ELSEVIER

# Reaxys®

## 資料庫簡介與應用

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2024

# 今日大綱

- 基本介紹與介面導覽
- 結構檢索
- 無機材料、實驗數據檢索
- 天然萃取物的生物活性應用
- 藥物靶點與藥物設計
- 逆合成 AI
- 實際操作小遊戲
- 線上自我學習資源

# Reaxys 全方位版 – 你值得更完整的研究體驗


針對未發表的有機分子
「預測」全合成路徑

專業的化學資料庫
- 找文獻
- 找化合物
- 找化學反應

整理化合物的生物活性數據，幫
化合物找應用，幫你的藥物靶點
蛋白質找化合物

全方位

# 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

**回答關鍵的研究問題:**

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

# Reaxys 涵蓋的範圍

| 287M | 68M | 116M | 44M | 48M |
| --- | --- | --- | --- | --- |
| Substances | Reactions | Documents | Patents | Bioactivities |

## 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

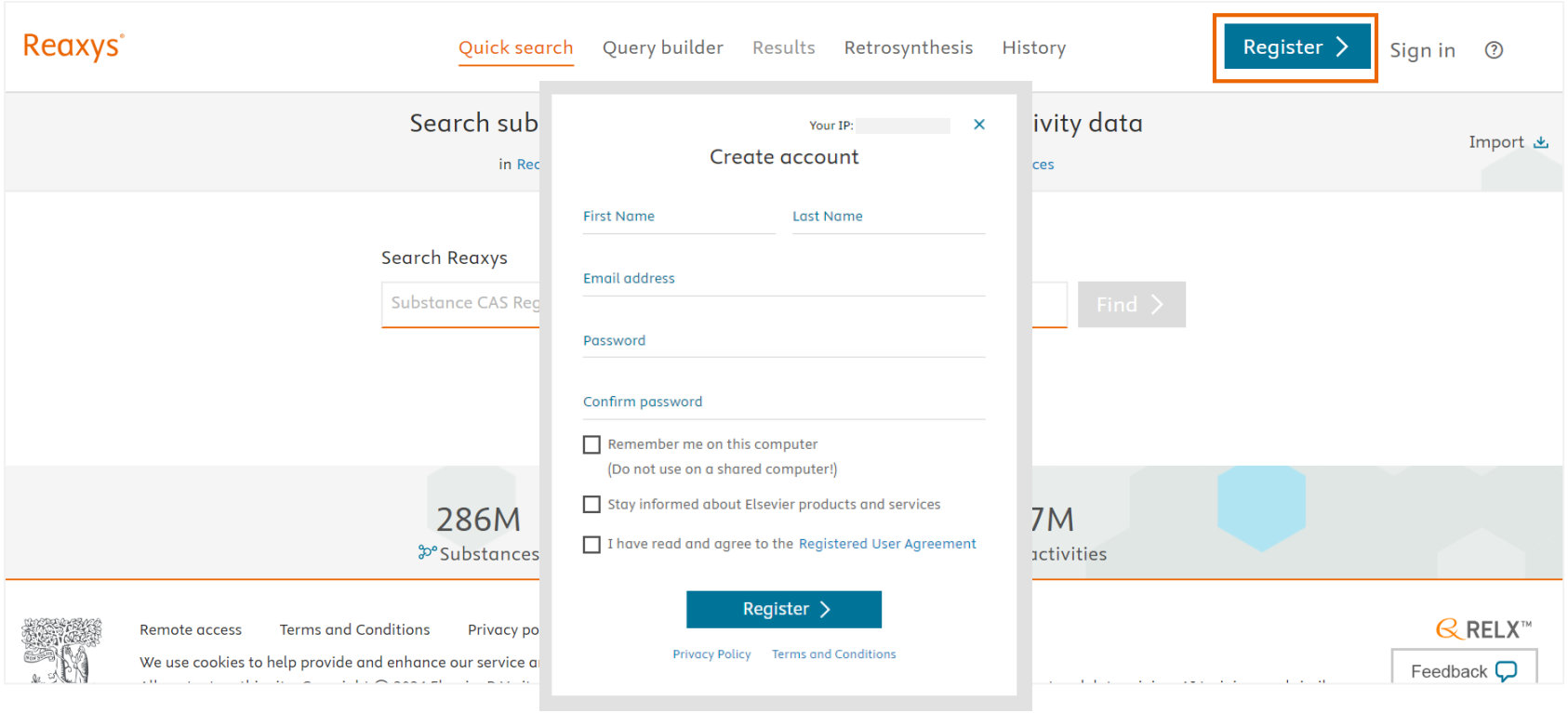
## 專利

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)

