



# Reaxys化學資料庫介紹

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2024.10



# 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

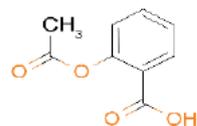
- 有機化学 1771年~
- 無機化学·有機金屬錯合物 1772年~

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，覆蓋範圍將擴大到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

# 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

[Quick search](#)

[Query builder](#)

[Results](#)

[Retrosynthesis](#)

[History](#)

[Register >](#)

[Sign in](#)

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances

Search Reaxys

Reactions, e.g. Suzuki coupling

Find >

AND

 Draw

[Content Overview](#) | Latest update: 09. October 2024 >

286M

 Substances

67M

 Reactions

116M

 Documents

44M

 Patents

47M

 Bioactivities

# Reaxys 檢索介面導覽

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Register &gt;

Sign in



Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Medicinal Chemistry, PubChem and Commercial Substance

Import 

Search Reaxys

關鍵字檢索

化學結構檢索  
(反應式、專利結構式)

AND



Draw

進階檢索 (實驗量測數據檢索)

逆合成AI工具  
預測複雜有機分子該如何合成

Content Overview | Latest update: 01. December 2022 >

257M

 Substances

60M

 Reactions

101M

 Documents

36M

 Patents

44M

 Bioactivities

# Reaxys 檢索介面導覽

## 可透過各種方式檢索

Search Reaxys

Caffeine

Search Reaxys

preparation Caffeine

Search Reaxys

"adenosine a2a receptor"

Results for Caffeine New Edit

	1,399	Substances	Structure :  as drawn <small>Edit in Query Builder Create Alert</small>	Preview Results <span style="float: right;">View Results &gt;</span>
	143,579	Documents	Structure :  as drawn Titles, Abstracts, Keywords : "Caffeine" <small>Edit in Query Builder Create Alert</small>	Preview Results <span style="float: right;">View Results &gt;</span>
	33	Commercial Substances	Structure :  as drawn <small>Edit in Query Builder Create Alert</small>	Preview Results <span style="float: right;">View Results &gt;</span>

實驗數值與參考出處

文獻、專利

供應商資訊

409 Reactions

Reaction Query :  as drawn  
Edit in Query Builder Create Alert

Preview Results View Results >

合成方法

80 Targets

Target(s) : adenosine a2a receptor  
Edit in Query Builder Create Alert

Preview Results View Results >

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

1,872 Documents with 3,563 Substances, 345 Reactions, 5 Targets

0 selected Limit To Exclude Export Sort by Publication Year ↓ Bioactivity Visualization

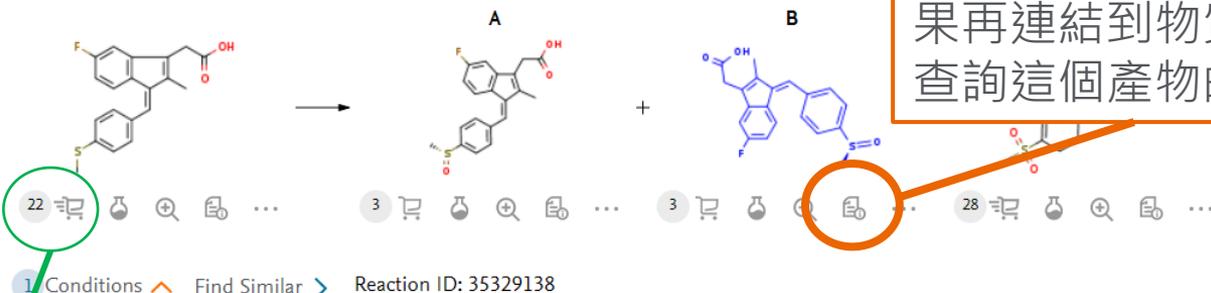
取得研究咸豐草的一千篇文獻中被我們人工索引的化合物清單。

1 Dual tolerance of ageratum (*Ageratum conyzoides*) and pot experiment  
 Wang, Zhongzhen; Wang, Hongbin; Wang, Haijuan; 2023, vol. 326, art. no. 116677  
 Abstract Index Terms Full Text  
 Abstract hit: {...and sticktight (*Bidens pilosa* L.) was relatively high, but the latter has been...}

2 Suitable light combinations enhance cadmium accumulation in *Bidens pilosa* L. by regulating the soil microbial communities  
 Xie, Junting; Lou, Xiuqin; Lu, Yezhen; Huang, Hai; Yang, Qing; Zhang, Zhipan; Zhao, Wenlu; (...) Du, Shaoting; Fang, Zhiguo [Environmental and Experimental Botany, 2023, vol. 205, art. no. 105128]  
 Abstract Index Terms Full Text  
 Abstract hit: {...accumulation in *Bidens pilosa* L. Compared with the control (fluorescent light), the translocation...}

3 Corrigendum to "Polyaspartic acid enhances the Cd phytoextraction efficiency of *Bidens pilosa* by remolding the rhizospheric environment and reprogramming plant metabolism" [Chemosphere 307 (Part 3) (2022) 136068] (Chemosphere (2022) 307(P3), (S0045653522025619), (10.1016/j.chemosphere.2022.136068))  
 Li, Xiong; Tian, Liyan; Li, Boqun; Chen, Huafang; Zhao, Gaojuan; Qin, Xiangshi; Liu, Yuanyuan; Yang, Yongping; Xu, Jianchu [Chemosphere, 2023, vol. 312, art. no. 137242]

# 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

Yield	Reference
A n/a	<a href="#">Srou, Hassan; Jalkh, Joanna; Le Maux, Paul; Chevance, Soizic;</a>
B n/a	<a href="#">Kobeissi, Marwan; Simonneaux, Gérard</a>
C n/a	<a href="#">[Journal of Molecular Catalysis A: Chemical, 2013, vol. 370, p. 75 - 79]</a> <a href="#">Full Text</a> <a href="#">Cited 37 times</a> <a href="#">Details</a> <a href="#">Abstract</a>

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<sub>4</sub>. 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

## Search Reaxys

"antibacterial coating" × Find >

AND

 7,010 Documents Titles, Abstracts, Keywords : "antibacterial coating" Preview Results ▾ View Results >

[Edit in Query Builder](#) [Create Alert](#) 

7,010 Documents with 3,063 Substances, 205 Reactions, 0 Targets

0 selected Limit To Exclude Export Sort by Publication Year ▾ Bioactivity Visualization 

**Filters**

- Limit to >
- Exclude >
- Publication Year ▾
- Document Type ▾
- Authors/Inventors ▾
- Current Patent Assignee ▾
- Patent Office ▾
- Journal Title ▾
- Substance Classes ▾
- Reaction Classes ▾
- Index Terms (List) ▾
- Index Terms (ReaxysTree) ▾
- Manually processed content only

**1** High efficiency photothermal cyclic self-healing **antibacterial coating** based on in-situ dual-functional BIOI@BI2S3 Cited 24 times

Feng, Huimeng; Wang, Tong; Wang, Wei; Ma, Chengcheng; Pu, Yanan; Chen, Shougang [Journal of Materials Science and Technology, 2024, vol. 173, p. 121 - 136]

[Abstract](#) [Index Terms](#) [Substances 3](#) [Full Text](#)

Abstract hit: {...cyclic self-healing **antibacterial coating**. The photothermal efficiency of BIOI@BI2S3 is improved by 38%...}

**2** Triple-function smart anticorrosion composite coating based on graphene and ZIF-8 with excellent pH-responsive self-healing and in vitro antimicrobial properties Cited 25 times

