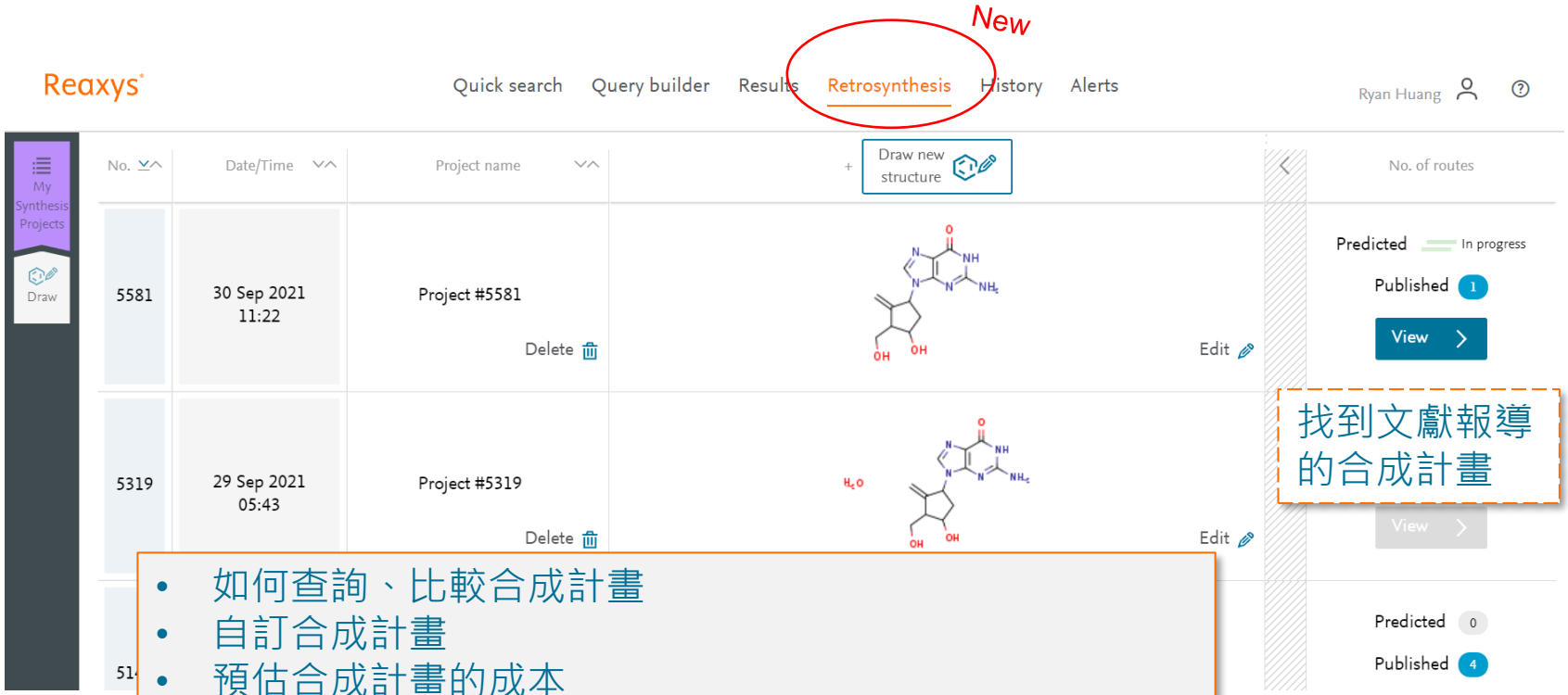
逆合成面板 (規劃合成路徑、合成材料與反應條件)



找到文獻報導的合成計畫

- 如何查詢、比較合成計畫
- 自訂合成計畫
- 預估合成計畫的成本
- 學習利用AI工具來輔助設計創新化合物的合成策略
- 儲存、資料匯出

(需登入個人帳號)

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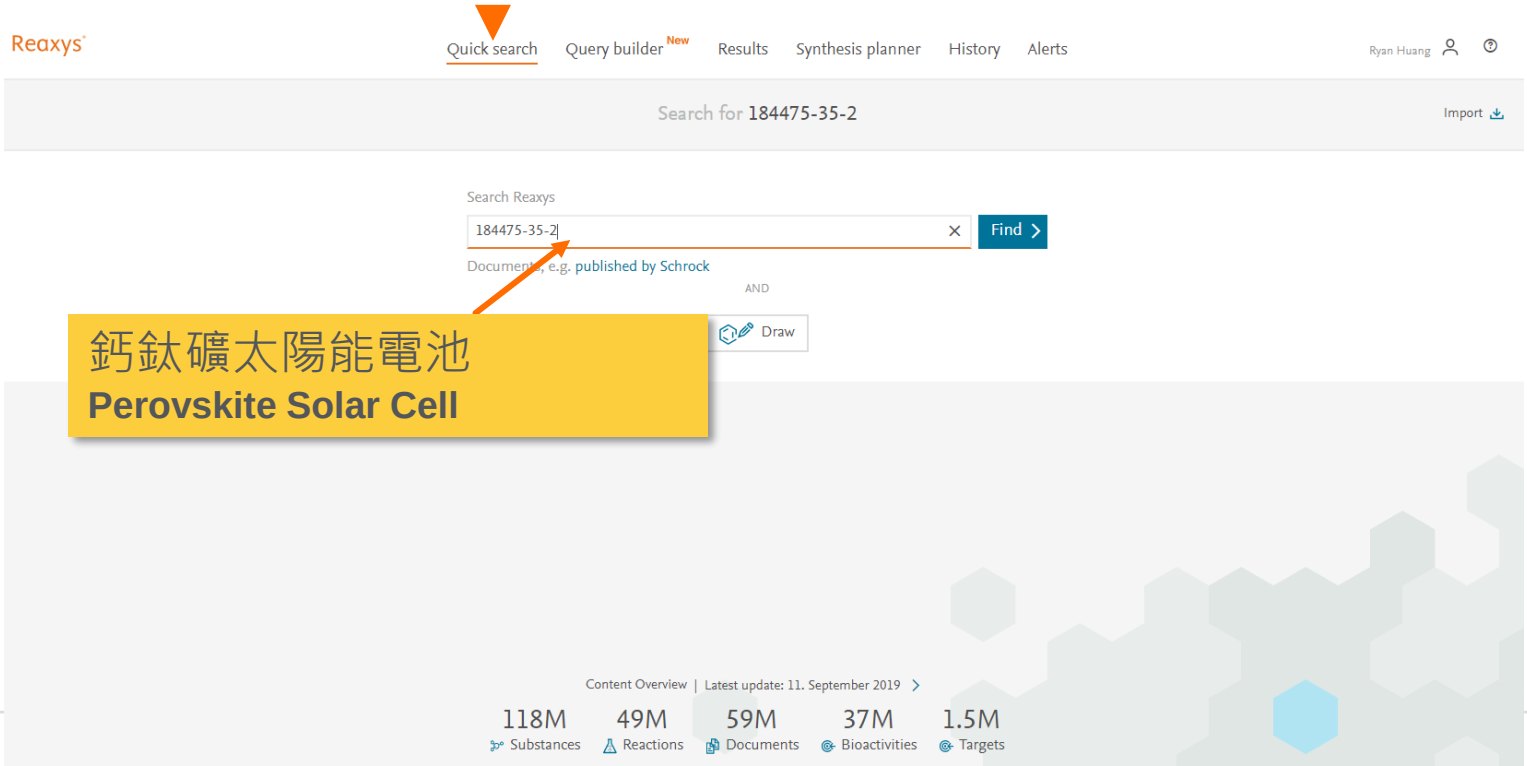
Quick Search

關鍵字查詢文獻

Quick Search 關鍵字查詢文獻



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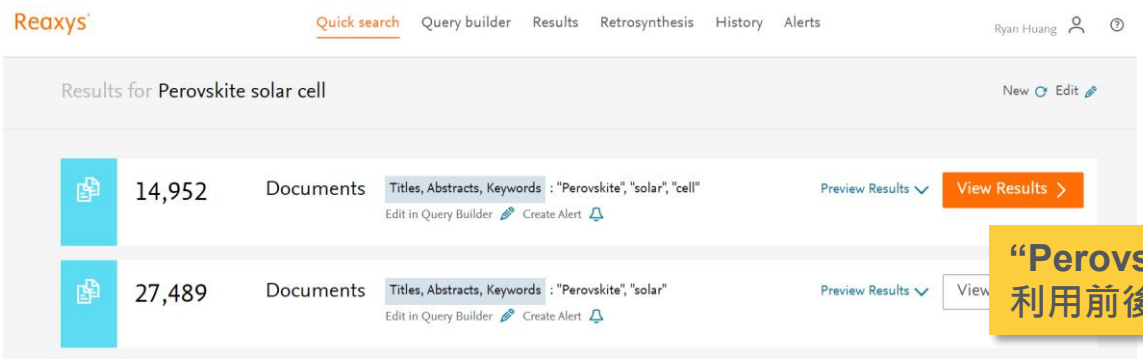
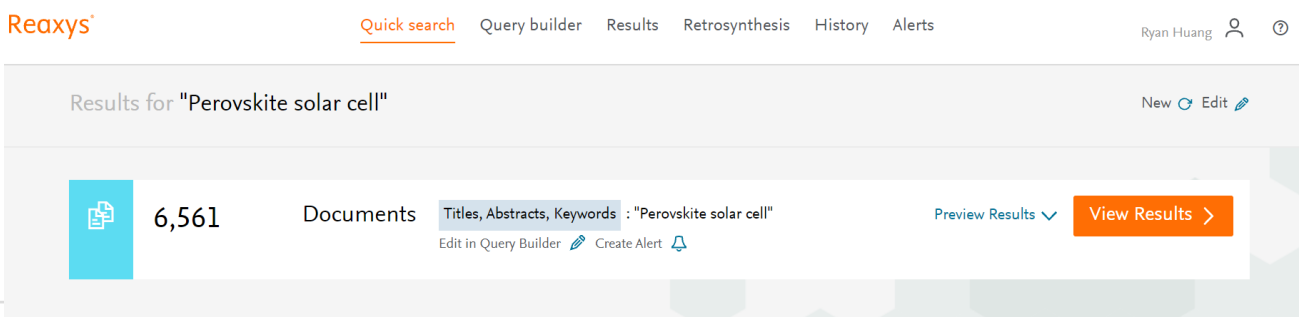
Quick Search 關鍵字查詢文獻



“Perovskite Solar Cell”
利用前後””限制搜尋範圍



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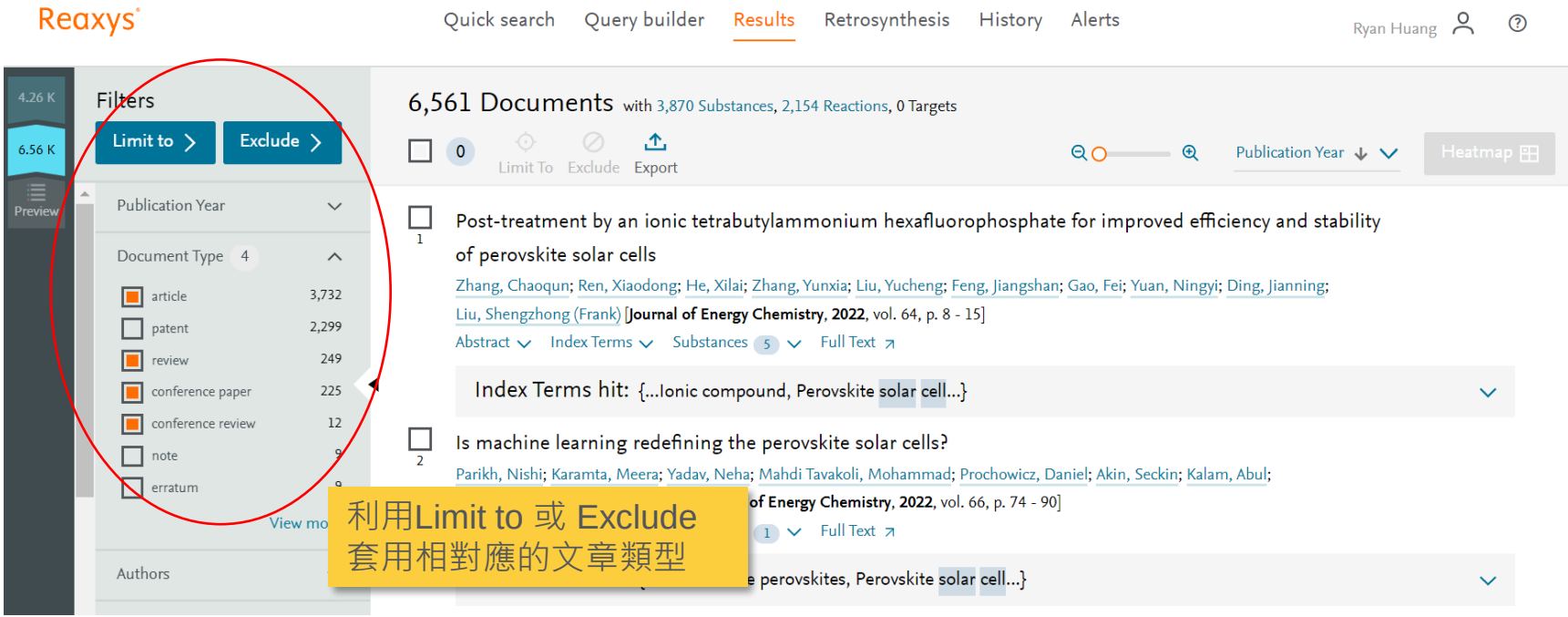
Quick Search 關鍵字查詢文獻

- 文章類型篩選 (Reaxys包含學術期刊與全世界105個專利局化學專利資料)



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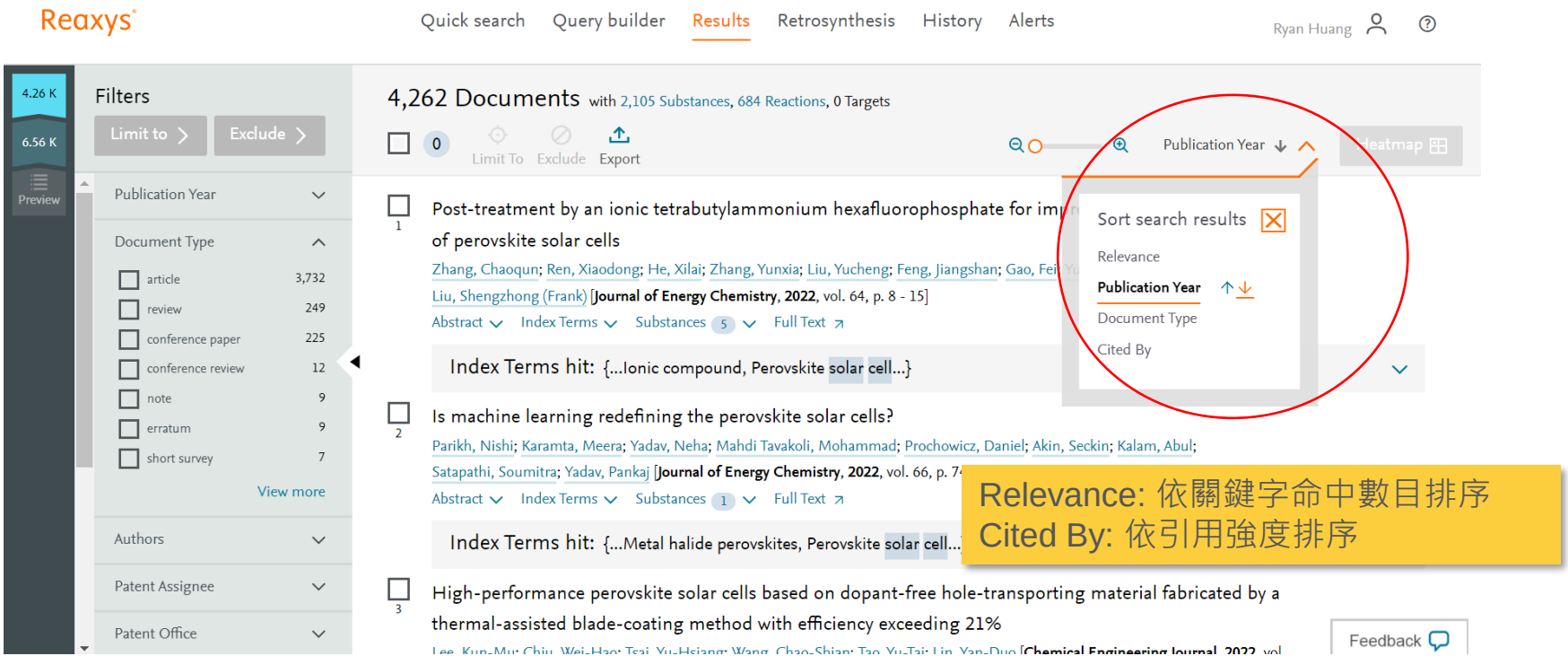
Quick Search 關鍵字查詢文獻
- 文章排序