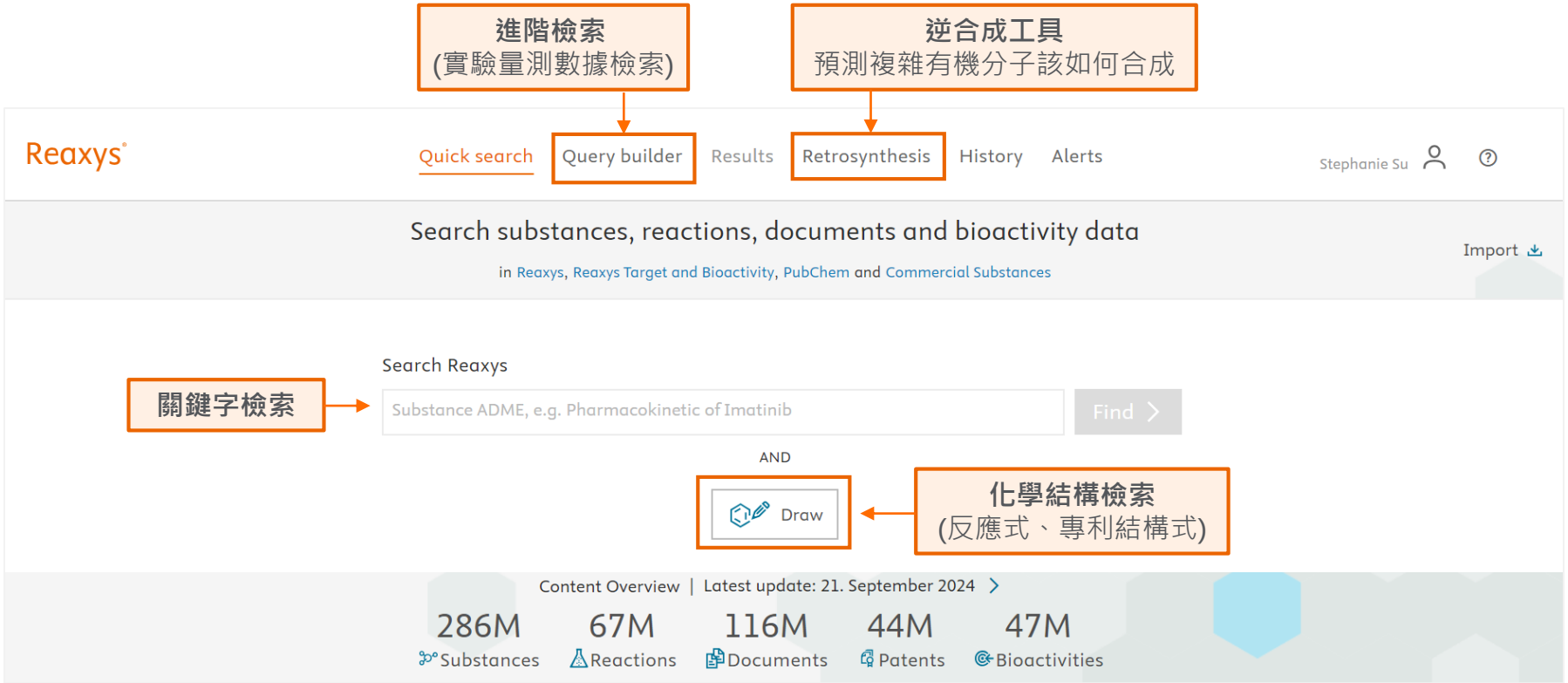
2021年起，覆盖範圍將擴大到105個專利局和所有化學品分類

# 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



# Reaxys 檢索介面導覽



# 多元搜尋指令

Search Reaxys

"paracetamol" Find

Substance Properties, e.g.solubility of vitamin D3

Search Reaxys

solubility of "vitamin d3" Find

Substance Effect, e.g.anticoagulant

Search Reaxys

synthesis of saccharose Find

Substance CAS Registry Number, e.g. 102625-70-7

Search Reaxys

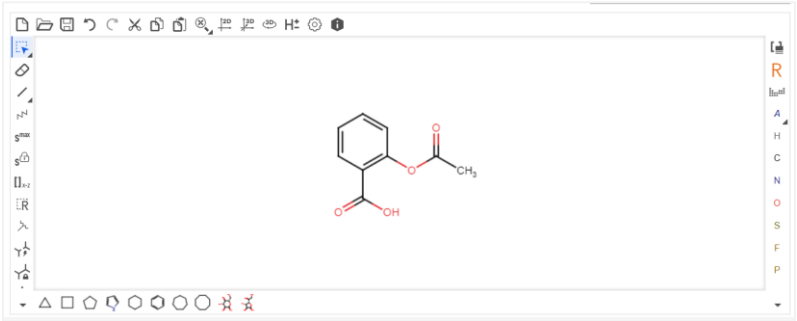
dissociation exponent of EDTA Find

Reactions, e.g.phosphorylation

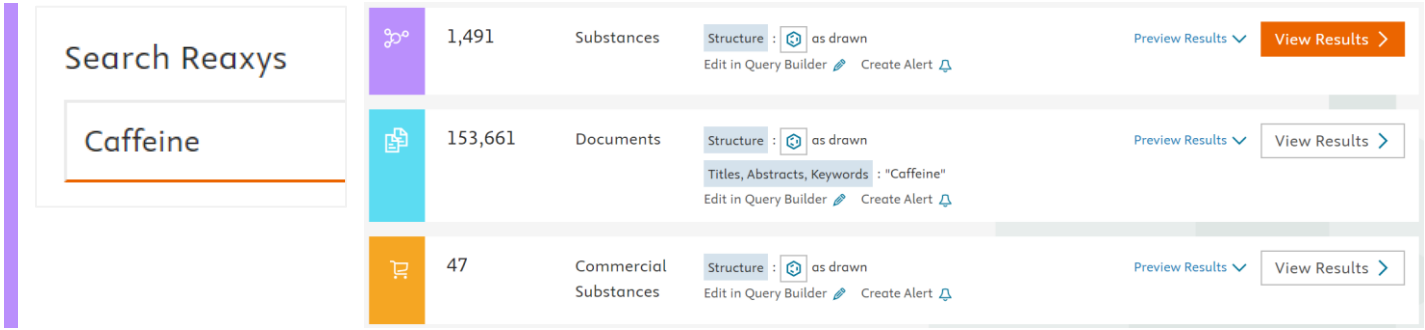
Search Reaxys

publications by "john white" Find

Documents, e.g.Tetrahedron, 2014, 70, 2343



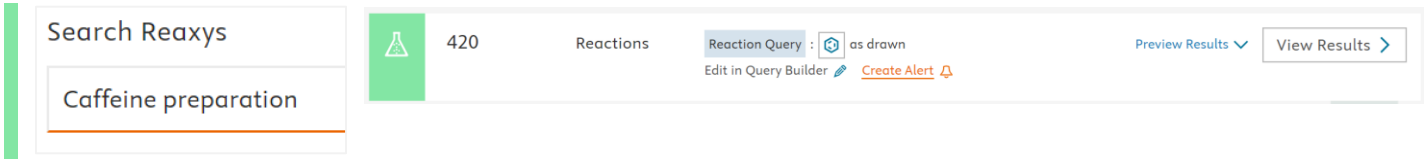
# Reaxys 檢索介面導覽



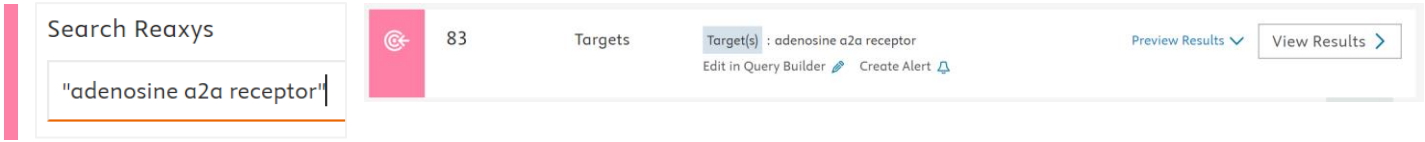

實驗數值與參考出處

文獻、專利

供應商資訊



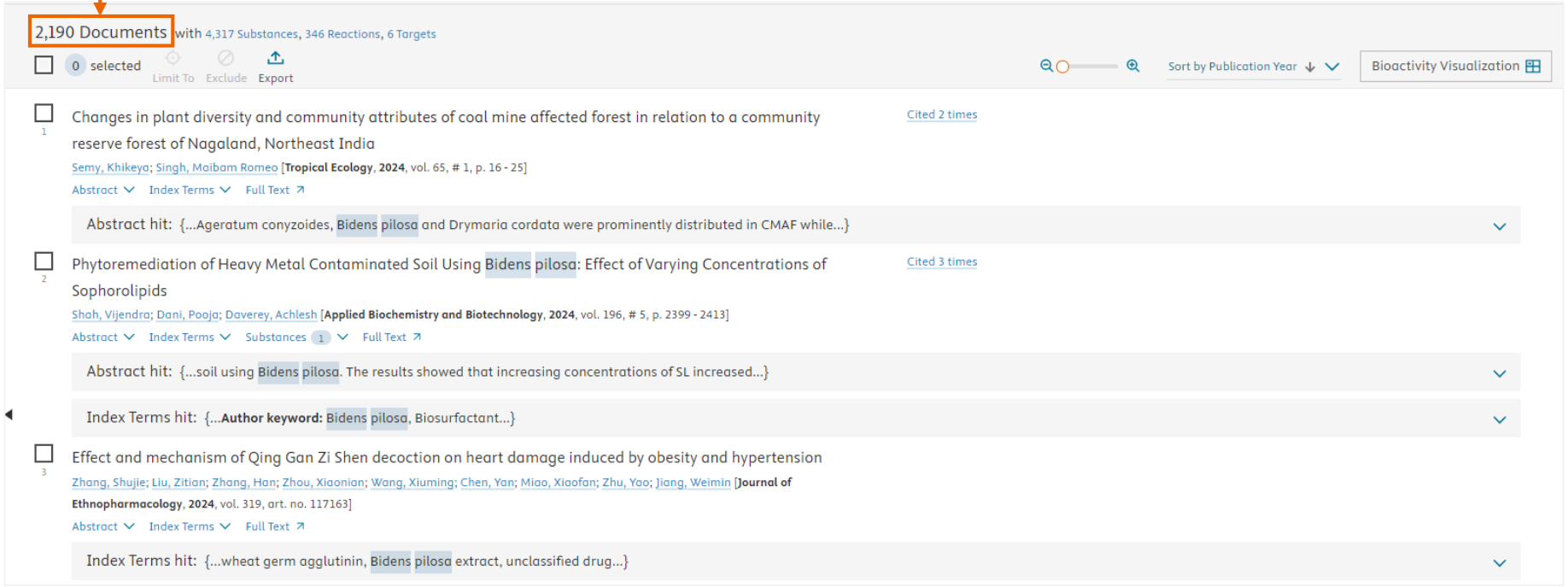

合成方法




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

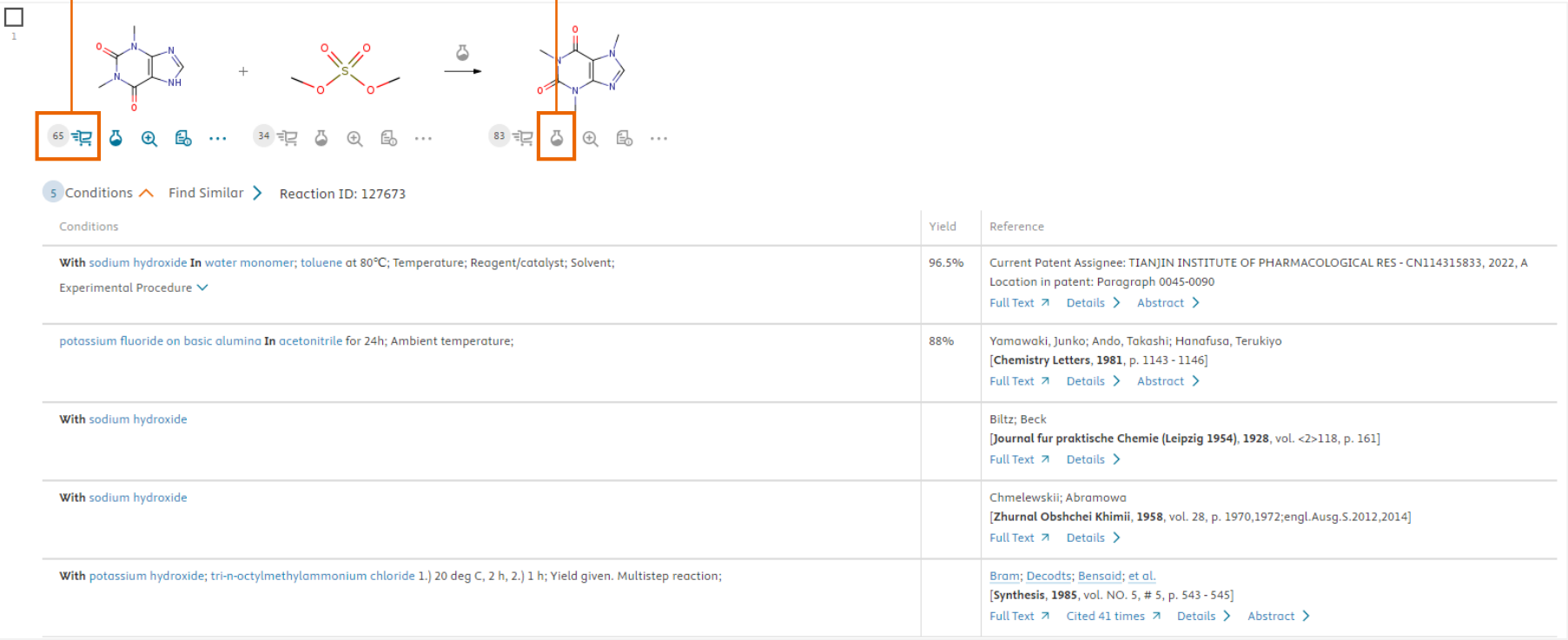
取得研究咸豐草的一千篇文獻中被我們**人工索引**的化合物清單。



# Reaxys 資料庫中的資料互相串連

從購物車連結到商用資料庫去評估實驗的成本

你可以從反應式的查詢結果再連結到物質資料庫，查詢這個產物的光譜數據。



5 Conditions | Find Similar | Reaction ID: 127673

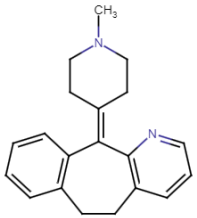
| Conditions | Yield | Reference |
|---|---|---|
| **With** sodium hydroxide **In** water monomer; toluene at 80°C; Temperature; Reagent/catalyst; Solvent; Experimental Procedure | 96.5% | Current Patent Assignee: TIANJIN INSTITUTE OF PHARMACOLOGICAL RES - CN114315833, 2022, A Location in patent: Paragraph 0045-0090 Full Text Details Abstract |
| potassium fluoride on basic alumina **In** acetonitrile for 24h; Ambient temperature; | 88% | Yamawaki, Junko; Ando, Takashi; Hanafusa, Terukiyo [**Chemistry Letters**, **1981**, p. 1143 - 1146] Full Text Details Abstract |
| **With** sodium hydroxide | | Biltz; Beck [**Journal fur praktische Chemie (Leipzig 1954)**, **1928**, vol. <2>118, p. 161] Full Text Details |
| **With** sodium hydroxide | | Chmelewskii; Abramowa [**Zhurnal Obshchei Khimii**, **1958**, vol. 28, p. 1970,1972;engl.Ausg.S.2012,2014] Full Text Details |
| **With** potassium hydroxide; tri-n-octylmethylammonium chloride 1.) 20 deg C, 2 h, 2.) 1 h; Yield given. Multistep reaction; | | Bram; Decodts; Bensaid; et al. [**Synthesis**, **1985**, vol. NO. 5, # 5, p. 543 - 545] Full Text Cited 41 times Details Abstract |

# 結構檢索

## Search Substance Structures

# Reaxys 三種結構搜尋與怎麼用

我感興趣的結構



Azatadine
CAS# 3964-81-6

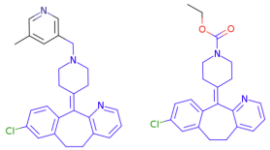
## As drawn

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



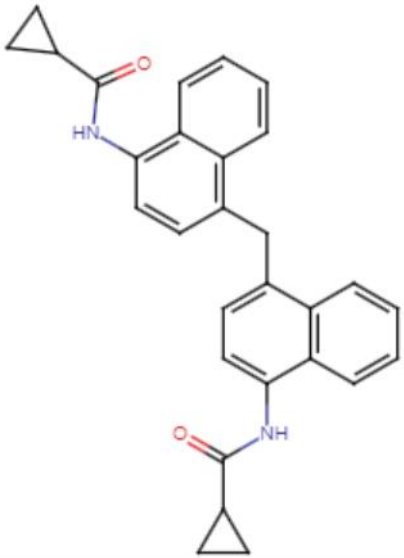
研究新的化合物，從已經發表的結構找線索，例如優化前導化合物 (lead compound)

## Similar

**「結構類似」**的化合物提供不同程度的結構變化

# 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

# 天然萃取物的生物活性應用

Organic Chemistry

# 天然萃取物檢索


**Question:** 探索藥用植物萃取物的生活性應用，已發表文獻中有哪些 Substances 紀錄?

**方法一:**

1. 檢索 Bidens Pilosa 的文獻
2. 取得文獻中人工提取的 Substances 清單

**方法二:**

1. 利用進階搜尋工具 Isolated from natural source

# 無機材料、實驗數據檢索

Inorganic Chemistry

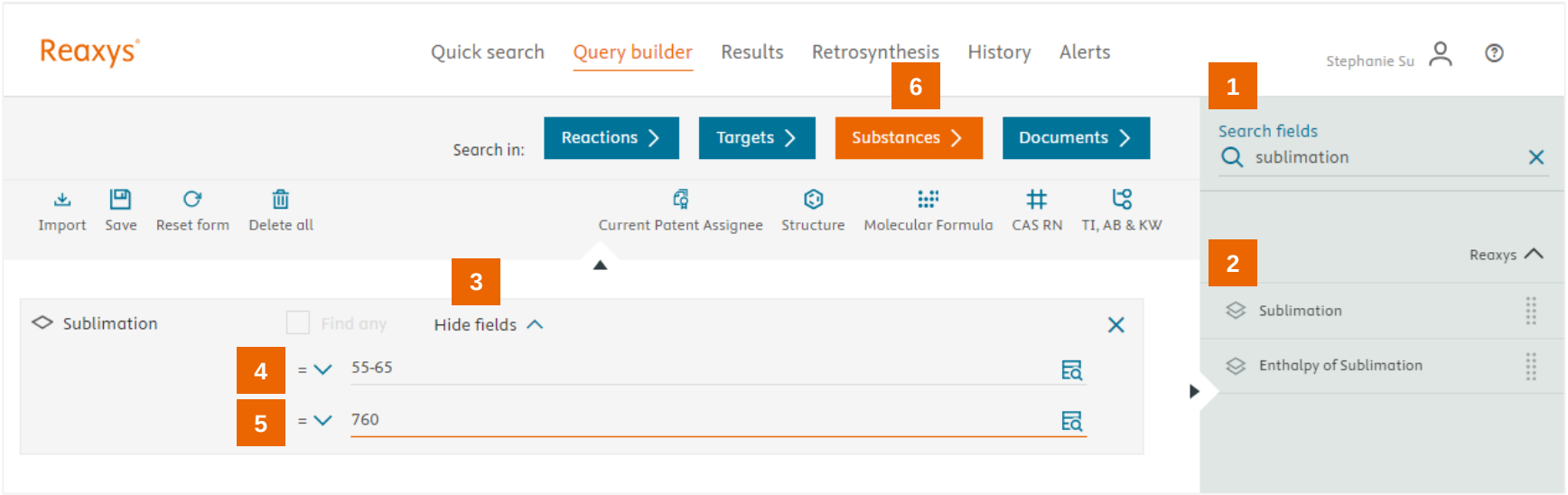
# Query builder: 實驗數據檢索

**Question:**

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

利用進階搜尋工具「**Sublimation**」

# Query builder: 實驗數據檢索




1 以關鍵字搜尋 Sublimation

2 左鍵點選 Sublimation

3 點擊 Show fields 顯示數據欄位

4 輸入溫度區間 55-65

5 可輸入 760 (torr) 或保持空白

6 點選 Substances 資料類型

# Query builder: 實驗數據檢索

160 Substances out of 327,427 Documents, containing 108,007 Reactions, 430 Targets

0 selected | Limit To | Exclude | Export | Preparations | Sort by No of References | Grid | Bioactivity Visualization