Zhou, Fan; Ma, Yanqi; Chen, Ying; Zhang, Li; Sheng, Xinxin [Progress in Organic Coatings, 2024, vol. 186, art. no. 108007]

[Abstract](#) [Index Terms](#) [Substances 4](#) [Full Text](#)

Index Terms hit: {...**Author keyword: Antibacterial coating**, Anticorrosion coating...}

**3** Antibacterial activity of additive manufactured NiTi alloy improved by zinc oxide-doped DCPD-PCL composite coating Cited 2 times

Zhang, Zhihui; Yang, Yanan; Zhang, Jundong; Sha, Pengwei; Xu, Zezhou; Li, Panpan; Yu, Zhenglei; Guo, Yunting; Ren, Luquan; Yan, Dandan [Ceramics International, 2024, vol. 50, # 1, p. 897 - 908]

[Abstract](#) [Index Terms](#) [Full Text](#)

Index Terms hit: {...**Author keyword: Antibacterial coating**, Biomineralization...}

# 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

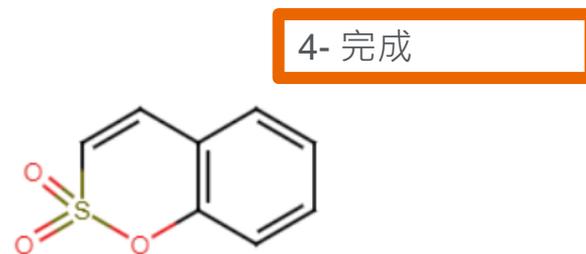
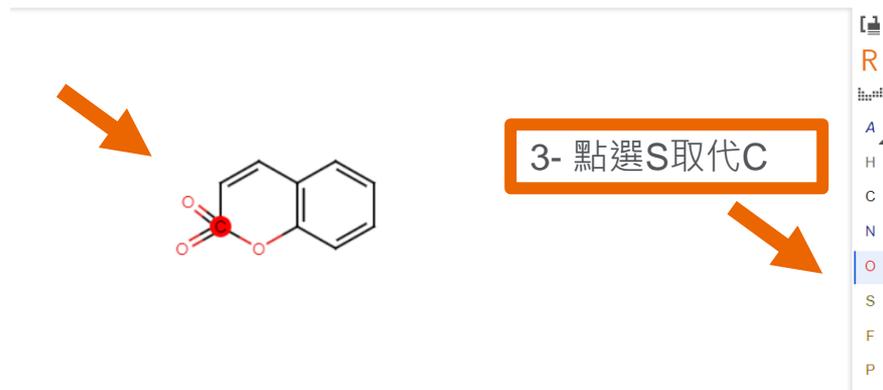
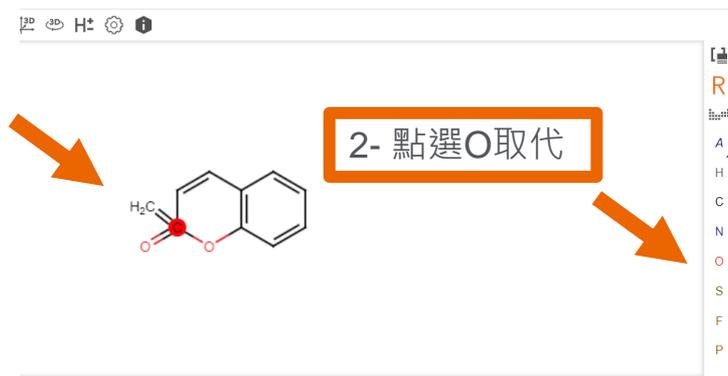
Mechanical Properties - 8 hits out of 362

Show/Hide columns ▾

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

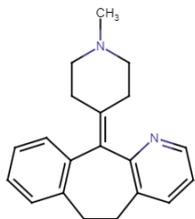
- 結構檢索 Draw

# 畫圖示範 Carbonyl Group to Sulfonyl Group



# Reaxys三種結構搜尋與怎麼用

我感興趣的結構



Azatadine  
CAS# 3964-81-6

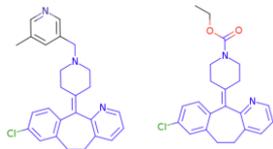
## As drawn

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)

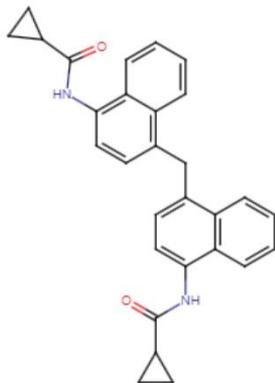
## Similar

「結構類似」的化合物  
提供不同程度的結構變化

線上示範

## 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。

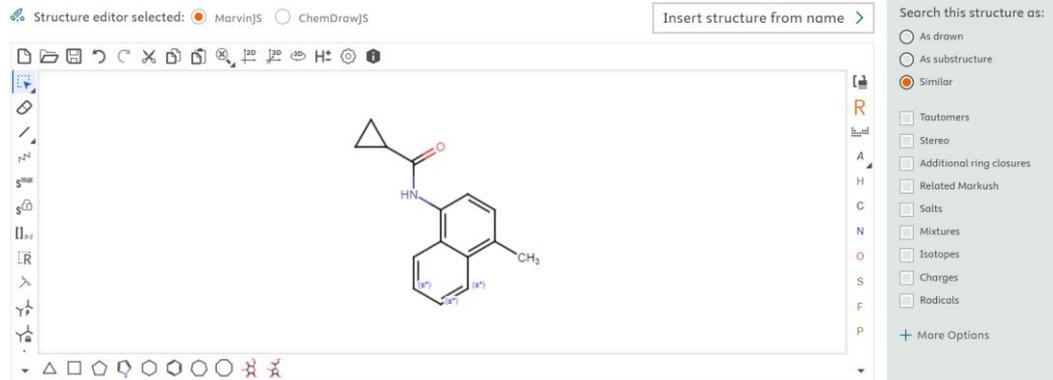


```
O=C(NC1=CC=C(CC2=C3C=CC=CC3=C(NC(=O)C3CC3)C=C2)C2=C1C=CC=C2)C1CC1
```

線上示範

Structure editor selected:  MarvinJS  ChemDrawJS

Insert structure from name >



Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals
- + More Options

修改結構, 點選 Similar

結果顯示

	2	Substances	Structure :  tight similarity Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>
	2	Substances	Structure :  near similarity Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>
	18	Substances	Structure :  average similarity Edit in Query Builder  Create Alert 	Preview Results 	<a href="#">View Results &gt;</a>

