



ELSEVIER

Reaxys[®]

資料庫簡介與應用

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Customer Success Manager, A&G Elsevier

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



Reaxys提供文章更著重於實驗數據

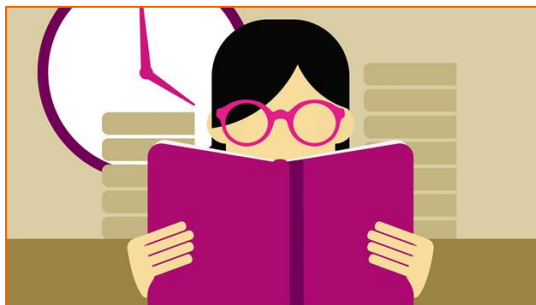
從化學相關的論文和專利中透過人工提取和整理
關鍵的「**實驗數據**」



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藥物靶點嗎?

Reaxys 涵蓋的範圍

287M



Substances

68M



Reactions

116M



Documents

44M



Patents

48M



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

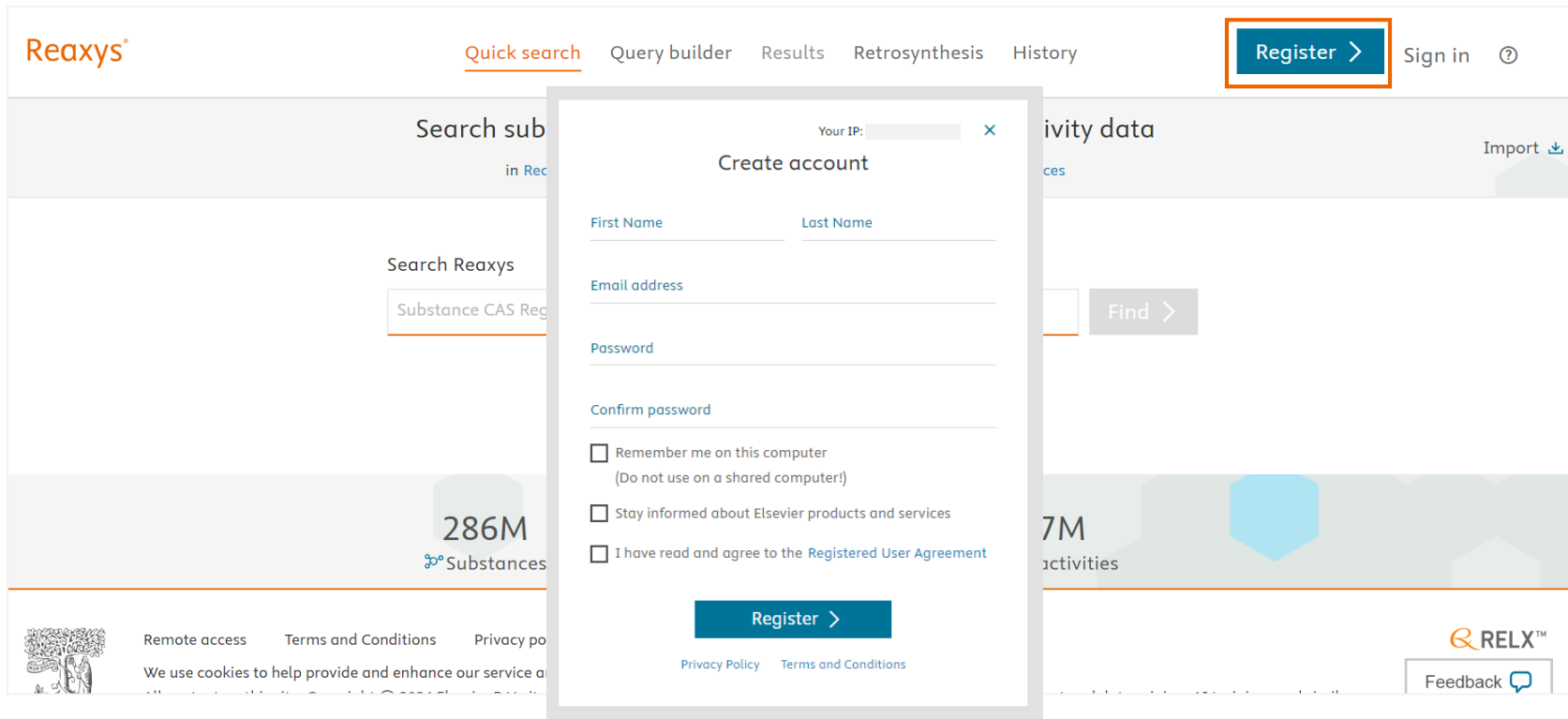
專利

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，覆蓋範圍將擴大到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®

Quick search Query builder Results Retrosynthesis History

Register > Sign in ?