carbon dioxide

OCO 44.0098 1900390 124-38-9

Hit Data - 2 | Bioactivity (All) | Other Data - 960

Identification | Physical Data - 27,313

Druglikeness | Spectra - 867

Preparations - 9,558

Reactions - 55,311

Targets - 53

Documents - 181,217

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

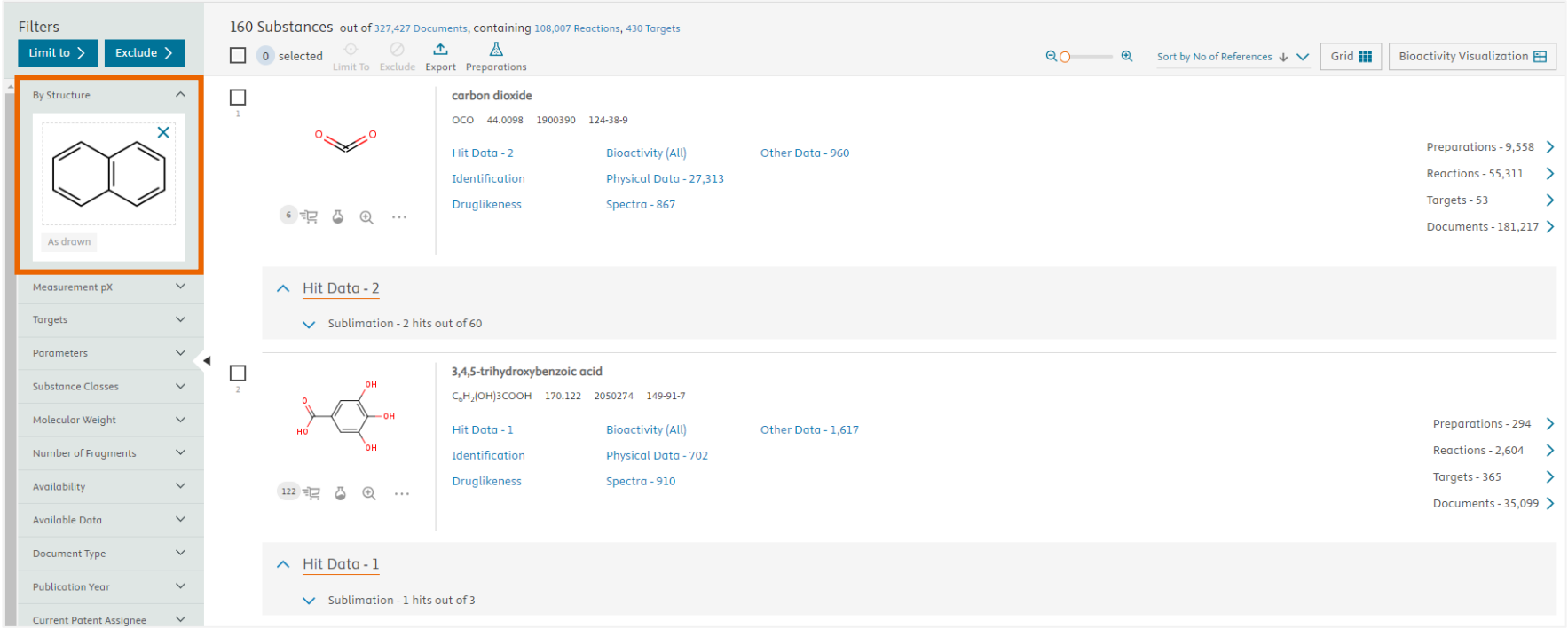
Hit Data - 2

Sublimation - 2 hits out of 60

Show/Hide columns

| Sublimation, °C | Pressure (Sublimation), Torr | Reference |
|---|---|---|
| -78.481 - -78.477 | 760 | Fernandez-Fassnacht, Enrique; Rio, Fernando del[**Journal of Chemical Thermodynamics**, **1984**, vol. 16, # 5, p. 469 - 474]<br>Full Text ↗ Cited 30 times ↗ Details > Abstract > |
| -78.514 | 760 | Meyers, C. H.; Dusen, M. S. van[**1933**, vol. 10, p. 381 - 412]<br>Full Text ↗ Details ><br>No author[**Gmelin Handbuch der Anorganischen Chemie**, Gmelin Handbook: C: MVol.C1, 151, page 363 - 365]<br>Full Text ↗ Details > |

# Query builder: 實驗數據檢索



# 藥物靶點與藥物設計

## Drug Targets and Drug Design

# 活性化合物的設計與優化

## 任務

- 建立 Structure-Activity Relationships (SAR)並辨認哪些結構特徵促進高活性和低活性
- 識別與化合物結構相似的化合物潛在非靶標活性
- 合理化並優化化合物系列的藥物代謝、藥物動力學和毒性特性

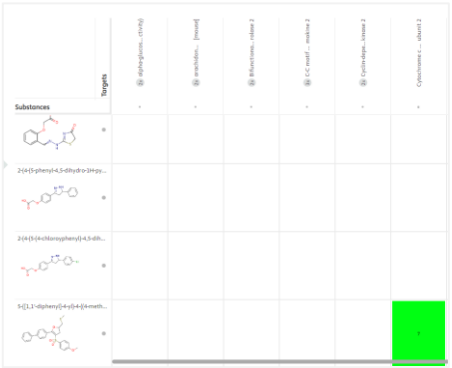
## Reaxys 如何協助

- 提供完整的生物活性 (bioactivity) 資訊，以幫助建立已知的結構-活性關係 (Structure-Activity Relationships)、藥物代謝藥物動力學 (DMPK) 和吸收、分佈、代謝、排泄及毒性(ADME-Tox)特性
- 提供生物活性熱圖，使結構及其對各種靶標的生物活性值能快速高效地展示

Toxicity/Safety Pharmacology - 81

**Quantitative Results**

| pX | Parameter | Value (quant) | Unit | Action on target | Target |
|---|---|---|---|---|---|
| 8.11 | IC50 | 7.7 | nM | | |
| 8.11 | IC50 | 7.8 | nM | | |
| 8 | IC50 | 10 | nM | Inhibitor | Bcr-ABL p210 (T315A):Wild |



# 藥物靶點檢索

## Question:

如何快速地取得靶點訊息並評估結構活性分析?

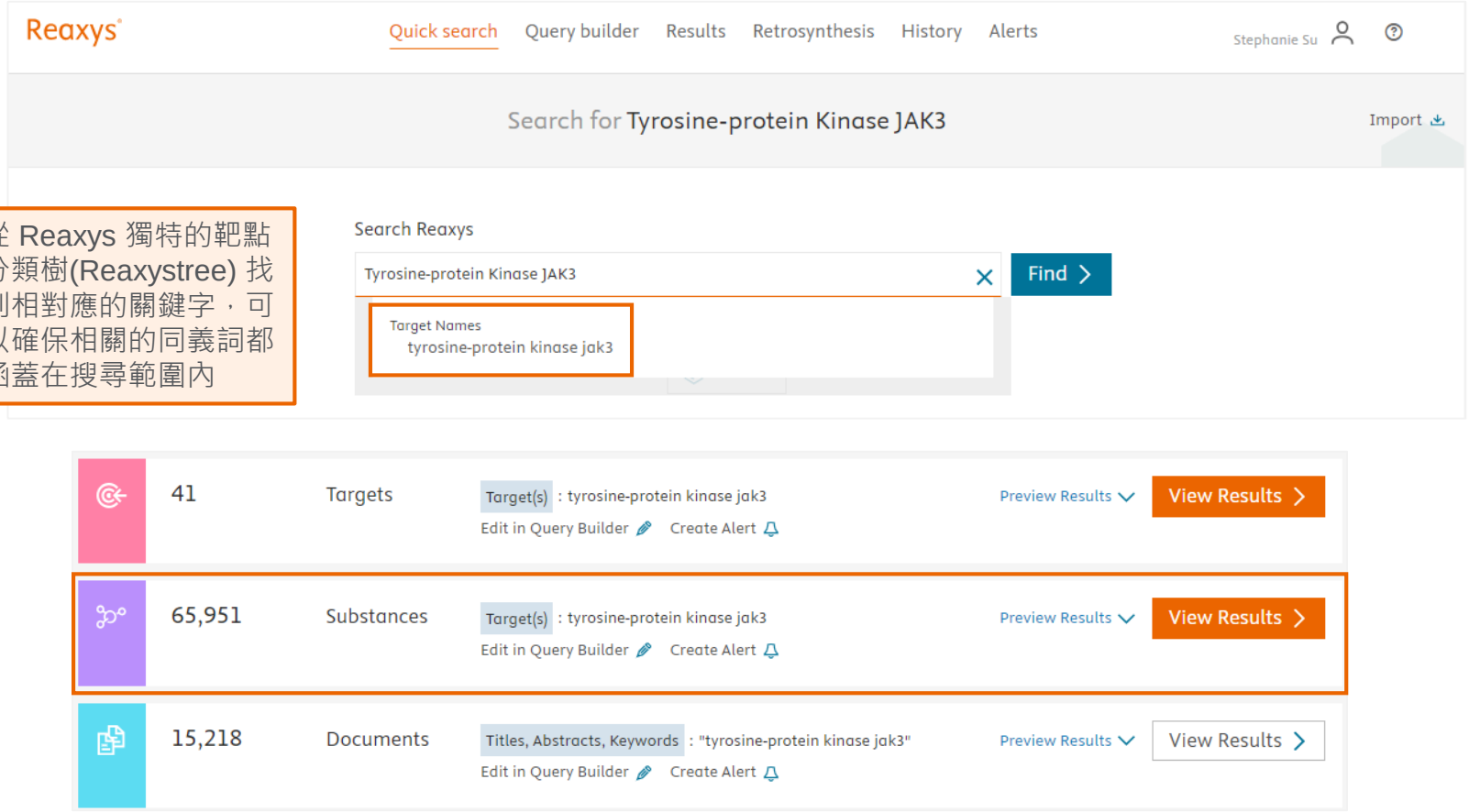
## 感興趣的靶點:

JAK3 (Tyrosine-protein Kinase JAK3)

與 JAK3 有 interaction 的 substances 有哪些?

結構特徵? 高活性的有那些?

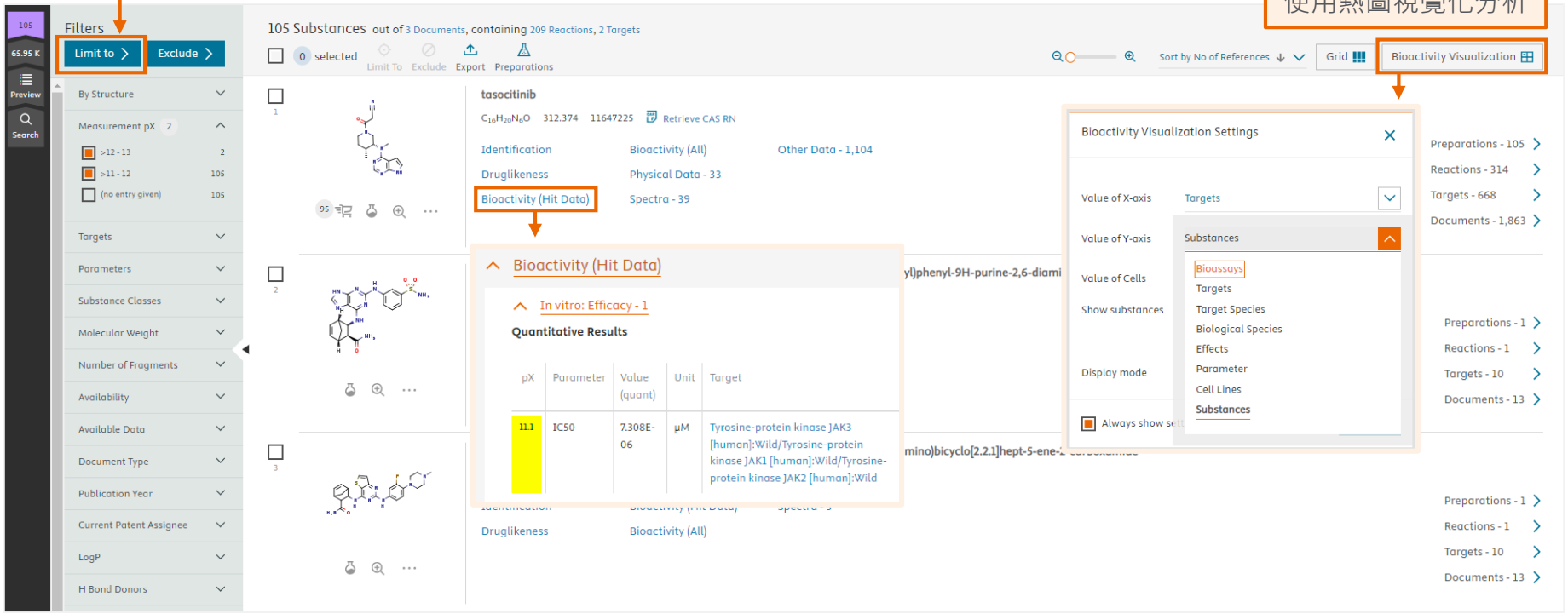
# 藥物靶點檢索


Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Stephanie Su
Search for Tyrosine-protein Kinase JAK3
Import
從 Reaxys 獨特的靶點分類樹(Reaxystree) 找到相對應的關鍵字，可以確保相關的同義詞都涵蓋在搜尋範圍內
Search Reaxys
Tyrosine-protein Kinase JAK3
Find
Target Names
tyrosine-protein kinase jak3
41
Targets
Target(s) : tyrosine-protein kinase jak3
Edit in Query Builder
Create Alert
Preview Results
View Results
65,951
Substances
Target(s) : tyrosine-protein kinase jak3
Edit in Query Builder
Create Alert
Preview Results
View Results
15,218
Documents
Titles, Abstracts, Keywords : "tyrosine-protein kinase jak3"
Edit in Query Builder
Create Alert
Preview Results
View Results