# 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

# 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」

# 分子式檢索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

Group 2 Ungroup

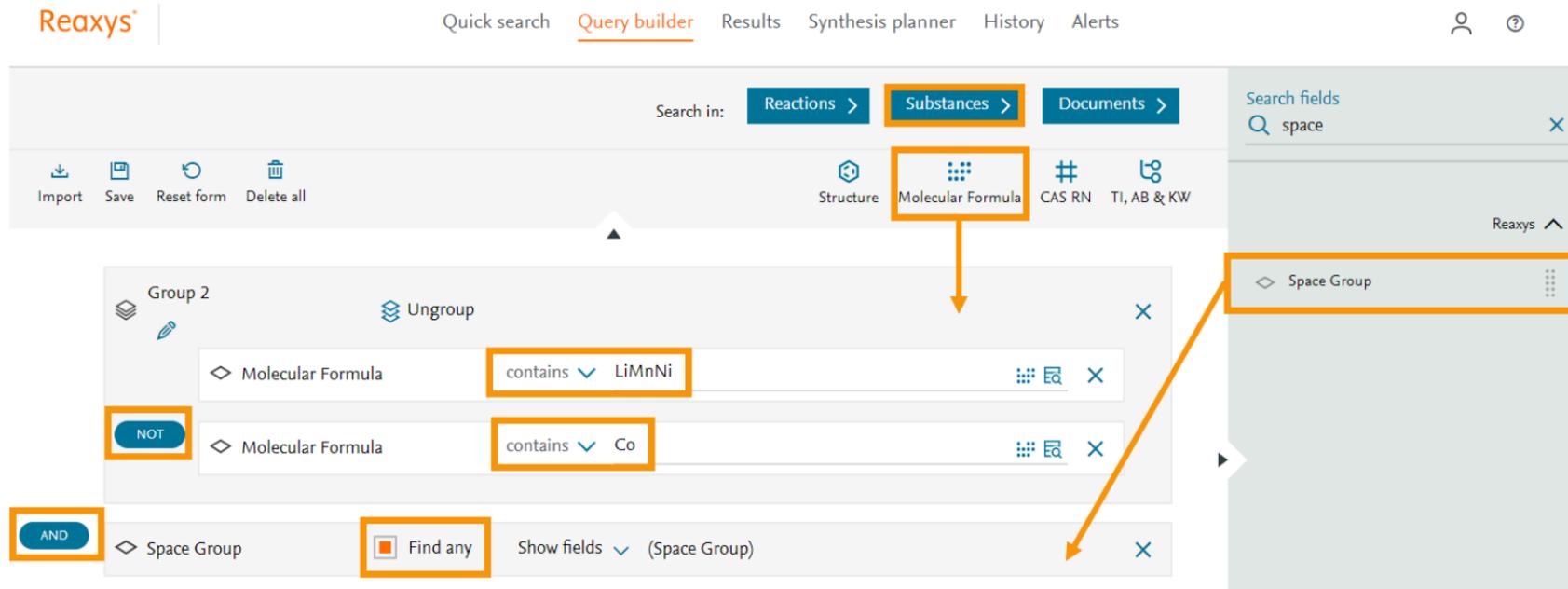
◇ Molecular Formula contains **LiMnNi**

**NOT** ◇ Molecular Formula contains **Co**

**AND** ◇ Space Group  Find any Show fields (Space Group)

Search fields  
Q space

◇ Space Group



# 分子式檢索②

438 Substances out of 458 Documents, containing 707 Reactions Reaxys - 438

0 Limit To Exclude Export Preparations No of References ↓ Grid

1 LiMn<sub>1.5</sub>Ni<sub>0.5</sub>O<sub>4</sub>

**lithium nickel manganese oxide**  
Li(Mn<sub>1.5</sub>Ni<sub>0.5</sub>)O<sub>4</sub> 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

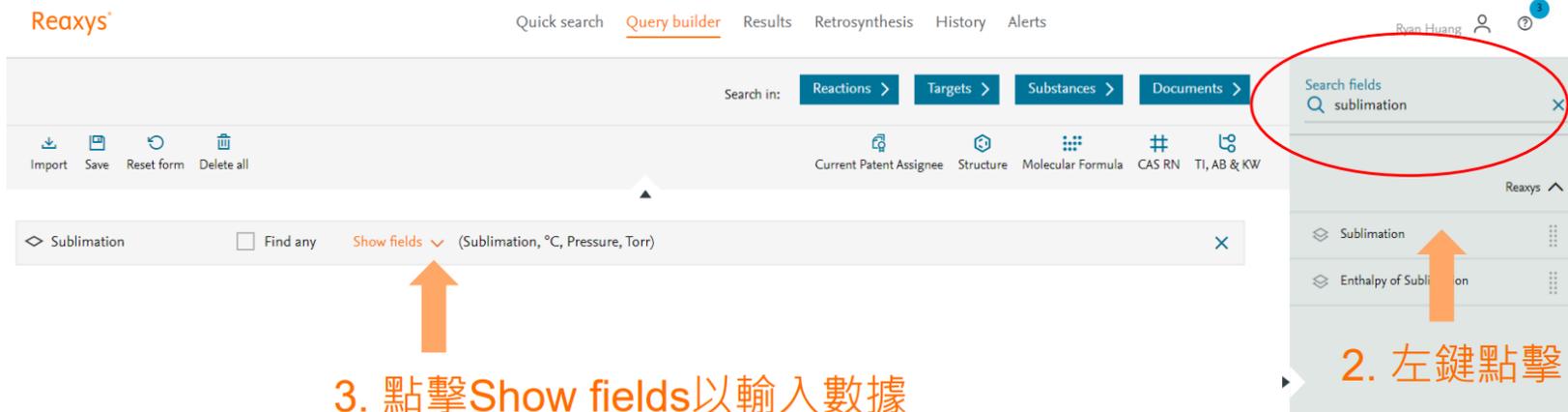
Space Group	Comment (Space Group)	Reference
227	a = 8.2 Å; Method = X-ray diffraction	Costa, Carlos M.; Ferdov, Stanislav; Gonçalves, Renato; Lanceros-Méndez, Senentxu; Ram, Pura; Sharma, Poonam; Sharma, Rakesh K.; Silva, M. Manuela; Singhal, Rahul[ <i>Journal of Alloys and Compounds</i> , 2021, vol. 853] <a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a>
227	a = 8.1789 Å; Method = Powder X-ray diffraction	Gong, Jijia; Yan, Shuipeng; Lang, Yaqiang; Zhang, Yuan; Fu, Shaoxiong; Guo, Jianling; Wang, Li; Liang, Guangchuan[ <i>Journal of Alloys and Compounds</i> , 2021, vol. 859, art. no. 157885]

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



The screenshot shows the Reaxys interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis, History, and Alerts. Below this is a search bar with the text 'Search in:' and four buttons: Reactions, Targets, Substances, and Documents. A dropdown menu is open, showing 'Search fields' with a search input containing 'sublimation'. Below the search bar, there are icons for Import, Save, Reset form, and Delete all. To the right, there are icons for Current Patent Assignee, Structure, Molecular Formula, CAS RN, and TI, AB & KW. At the bottom, there is a search result card for 'Sublimation' with a 'Find any' checkbox and a 'Show fields' dropdown menu. An orange arrow points to the 'Show fields' dropdown. To the right, a separate panel shows a list of search fields: 'Sublimation' and 'Enthalpy of Sublimation'. An orange arrow points to the 'Sublimation' entry in this list.

3. 點擊Show fields以輸入數據

2. 左鍵點擊

# 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 Molecular Formula CAS RN TI, AB & KW

Sublimation  Find any Hide fields ^

= v 55-65 

= v 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)

Search fields 

Fields Forms History

Reaxys ^

Topics and Keywords v

Identification v

Physical Properties v

Spectra v

MedChem v

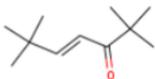
Other v

Reactions v

Bibliography v

# 實驗數據檢索③

4



(E)-2,2,6,6-tetramethylhept-4-en-3-one

(CH3)3CCCHCOC(CH3)3 168.279 1904245 20859-13-6

Hit Data - 1

Druglikeness

Spectra - 25

Preparations - 14 >

Identification

Physical Data - 12

Reactions - 62 >

Documents - 37 >

## Hit Data - 1

Sublimation - 1 hits out of 1

Show/Hide columns v

Sublimation, °C	Pressure (Sublimation), Torr	Reference
-----------------	------------------------------	-----------