Relevance: 依關鍵字命中數目排序
Cited By: 依引用強度排序

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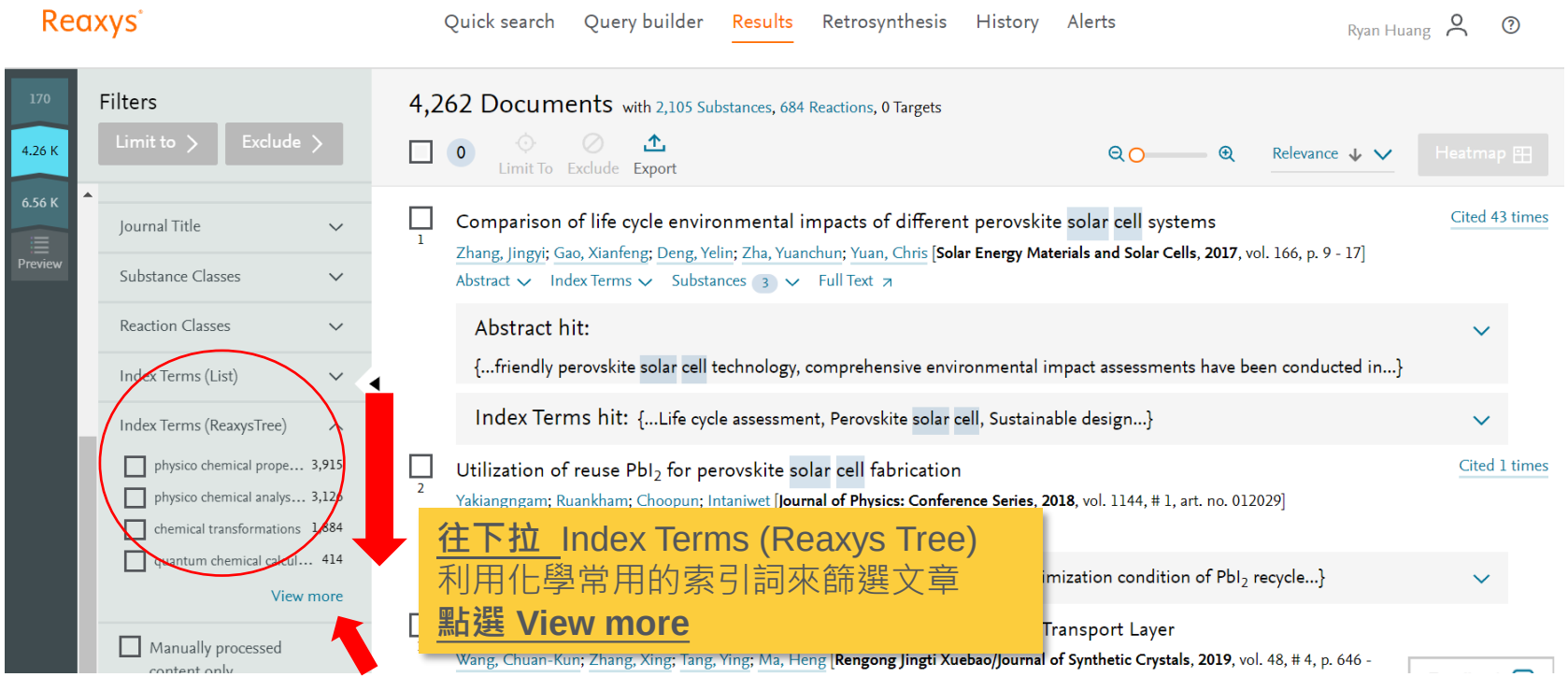
Quick Search 關鍵字查詢文獻
- 索引詞篩選 (Index Terms Reaxys Tree)



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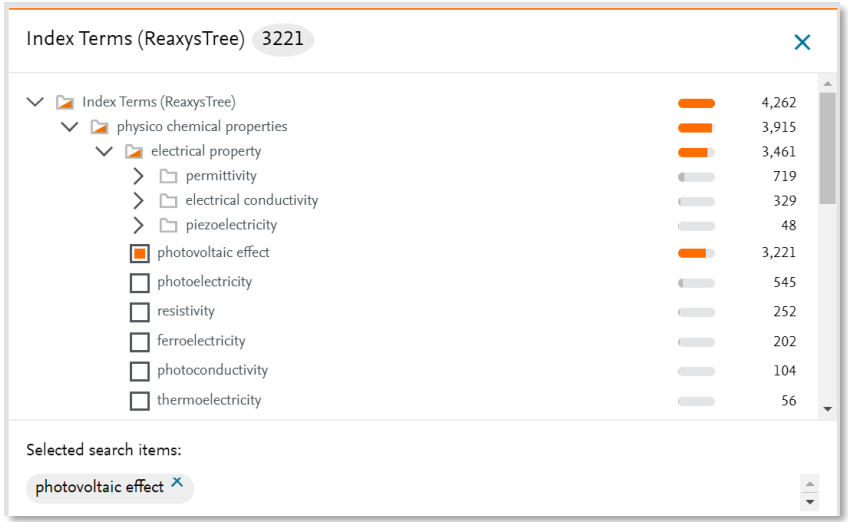
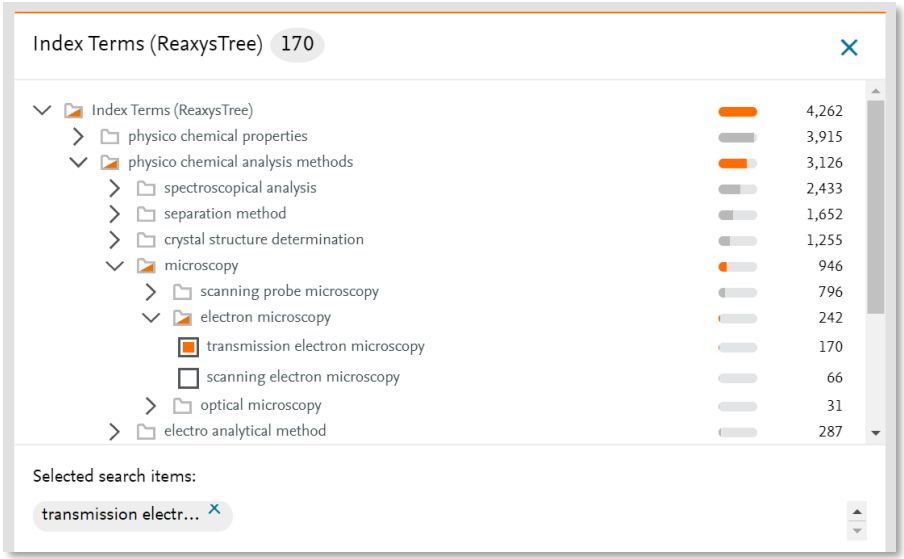
Quick Search 關鍵字查詢文獻
- 索引詞篩選 (Index Terms Reaxys Tree)





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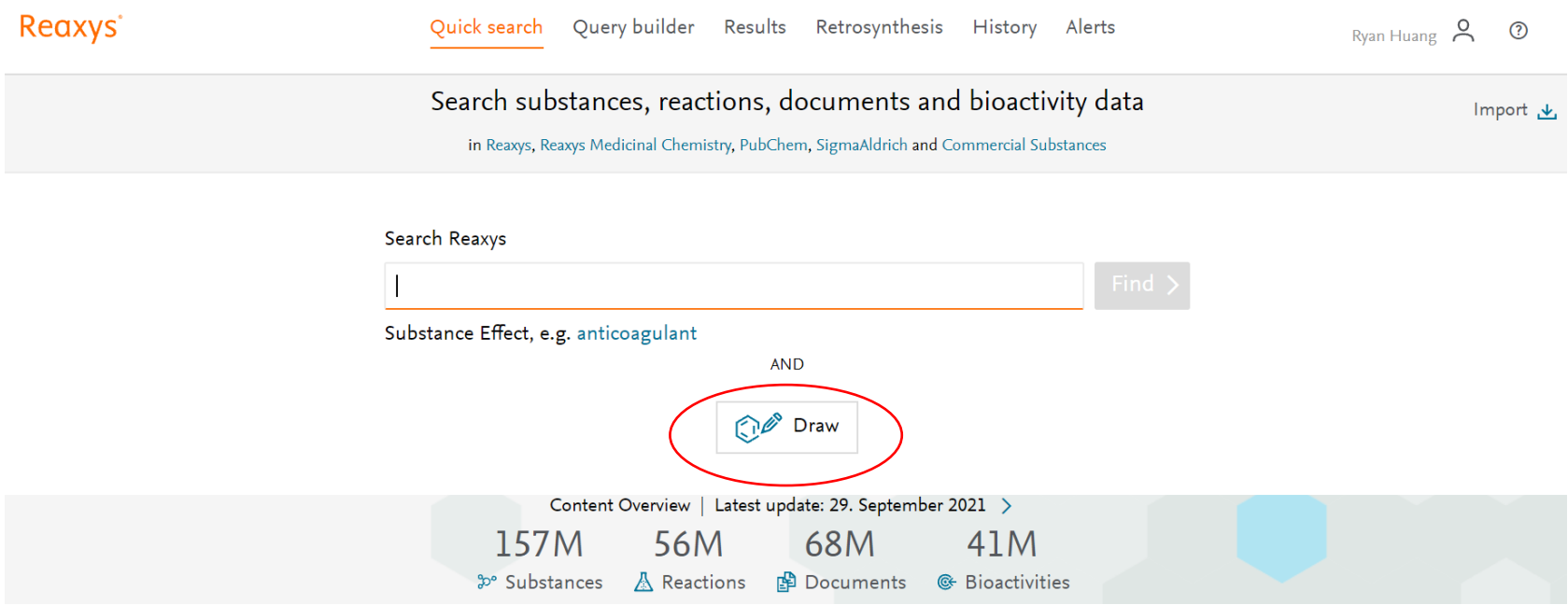
Quick Search

結構搜尋

Quick Search 結構搜尋



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MarvinJS 結構編輯器

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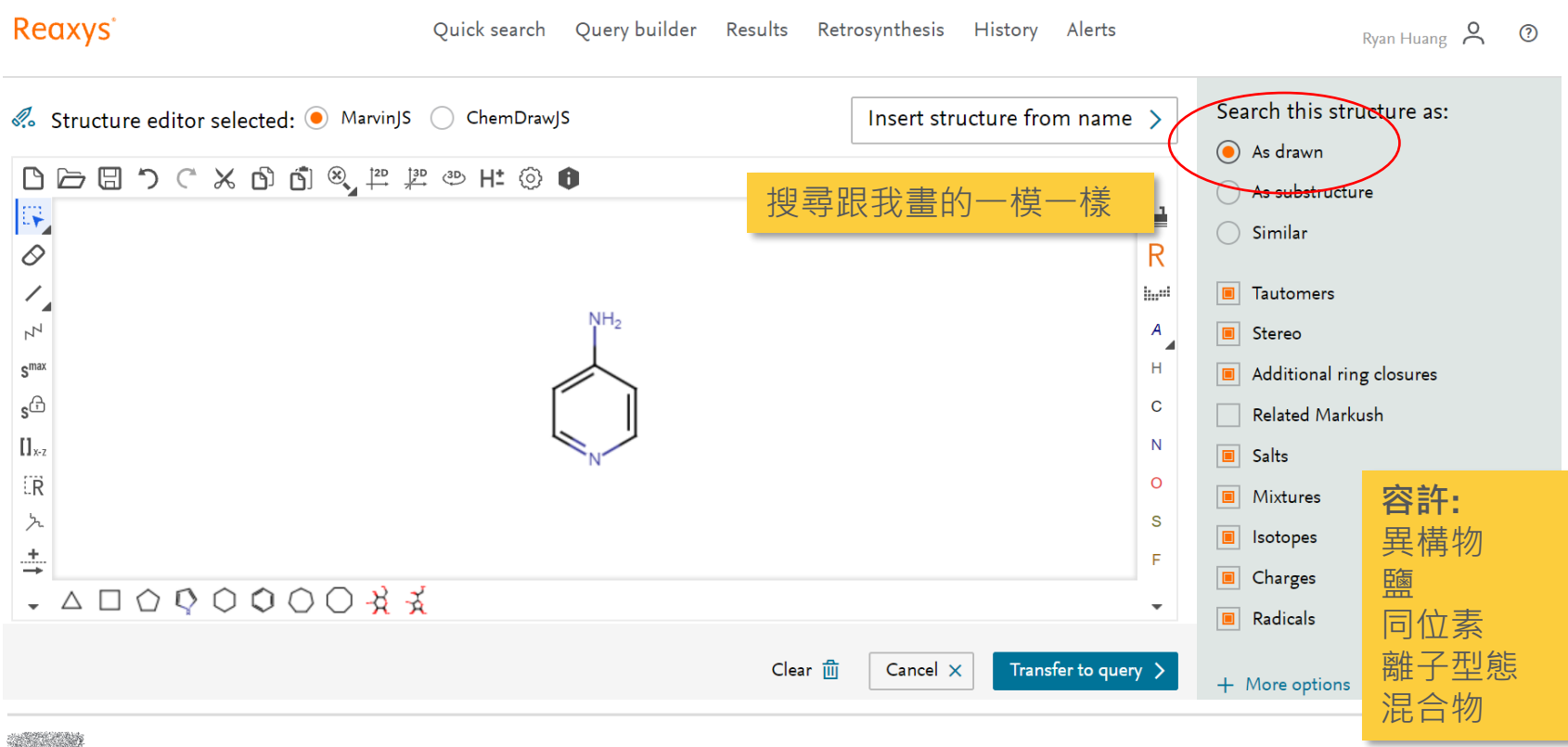
絕對結構搜尋 As drawn



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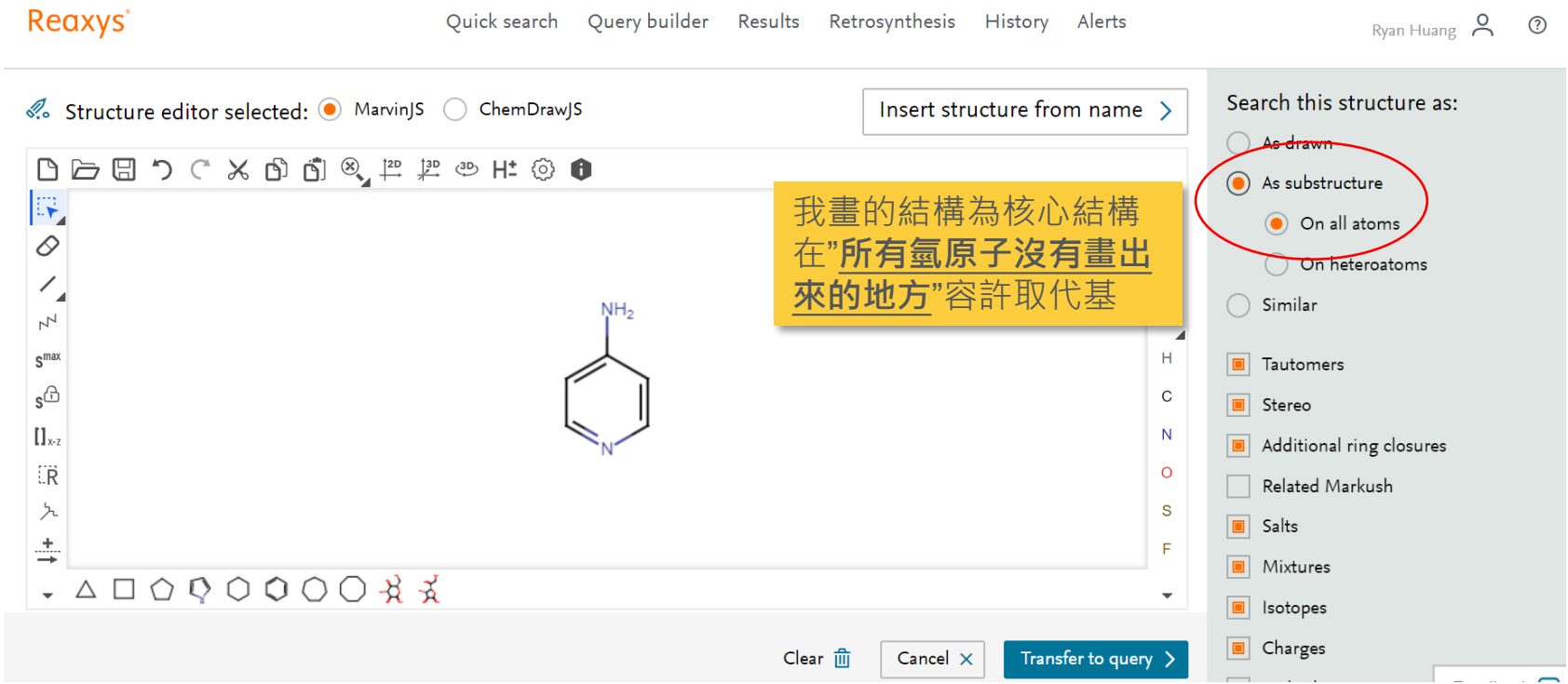
相似結構搜尋 As substructure