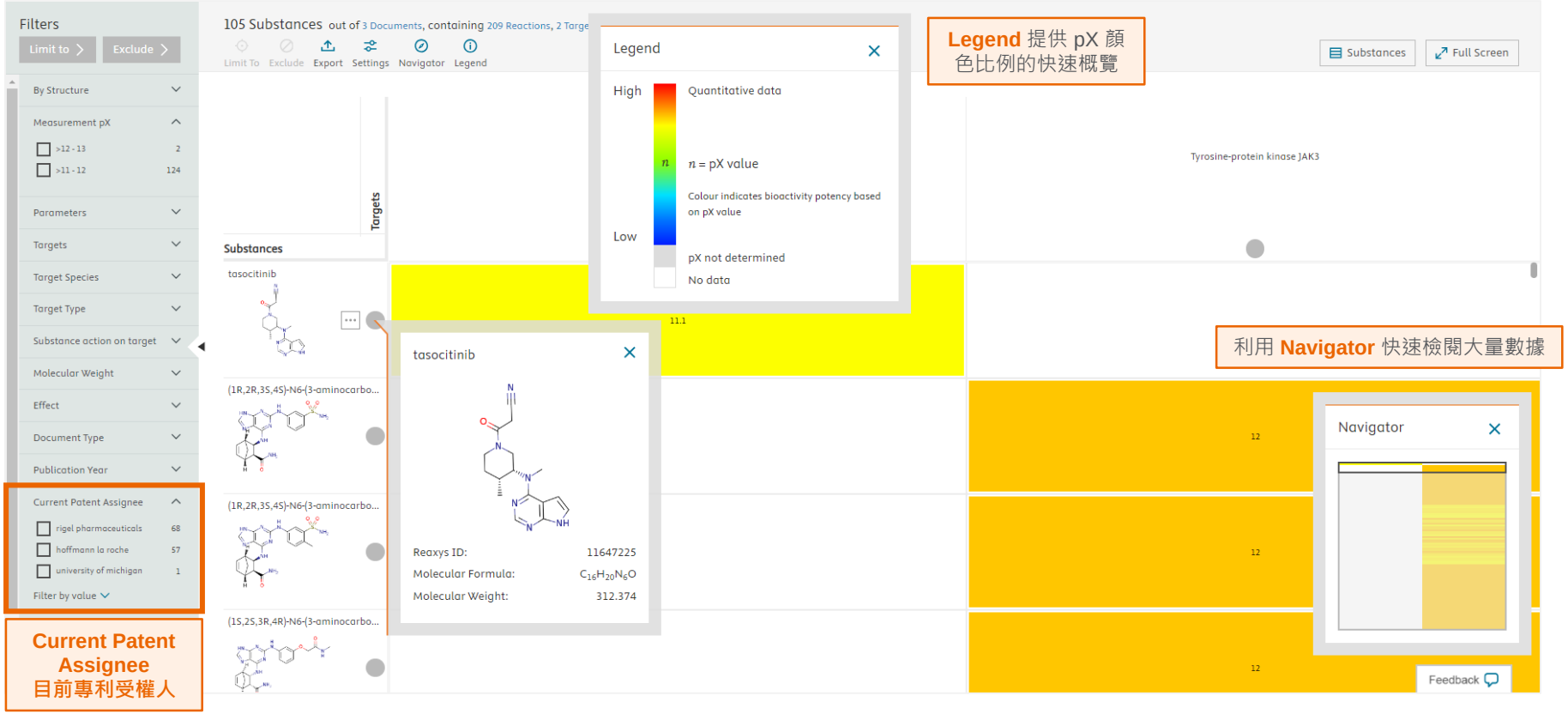
# 藥物靶點檢索

利用生物活性專屬的過濾工具

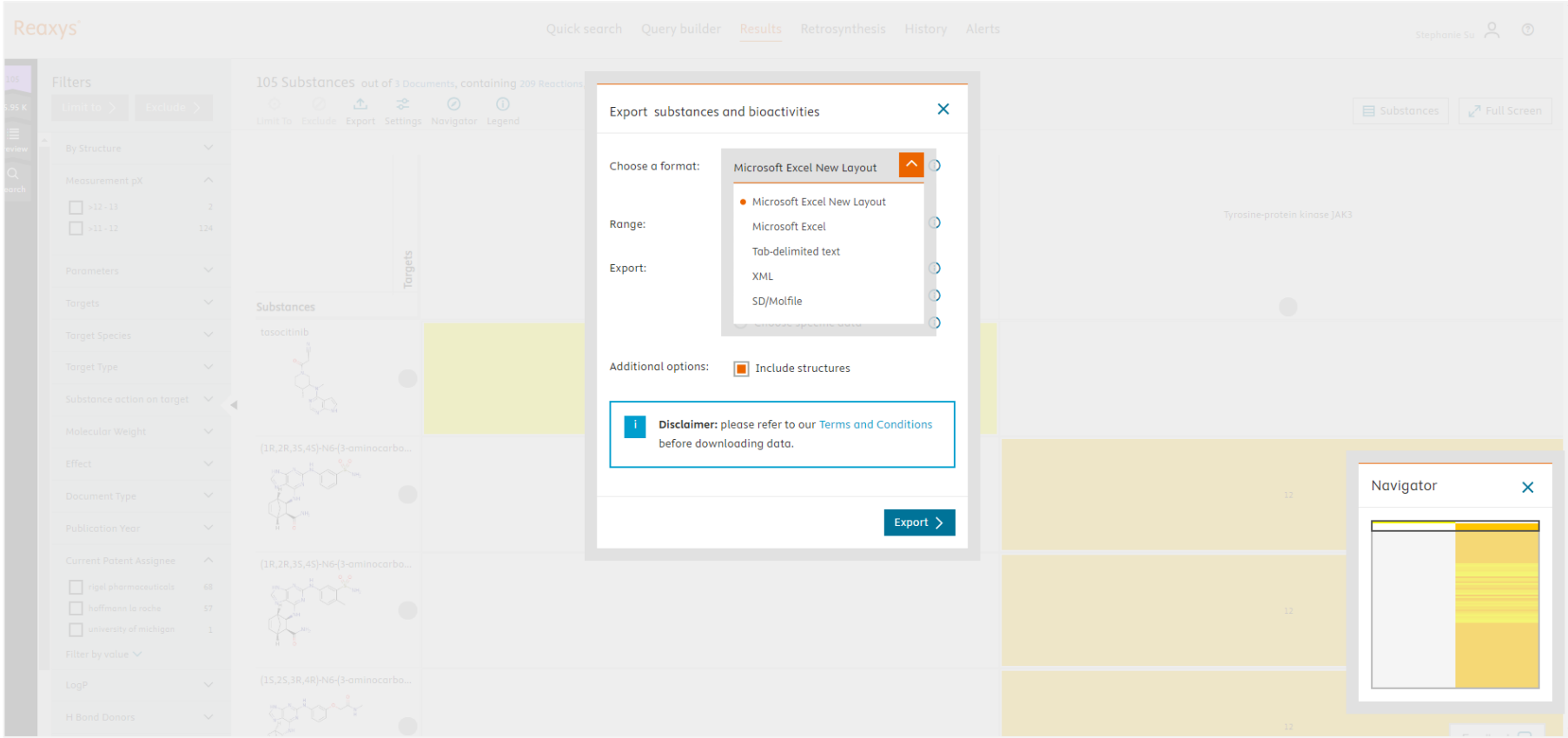
使用熱圖視覺化分析



# 藥物靶點檢索: 使用熱圖視覺化分析



# 藥物靶點檢索: 匯出 SAR 資料做更多分析

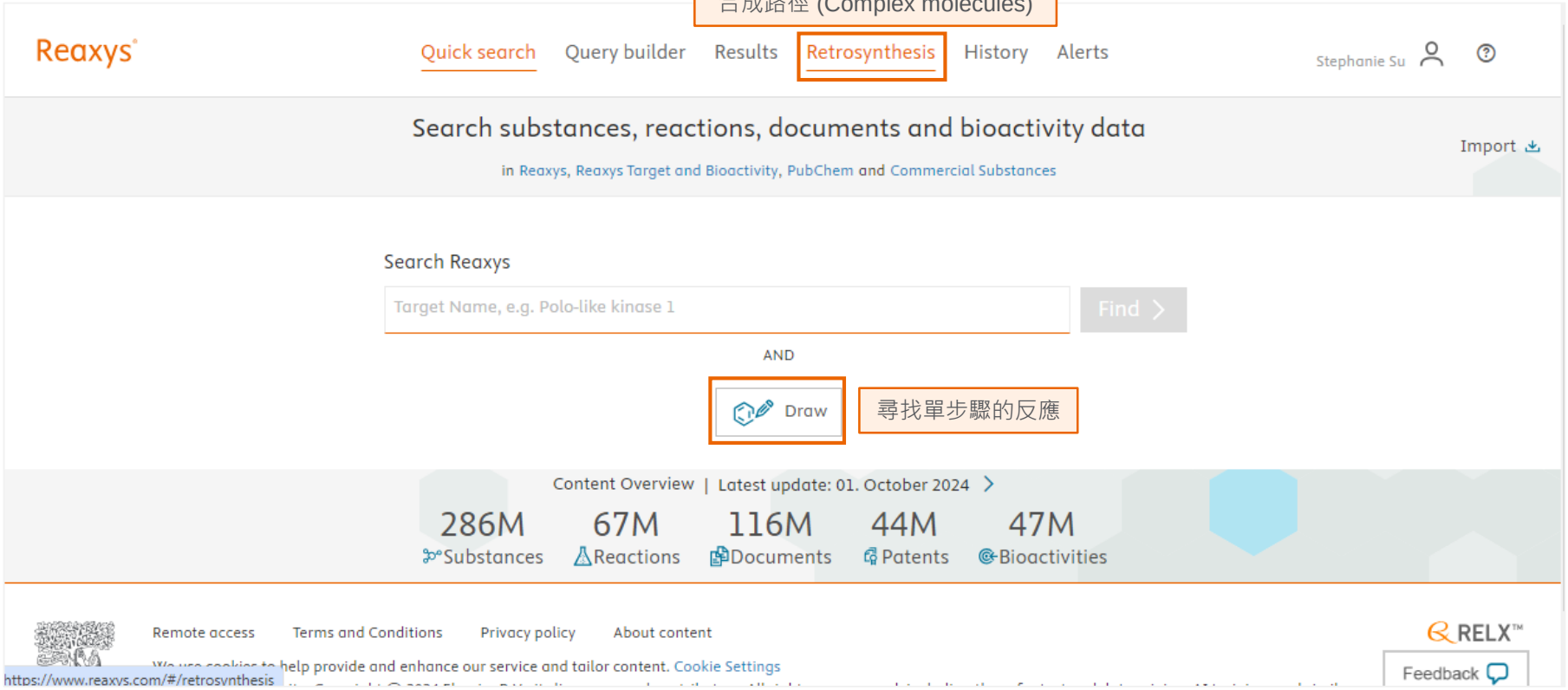


# 逆合成工具

## Retrosynthesis

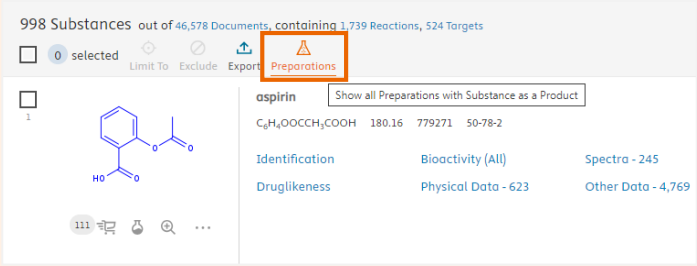
# Retrosynthesis

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

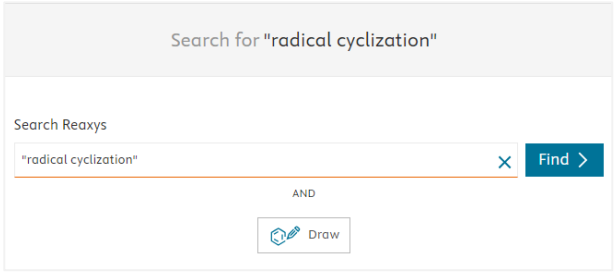


# 尋找反應式 (Chemical equation) 的方法

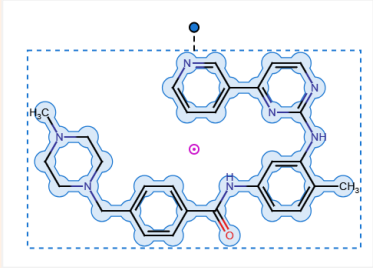
1. **已知物質的製備方式**
   (從 substance介面連結 preparations)



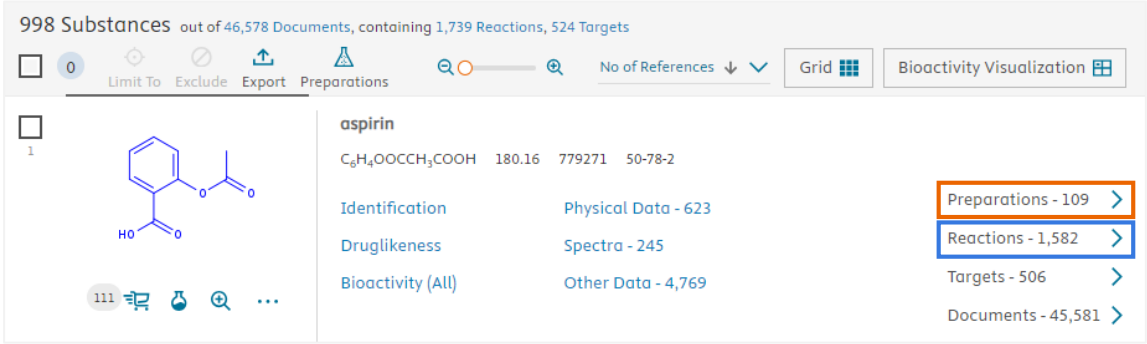

2. **關鍵字檢索** (例：radical cyclization)、命名反應式 (例：Suzuki coupling)



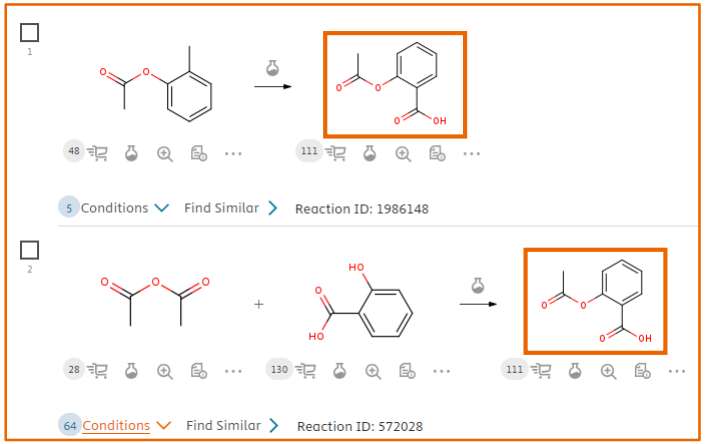

3. **直接畫出反應式**
   (完整、半個反應式)