55

760

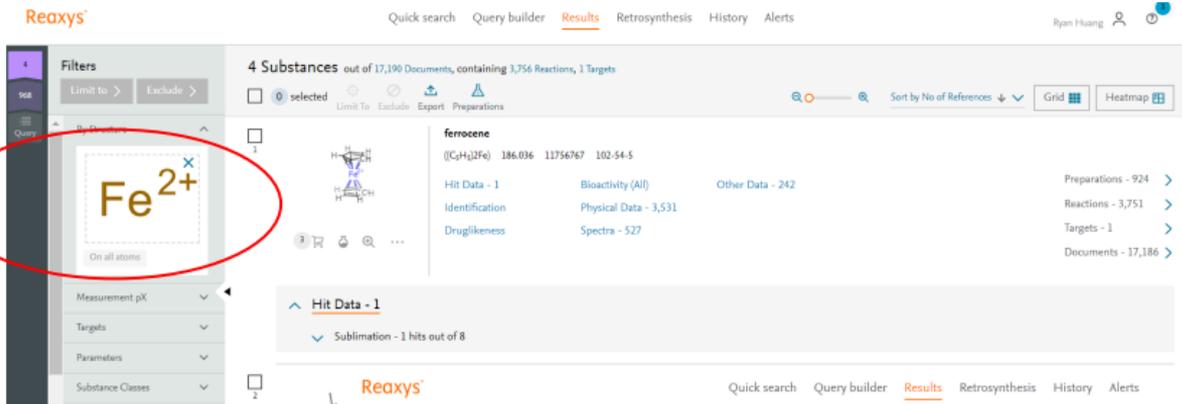
Reference

Overman, L.E.; Clizbe, L.A.; Freerks, R.L. [Journal of the American Chemical Society, 1981, vol. 103, p. 2807]

Full Text ↗ Cited 67 times ↗ Details >

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

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

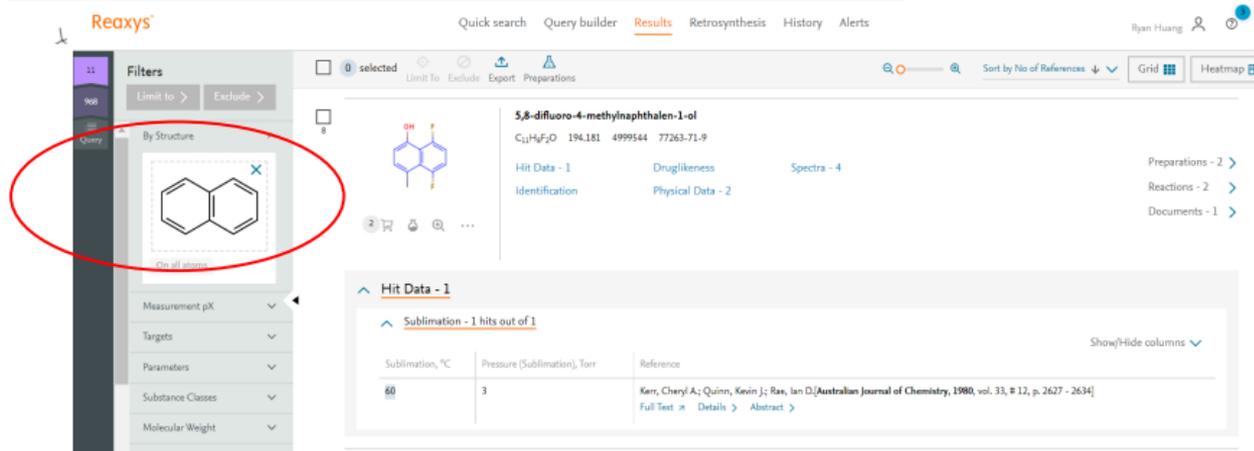
**ferrocene**  
[[C<sub>10</sub>H<sub>10</sub>2Fe] 186.036 11756767 102-54-5

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

Filters: By Structure, On all atoms, Measurement pK, Targets, Parameters, Substance Classes



Reaxys Quick search Query builder **Results** Retrosynthesis History Alerts Ryan Huang

5,8-difluoro-4-methylnaphthalen-1-ol  
C<sub>11</sub>H<sub>7</sub>F<sub>2</sub>O 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

Sublimation, °C	Pressure (Sublimation), Torr	Reference
80	3	Kerr, Cheryl A.; Quinn, Kevin J.; Ras, Ian D. <i>Australian Journal of Chemistry</i> , 1980, vol. 33, # 12, p. 2627 - 2634 <a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a>

Filters: By Structure, On all atoms, Measurement pK, Targets, Parameters, Substance Classes, Molecular Weight



- 進階搜尋 Query Builder
- 天然萃取物的生物活性應用

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

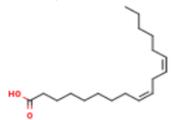
方法二

- 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" 

1  
  


**linoleic acid**  
 $C_5H_{11}CHCHCH_2CHCHC_7H_{14}C(O)OH$  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 v

Isolated from Natural Source	Reference
plant of <b>Bidens pilosa</b> L. var. minor (Blume) sherff collected at the roadside of Tung-Shih	Chang, Ming-Huey; Wang, Guei-Jane; Kuo, Yueh-Hsiung; Lee, Ching-Kuo] <b>Journal of the Chinese Chemical Society</b> , 2000, vol. 47, # 5, p. 1131 - 1136 <a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a> >

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。

需要註冊登入

Reaxys<sup>®</sup>

[Quick search](#) [Query builder](#) [Results](#) **Retrosynthesis** [History](#)

[Register >](#) [Sign in](#) 10

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Medicinal Chemistry, PubChem and Commercial Substance