Your IP: [] x

Create account

First Name Last Name

Email address

Password

Confirm password

☐ Remember me on this computer
(Do not use on a shared computer!)

☐ Stay informed about Elsevier products and services

☐ I have read and agree to the [Registered User Agreement](#)

Register >

Privacy Policy Terms and Conditions

Search sub in Rec

Search Reaxys

Substance CAS Reg

286M
Substances

Activity data Import

Find >

7M
activities

Remote access Terms and Conditions Privacy po

We use cookies to help provide and enhance our service a

RELX™

Feedback

Reaxys 檢索介面導覽



進階檢索
(實驗量測數據檢索)

逆合成工具
預測複雜有機分子該如何合成

Reaxys®

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Stephanie Su

Search substances, reactions, documents and bioactivity data

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

Import

Search Reaxys

關鍵字檢索

Substance ADME, e.g. Pharmacokinetic of Imatinib

Find >

AND



Draw

化學結構檢索
(反應式、專利結構式)

Content Overview | Latest update: 21. September 2024 >

286M

Substances

67M

Reactions

116M

Documents

44M

Patents

47M

Bioactivities

多元搜尋指令

Search Reaxys

Reaxys 檢索介面導覽

Search Reaxys Caffeine	1,491 Substances Structure :  as drawn Edit in Query Builder  Create Alert  Preview Results  View Results 	實驗數值與 參考出處
Search Reaxys Caffeine preparation	153,661 Documents Structure :  as drawn Titles, Abstracts, Keywords : "Caffeine" Edit in Query Builder  Create Alert  Preview Results  View Results 	文獻、專利
Search Reaxys "adenosine a2a receptor"	47 Commercial Substances Structure :  as drawn Edit in Query Builder  Create Alert  Preview Results  View Results 	供應商資訊
Search Reaxys Caffeine preparation	420 Reactions Reaction Query :  as drawn Edit in Query Builder  Create Alert  Preview Results  View Results 	合成方法
Search Reaxys "adenosine a2a receptor"	83 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



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。

2,190 Documents with 4,317 Substances, 346 Reactions, 6 Targets

☐ 0 selected Limit To Exclude Export

Search Sort by Publication Year Bioactivity Visualization

☐ 1 Changes in plant diversity and community attributes of coal mine affected forest in relation to a community reserve forest of Nagaland, Northeast India [Cited 2 times](#)
[Semy, Khikeya; Singh, Maibam Romeo](#) [Tropical Ecology, 2024, vol. 65, # 1, p. 16 - 25]
Abstract Index Terms Full Text

Abstract hit: {...Ageratum conyzoides, Bidens pilosa and Drymaria cordata were prominently distributed in CMAF while...}

☐ 2 Phytoremediation of Heavy Metal Contaminated Soil Using Bidens pilosa: Effect of Varying Concentrations of Sophorolipids [Cited 3 times](#)
[Shah, Vijendra; Dani, Pooja; Davey, Achlesh](#) [Applied Biochemistry and Biotechnology, 2024, vol. 196, # 5, p. 2399 - 2413]
Abstract Index Terms Substances 1 Full Text

Abstract hit: {...soil using Bidens pilosa. The results showed that increasing concentrations of SL increased...}

Index Terms hit: {...Author keyword: Bidens pilosa, Biosurfactant...}

☐ 3 Effect and mechanism of Qing Gan Zi Shen decoction on heart damage induced by obesity and hypertension [Cited 3 times](#)
[Zhang, Shujie; Liu, Zitian; Zhang, Han; Zhou, Xiaonian; Wang, Xiuming; Chen, Yan; Miao, Xiaofan; Zhu, Yao; Jiang, Weimin](#) [Journal of Ethnopharmacology, 2024, vol. 319, art. no. 117163]
Abstract Index Terms Full Text

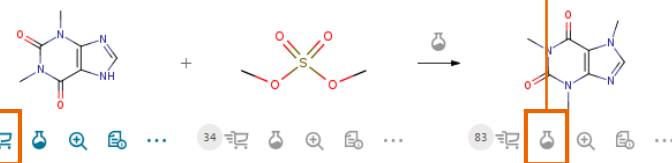
Index Terms hit: {...wheat germ agglutinin, Bidens pilosa extract, unclassified drug...}

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。

1



65

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 für praktische Chemie (Leipzig 1954), 1928, vol. <Z>118, p. 161] Full Text Details
With sodium hydroxide		Chmielewski; 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