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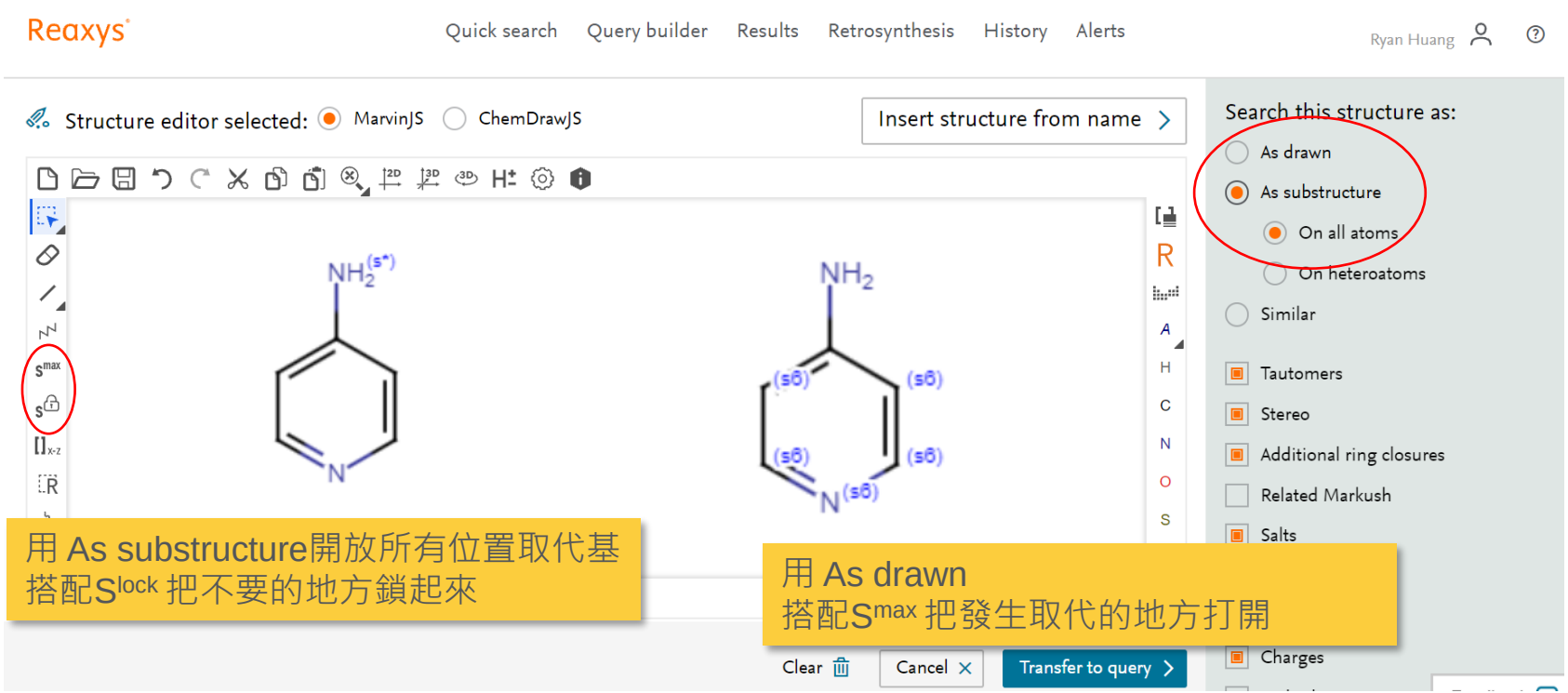
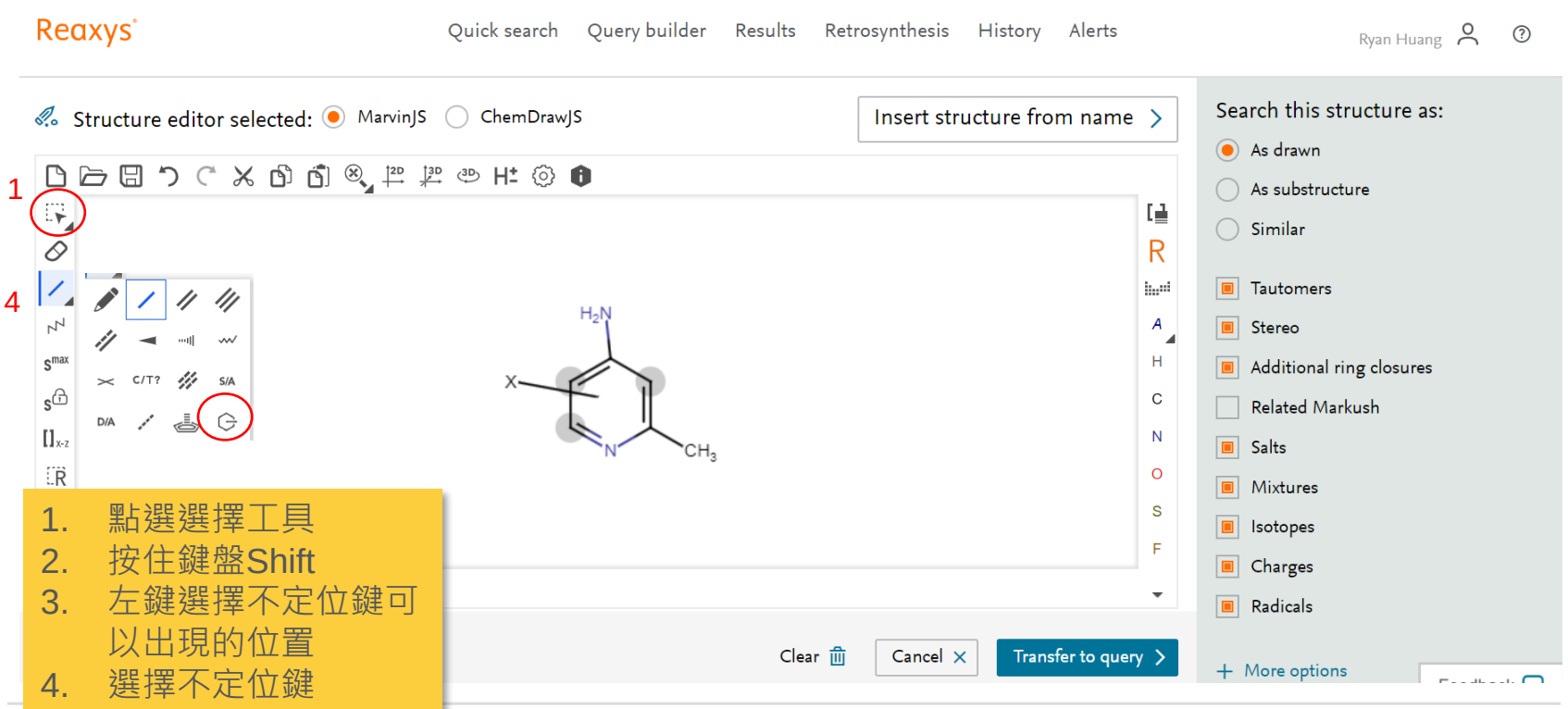
相似結構搜尋 S^{lock} & S^{max}



[(151) Reaxys 結構編輯器 - 相似結構搜尋 原子鎖工具 - YouTube]

不定位鍵的使用



1. 點選選擇工具
2. 按住鍵盤Shift
3. 左鍵選擇不定位鍵可以出現的位置
4. 選擇不定位鍵

[(151) Reaxys 結構編輯器 - 不定位鍵 - YouTube]

更多關於結構編輯器的進階技巧

(151) Reaxys 結構編輯器 - 縮寫官能基團 - YouTube

(151) Reaxys 結構編輯器 - 原子屬性列表 - YouTube

(151) Reaxys 結構編輯器 - G 任意官能基工具定義 - YouTube

(151) Reaxys 結構編輯器 - R 基團與末端定義工具 - YouTube

(151) Reaxys 結構編輯器 - 原子列表與原子列表非 - YouTube

(151) Reaxys 結構編輯器 - 鹽類與同位素 - YouTube

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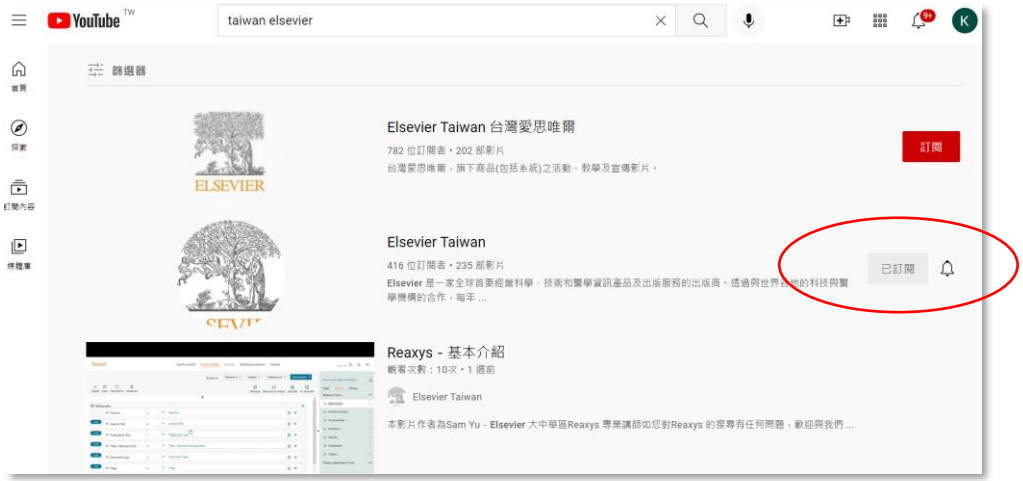
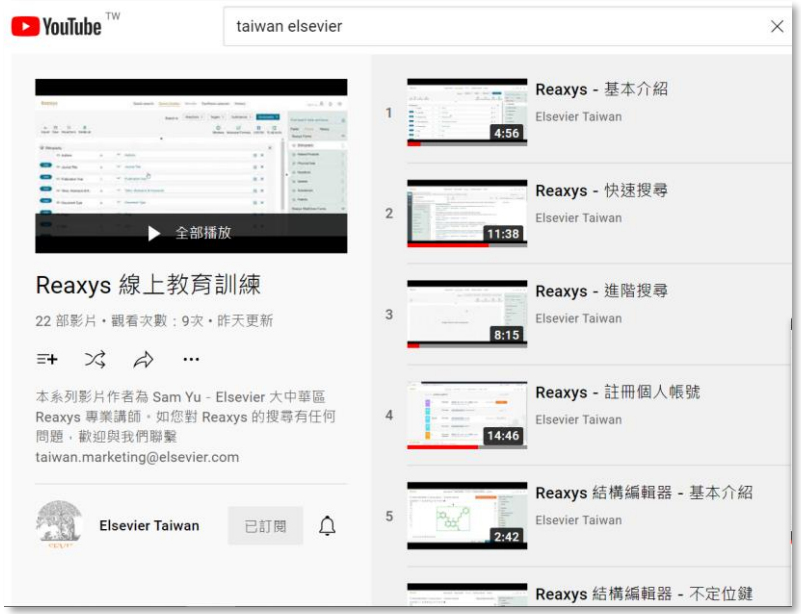
訂閱Elsevier Taiwan 自學線上資源



無廣告、持續更新中



https://www.youtube.com/playlist?list=PLBSTWvuNnJAl4laTo5zNkqaJ9va-LUtj0

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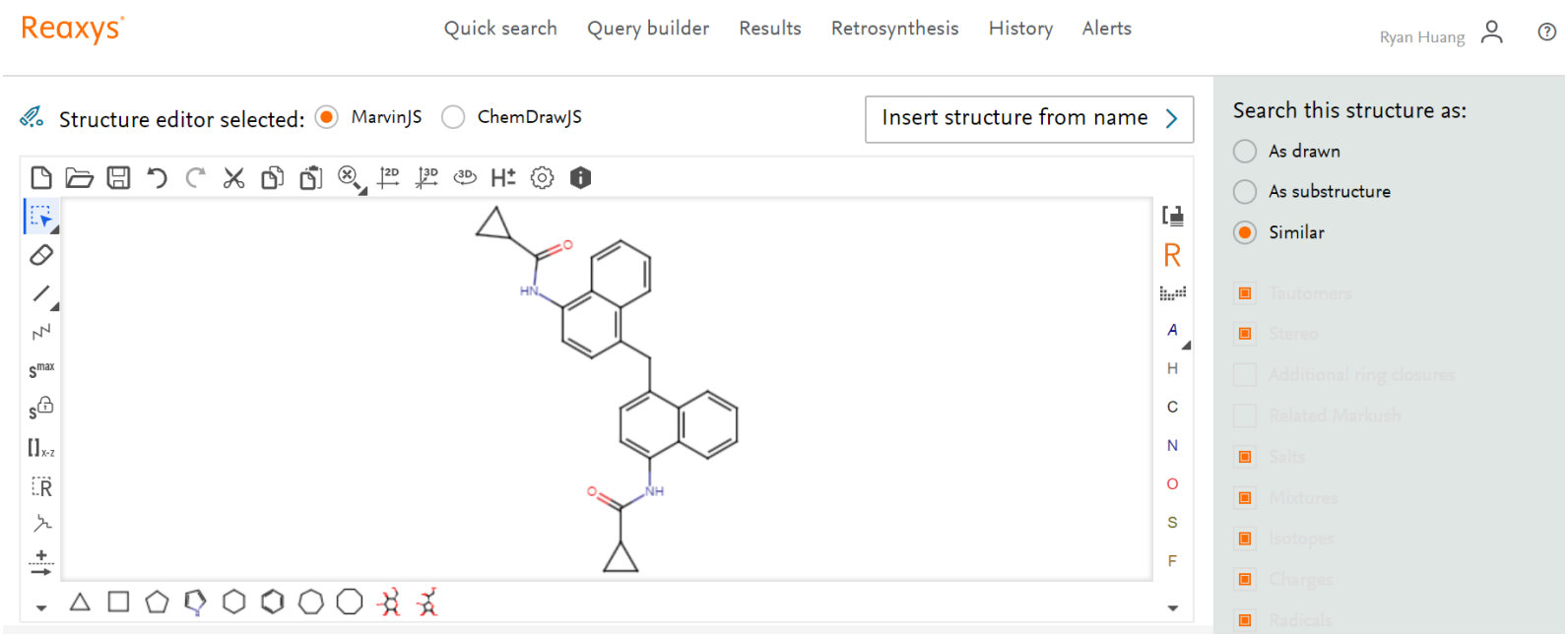
應用案例- 新穎性搜尋Novelty Search



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

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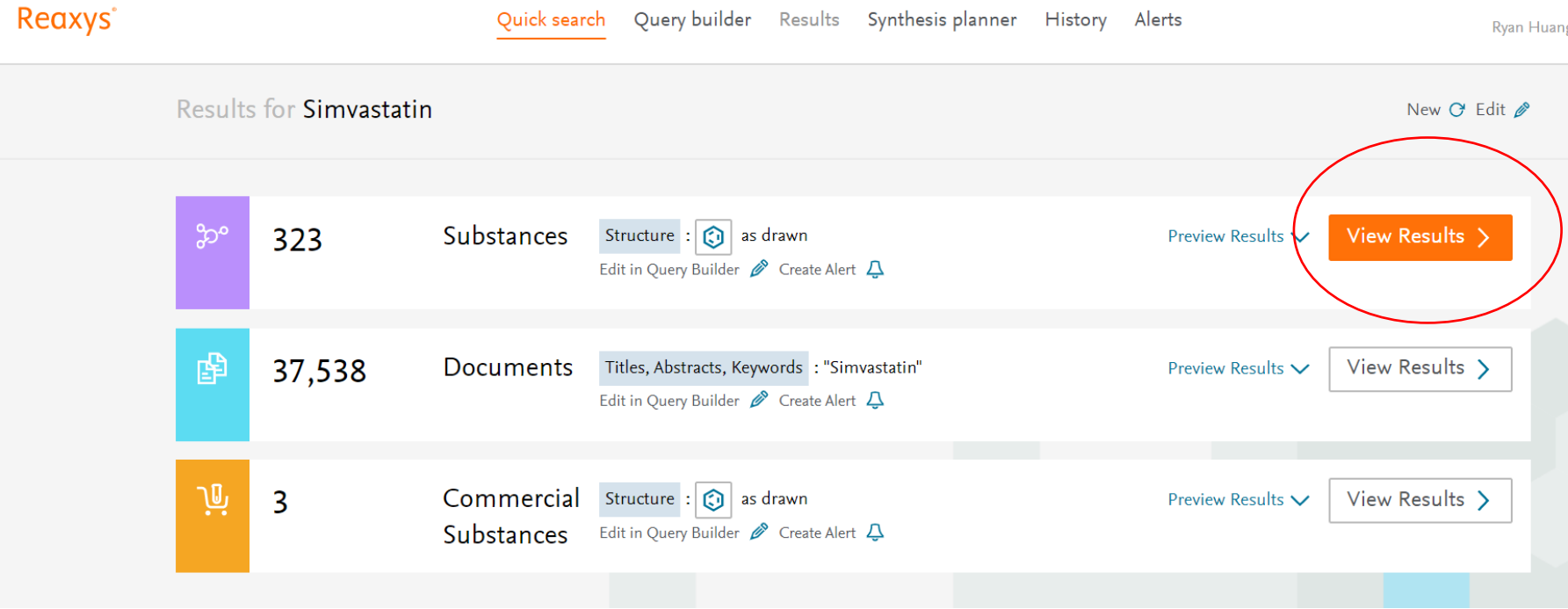
Substance Page