Import 

Search Reaxys

Reactions, e.g. phosphorylation

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

AND

 Draw

尋找單步驟的反應

Content Overview | Latest update: 01. December 2022 >

257M

 Substances

60M

 Reactions

101M

 Documents

36M

 Patents

44M

 Bioactivities

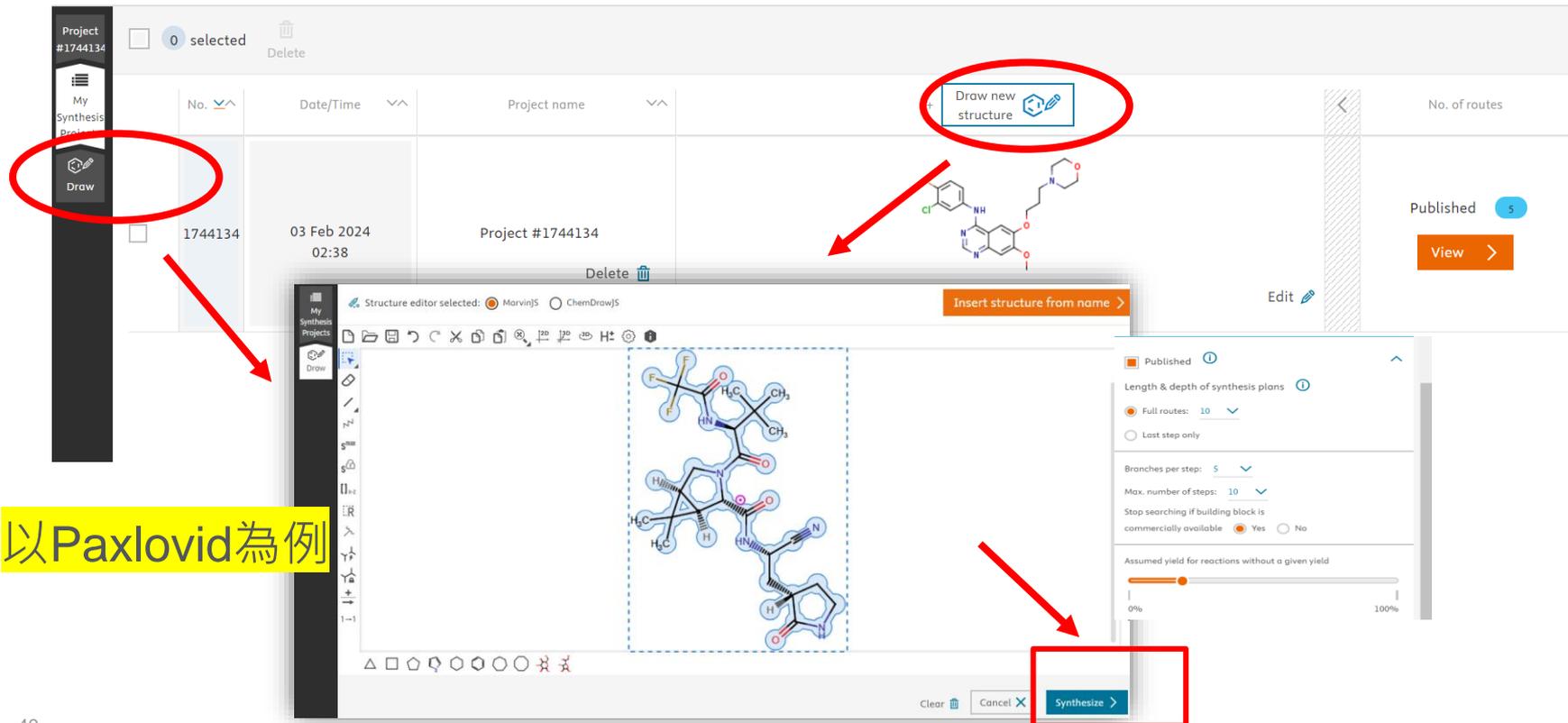
# 畫出分子架構, 選擇條件, 並點選 Synthesize 合成

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang

2



The screenshot displays the Reaxys Retrosynthesis interface. On the left, a sidebar contains a 'Draw' button circled in red. The main area features a table with columns for 'No.', 'Date/Time', 'Project name', and 'No. of routes'. The first row shows project #1744134 from 03 Feb 2024. A red arrow points from the 'Draw' button to the 'Draw new structure' button in the table's header, which is also circled in red. Below the table, a chemical structure editor is open, showing the structure of Paxlovid. A red arrow points from the 'Draw new structure' button to the editor. On the right, a settings panel is visible, and a red arrow points from the 'Synthesize' button at the bottom of the editor to the 'Synthesize' button in the settings panel, which is also circled in red.

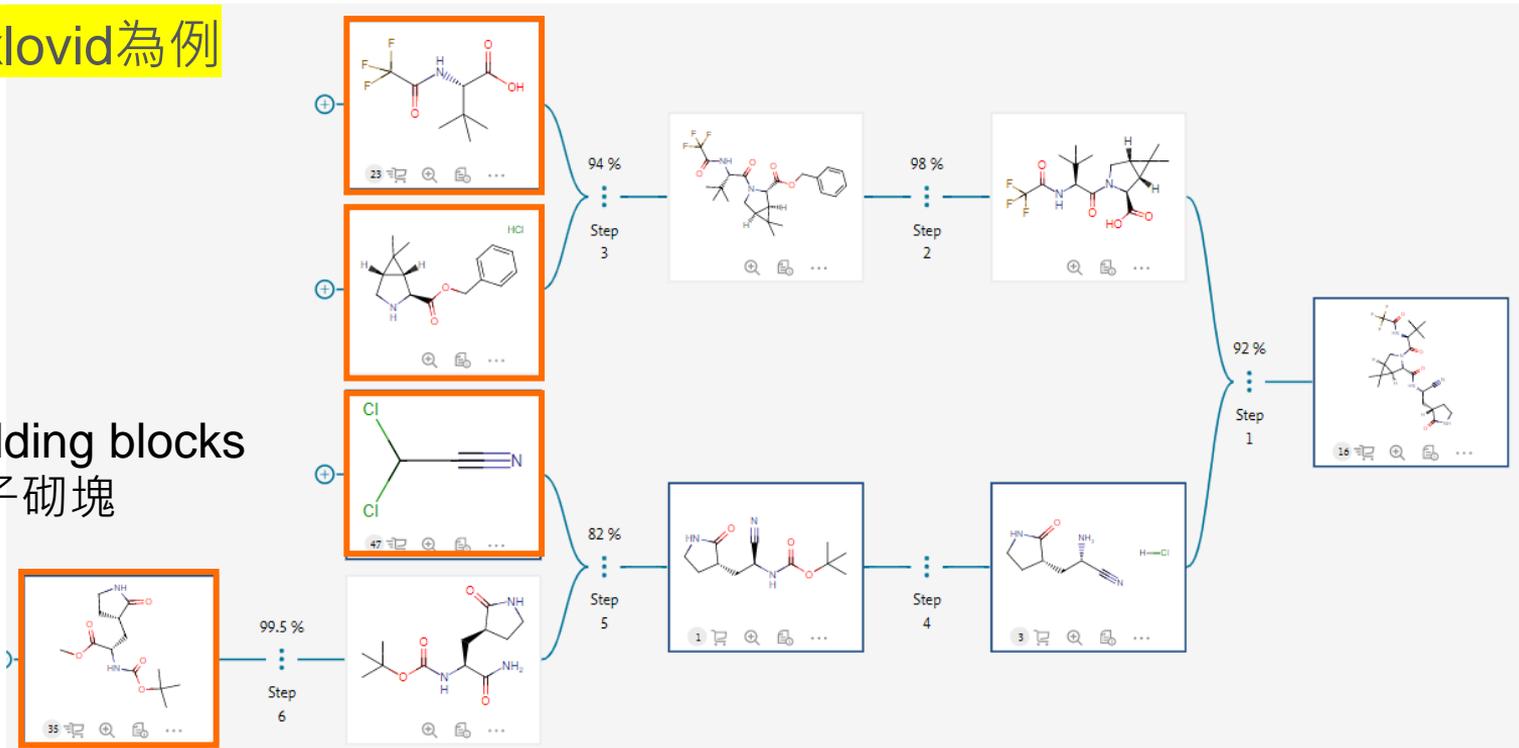
No.	Date/Time	Project name	No. of routes
1744134	03 Feb 2024 02:38	Project #1744134	Published 5