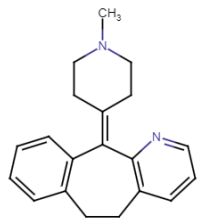


結構檢索

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

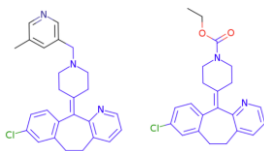
As drawn

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



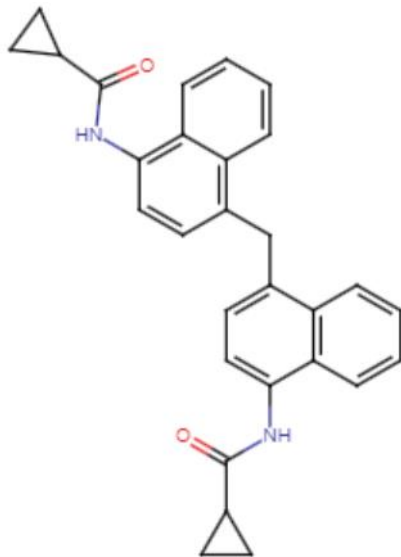
研究新的化合物，從已經發表的結構找線索，例如優化前導化合物 (lead compound)

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

Black-jack (鬼針草)

Plant ⓘ

Overview

Benefits



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

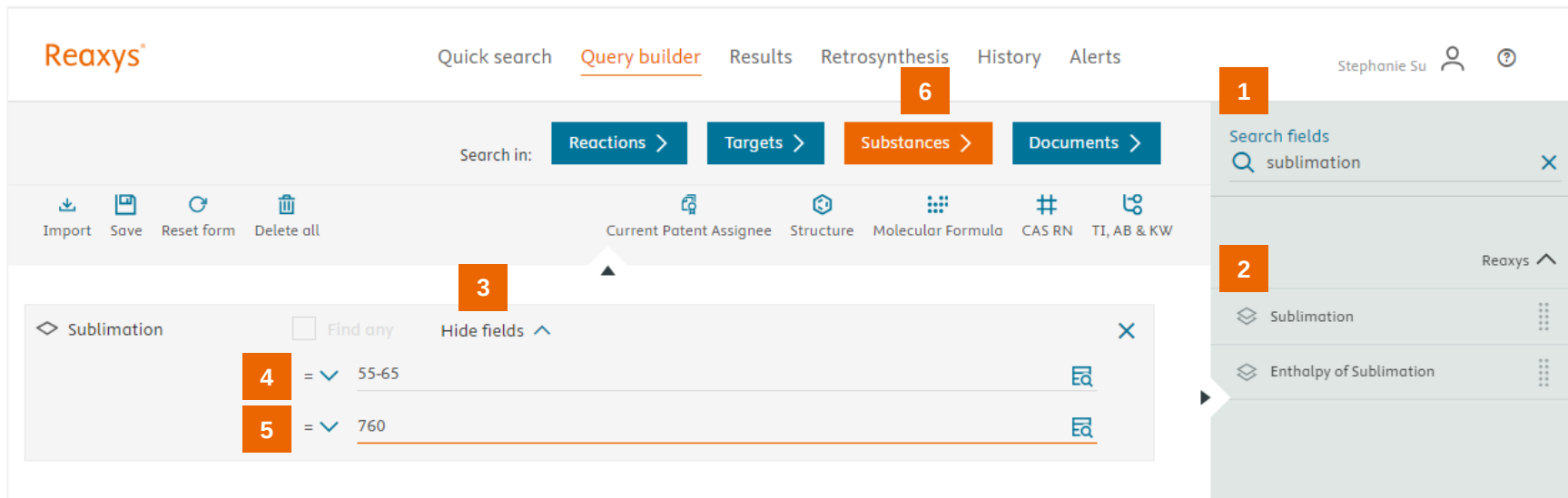
Inorganic Chemistry

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



The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (highlighted with orange), Results, Retrosynthesis, History, and Alerts. Below these are search filters: Reactions, Targets, Substances (highlighted with orange), and Documents. A search bar contains the text 'sublimation'. On the right, a sidebar shows search fields: Sublimation and Enthalpy of Sublimation. The main area displays a table with columns for Sublimation, Find any, and Hide fields. The table has two rows: one with '55-65' and another with '760'. The interface is annotated with numbered callouts: 1 points to the search bar, 2 points to the Sublimation field in the sidebar, 3 points to the 'Find any' checkbox, 4 points to the '55-65' input, 5 points to the '760' input, and 6 points to the 'Substances' filter.