物質數據整理

預覽頁面選擇Substances



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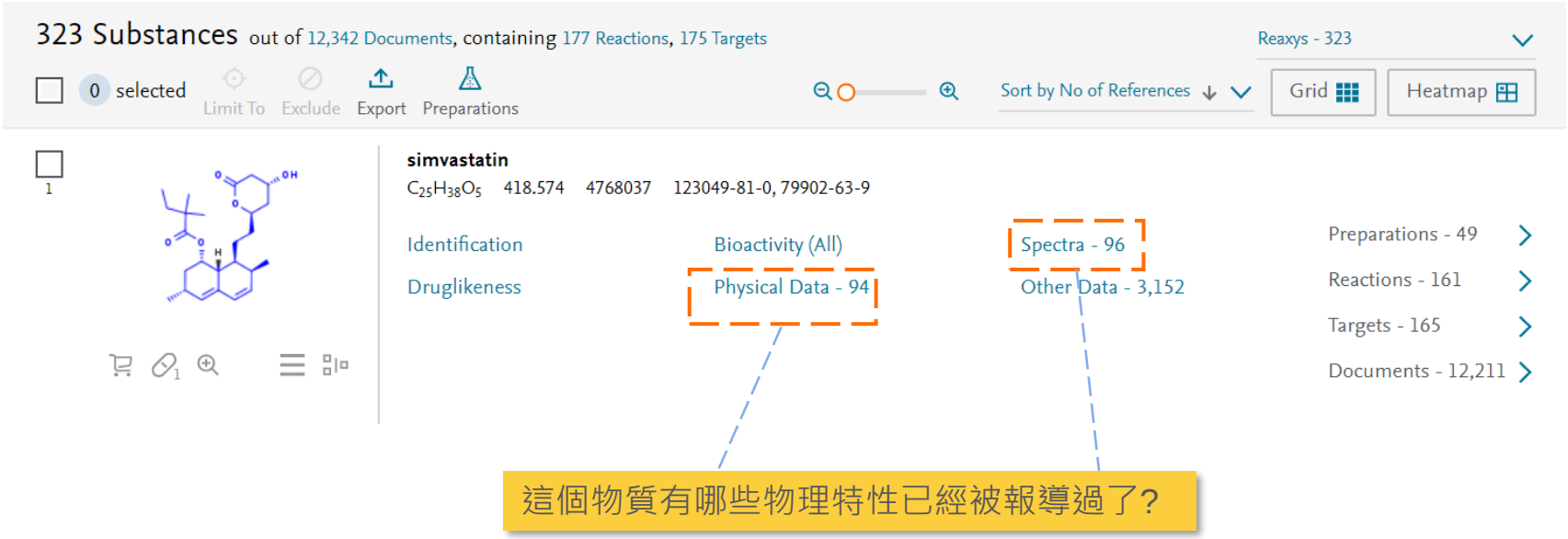
Reaxys人工擷取重要的實驗數據，並保留原始文獻出處
- 物理性質、光譜



Reaxys人工擷取重要的實驗數據，並保留原始文獻出處
- 物理性質、光譜

Solubility, $g \cdot l^{-1}$	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					organic solvents	[Macromolecular Bioscience, 2014, vol. 14, # 11, p. 1556 - 1568] Full Text ↗ Cited 27 times ↗ Details > Abstract >
6.73904	in pure solvent		aq. phosphate buffer	supporting information		Chung, Sanny S. W.; Cuellar, Rebecca A. D.; Wang, Xiangyuan; Reczek, Peter R. ; Georg, Gunda I.; Wolgemuth, Debra J.[**ACS Medicinal Chemistry Letters, 2013**, vol. 4, # 5, p. 446 - 450] Full Text ↗ Cited 8 times ↗ Details > Abstract >
15	in solution	25	aq. phosphate buffer			Ambike, Anshuman A.; Mahac ch, **2005**, vol. 22, # 6, p. 990 - 998] Full Text ↗ Cited 149 times ↗ Details > Abstract >
7.3E-05	in pure solvent	25	H2O			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[**Biological and pharmaceutical bulletin, 2002**, vol. 25, # 3, p. 346 - 350] Full Text ↗ Details > Abstract >
79.55	in pure solvent	25	propan-2-ol			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[**Biological and pharmaceutical bulletin, 2002**, vol. 25, # 3, p. 346 - 350] Full Text ↗ Details > Abstract >
19.09	in pure solvent	25	diethyl ether			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[**Biological and**

提供原始文獻連結

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- 專利出處、純化方法、專利名稱

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Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處
- 合成反應 & 購物車

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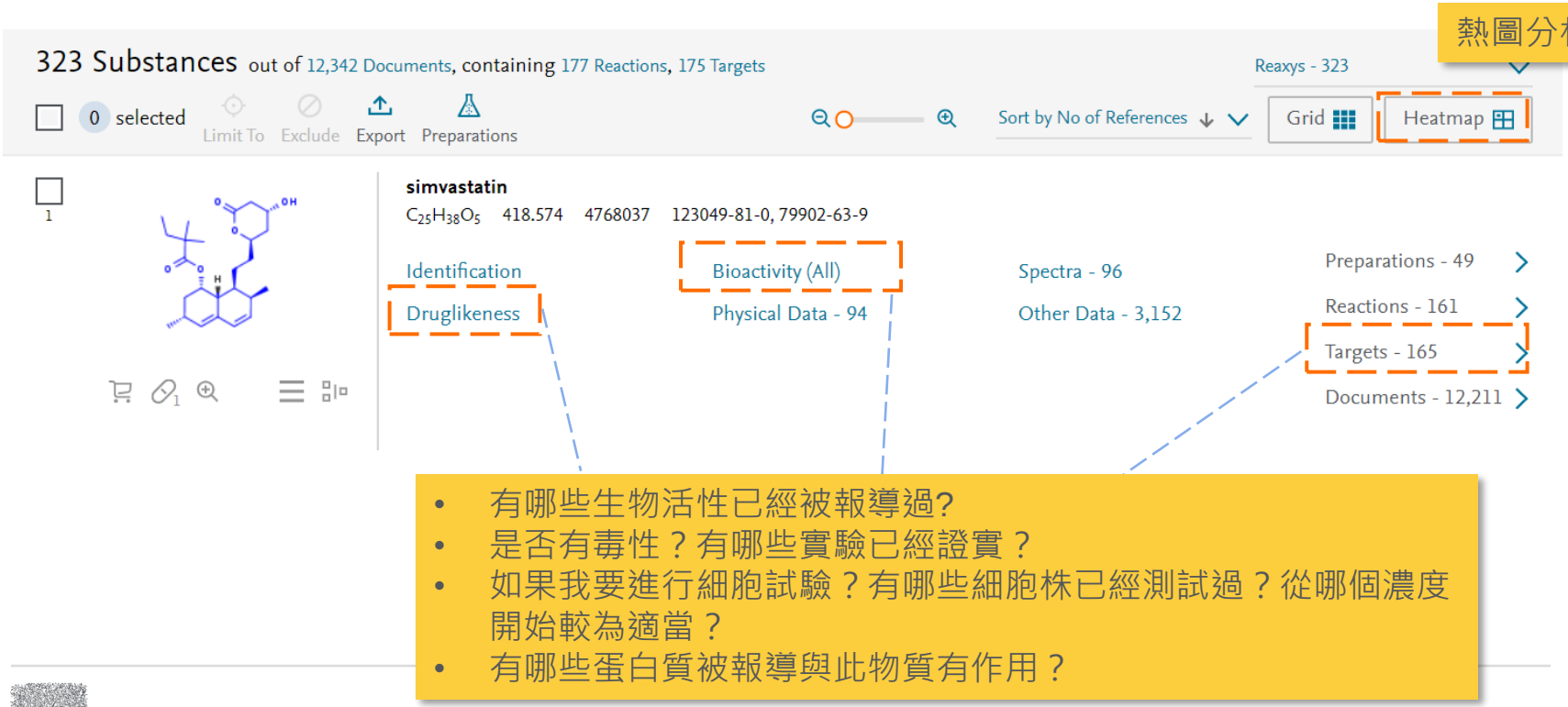
Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處
- 生物活性應用



Reaxys以人工擷取重要的實驗數據，並保留原始文獻出處
- 天然萃取物、應用

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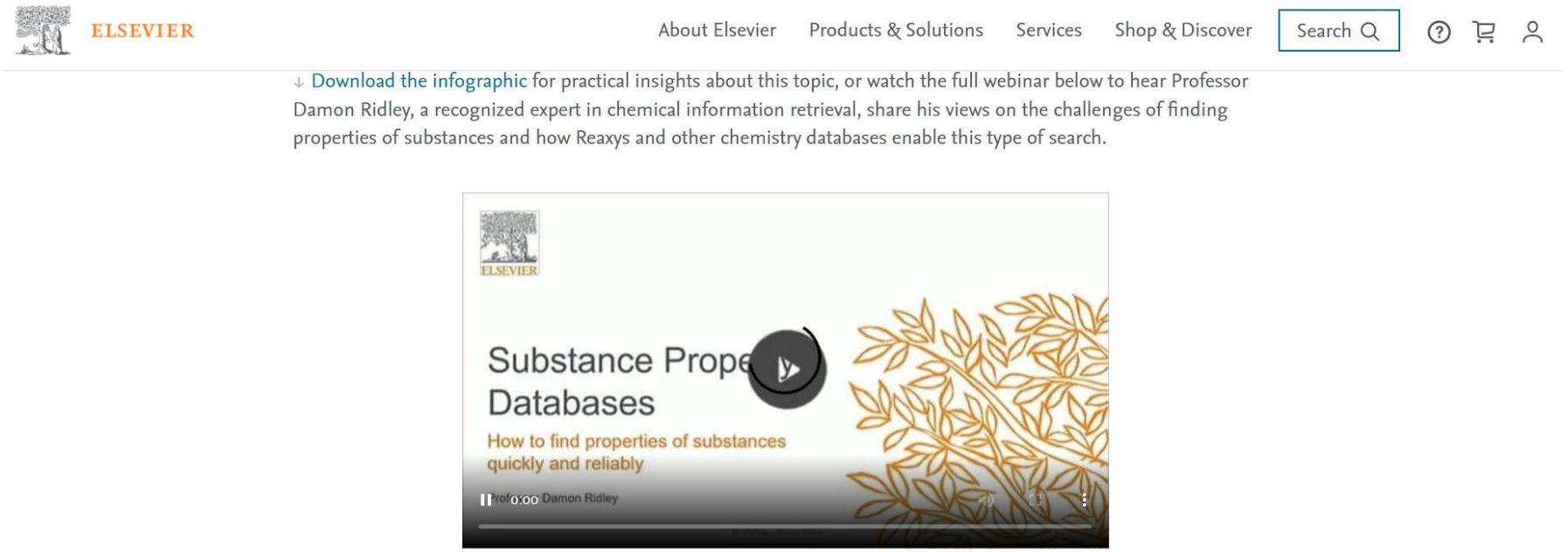
如何訓練學生學習用資料庫尋找化學關鍵資訊



[Finding physical and chemical properties of substances in Reaxys and other chemistry databases – Webinar and Infographic (elsevier.com)]

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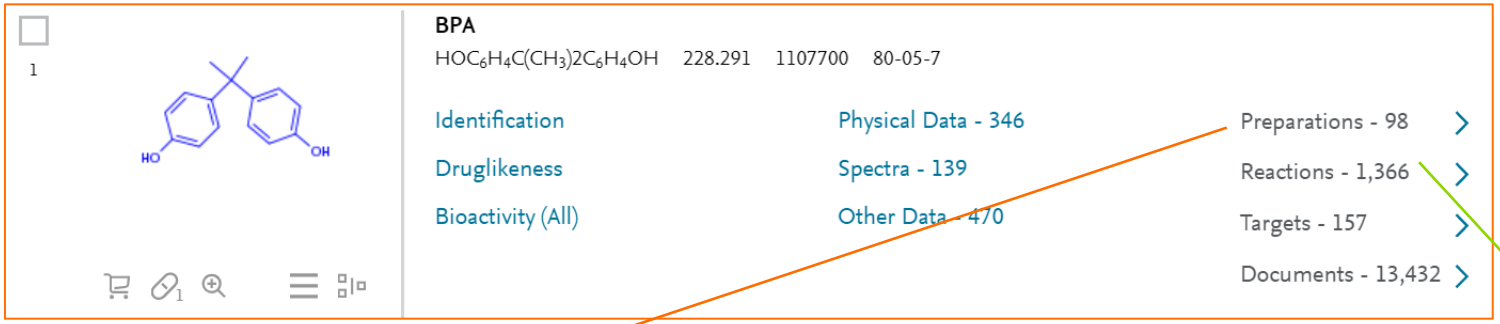
Reactions Search