以Paxlovid為例

# Retrosynthesis 逆合成計畫

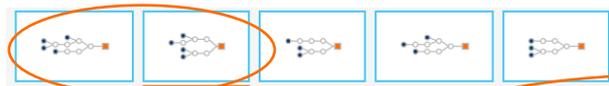
以Paxlovid為例

Building blocks  
分子砌塊



# Retrosynthesis 逆合成計畫

匯出資料



查看步驟  
資訊

Rotate Fit view Copy route

## 比較路徑

Published route #2

Conditions	Yield	Reference
<p><b>With</b> 1-hydroxy-7-aza-benzotriazole; N-[3-(N,N-dimethylamino)-propyl]-N'-ethyl-carbodiimide hydrochloride; N-ethyl-N,N-diisopropylamine In dichloromethane at 0 - 25°C; for 16h; Solvent; Temperature; Reagent/catalyst;</p> <p><a href="#">Experimental Procedure</a></p>	92%	<p>Current Patent Assignee: ZHEJIANG LEPP PHARMACOLOGICAL STOCK - CN114437043, 2022, A</p> <p>Location in patent: Paragraph 0011; 0058-0068</p> <p><a href="#">Full Text</a> <a href="#">Details</a> <a href="#">Abstract</a></p>
<p><b>8; 9; 10 Preparation of compound I</b></p> <p>364g of compound V, 207g of compound VI, 164g of 1-hydroxy-7-azabenzotriazole (HOAT) and 260g of diisopropylethylamine were dissolved in 3L of dichloromethane, stirred and cooled to 0°C, and then added 187 g of 1-ethyl-3-(3-dimethylpropylamine)carbodiimide (EDCI) was stirred at 25°C for 16 hours. The temperature was lowered to 0°C, 500 mL of water was added dropwise, and the solution was separated after stirring for 1 h. The organic phase was washed with dilute acid, dried over anhydrous magnesium sulfate, and concentrated to dryness under reduced pressure. The crude product was recrystallized from isopropyl acetate/n-heptane to obtain 459.5 g of compound I with a yield of 92% and a HPLC purity of 99.4%.</p>		
<p><b>Stage #1:</b> (S)-2-amino-3-((S)-2-oxopyrrolidin-3-yl)propanenitrile hydrochloride; (1R,2S,5S)-6,6-dimethyl-3-[3-methyl-N-(trifluoroacetyl)-L-valyl]-3-</p>	10 kg	<p>Current Patent Assignee: SHANDONG ZONGKENG BLUE SEA MEDICINE SCIENCE AND TECH - CN114437044, 2022, A</p>

增加步驟

刪除/增加步驟

- 反應式 Reactions 搜尋

# Reaxys尋找反應式的方法

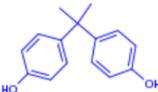
1. 已知物質的製備方式 (從substance介面連結preparations)
2. 關鍵字檢索 (例：radical cyclization)、命名反應式(例：Suzuki coupling)
3. 直接畫出反應式 (完整、半個反應式)



# Reaxys尋找反應式的方法

## ~已知物質的製備方式~

1



**BPA**  
HOC6H4C(CH3)2C6H4OH 228.291 1107700 80-05-7

Identification      Physical Data - 346

Druglikeness        Spectra - 139

Bioactivity (All)    Other Data - 470

Preparations - 98 >

Reactions - 1,366 >

Targets - 157 >

Documents - 13,432 >

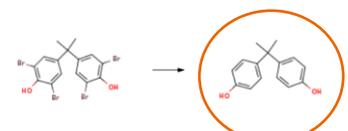
只出現在產物 (Product)

產物或起始物 (Reactants or Products)

99 Reactions out of 236 Documents containing 132 Substances, 436 Targets

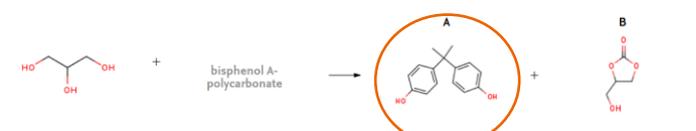
0 selected    Limit To    Exclude    Export    Syn-Plan    Show Conditions

1



4 Conditions    Find Similar    Reaction ID: 46083924

2



1 Conditions    Find Similar    Reaction ID: 44100782

1,402 Reactions out of 1,138 Documents containing 1,923 Substances, 1,080 Targets

0 selected    Limit To    Exclude    Export    Syn-Plan    Show Conditions

1



8 Conditions    Find Similar    Reaction ID: 70732

2



4 Conditions    Find Similar    Reaction ID: 46083924

# Reaxys尋找反應式的方法

## ~關鍵字檢索①~

Reaxys<sup>®</sup> [Quick search](#) Query builder Results Retrosynthesis History [Register >](#) [Sign in](#) 

Search for "radical cyclization" [Import](#) 

Search Reaxys

"radical cyclization"  [Find >](#)

AND

 Draw

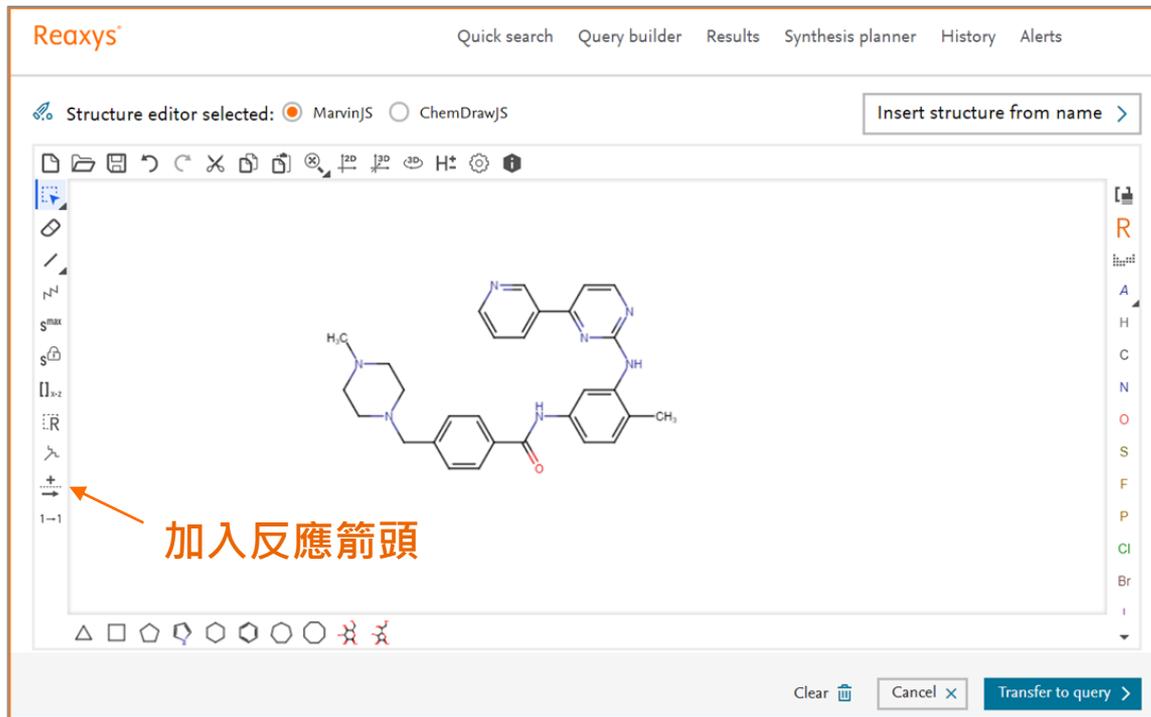
Results for "radical cyclization" [New](#)  [Edit](#) 

	75	Reactions	<b>Condition</b> : radical cyclization <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a>  <a href="#">View Results &gt;</a>
	7,895	Documents	<b>Titles, Abstracts, Keywords</b> : "radical cyclization" <a href="#">Edit in Query Builder</a>  <a href="#">Create Alert</a> 	<a href="#">Preview Results</a>  <a href="#">View Results &gt;</a>



# Reaxys尋找反應式的方法

## ~繪製反應式①~



Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Structure editor selected:  MarvInJS  ChemDrawJS