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 >

Hit Data - 2

Sublimation - 2 hits out of 60

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] Full Text Cited 30 times Details Abstract
-78.514	760	Meyers, C. H.; Dusen, M. S. van[1933 , vol. 10, p. 381 - 412] Full Text Details No author[Gmelin Handbuch der Anorganischen Chemie , Gmelin Handbook: C: MVolC1, 151, page 363 - 365] Full Text Details

Show/Hide columns

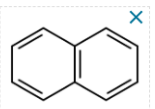
系統會將 Sublimation 資料標示於 Hit Data
>> 方便比較並列出文獻出處

Query builder: 實驗數據檢索

Filters

Limit to > Exclude >

By Structure


As drawn

Measurement pX

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Available Data

Document Type

Publication Year

Current Patent Assignee

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

0 selected Limit To Exclude Export Preparations

Search Sort by No of References Grid Bioactivity Visualization

1



carbon dioxide

OCO 44,0098 1900390 124-38-9

Hit Data - 2

Identification

Druglikeness

Bioactivity (All)

Physical Data - 27,313

Spectra - 867

Other Data - 960

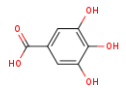
Preparations - 9,558

Reactions - 55,311

Targets - 53

Documents - 181,217

2



3,4,5-trihydroxybenzoic acid

C₆H₂(OH)₃COOH 170.122 2050274 149-91-7

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)

Physical Data - 702

Spectra - 910

Other Data - 1,617

Preparations - 294

Reactions - 2,604

Targets - 365

Documents - 35,099

Hit Data - 2

Sublimation - 2 hits out of 60

Hit Data - 1

Sublimation - 1 hits out of 3



藥物靶點與藥物設計

Drug Targets and Drug Design

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

[illegible]

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

Preview Results ▾

View Results >

Edit in Query Builder Create Alert



65,951

Substances

Target(s) : tyrosine-protein kinase jak3

Preview Results ▾

View Results >

Edit in Query Builder Create Alert



15,218

Documents

Titles, Abstracts, Keywords : "tyrosine-protein kinase jak3"

Preview Results ▾

View Results >

Edit in Query Builder Create Alert

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

105 Substances out of 3 Documents, containing 209 Reactions, 2 Targets

0 selected Limit To Exclude Export Preparations

Limit to > Exclude >

By Structure

Measurement pX 2

>12 - 13 2

>11 - 12 105

(no entry given) 105

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Available Data

Document Type

Publication Year

Current Patent Assignee

LogP

H Bond Donors

tasocitinib

C10H20N4O 312.374 11647225 Retrieve CAS RN

Identification Bioactivity (All) Other Data - 1,104

Druglikeness Physical Data - 33 Spectra - 39

Bioactivity (Hit Data)

Bioactivity (Hit Data)

In vitro: Efficacy - 1

Quantitative Results

pX	Parameter	Value (quant)	Unit	Target
11.1	IC50	7.308E-06	μM	Tyrosine-protein kinase JAK3 [human];Wild/Tyrosine-protein kinase JAK1 [human];Wild/Tyrosine-protein kinase JAK2 [human];Wild