反應式查詢

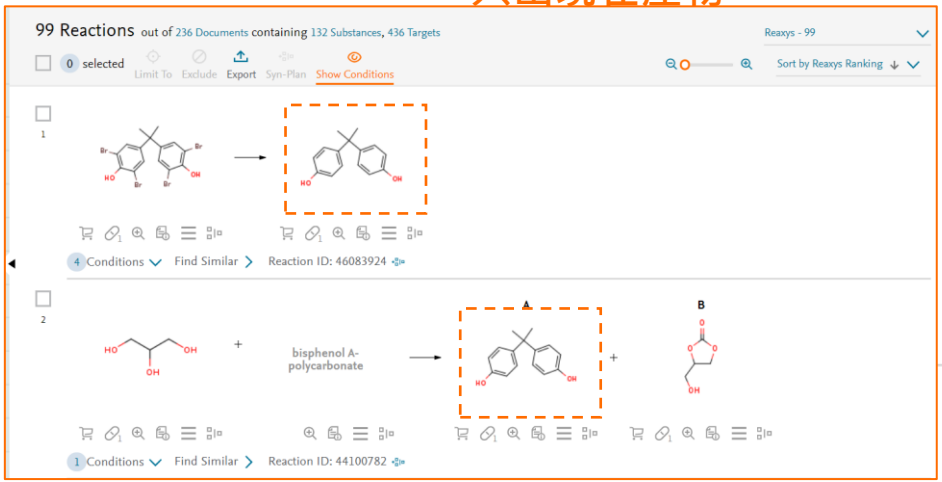
您可以用各種方式搜尋Reaction

1. 從物質資訊頁面連結到製備方式
2. 關鍵字搜尋、命名反應搜尋 (例如 Suzuki coupling)
3. 畫出反應式搜尋

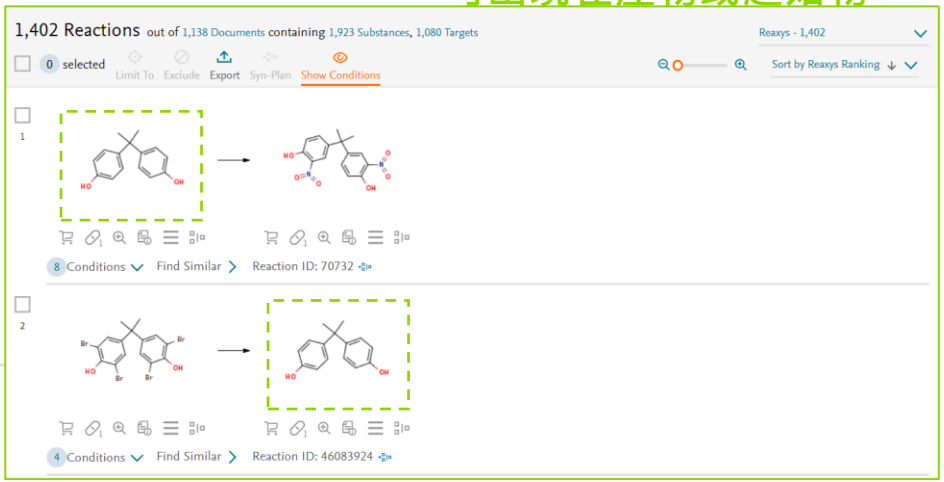
方法一、由物質頁面連結到製備方式 Preparation



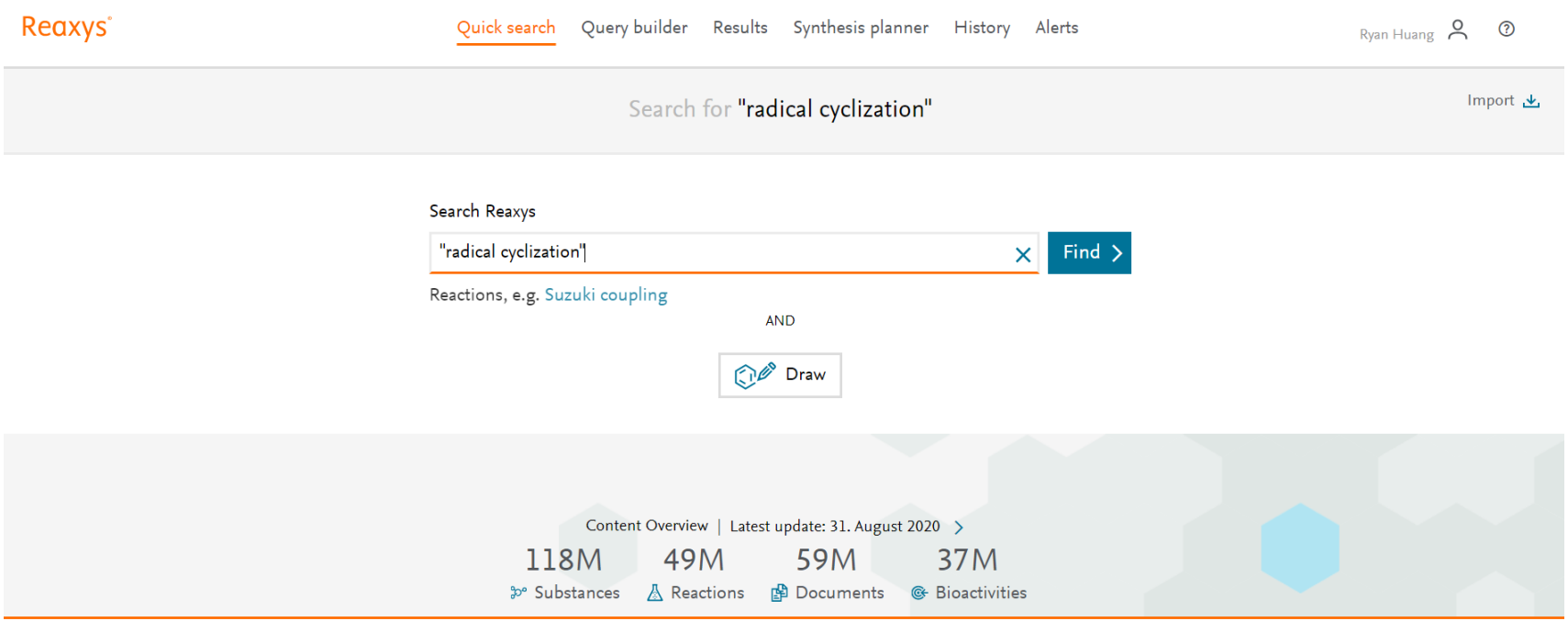
只出現在產物



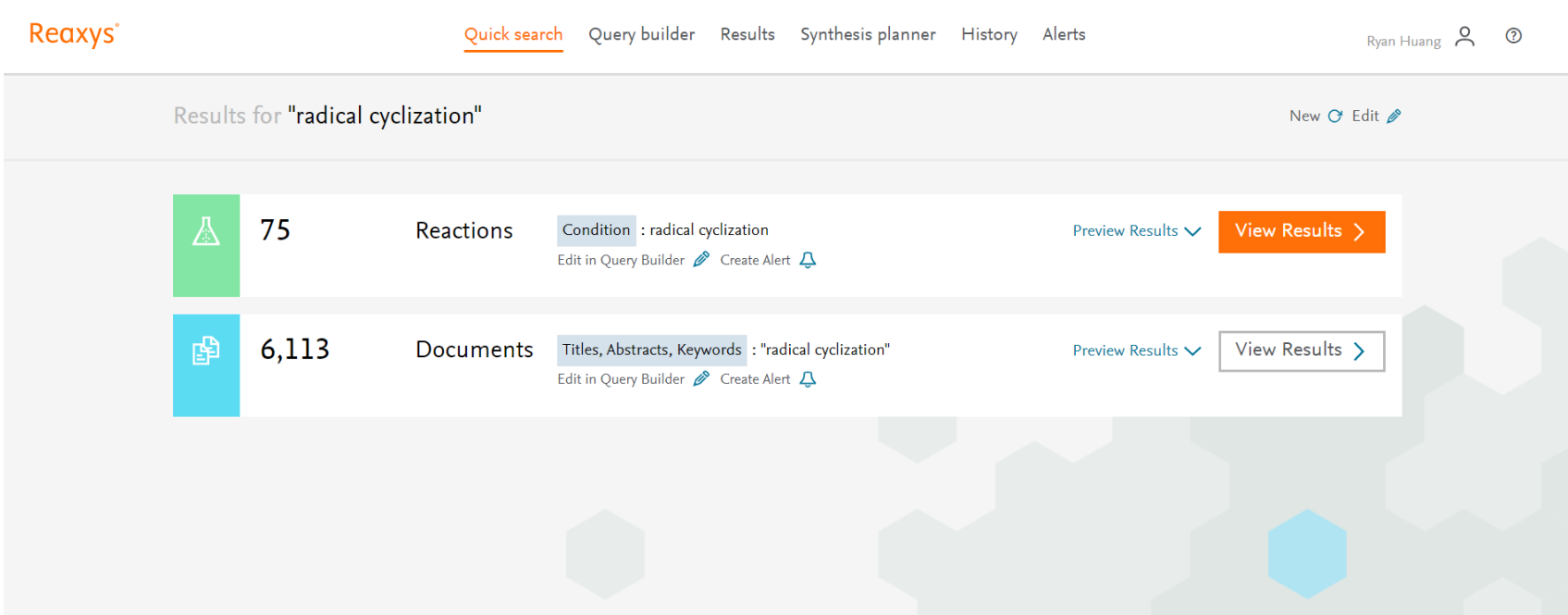
可出現在產物或起始物



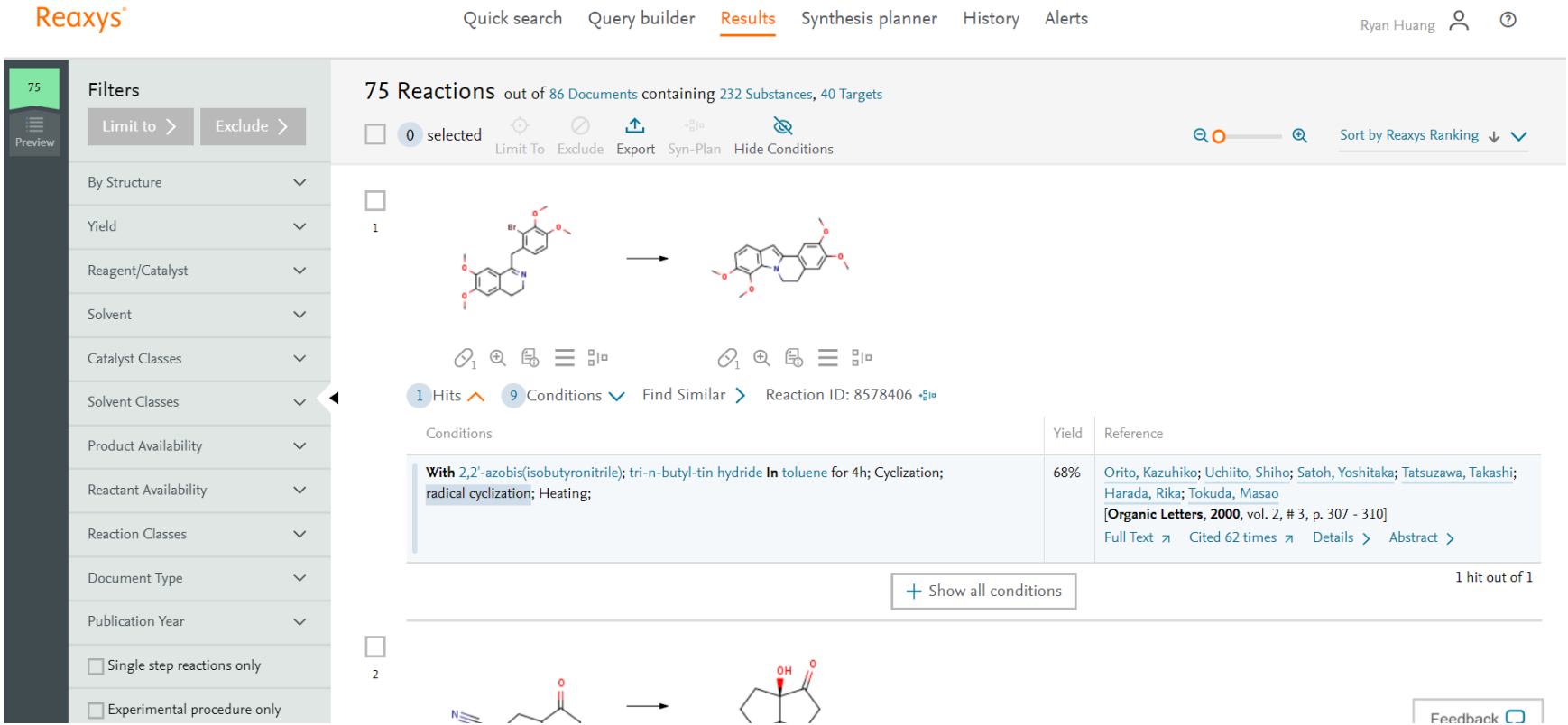
方法二、直接輸入反應關鍵字或是命名反應



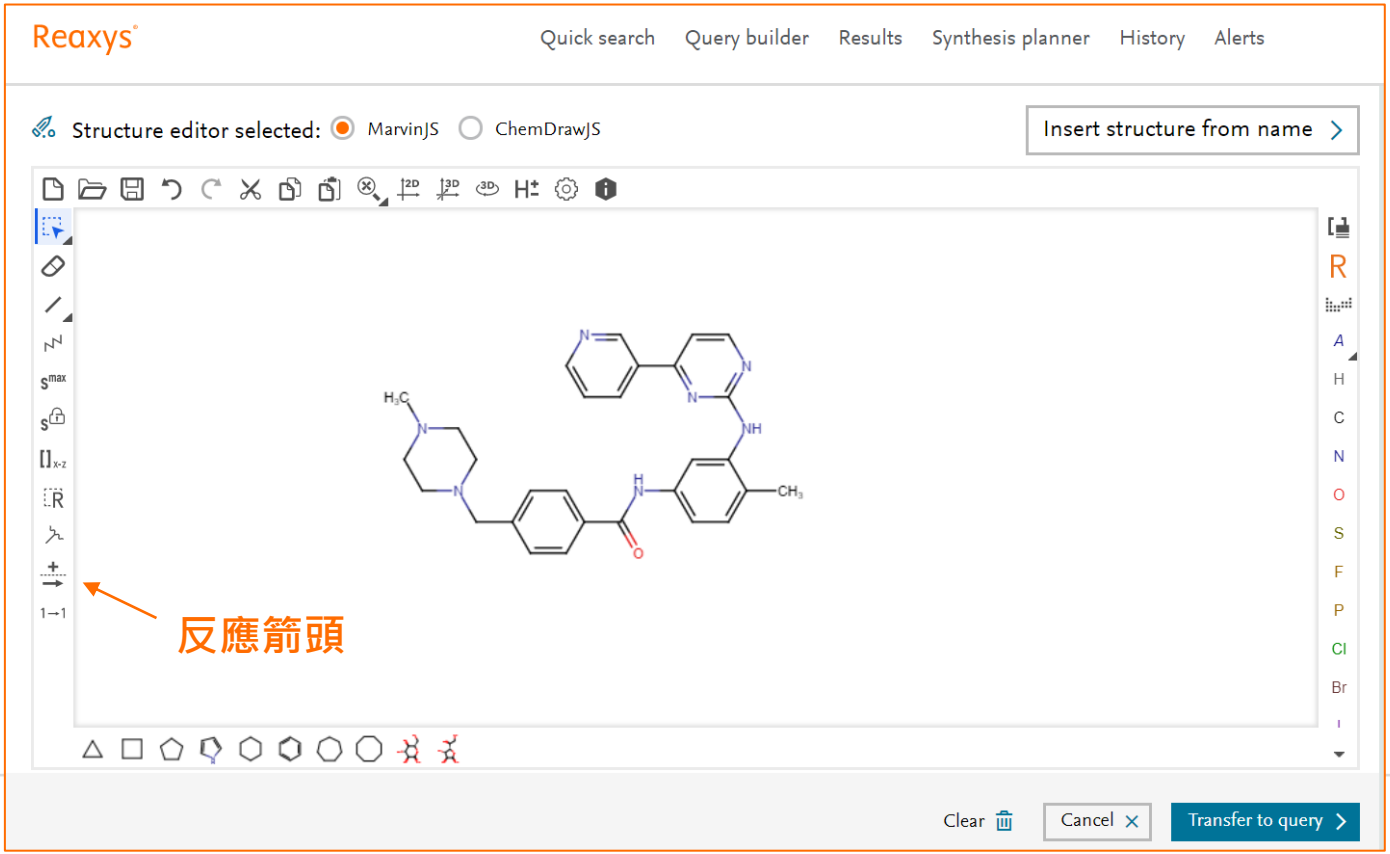
方法二、直接輸入反應關鍵字或是命名反應



方法二、直接輸入反應關鍵字或是命名反應



方法三、結構編輯器畫反應式



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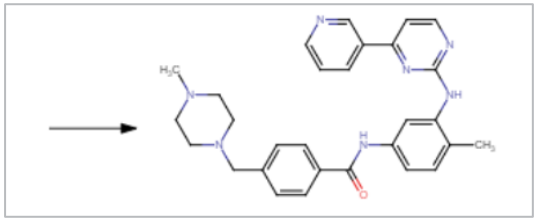
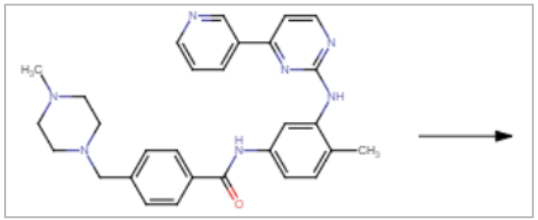
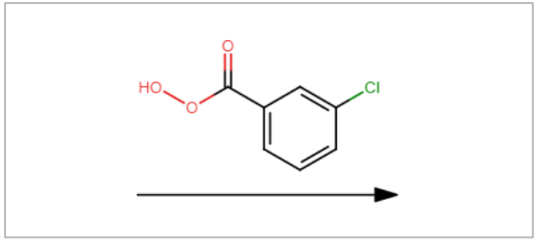
方法三、結構編輯器畫反應式



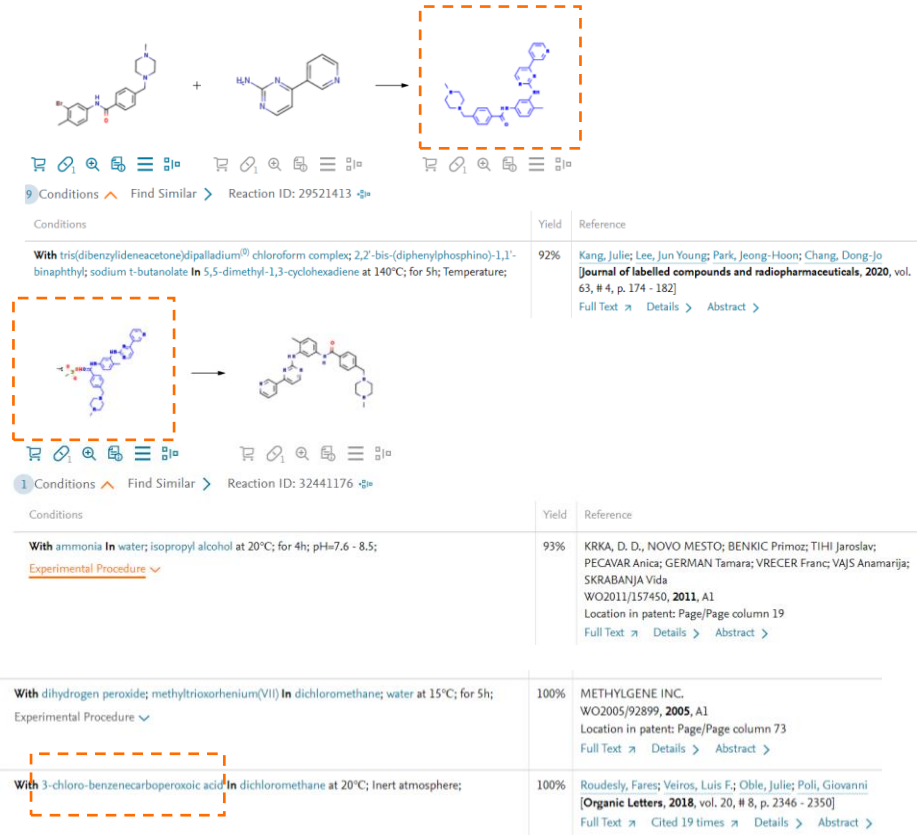
箭頭在左
產物



箭頭在右
起始物



箭頭在下
催化劑或溶劑



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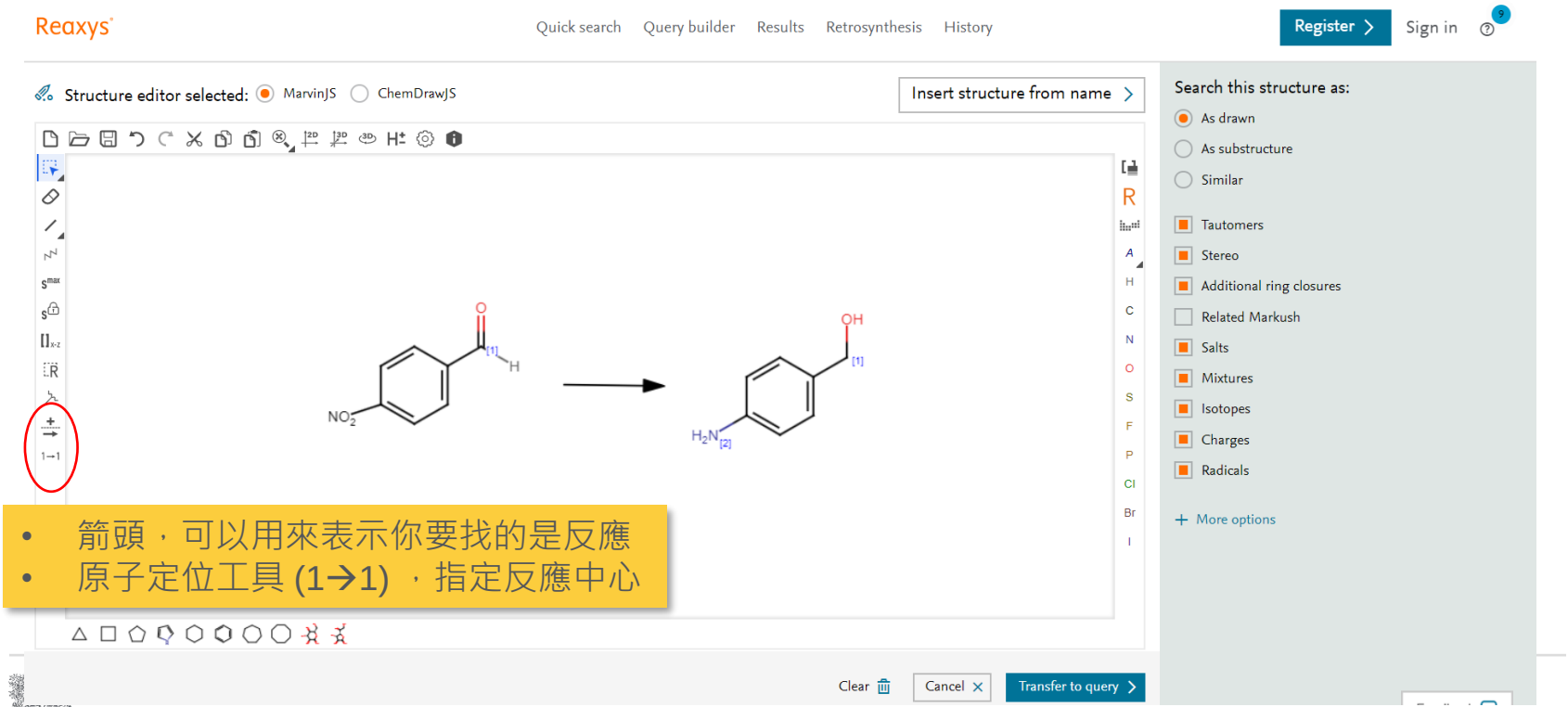
方法三、結構編輯器畫反應式