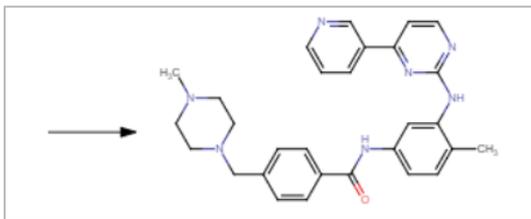
Insert structure from name >

加入反應箭頭

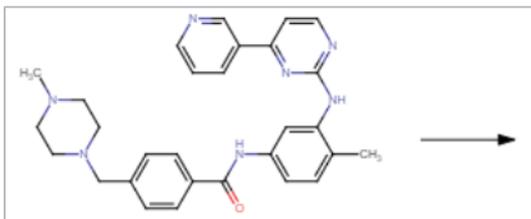
Clear  Transfer to query >

# Reaxys尋找反應式的方法

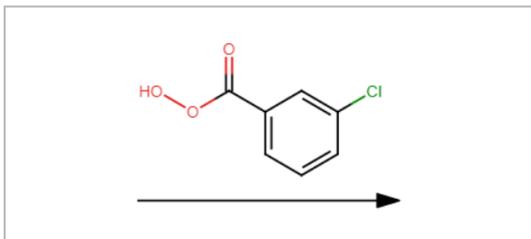
## ~繪製反應式②~



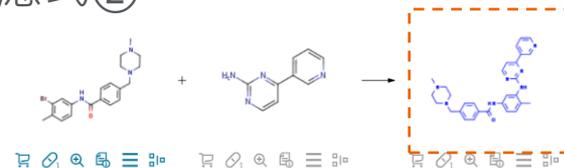
箭頭在左  
產物



箭頭在右  
起始物

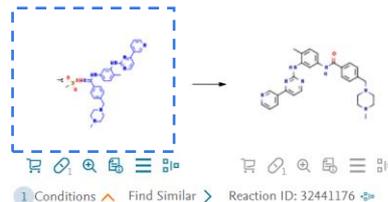


箭頭在下  
催化劑或溶劑



Conditions Find Similar Reaction ID: 29521413

Conditions	Yield	Reference
With tris(dibenzylideneacetone)dipalladium <sup>0</sup> chloroform complex; 2,2'-bis-(diphenylphosphino)-1,1'-binaphthyl; sodium t-butanolate In 5,5-dimethyl-1,3-cyclohexadiene at 140°C; for 5h; Temperature;	92%	Kang, Julie; Lee, Jun Young; Park, Jeong-Hoon; Chang, Dong-jo [Journal of labelled compounds and radiopharmaceuticals, 2020, vol. 63, # 4, p. 174 - 182] Full Text Details Abstract



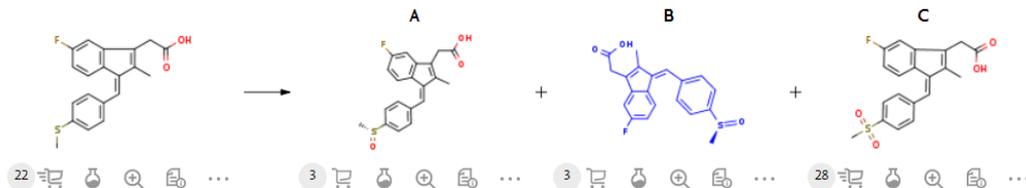
Conditions Find Similar Reaction ID: 32441176

Conditions	Yield	Reference
With ammonia In water; isopropyl alcohol at 20°C; for 4h; pH=7.6 - 8.5; <a href="#">Experimental Procedure</a>	93%	KRKA, D. D., NOVO MESTO; BENKIC Primoz; TIHI Jaroslav; PECAVAR Anica; GERMAN Tamara; VRECEK Franc; VAJS Anamarija; SKRABANJA Vida WO2011/157450, 2011, A1 Location in patent: Page/Page column 19 Full Text Details Abstract

Conditions	Yield	Reference
With dihydrogen peroxide; methyltrioxorhenium(VII) In dichloromethane; water at 15°C; for 5h; <a href="#">Experimental Procedure</a>	100%	METHYLGENE INC. WO2005/92899, 2005, A1 Location in patent: Page/Page column 73 Full Text Details Abstract

Conditions	Yield	Reference
With 3-chloro-benzenecarboxylic acid In dichloromethane at 20°C; Inert atmosphere;	100%	Roudesly, Fares; Veiros, Luis F.; Obie, Julie; Poli, Giovanni [Organic Letters, 2018, vol. 20, # 8, p. 2346 - 2350] Full Text Cited 19 times Details Abstract

## 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

With 2-methylimidazole;  $C_{84}H_{72}ClFeN_4O_{12}S_4^{(4-)} \cdot 4Na^{(+)}$ ; dihydrogen peroxide In methanol; aq. phosphate buffer at -20°C; for 1h; Inert atmosphere; Overall yield = 100 %Spectr.; enantioselective reaction;

[Experimental Procedure](#)

Yield

Reference

A n/a	Slour, Hassan; Jalkh, Joanna; Le Maux, Paul; Chevance, Soizic;
B n/a	Kobeissi, Marwan; Simonneaux, Gérard
C n/a	<b>Journal of Molecular Catalysis A: Chemical</b> , 2013, vol. 370, p. 75 - 79] <a href="#">Full Text</a> <a href="#">Cited 37 times</a> <a href="#">Details</a> <a href="#">Abstract</a>

### 2.3 General procedure for asymmetric sulfoxidation

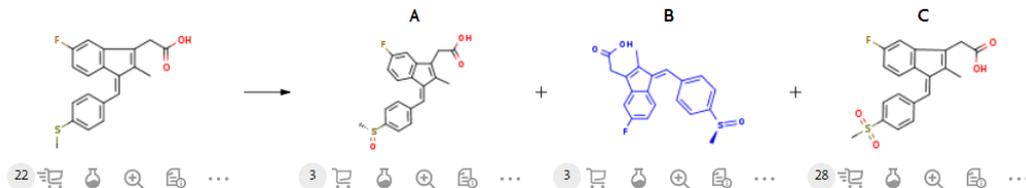
General procedure: Methyl phenyl sulfoxide. Manganese porphyrin complex 1 (1.6 mg, 1 μmol) and imidazole (1.7 mg, 25 μmol) were placed in a test tube under argon. The solvent (375 μL MeOH + 125 μL PBS, pH 7) was then added via syringe, followed by the sulfide (5 μL, 42.3 μmol). Finally, hydrogen peroxide (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

# 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

With 2-methylimidazole;  $C_{84}H_{72}ClFeN_4O_{12}S_4^{14-} \cdot 4Na^{1+}$ ; dihydrogen peroxide In methanol; aq. phosphate buffer at  $-20^\circ C$ ; for 1h; Inert atmosphere; Overall yield = 100 %Spectr.; enantioselective reaction;

[Experimental Procedure](#)

Yield

Reference

A n/a	<a href="#">Srouf, Hassan; Jalkh, Joanna; Le Maux, Paul; Chevance, Soizic;</a>
B n/a	<a href="#">Kobeissi, Marwan; Simonneaux, Gérard</a>
C n/a	<a href="#">Journal of Molecular Catalysis A: Chemical, 2013, vol. 370, p. 75 - 79]</a> <a href="#">Full Text</a> <a href="#">Cited 37 times</a> <a href="#">Details</a> <a href="#">Abstract</a>

### 2.3 General procedure for asymmetric sulfoxidation

General procedure: Methyl phenyl sulfoxide. Manganese porphyrin complex 1 (1.6 mg, 1  $\mu$ mol) and imidazole (1.7 mg, 25  $\mu$ mol) were placed in a test tube under argon. The solvent (375  $\mu$ L MeOH + 125  $\mu$ L PBS, pH 7) was then added via syringe, followed by the sulfide (5  $\mu$ L, 42.3  $\mu$ mol). Finally, hydrogen peroxide (1.8  $\mu$ L, 21.2  $\mu$ mol) 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(HPLC)、數值

# Reaxys進階反應式檢索

~利用Query builder進一步「加工」搜尋條件~

Reaxys<sup>®</sup>[Quick search](#) [Query builder](#) [Results](#) [Retrosynthesis](#) [History](#)[Register >](#)[Sign in](#)Results for 