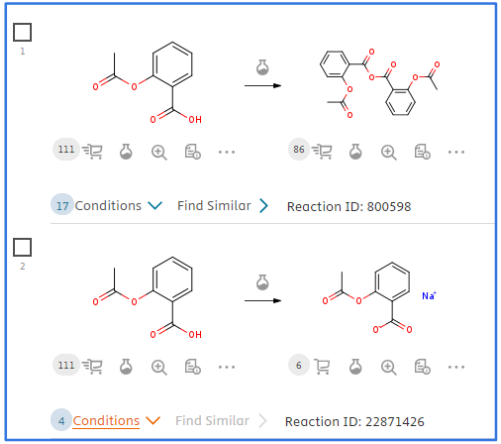
# 尋找反應式的方法: 已知物質的製備方式



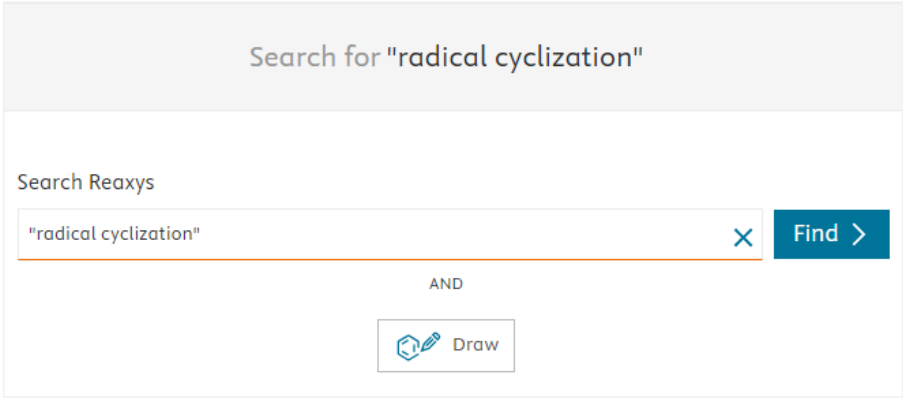

**Preparations 指出現在產物 (Product)**

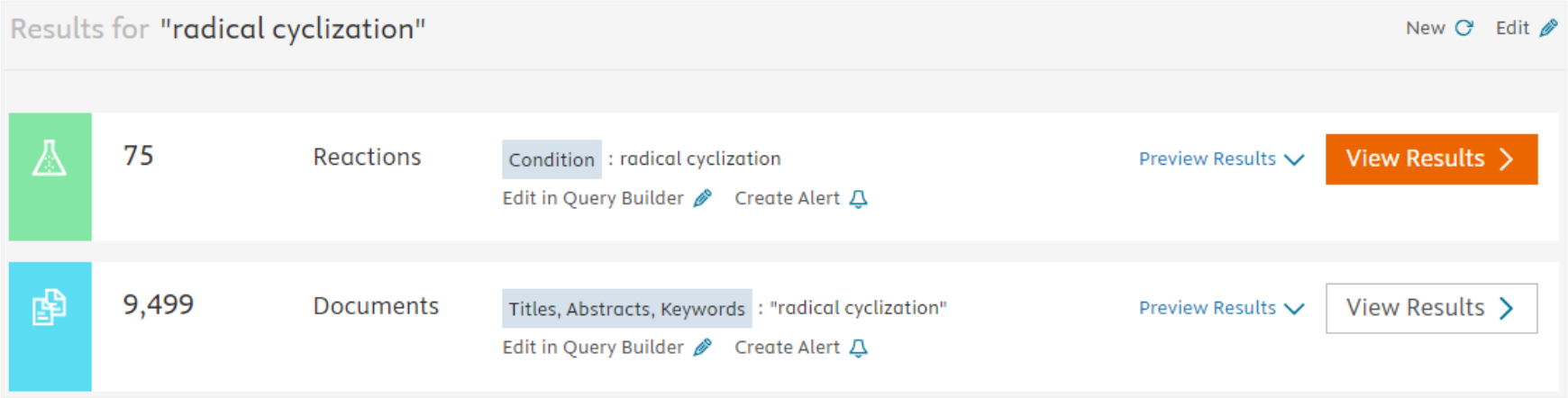



**Reactions 產物或起始物 (Reactants or Products)**

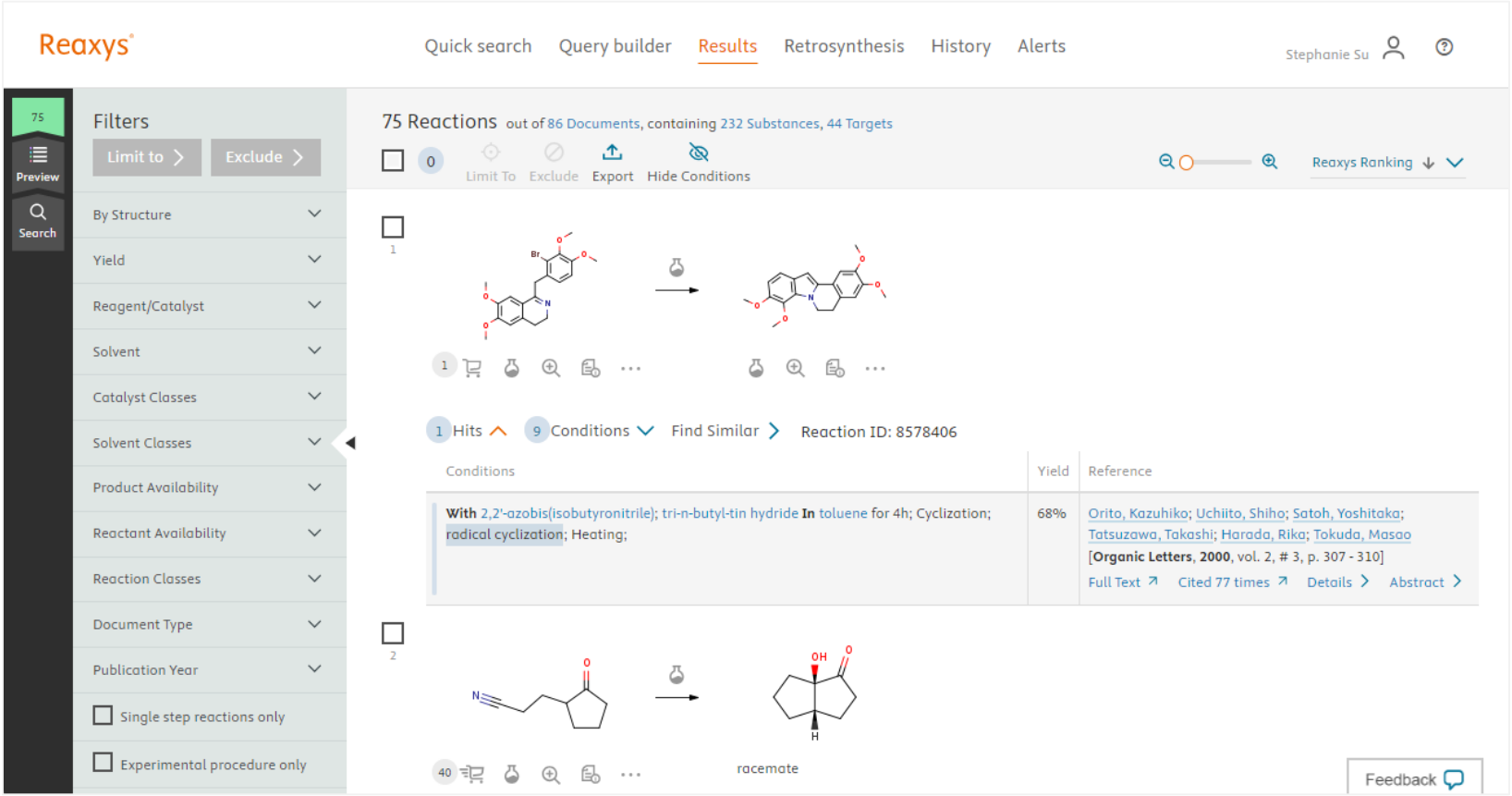


# 尋找反應式的方法: 關鍵字檢索

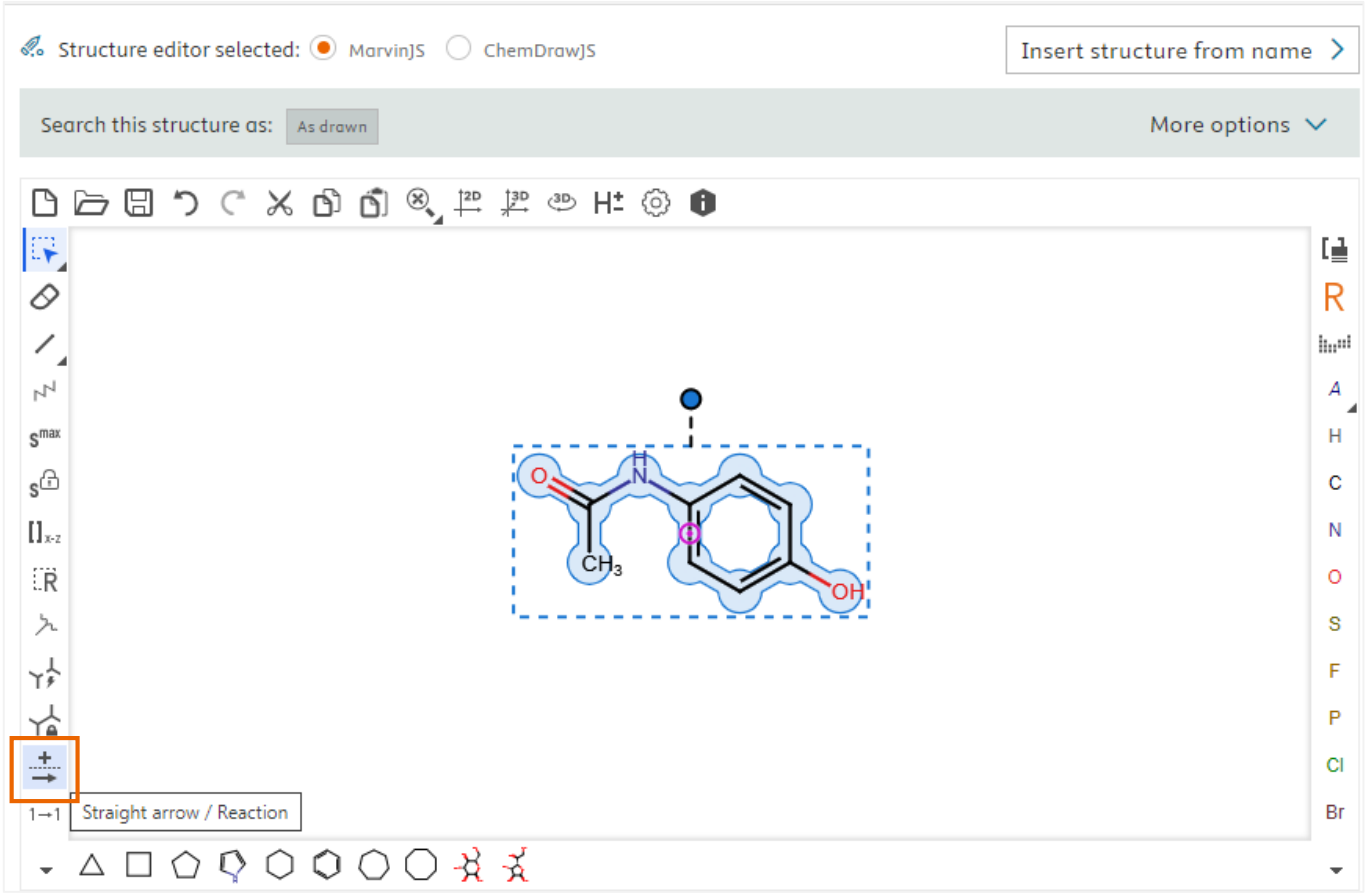


# 尋找反應式的方法: 關鍵字檢索

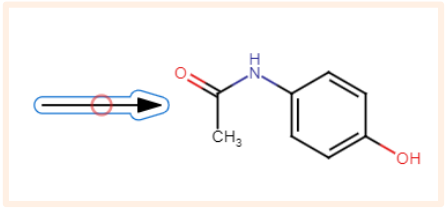


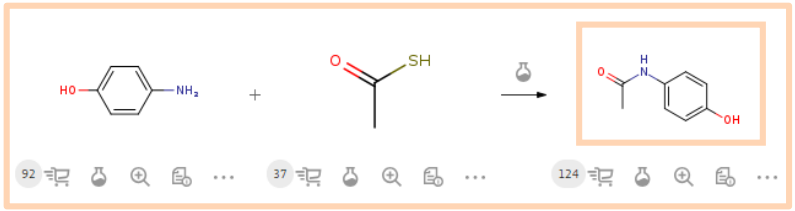
# 尋找反應式的方法: 繪製反應式



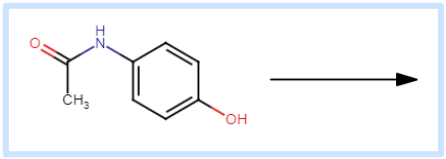
# 尋找反應式的方法: 繪製反應式

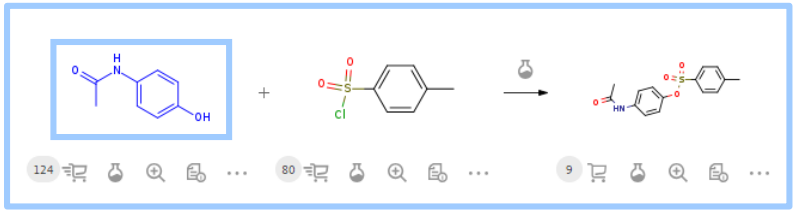
**產物:** 箭頭在左



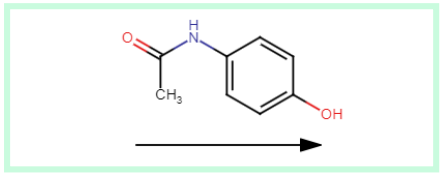


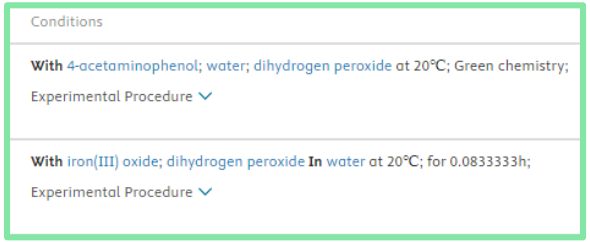

**起始物:** 箭頭在右






**催化劑或溶劑:** 箭頭在下

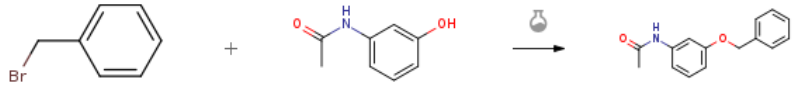




# 進階反應式檢索: 介面資訊

**人工索引欄位**
**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




53 113 19

7 Conditions | Find Similar | Reaction ID: 9076900

| Conditions | Yield | Reference |
|---|---|---|
| **With** caesium carbonate **In** N,N-dimethyl-formamide at 40°C; | 98% | Maignan, Jordany R.; Lichorowic, Cynthia L.; Giarrusso, James; Blake, Lynn D.; Casandra, Debora; Mutka, Tina S.; LaCrue, Alexis N.; (...) Kyle, Dennis E.; Manetsch, Roman<br>[**Journal of Medicinal Chemistry**, **2016**, vol. 59, # 14, p. 6943 - 6960]<br>Full Text ↗ Cited 22 times ↗ Details › Abstract › |