Bioactivity Visualization Settings

Value of X-axis Targets

Value of Y-axis Substances

Value of Cells

Show substances

Display mode

Always show settings

Preparations - 105 >

Reactions - 314 >

Targets - 668 >

Documents - 1,863 >

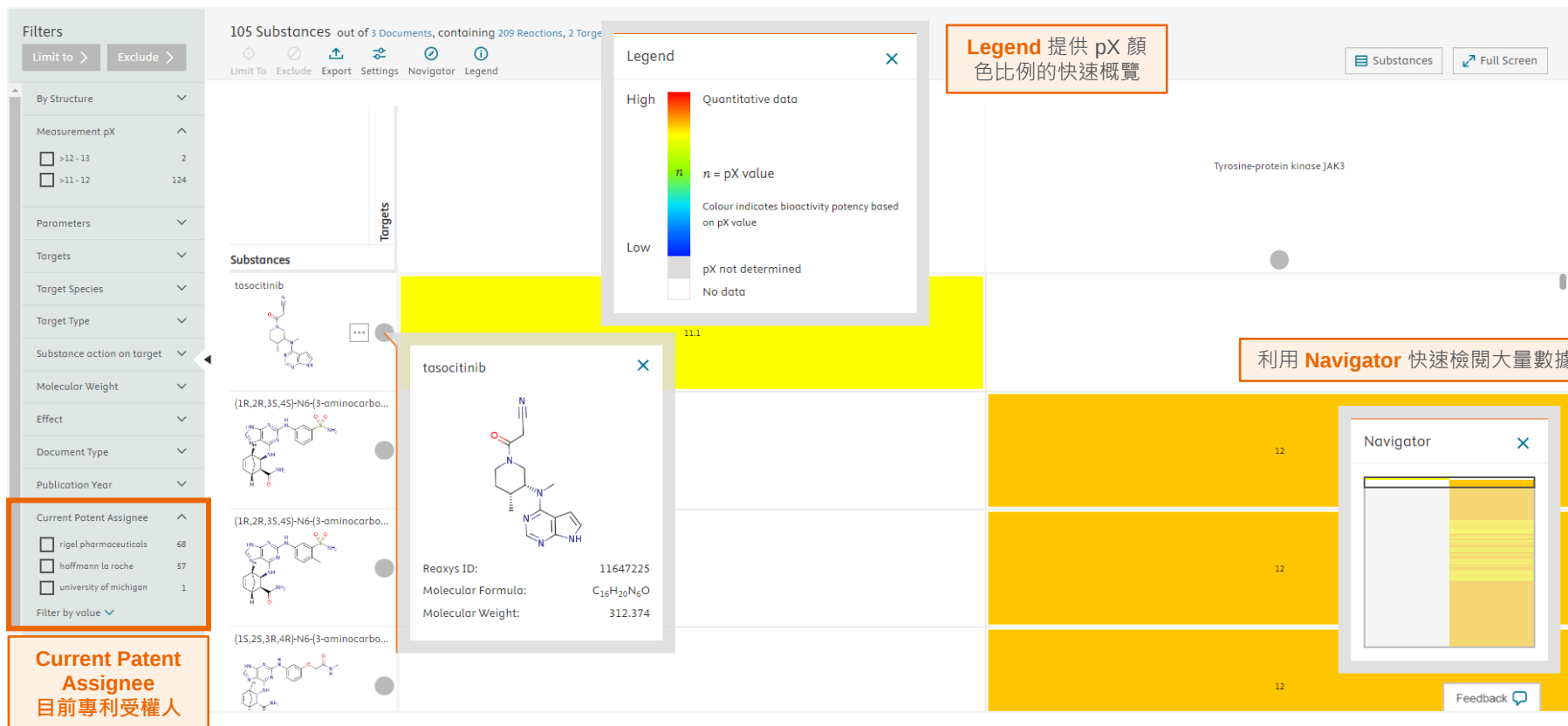
Preparations - 1 >

Reactions - 1 >

Targets - 10 >

Documents - 13 >

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

Reaxys® Quick search Query builder **Results** Retrosynthesis History Alerts Stephanie Su

105 Substances out of 3 Documents, containing 209 Reactions

Limit To Exclude Export Settings Navigator Legend

Filters

- By Structure
- Measurement pK
 - >12 - 13 2
 - >11 - 12 124
- Parameters
- Targets
- Target Species
- Target Type
- Substance action on target
- Molecular Weight
- Effect
- Document Type
- Publication Year
- Current Patent Assignee
 - rigel pharmaceuticals 68
 - hoffmann la roche 57
 - university of michigan 1
- Filter by value
- LogP
- H Bond Donors

Substances

tosocitinib

(1R,2R,3S,4S)-N6-(3-aminocarba...

(1R,2R,3S,4S)-N6-(3-aminocarba...

(1S,2S,3R,4R)-N6-(3-aminocarba...

Export substances and bioactivities

Choose a format:

- Microsoft Excel New Layout
- Microsoft Excel
- Tab-delimited text
- XML
- SD/Molfile

Range:

Export:

Additional options: ☒ Include structures

Disclaimer: please refer to our [Terms and Conditions](#) before downloading data.

Export

Tyrosine-protein kinase JAK3

Navigator



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)

Reaxys®

[Quick search](#)

[Query builder](#)

[Results](#)

[Retrosynthesis](#)

[History](#)

[Alerts](#)

Stephanie Su



Search substances, reactions, documents and bioactivity data

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

Import

Search Reaxys

Target Name, e.g. Polo-like kinase 1

Find >

AND



Draw

尋找單步驟的反應

Content Overview | Latest update: 01. October 2024 >

286M

Substances

67M

Reactions

116M

Documents

44M

Patents

47M

Bioactivities



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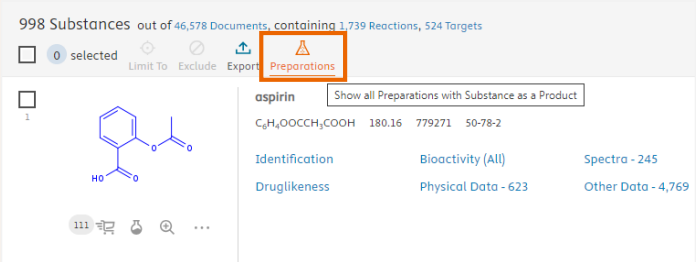
<https://www.reaxys.com/#/retrosynthesis>

RELX™

Feedback

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)