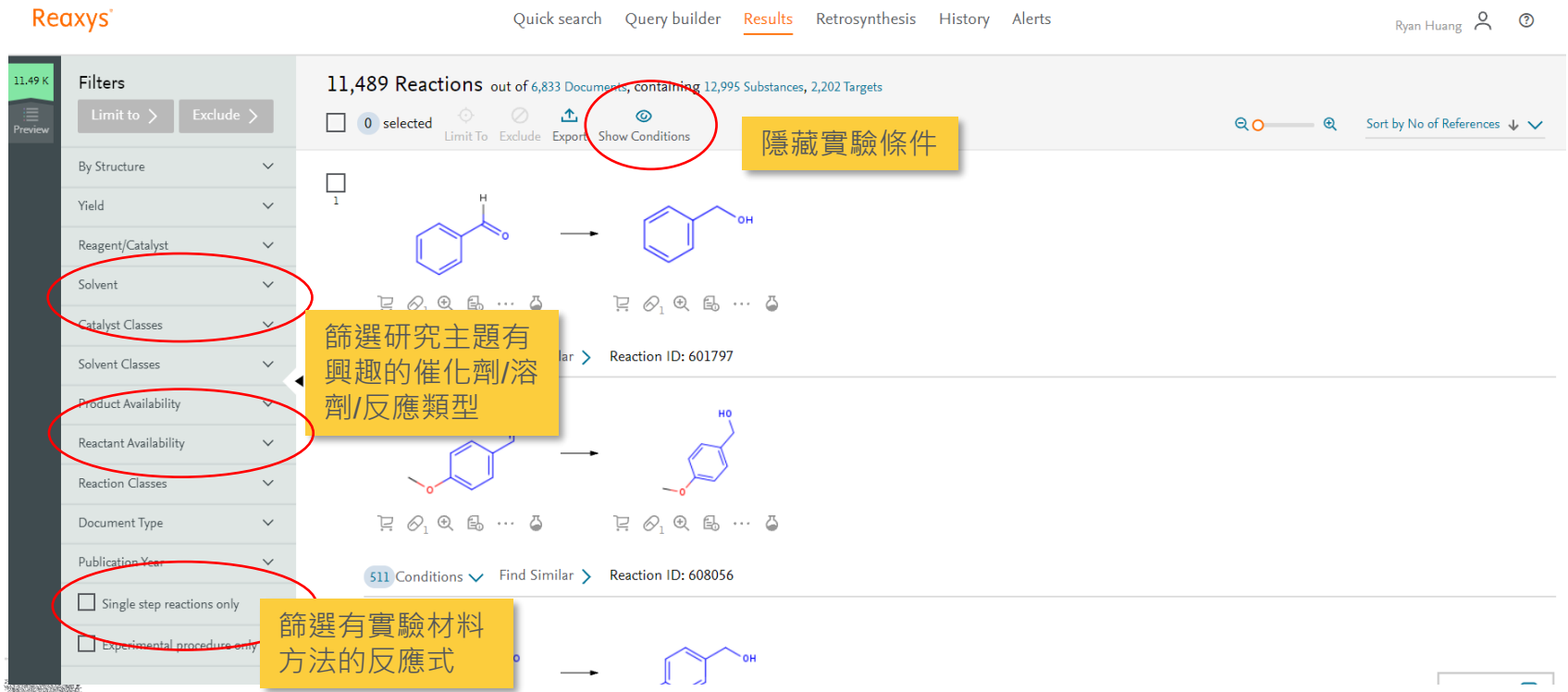
- 指定反應中心



- 箭頭，可以用來表示你要找的是反應
- 原子定位工具 (1→1) ，指定反應中心

方法三、結構編輯器畫反應式

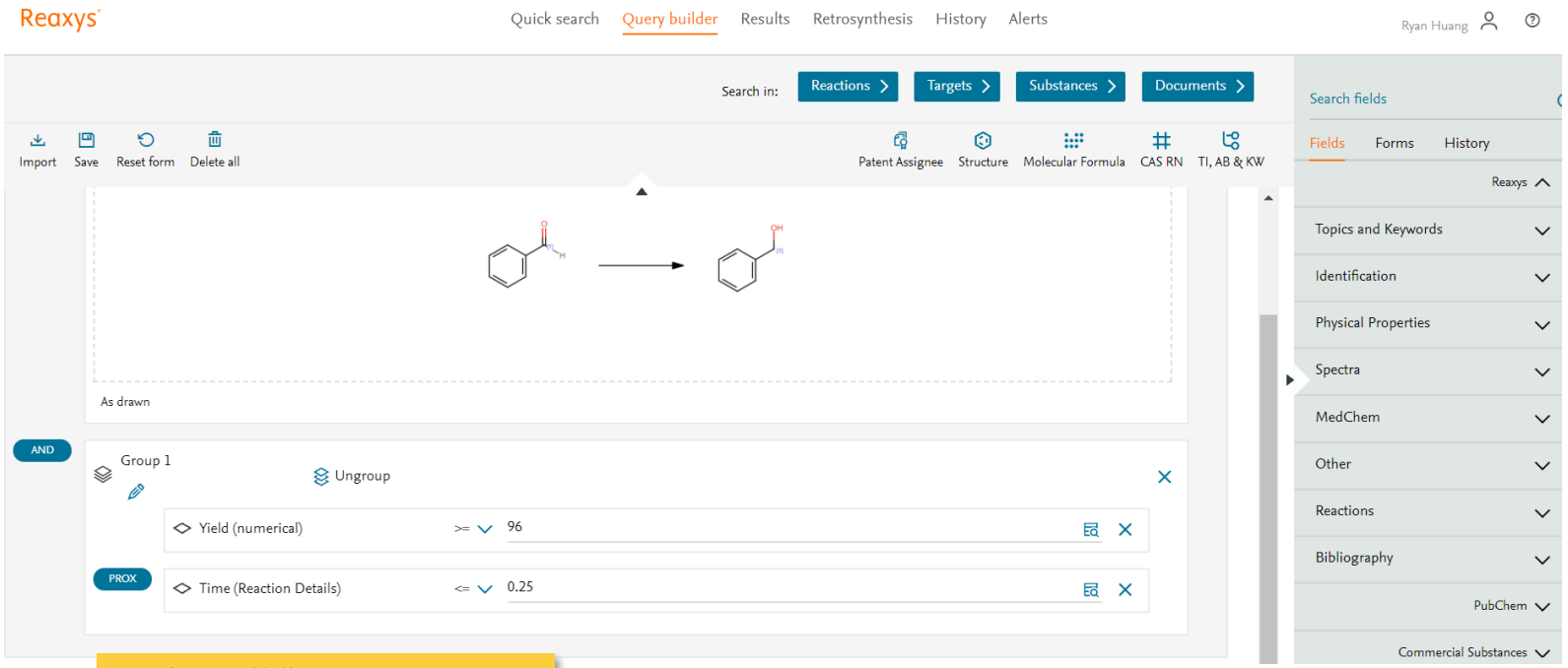
- 記得探索左邊的反應過濾器



[(152) Reaxys 反應式搜尋 - 基本過濾工具 - YouTube]

方法三、結構編輯器畫反應式

- 利用進階搜尋 (Query Builder來限制反應條件)



- 時間單位為Hr
- 同一個資料格裡面必須用Proximity (相鄰)串在一起

[(152) Reaxys 反應式搜尋 - 如何定義反應條件 - YouTube]

使用Query Builder 搜尋使用”特定催化劑”的反應式

Query > Forms > Reactions

或使用自由字元*來增加搜尋效率
例如：
Pd*
Pd*Pt

免費的有機反應APP – 你需要知道的命名反應都在這裡

ReactionFlash® gives access to over 1,000 Named Reactions, their mechanisms and examples published in peer-reviewed literature.

Developed in collaboration with the renowned research group of Prof. Dr. Carreira of ETH Zurich.

Available for free on:

Download on the App Store

GET IT ON Google Play

自學

實驗室查詢

闖關

[ReactionFlash - Need to know everything about named reactions? (elsevier.com)]

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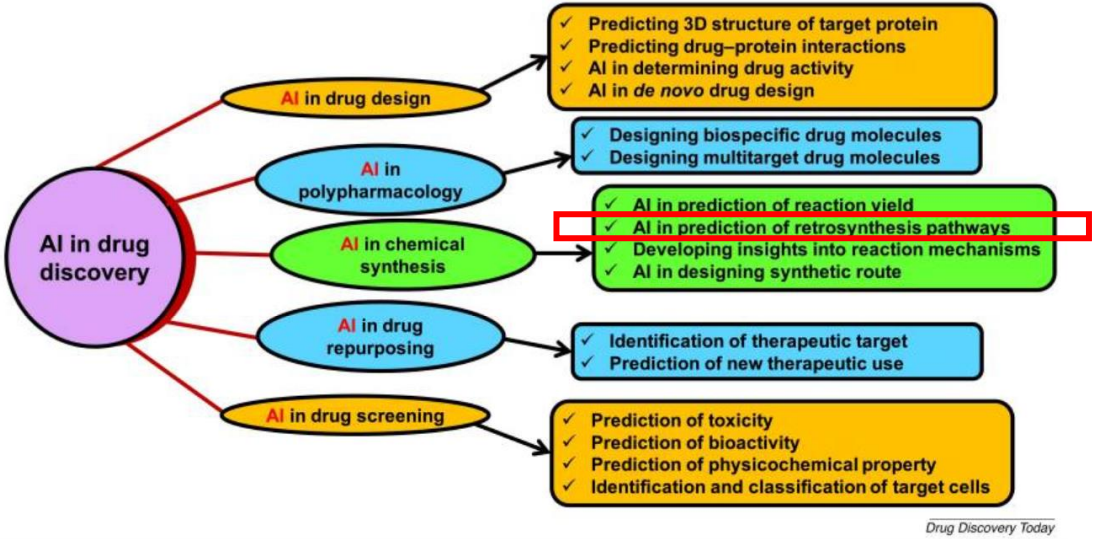
Reaxys Retrosynthesis Page

逆合成工具

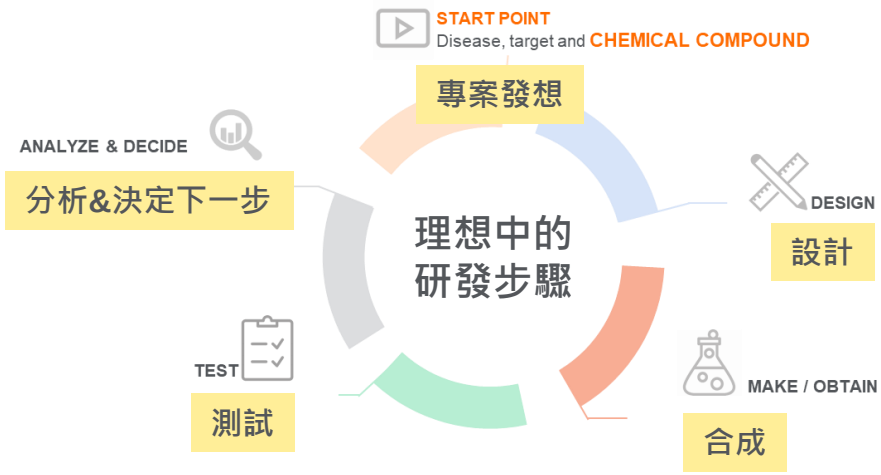
Reaxys retrosynthesis要解決的問題

- 如何有效率的合成目標分子

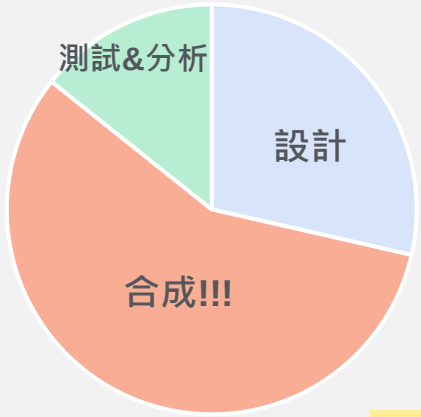


Paul, Debleena et al. “Artificial intelligence in drug discovery and development.” *Drug discovery today* vol. 26,1 (2021): 80-93. doi:10.1016/j.drudis.2020.10.010

合成步驟正在拖慢你的腳步



現實狀況



合成是瓶頸步驟
花了>50%的時間

能不能有電腦輔助的工具來加快合成的步驟?

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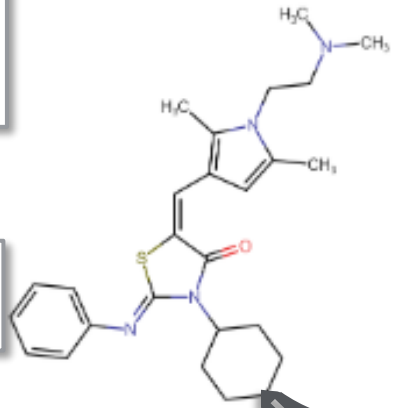
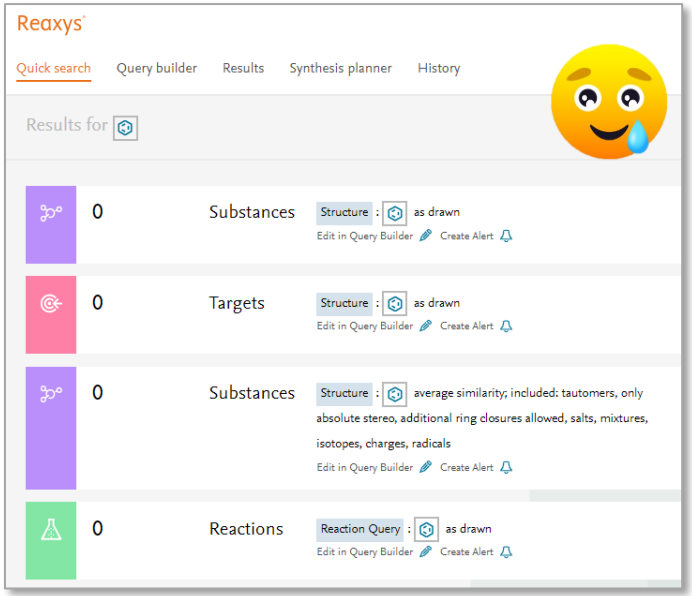
新分子的合成路徑是如何以人工設計的?