| **Stage #1:** 3-Hydroxyacetanilid **With** potassium carbonate **In** acetone at 20°C; for 0.5h; Inert atmosphere;<br>**Stage #2:** benzyl bromide **In** acetone for 2h; Inert atmosphere;<br>Experimental Procedure ^ | 98% | Damodar, Kongara; Gim, Ji Geun; Jeon, Seong Ho; Lee, Jeong Tae; Lee, Yeontaek; Nam, Ki Yoon; Park, Jae Phil; Park, Lee Seul<br>[**Molecules**, **2021**, vol. 26, # 3]<br>Full Text ↗ Cited 6 times ↗ Details › Abstract › |

**Full text of reaction**

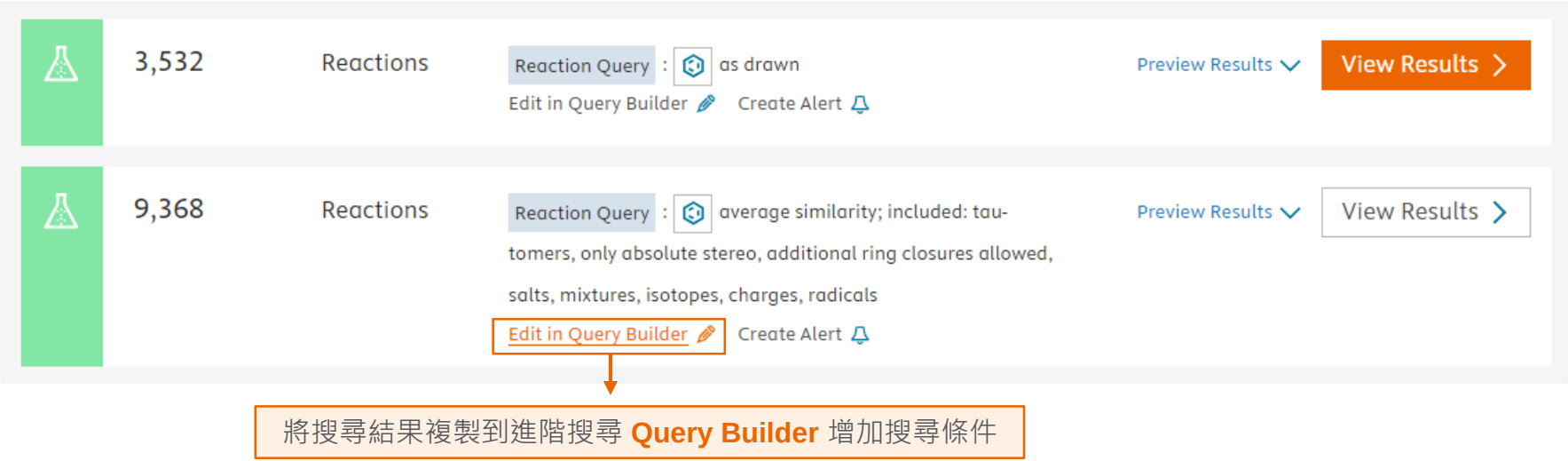
詳細實驗步驟
(文獻原文移植)
資訊量最豐富，包含詳細步驟、分析方法 (HPLC)、數值

Synthesis of N-(3-(benzyloxy)phenyl)acetamide (14)

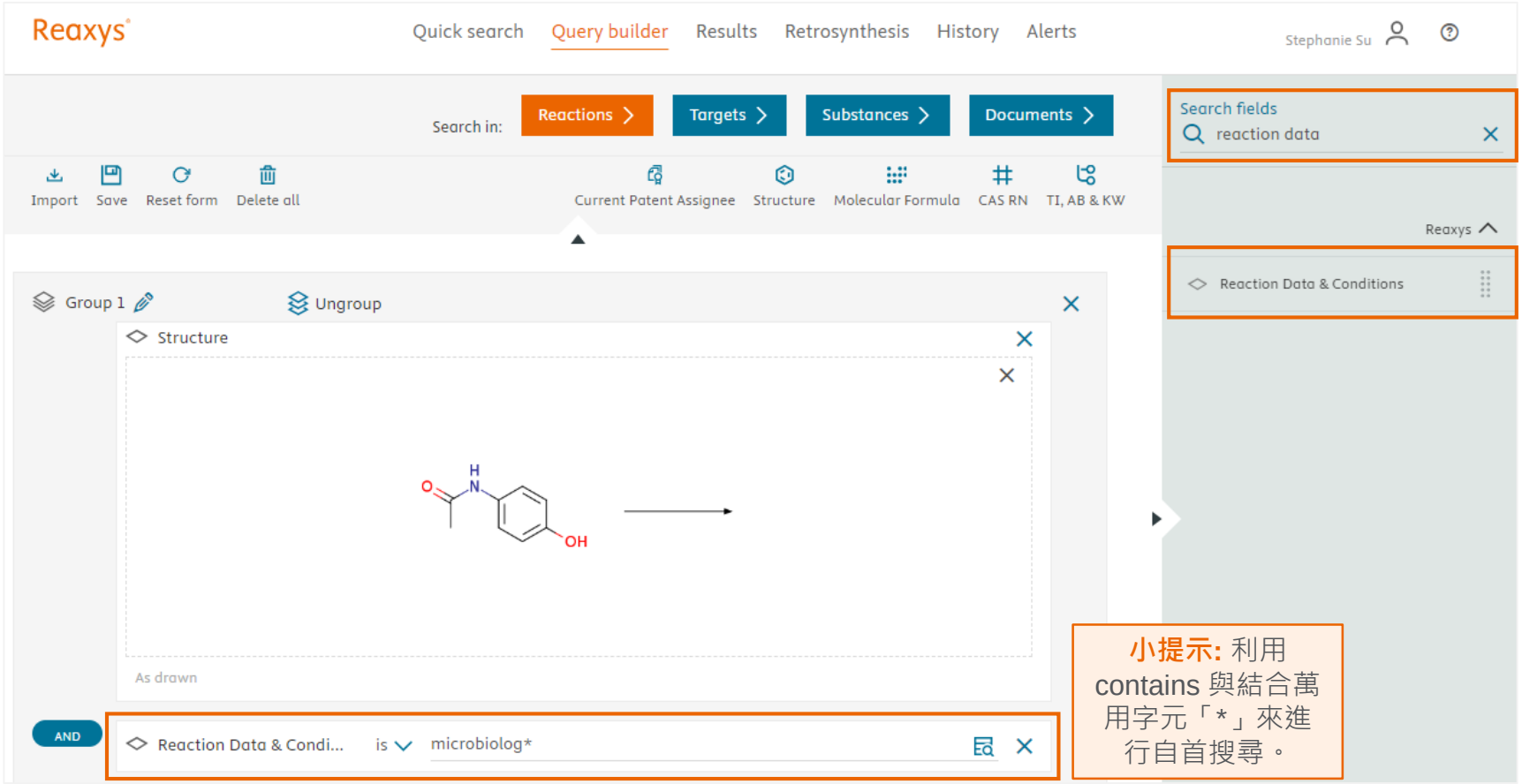
To a stirred solution of N-(3-hydroxyphenyl)acetamide (5.0 g, 33.08 mmol) in acetone (130mL) was added K2CO3 (18.23 g, 132.31 mmol) under argon atmosphere and stirred for 30min at room temperature. Benzyl bromide (3.93 mL, 33.08 mmol) was added dropwise andstirred for 2 h. After completion of the reaction, the solid was filtered off and the filtrate wasconcen-trated under reduced pressure. The residue was dissolved in EtOAc (70 mL), washedwith 2N HCl (2 x 15 mL), H2O (2 x 20 mL) and brine (20 mL), dried over anhyd. Na2SO4and concentrated in vacuo. The crude was purified by column chromatography(MeOH/CH2Cl2 = 1:19) afford the desired product 14 (7.82 g, 98.0 %) as white solid.