將搜尋結果複製到進階搜尋Query Builder增加搜尋條件

	52	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	<a href="#">Preview Results</a> 	<a href="#">View Results &gt;</a>
Top 3 results					
	81	Reactions	Reaction Query :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	<a href="#">Preview Results</a> 	<a href="#">View Results &gt;</a>

# Reaxys進階反應式檢索

~利用Query builder進一步「加工」搜尋條件~

Reaxys<sup>®</sup> 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

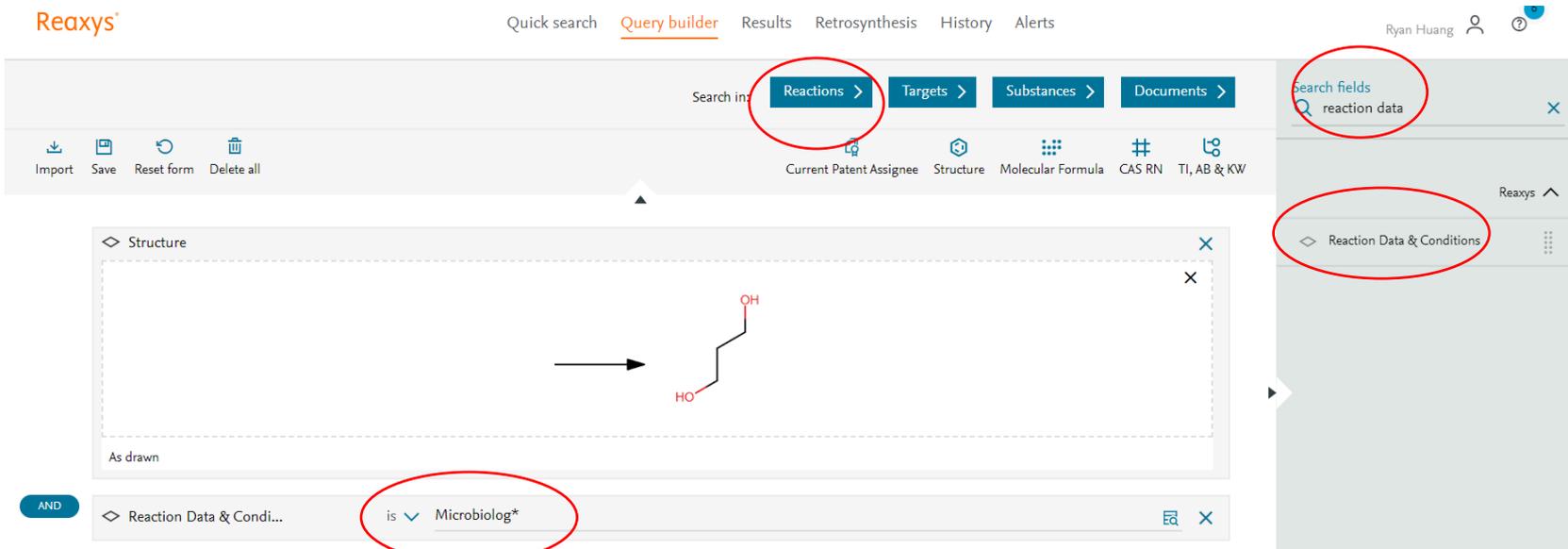
Structure

As drawn

Reaction Data & Conditions is **Microbiolog\***

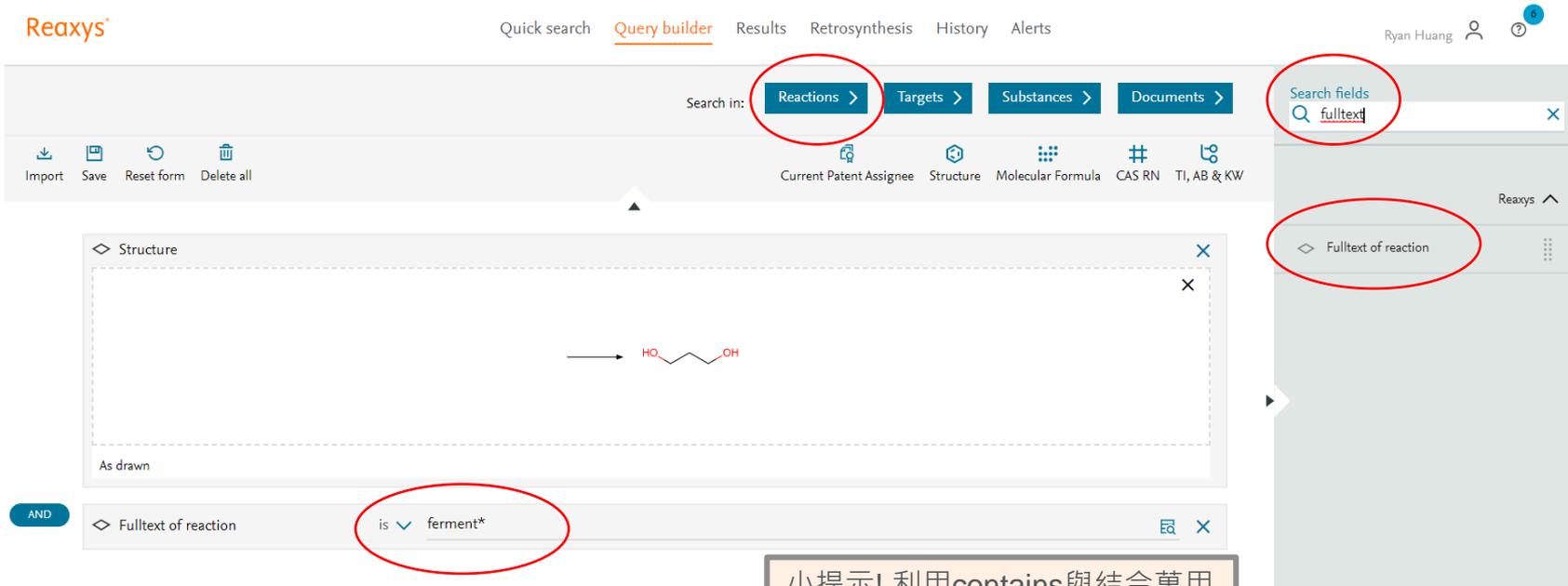
Search fields: reaction data

Reaction Data & Conditions



# Reaxys進階反應式檢索

~利用Query builder進一步「加工」搜尋條件~



The screenshot shows the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected. The search criteria are defined as follows:

- Search in:** Reactions > Targets > Substances > Documents >
- Search fields:** fulltext
- Structure:** As drawn (Chemical structure of 1,3-butanediol: OCC(O)CO)
- Fulltext of reaction:** is ferment\*

Red circles highlight the 'Reactions' dropdown, the 'Search fields' dropdown, the 'Fulltext of reaction' dropdown, and the 'is ferment\*' search term.

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>

## Reaxys Academy

The Reaxys Academy is designed to provide you educational material to support learning chemistry concepts and digital chemistry literacy with Reaxys. In these courses you will learn how to get started with Reaxys and how to apply this knowledge to enhance your learning on analytical, organic and inorganic chemistry.

Test your knowledge and share your accomplishments:

- Review the materials below
- 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

Reaxys 101

Self-paced course

The

...based, chemical  
...research for chemical  
...chemical structures and substance  
... approximate time to complete – 30-45

Chemistry 101 with Reaxys

Self-paced course

Reaxys can broaden the understanding of chemistry for any level of student: from undergraduate and graduate to post-graduate and beyond.



Chemists need exposure to relevant chemistry databases early in their careers to effectively learn chemistry, gain chemistry digital literacy skills, and be well-prepared for their research projects and labs. Approximate time to complete – 45-60 minutes.

Reaxys  
Certification



Thank you