998 Substances out of 46,578 Documents, containing 1,739 Reactions, 524 Targets

0 selected Limit To Exclude Export Preparations

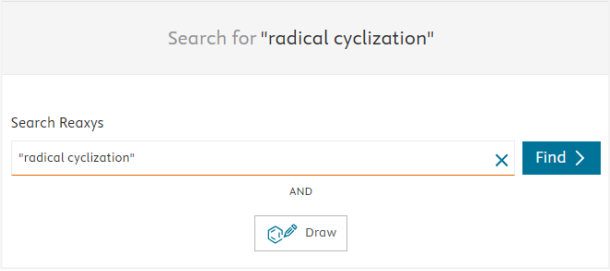
aspirin Show all Preparations with Substance as a Product

CC(=O)OC1=CC=CC=C1C(=O)O 180.16 779271 50-78-2

Identification Bioactivity (All) Spectra - 245

Druglikeness Physical Data - 623 Other Data - 4,769

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



Search for "radical cyclization"

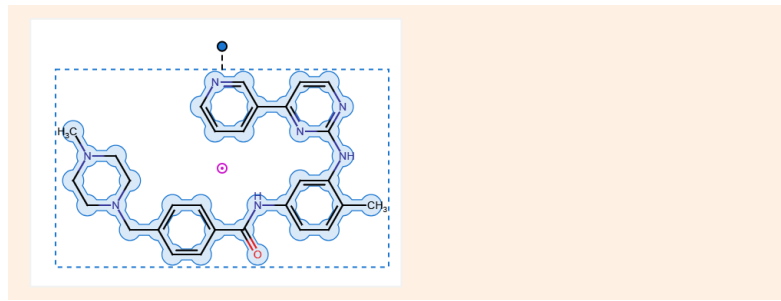
Search Reaxys

"radical cyclization" X Find >

AND

Draw

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

998 Substances out of 46,578 Documents, containing 1,739 Reactions, 524 Targets

Limit To Exclude Export Preparations

No of References ↓

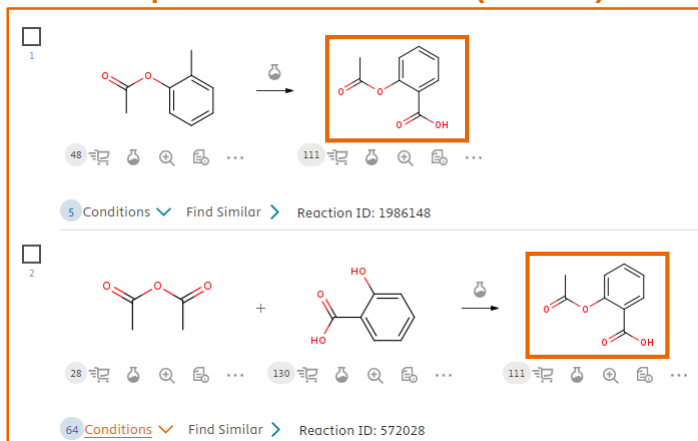
Grid Bioactivity Visualization

aspirin
CC(=O)Oc1ccccc1C(=O)O 180.16 779271 50-78-2

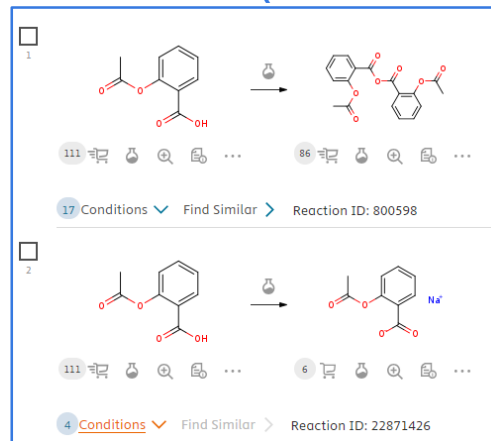
Identification Physical Data - 623
 Druglikeness Spectra - 245
 Bioactivity (All) Other Data - 4,769

Preparations - 109
 Reactions - 1,582
 Targets - 506
 Documents - 45,581

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

Search for "radical cyclization"

Search Reaxys

"radical cyclization" × Find >

AND

 Draw

Results for "radical cyclization"						New 	Edit 
	75	Reactions	Condition : radical cyclization	Preview Results 	View Results >		
			Edit in Query Builder 	Create Alert 			
	9,499	Documents	Titles, Abstracts, Keywords : "radical cyclization"	Preview Results 	View Results >		
			Edit in Query Builder 	Create Alert 			

尋找反應式的方法: 關鍵字檢索

Reaxys®

Quick searchQuery builder**Results**RetrosynthesisHistoryAlerts

Stephanie Su

75

Preview

Search

Filters

Limit to >Exclude >

By Structure >

Yield >

Reagent/Catalyst >

Solvent >

Catalyst Classes >

Solvent Classes >

Product Availability >

Reactant Availability >

Reaction Classes >

Document Type >

Publication Year >

☐ Single step reactions only

☐ Experimental procedure only

75 Reactions out of 86 Documents, containing 232 Substances, 44 Targets

☐ 0Limit ToExcludeExportHide Conditions

Reaxys Ranking >

1



1 Hits9 ConditionsFind Similar >Reaction ID: 8578406

Conditions	Yield	Reference
With 2,2'-azobis(isobutyronitrile); tri-n-butyl-tin hydride In toluene for 4h; Cyclization; radical cyclization; Heating;	68%	Orito, Kazuhiko; Uchiito, Shiho; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao [Organic Letters, 2000, vol. 2, # 3, p. 307 - 310] Full Text Cited 77 times Details Abstract >