- Thinking chemistry
- 搜尋可以參考的反應式
- 搜尋可以參考的起始材料
- 上實驗桌

- Thinking chemistry
- 上實驗桌





✓ 拓展更多可行的合成策略/合成材料
✓ 節省查詢時間
✓ 加速學習曲線

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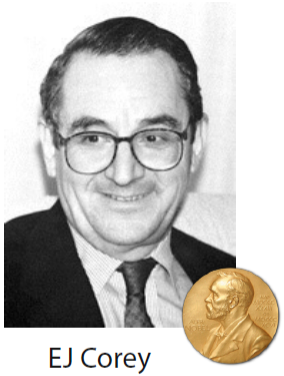
諾貝爾獎得主EJ Corey以電腦輔助化學合成規劃

The roots of Computer Aided Synthesis Planning



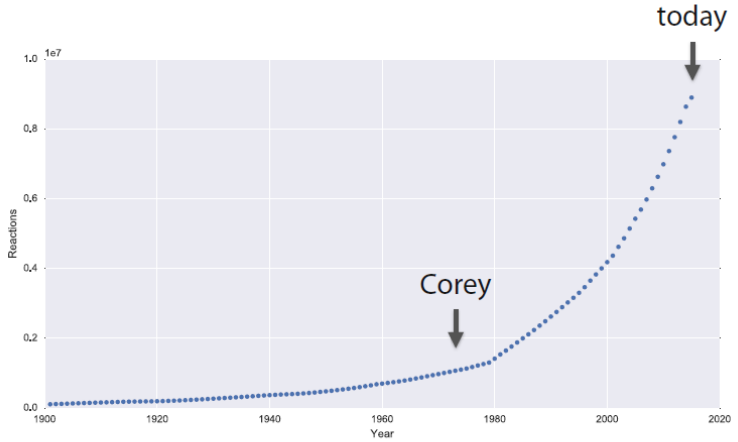
EJ Corey
Nobel prize 1990

Vleduts (1963), Corey (1968)
Write down all of chemical knowledge in logic form

Great for humans!
Not so much for machines…

Vléduts,G. *Inform. Storage Retrieval* 1, 117–146 (1963).
Corey, *The Logic of Chemical Synthesis*

Manual coding cannot work on scale



- chemical knowledge grows exponentially, doubles every decade

兩個超越90年代的成功障礙：
1. 電腦的硬體尚未發展到可以解決預測化學合成的計算規模。
2. 以人工編寫合成規則，需要大量的時間且跟不上新反應發表的速度。

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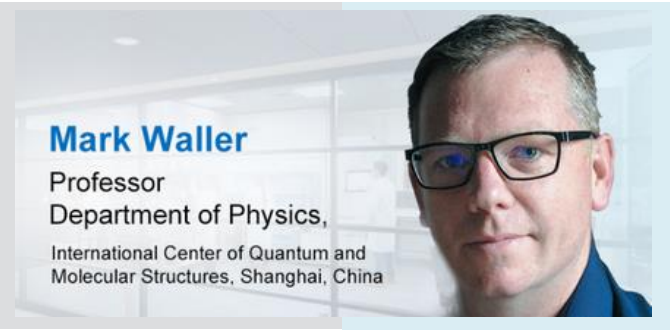
Reaxys使用的策略

–結合 高品質的Reaxys reactions資料 與 神經網路 (Neural Network) 3N-MCTS 科技



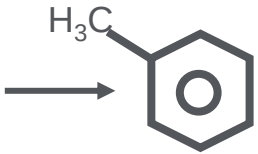
NEWS

AI in Action: Neural networks learn the art of chemical synthesis

Robert F. Service

+ See all authors and affiliations

Science 07 Jul 2017:
Vol. 357, Issue 6346, pp. 27
DOI: 10.1126/science.357.6346.27



Reaxys®

3N-MCTS : 3 layers Neural Network - Monte-Carlo-Tree-Search

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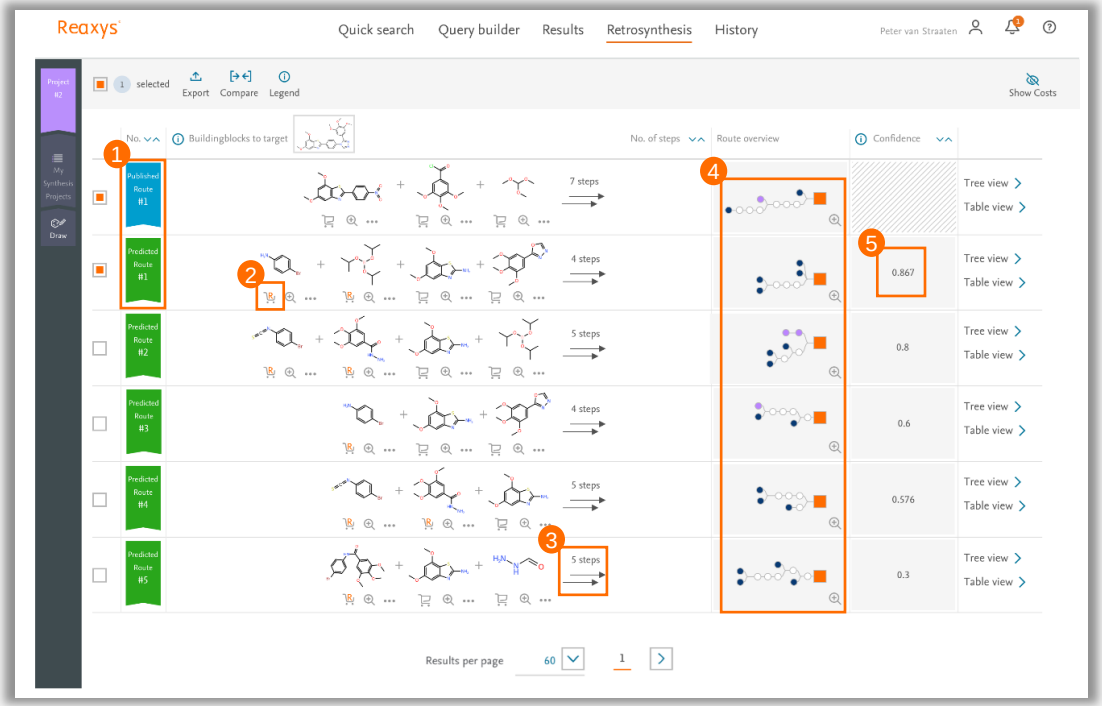
簡單的介面，只要10分鐘的預測時間

–只要畫出目標分子，Reaxys 15M的反應式做後盾



1. 同時呈現文獻發表的合成路徑與AI預測路徑進行比較
2. AI會確定合成路徑起點是買的到的商用材料
3. 以合成路徑長短排序
4. 以圖形讓你判斷合成策略的複雜度
5. 內建的評分系統輔助您判斷AI的可信度

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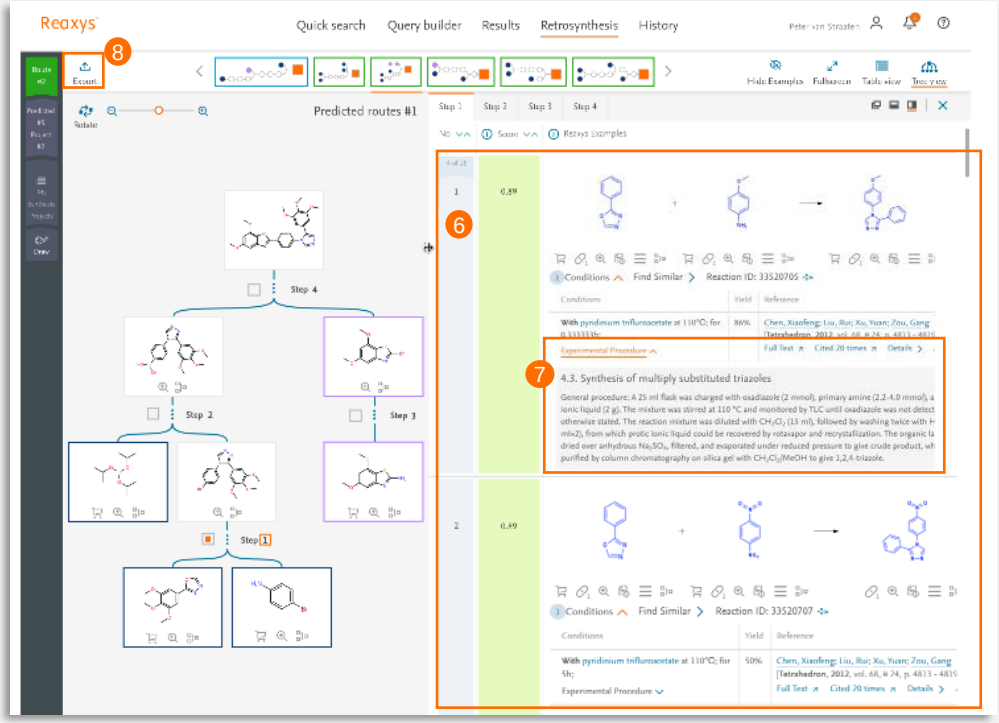
簡單的介面，只要10分鐘的預測時間

–只要畫出目標分子，Reaxys 15M的反應式做後盾



6 自動搜尋呈現文獻中"相似"的反應，畫面(左側)呈現預測路徑，(右側)呈現Reference路徑，讓您輕鬆判斷可行性

7 提供完整的實驗材料方法Experimental Procedure讓您參考如何規劃實驗細節

8 各種輸出格式，PDF並支援各式電子實驗記錄

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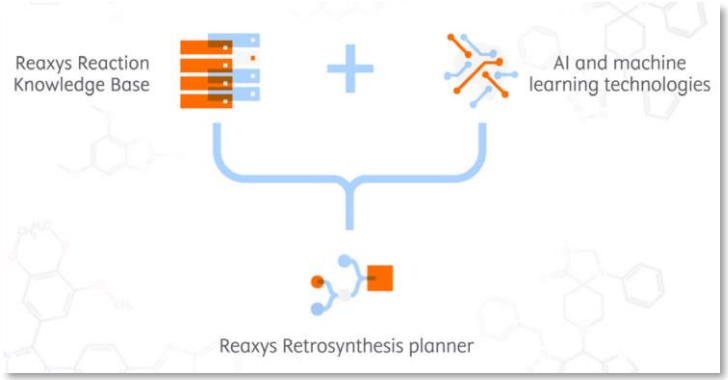
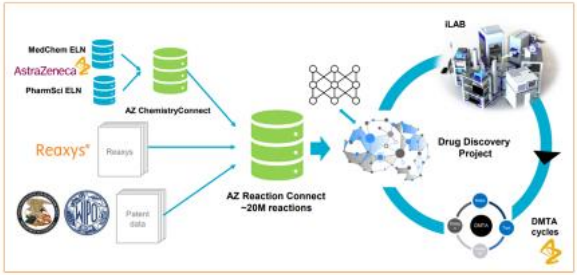
知名研究團隊的AI進展

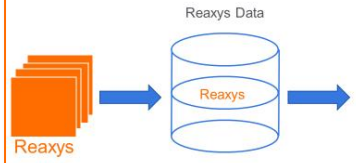


Reaxys data is key component of reaction knowledge base that is helping AstraZeneca to embed predictive algorithms in their drug development projects



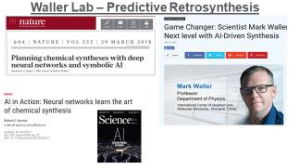
European Laboratory Research & Innovation Group: https://elrig.org/downloads/ri19/Ola_Engkvist.pdf

Elsevier collaboration with leading academics and and the use of Reaxys data powers the most siginificant developments in predictive retrosynthesis algorithms

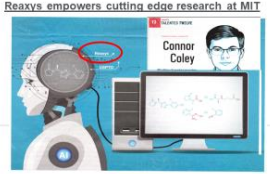


- >12.5 M reactions data
- Organic, single step reactions
- Harmonized, curated and AI/ML ready data

Waller Lab – Predictive Retrosynthesis

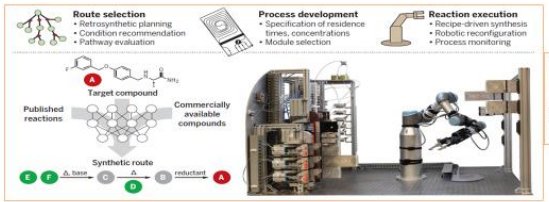


Reaxys empowers cutting edge research at MIT



Reaxys data is helping Jensen group transform the design of industrial processes for chemical and drug manufacturing

MIT Jensen Research Group
MIT Department of Chemical Engineering



From 12.5 million published single-step reactions tabulated in the **Reaxys** database, they prepared a library of **163,723 rules**. Transformations with **stereochemistry** were included in the rules.

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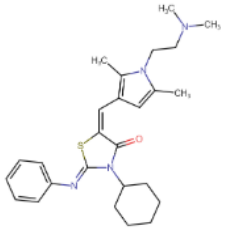
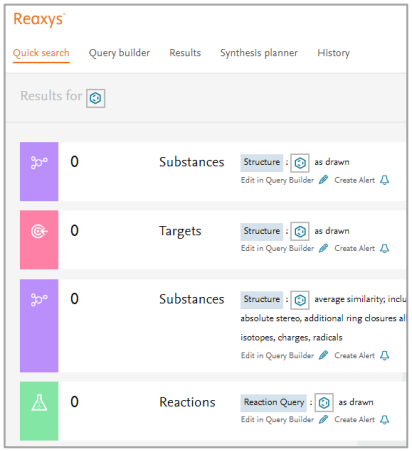
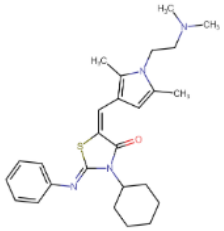
人工查詢規劃逆合成路徑



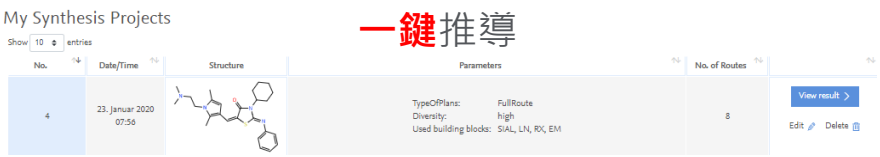


1. Thinking about chemistry
2. **Reaction & Literature Search**
3. **Start Material Search**
4. Work at the Bench

以數位工具輔助逆合成規劃路徑

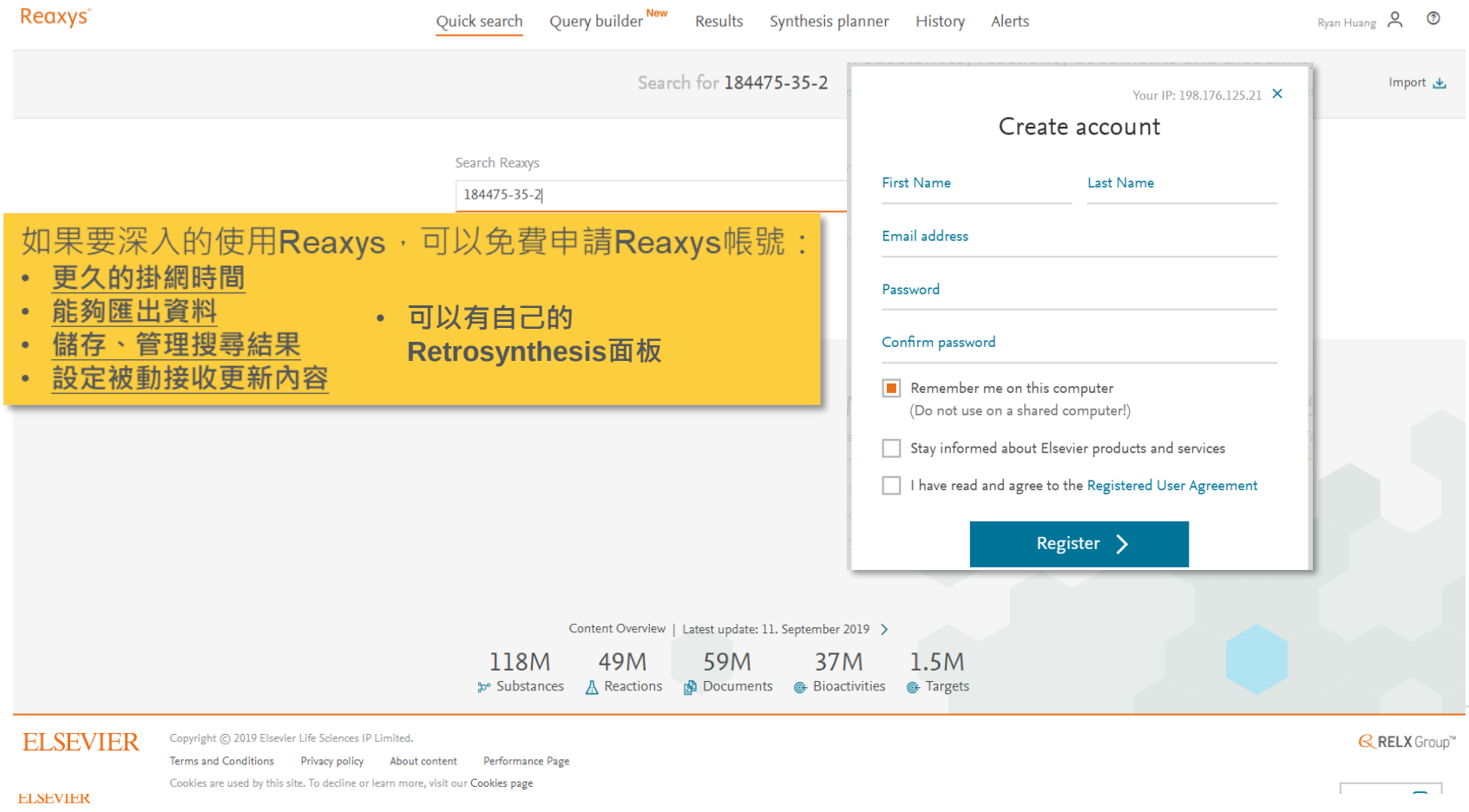


一鍵推導

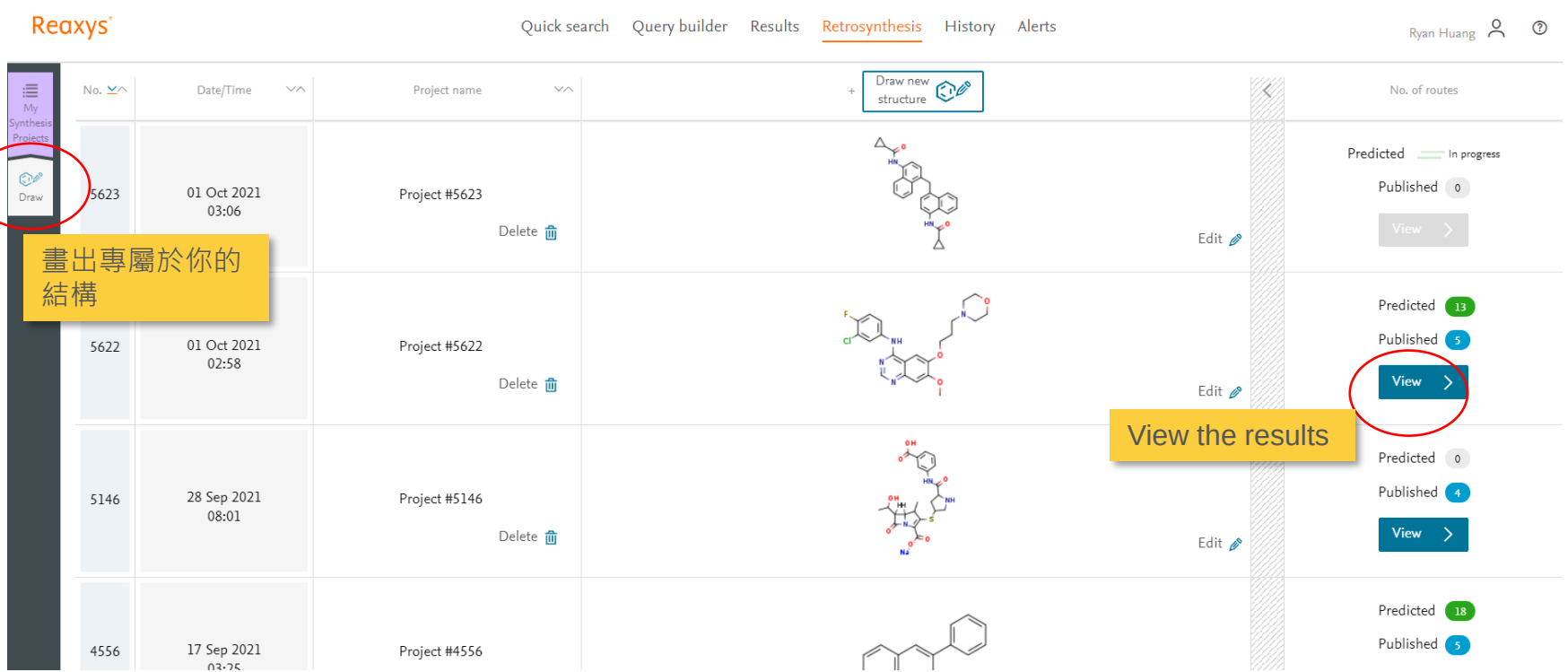


- **Thinking about chemistry**
- **Work at the Bench**

登入Reaxys –註冊**免費帳號**



逆合成面板 (規劃合成路徑、合成材料與反應條件)