# 進階反應式檢索: Query builder

## 利用 **Query builder** 進一步「加工」搜尋條件

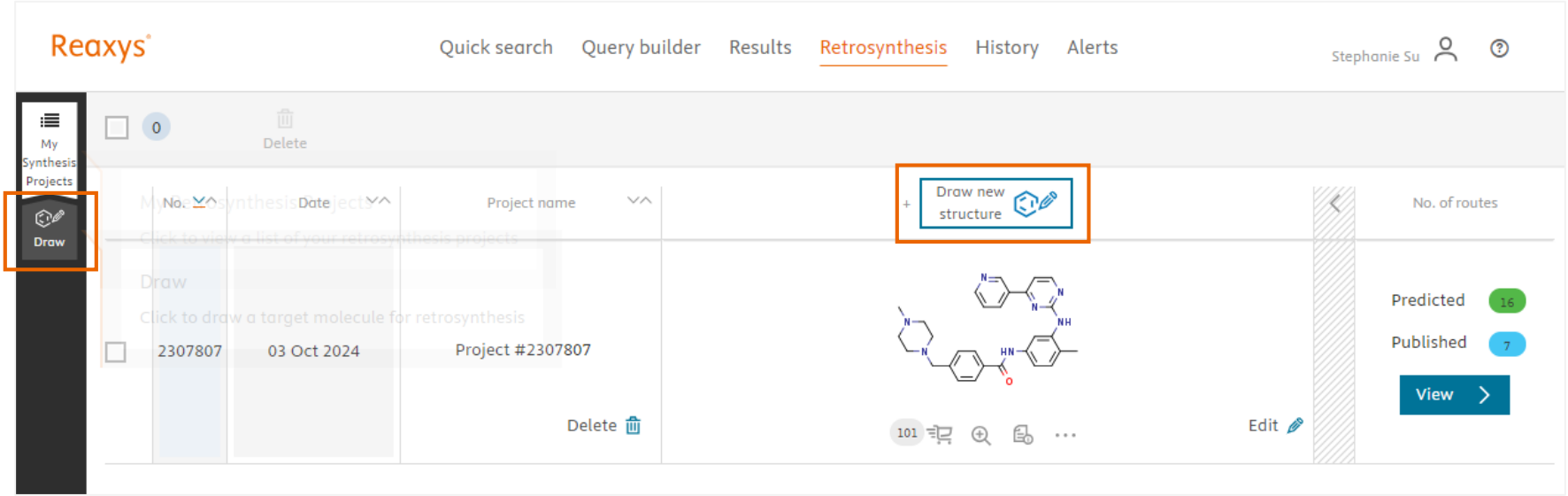


# 進階反應式檢索: Query builder

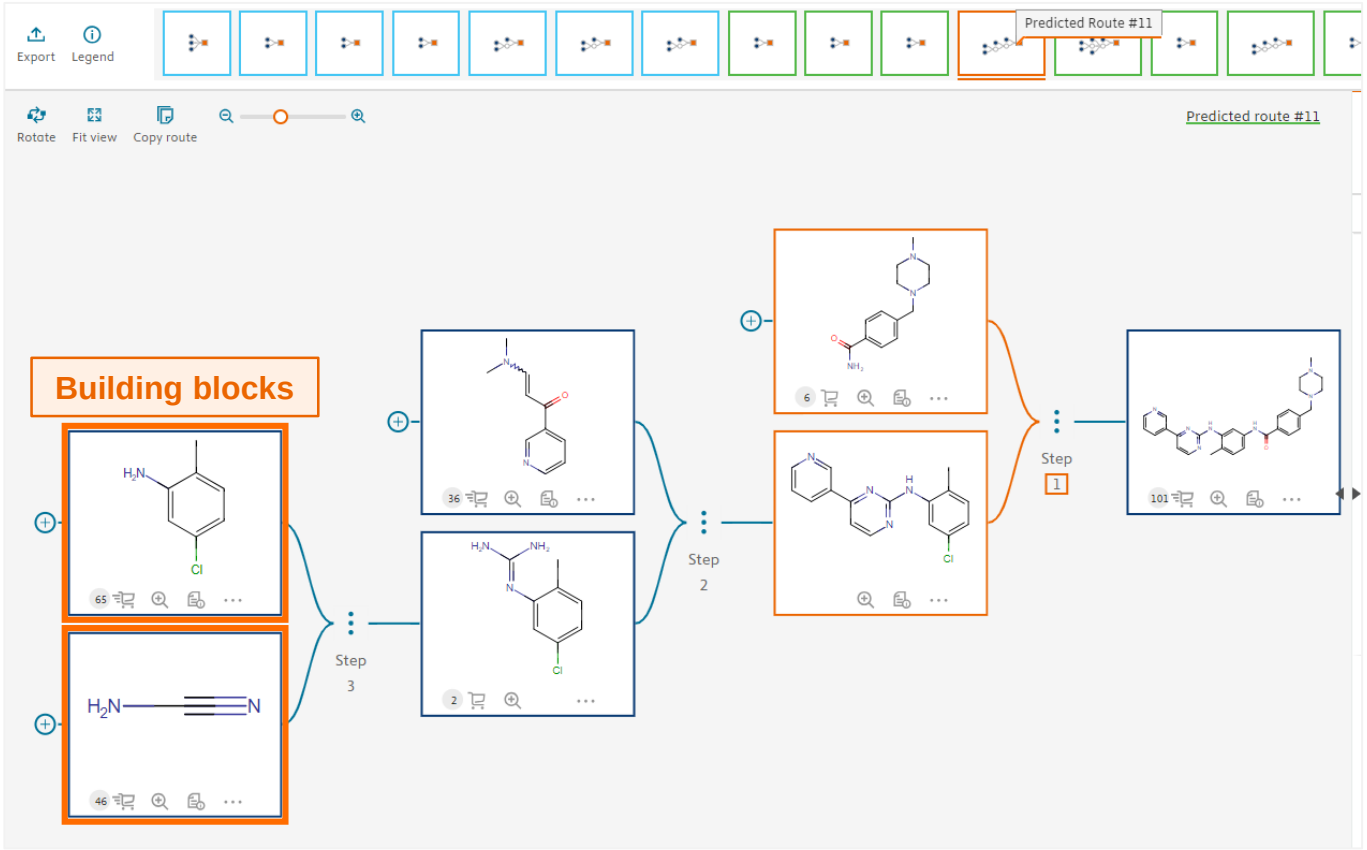



**小提示:** 利用 contains 與結合萬用字元「*」來進行自首搜尋。

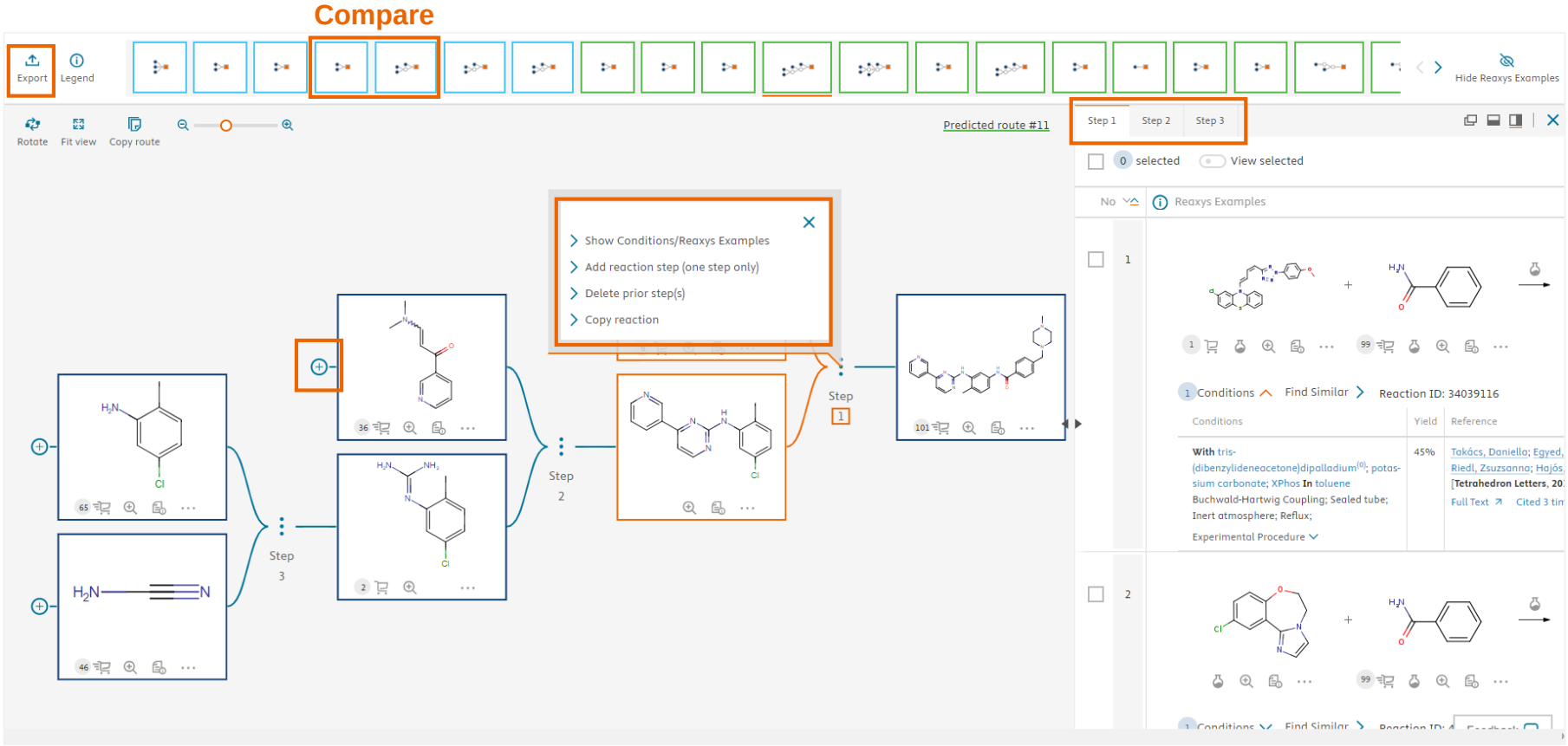
# Retrosynthesis: 繪製分子



# Retrosynthesis: Paxlovid



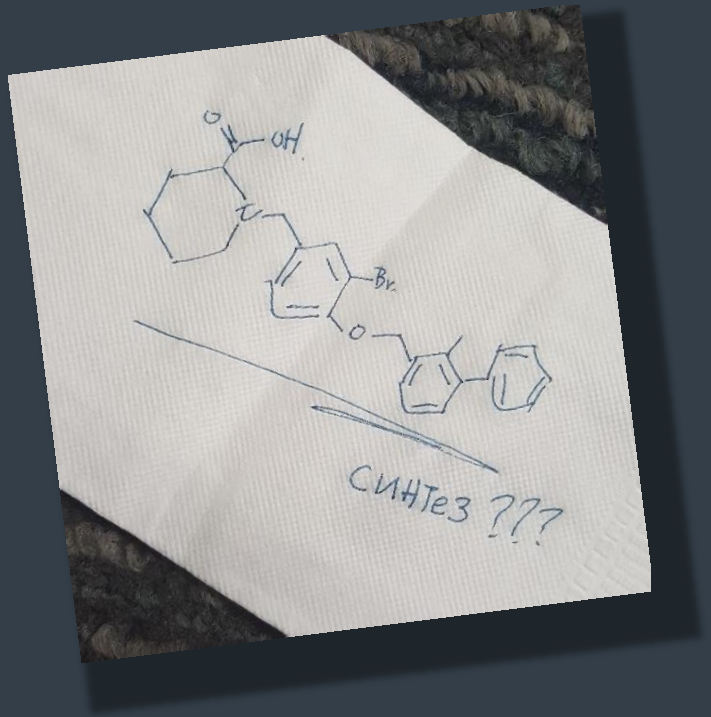
# Retrosynthesis: other features



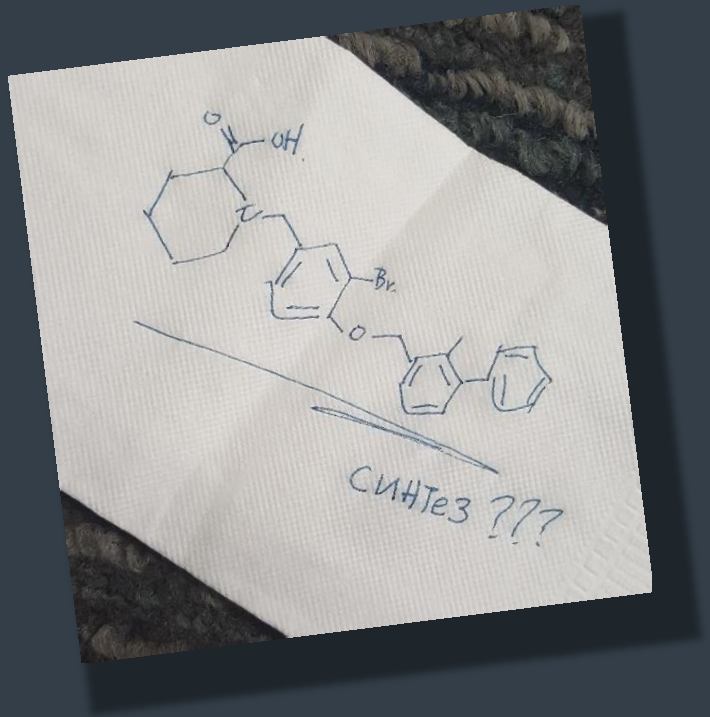
# 實際操作小遊戲

# 小遊戲: 神秘的科學家

一位穿著實驗衣的科學家搖搖晃晃的從你旁邊的吧檯走出去，你轉身看到吧檯留下了一張寫著一串文字及圖案的餐巾紙。你撿起餐巾紙站起來朝門口走去找那位科學家，但他卻不見蹤影。突然，你意識到從在 Reaxys 上搜尋，你可能能找到餐巾紙上圖樣的更多線索。



# 題目一




**在餐巾紙上的化合物有哪些已知的應用方式:**

A. High temperature resistant coating from aerospace R&D Dept. (航空研發部研發出的抗高溫塗層)

B. Anti-cancer medication in Pharmaceutical R&D Dept. (藥物研發部在研究的抗癌藥物)

C. New antioxidant extract from Health Food R&D Dept. (健康食品部所研發的新型抗氧化萃取物)

D. Evidence of a new narcotic discovered in the criminal investigation laboratory (刑事調查實驗室新發現的新型毒品證據)

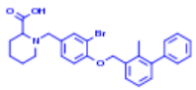
答案: B

## 1 Substances out of 4 Documents, containing 6 Reactions, 2 Targets

Reaxys - 1

0 | Limit To | Exclude | Export | Preparations | No of References | Grid | Heatmap

1



**1-({3-bromo-4-[(2-methyl-3-phenyl-phenyl)methoxy]phenyl}methyl)piperidine-2-carboxylic acid**

$C_{27}H_{28}BrNO_3$ 494.428 27956541

Identification | Physical Data - 5 | Preparations - 6

Druglikeness | Spectra - 10 | Reactions - 6

Bioactivity (All) | Targets - 2

Documents - 4

## 4 Documents with 535 Substances, 668 Reactions, 3 Targets

Reaxys - 4

0 | Limit To | Exclude | Export | Publication Year | Heatmap

1

Novel multitarget inhibitors with antiangiogenic and immunomodulator properties

Cited 2 times

Conesa-Milián, Laura; Falomir, Eva; Murga, Juan; Carda, Miguel; Marco, J. Alberto [**European Journal of Medicinal Chemistry, 2019**, vol. 170, p. 87 - 98]

Abstract | Index Terms | Substances 56 | Reactions 110 | Targets | Full Text

Hit Substances 1

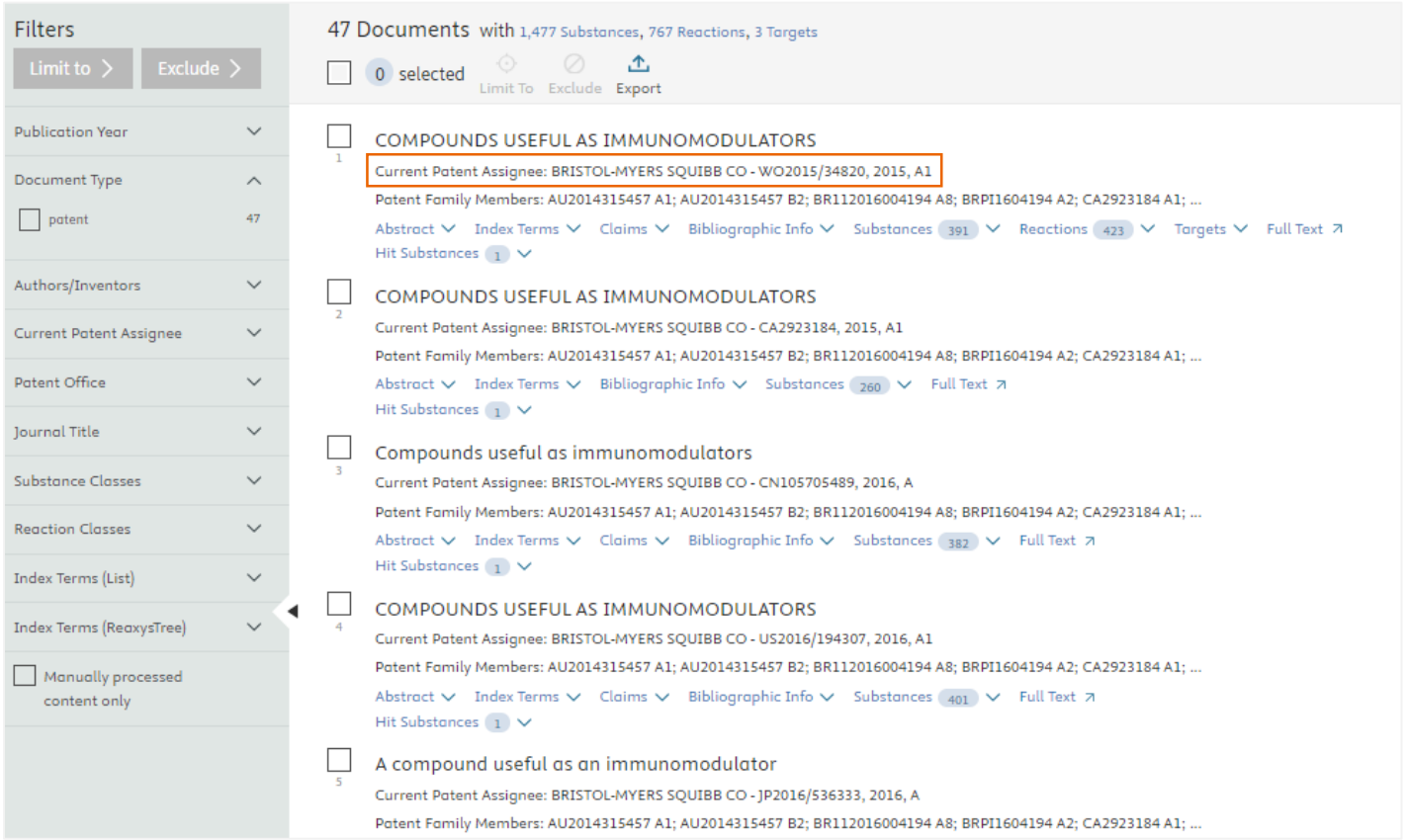
### Abstract

By means of docking studies, seventeen compounds T.1-T17 have been designed and evaluated as multitarget inhibitors of VEGFR-2 and PD-L1 proteins in order to overcome resistance phenomena offered by cancer. All these designed molecules display a urea moiety as a common structural feature and eight of them (T.1-T8) further contain a 1,2,3-triazol moiety. The antiproliferative activity of these molecules on several tumor cell lines (HT-29, MCF-7, HeLa, A549, HL-60), on the endothelial cell line HMEC-1 and on the