2



40racemate

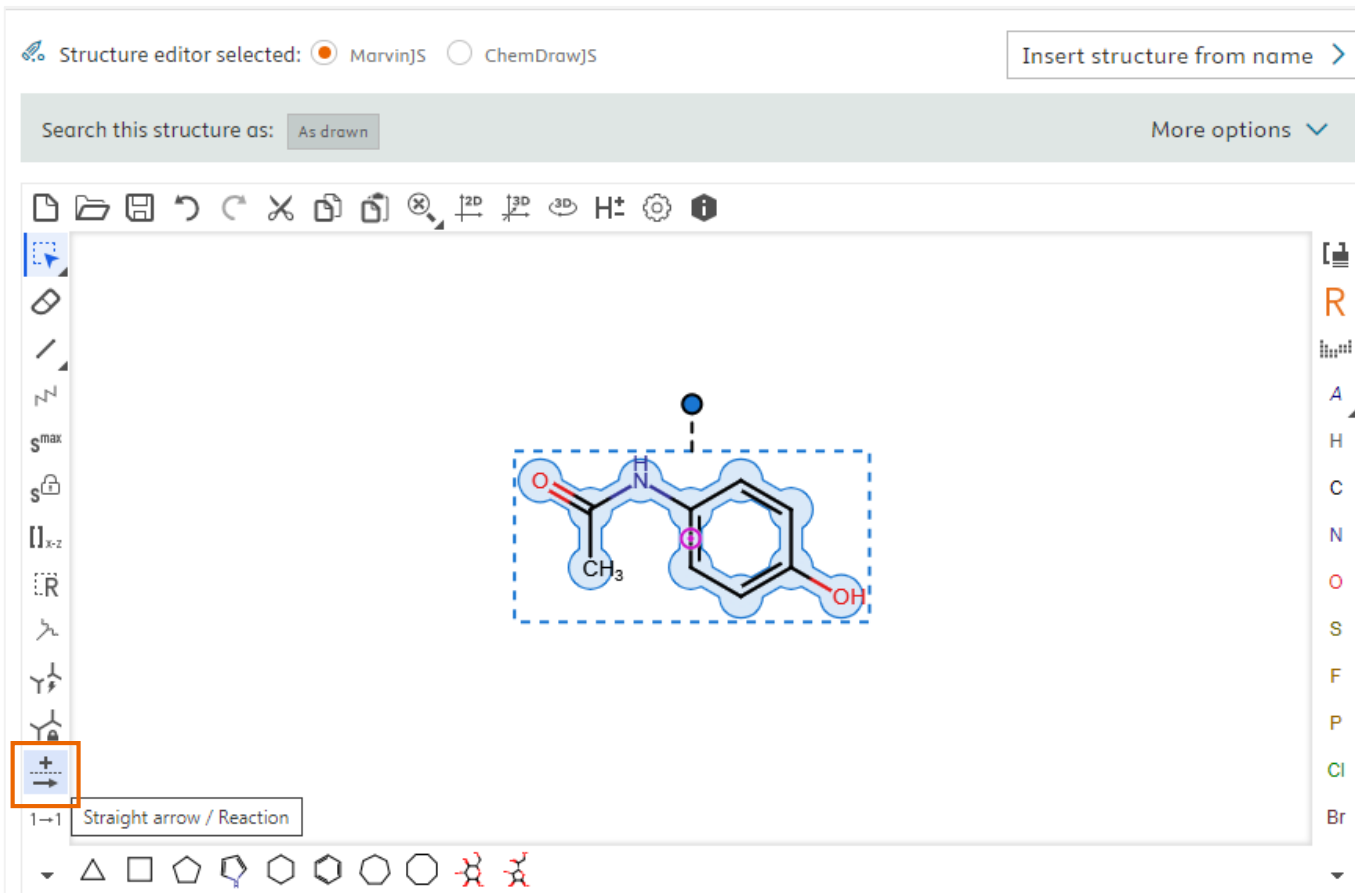
Feedback

尋找反應式的方法: 繪製反應式

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

Insert structure from name >

Search this structure as: As drawn More options ▾

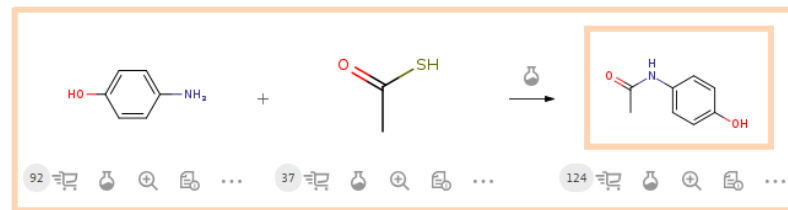
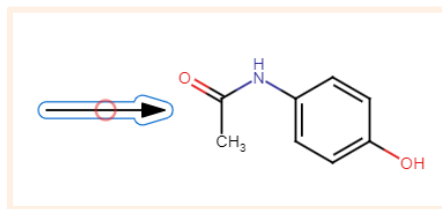


加入反應箭頭

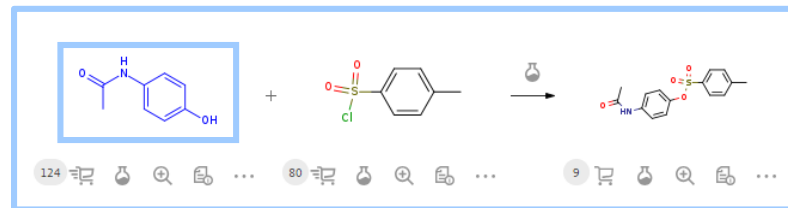
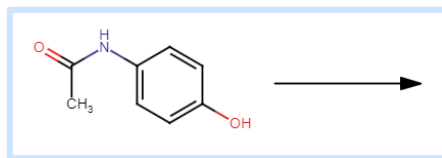
1→1 Straight arrow / Reaction

尋找反應式的方法：繪製反應式

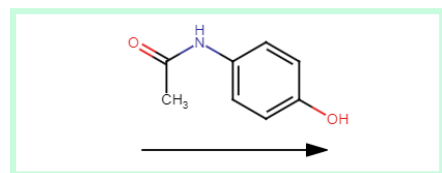
產物：箭頭在左



起始物：箭頭在右



催化劑或溶劑：箭頭在下



Conditions
With 4-acetaminophen; water; dihydrogen peroxide at 20°C; Green chemistry; Experimental Procedure ▼
With iron(III) oxide; dihydrogen peroxide In water at 20°C; for 0.0833333h; Experimental Procedure ▼

進階反應式檢索: 介面資訊

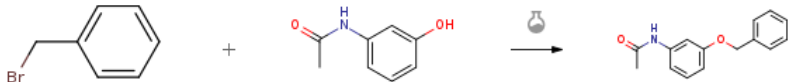
人工索引欄位

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

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



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.; Lichorowicz, Cynthia L.; Giarrusso, James; Blake, Lynn D.; Casandra, Debora; Mutka, Tina S.; LaCrue, Alexis N.; (...) Kyle, Dennis E.; Manetsch, Roman [Journal of Medicinal Chemistry, 2016, vol. 59, # 14, p. 6943 - 6960] Full Text Cited 22 times Details Abstract
Stage #1: 3-Hydroxyacetanilid With potassium carbonate In acetone at 20°C; for 0.5h; Inert atmosphere; Stage #2: benzyl bromide In acetone for 2h; Inert atmosphere; 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 [Molecules, 2021, vol. 26, # 3] Full Text Cited 6 times Details Abstract