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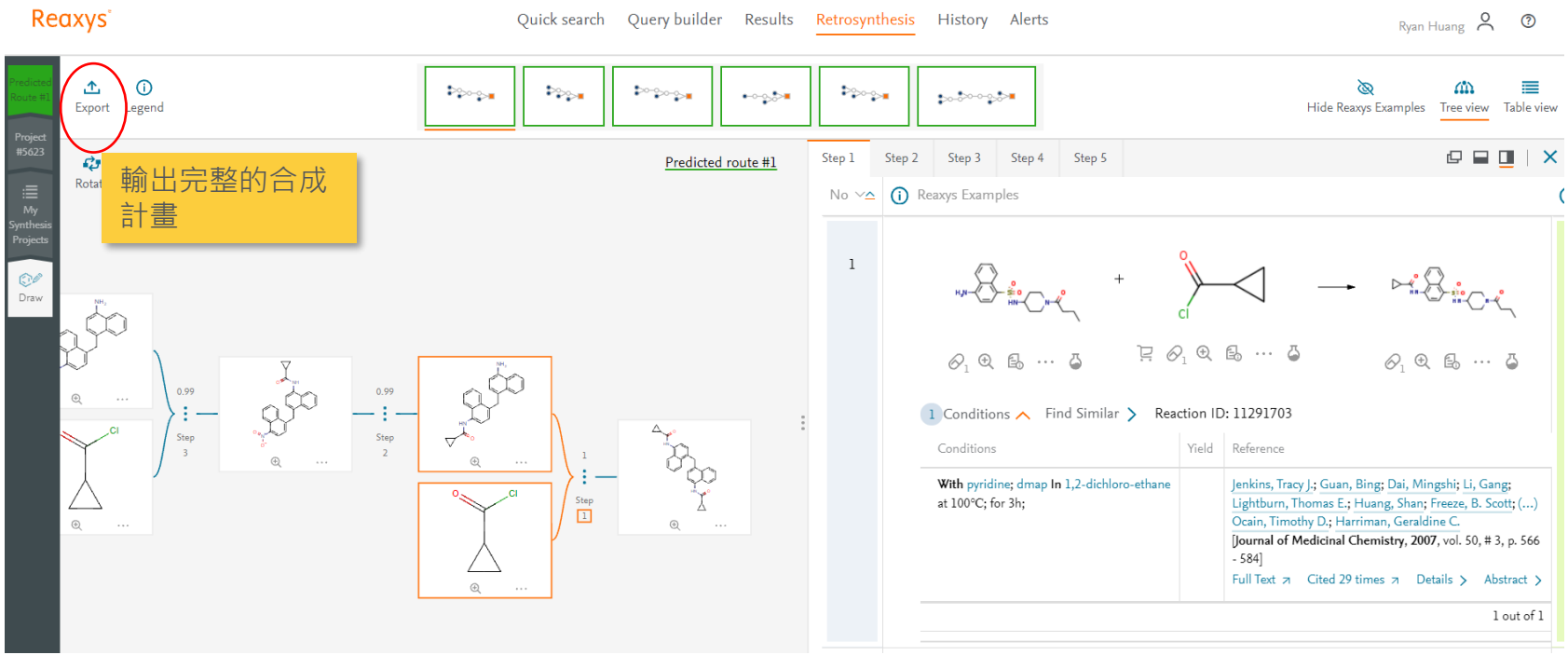
逆合成面板 (規劃合成路徑、合成材料與反應條件)



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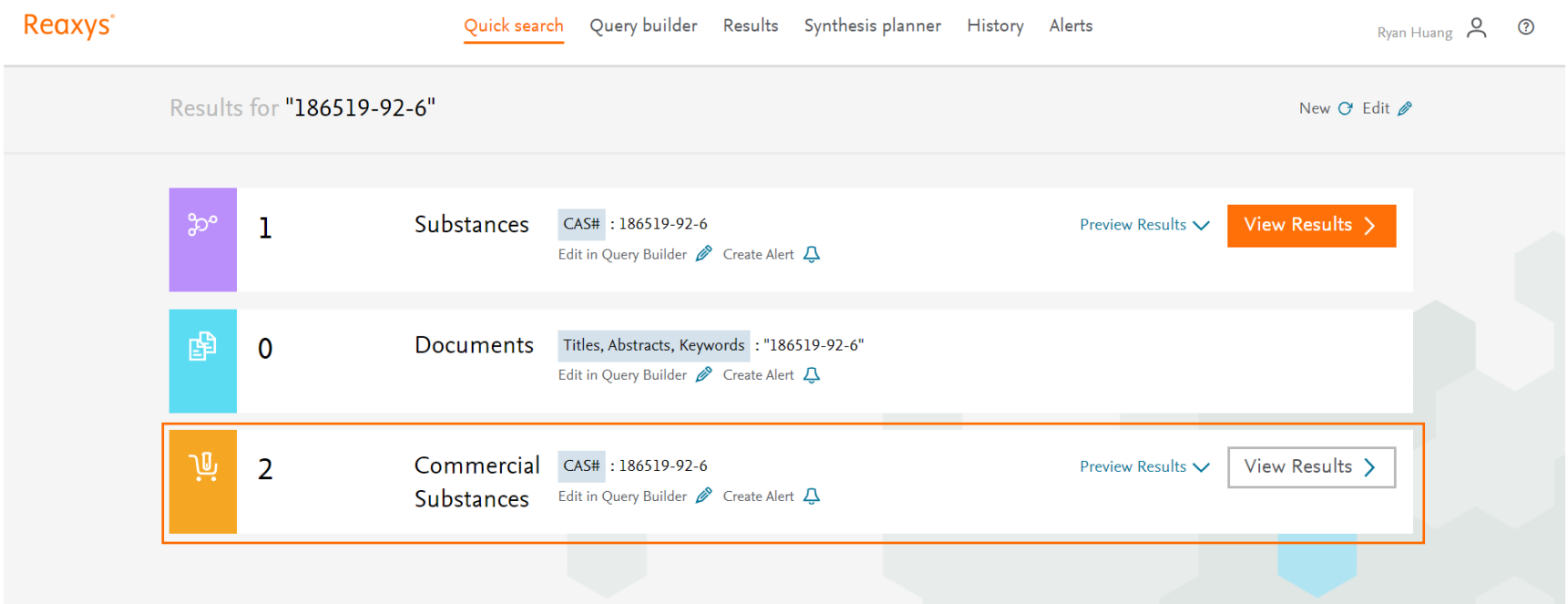
Reaxys Commercial Substances

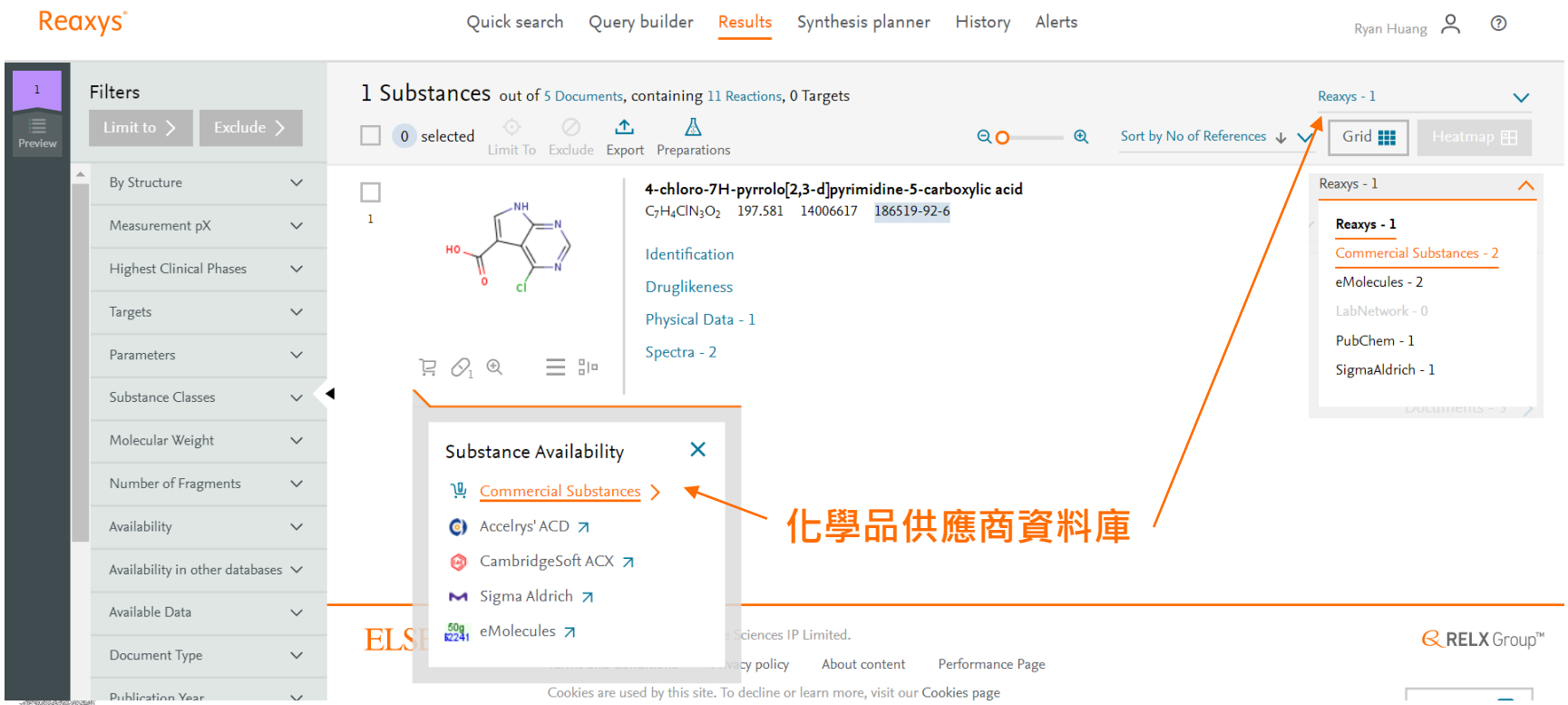
供應商物質資料庫

新增分類”Commercial Substances”於預視頁面

- Quick Search輸入CAS#，或畫結構搜尋您要購買的物質



物質頁面購物車新增分類”Commercial Substances”
- 或點擊右上方切換資料庫為Commercial Substances



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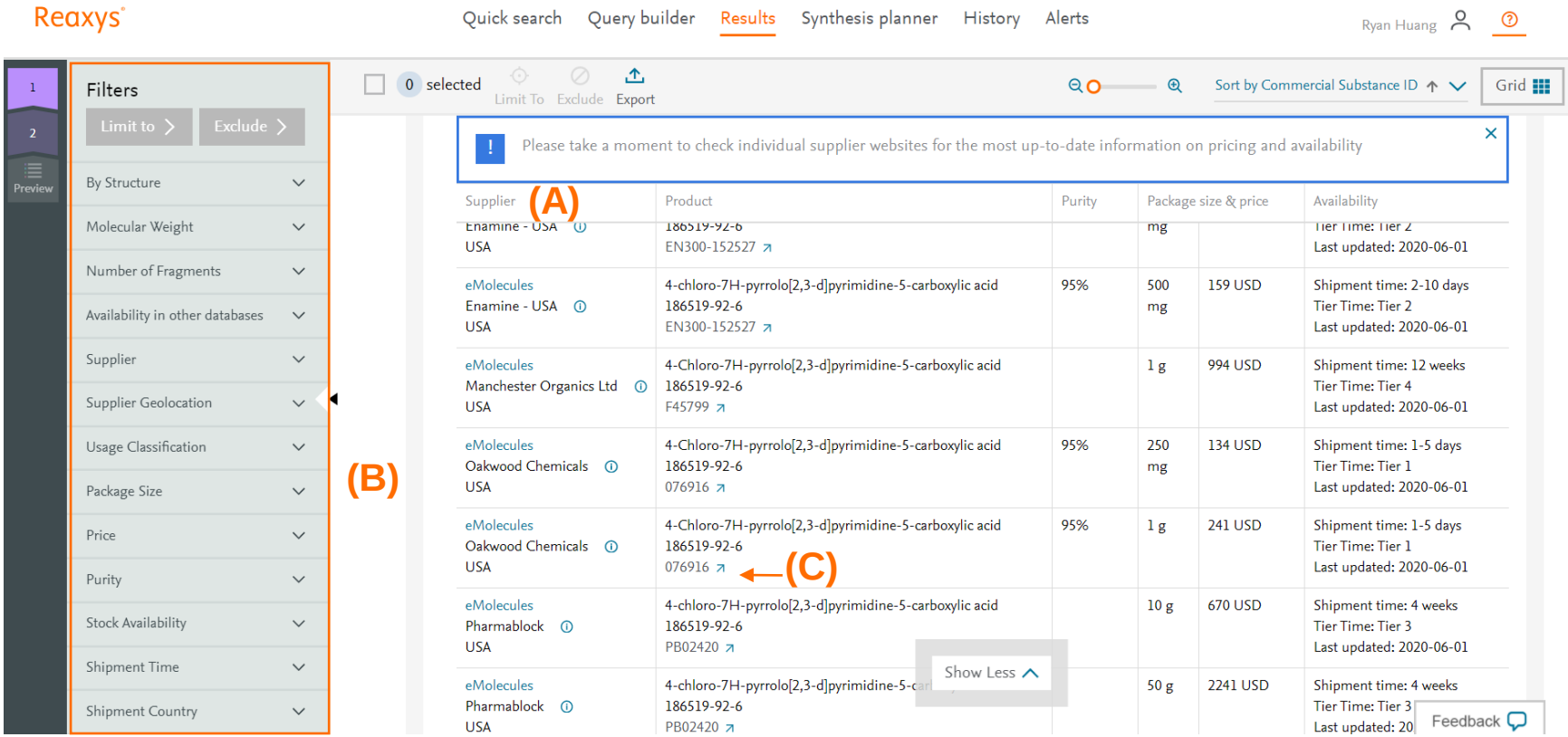
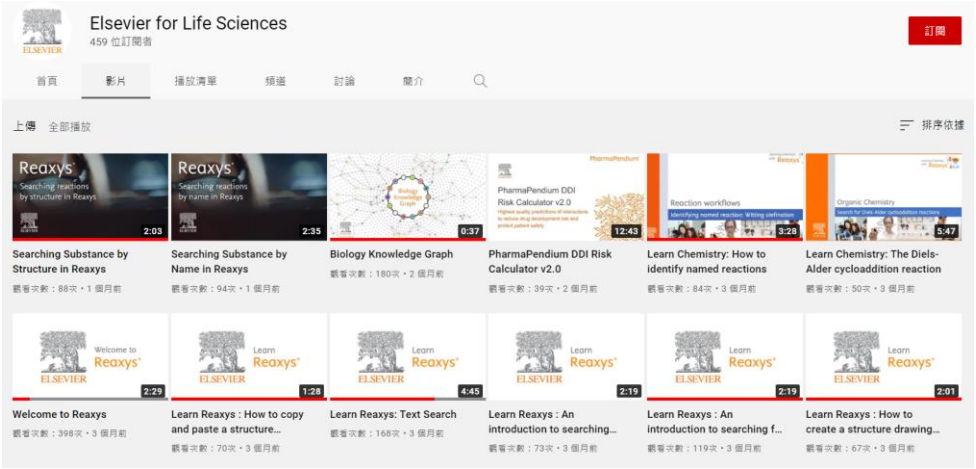
Reaxys Commercial Substances 為每一筆物質提供詳細的供應商列表(A)包括純度、價格、包裝及到貨時間。您可利用篩選工具(B)加速挑選過程，並點擊供應商品頁面連結(C)造訪供應商網頁。



其他自學線上資源



RxED Learning Chemistry with Reaxys（English）

[(152) RxED: Learning Chemistry with Reaxys - YouTube]

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邀請您填寫課後問卷~

歡迎來信留下您對Reaxys的所有問題~

r.huang@elsevier.com