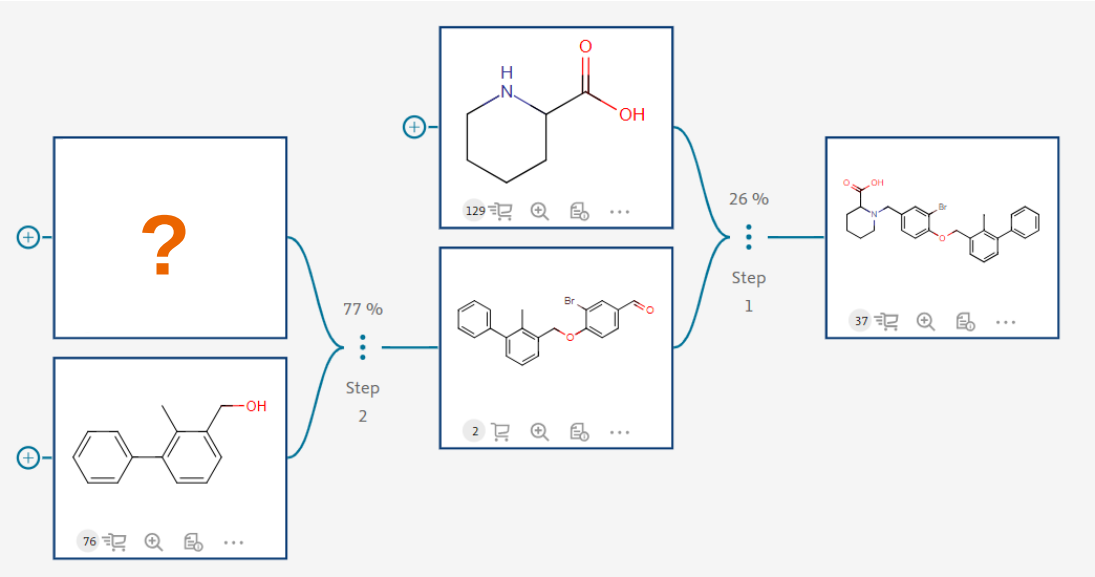
# 題目二

哪一家公司最早持有這類化合物的專利? 年份是哪一年?

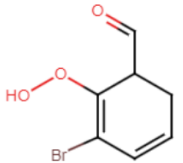
# 答案: BRISTOL-MYERS SQUIBB CO - WO2015/34820, 2015, A1



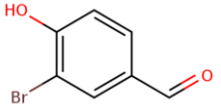
**題目三:** 跟著線索，你在 BMS 大樓裡找到了科學家，並將餐巾紙還給他。當你轉身離開，科學家追了上來，問你是否會用 Reaxys，並協助他解決困擾他幾天的合成方法，並找到化合物的合成路徑。



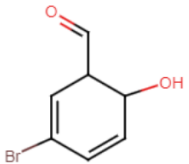

A

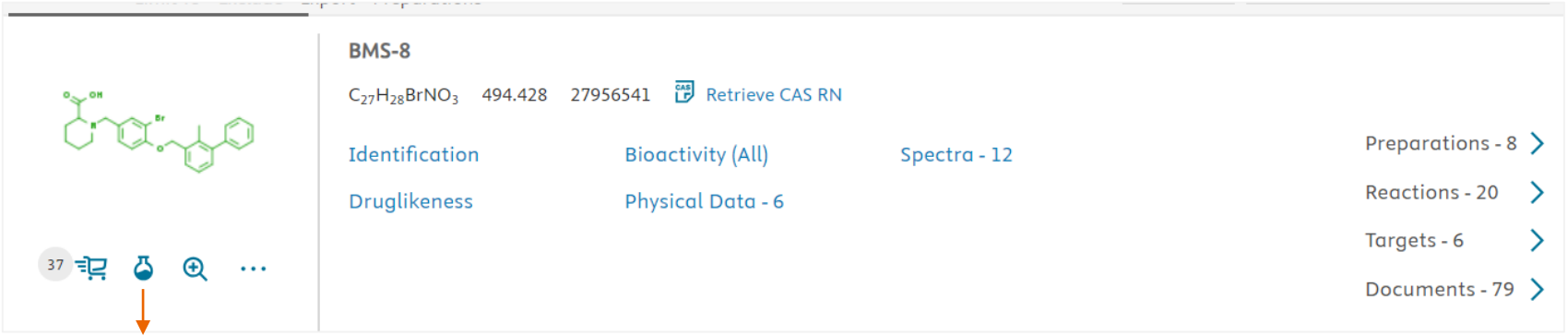


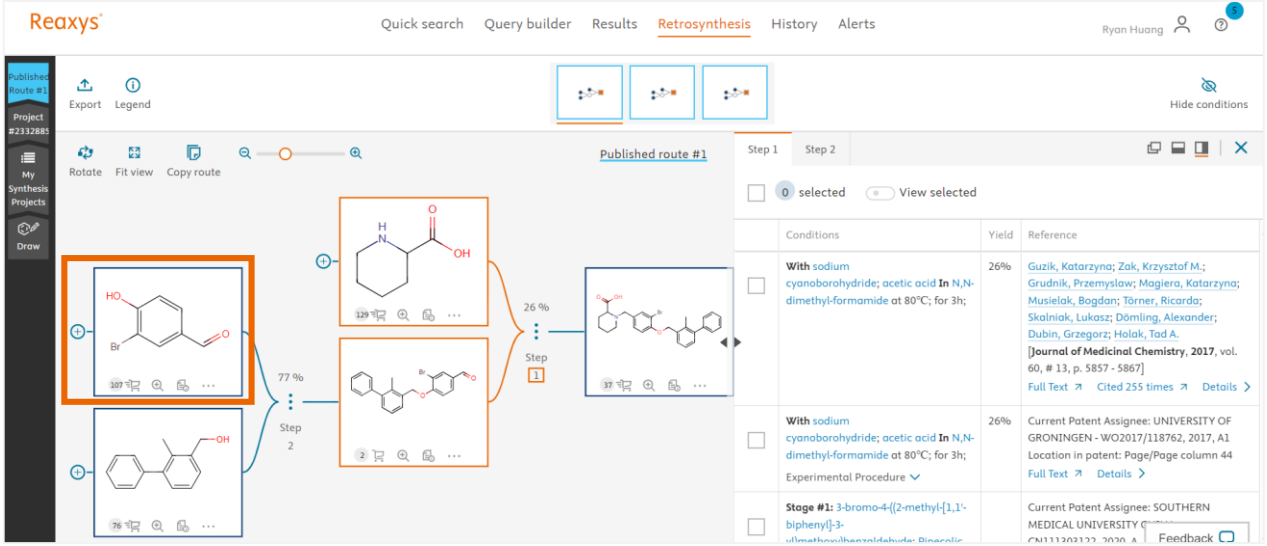

B




C




BMS-8
$C_{27}H_{28}BrNO_3$ 494.428 27956541 Retrieve CAS RN
Identification
Bioactivity (All)
Spectra - 12
Druglikeness
Physical Data - 6
Preparations - 8
Reactions - 20
Targets - 6
Documents - 79
37
Synthesize
Find preparations
Create retrosynthesis plans


Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Ryan Huang
Export
Legend
Hide conditions
Rotate
Fit view
Copy route
Published route #1
Step 1
Step 2
0 selected
View selected
Conditions
Yield
Reference
With sodium cyanoborohydride; acetic acid In N,N-dimethyl-formamide at 80°C; for 3h;
26%
Guzik, Katarzyna; Zak, Krzysztof M.; Grudnik, Przemyslaw; Magiera, Katarzyna; Musielak, Bogdan; Törner, Ricarda; Skalniak, Lukasz; Dömling, Alexander; Dubin, Grzegorz; Holak, Tad A.
Journal of Medicinal Chemistry, 2017, vol. 60, # 13, p. 5857 - 5867
Full Text
Cited 255 times
Details
With sodium cyanoborohydride; acetic acid In N,N-dimethyl-formamide at 80°C; for 3h;
Experimental Procedure
Current Patent Assignee: UNIVERSITY OF GRONINGEN - WO2017/118762, 2017, A1
Location in patent: Page/Page column 44
Stage #1: 3-bromo-4-((2-methyl-[1,1'-biphenyl]-3-
Current Patent Assignee: SOUTHERN MEDICAL UNIVERSITY
77 %
Step 2
26 %
Step 1
Feedback

答案: B

# 線上自我學習資源

# Reaxys 學院: 線上學習與認證平台

## Reaxys Academy

加入我們為學生和教育工作者提供的自訂進度線上化學培訓。了解如何使用 Reaxys 加深您對分析、有機和無機化學的理解。

### Reaxys 101

預估完成時間：30-45 分鐘

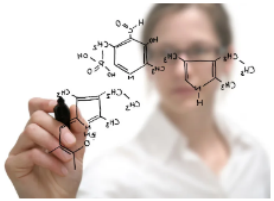
這個自訂進度課程非常適合圖書館員、教育工作者、研究員和學生，可簡單了解 Reaxys，也能提升自己的技能和對研究平台 Reaxys 的理解。

開始測驗

### Reaxys 化學 101

預估完成時間：45-60 分鐘

這門自訂進度課程展示，Reaxys 能拓展各層級學生對於化學的了解，從大學生到研究生，甚或更高的層級。

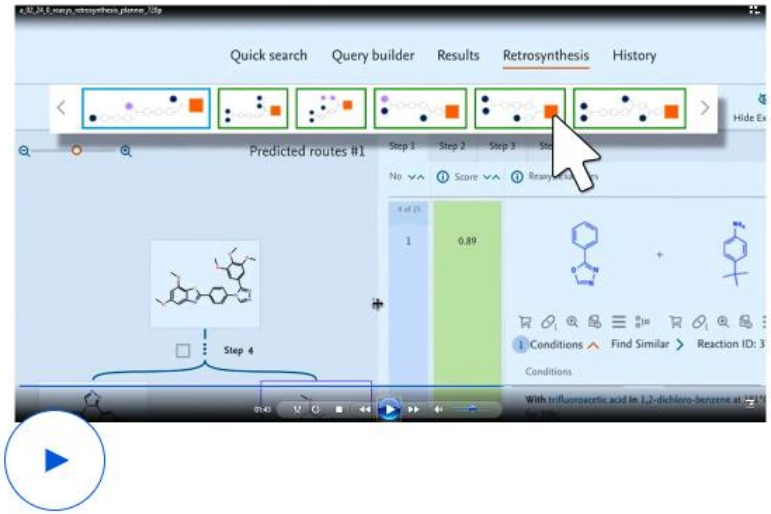


開始測驗

# 預測逆合成

## Reaxys 預測逆合成加速逆合成分析和預測 (網址)

Get a video overview of Predictive Retrosynthesis




### 觀看 Reaxys 預測逆合成短片

過去，逆合成分析只能完全依靠化學家的專業知識和時間，但是，Reaxys 預測逆合成卻改變了這個模式，並贏得獎項。本產品將人工智慧應用於世界最大的化學反應資料庫，提供強大的預測路徑，從而增強你的知識水準。運用 Reaxys 預測逆合成，能以更快的速度，獲得更廣泛的分子答案。

# 用戶資源

## 線上講座

### Big data in chemistry

- A universal approach to reaction informatics
- Understanding the history of chemical space through big data
- Reaction condition prediction using Reaxys: from raw data to best-in-class model
- Charting the chemical reaction space for DNA-encoded library design

### Reaxys Predictive Retrosynthesis

- Reaxys Predictive Retrosynthesis — speed matters
- AI-enabled predictive retrosynthesis tool to advance drug discovery
- Next generation synthesis planning using AI for chemists

## 線上資源

**Chemistry & Bioactivity data factsheet**


**Reaxys Quick reference guide**


**Bioactivity Visualization**


**Reaxys 支援中心**

ELSEVIER

# Thank you