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 and stirred for 2 h. After completion of the reaction, the solid was filtered off and the filtrate was concentrated under reduced pressure. The residue was dissolved in EtOAc (70 mL), washed with 2N HCl (2 x 15 mL), H₂O (2 x 20 mL) and brine (20 mL), dried over anhyd. Na₂SO₄ and concentrated in vacuo. The crude was purified by column chromatography (MeOH/CH₂Cl₂ = 1:19) to 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

	3,532	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	9,368	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 	Preview Results 	View Results 

將搜尋結果複製到進階搜尋 **Query Builder** 增加搜尋條件

進階反應式檢索: Query builder

Reaxys® Quick search Query builder Results Retrosynthesis History Alerts Stephanie Su

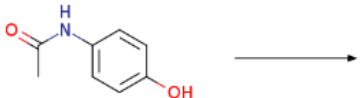
Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Current Patent Assignee Structure Molecular Formula CAS RN TI, AB & KW

Group 1 Ungroup

Structure



As drawn

Reaction Data & Conditions is microbiolog*

Search fields
reaction data

Reaction Data & Conditions

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

Reaxys®

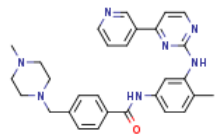
Quick search Query builder Results Retrosynthesis History Alerts

Stephanie Su

My Synthesis Projects

Draw

0 Delete

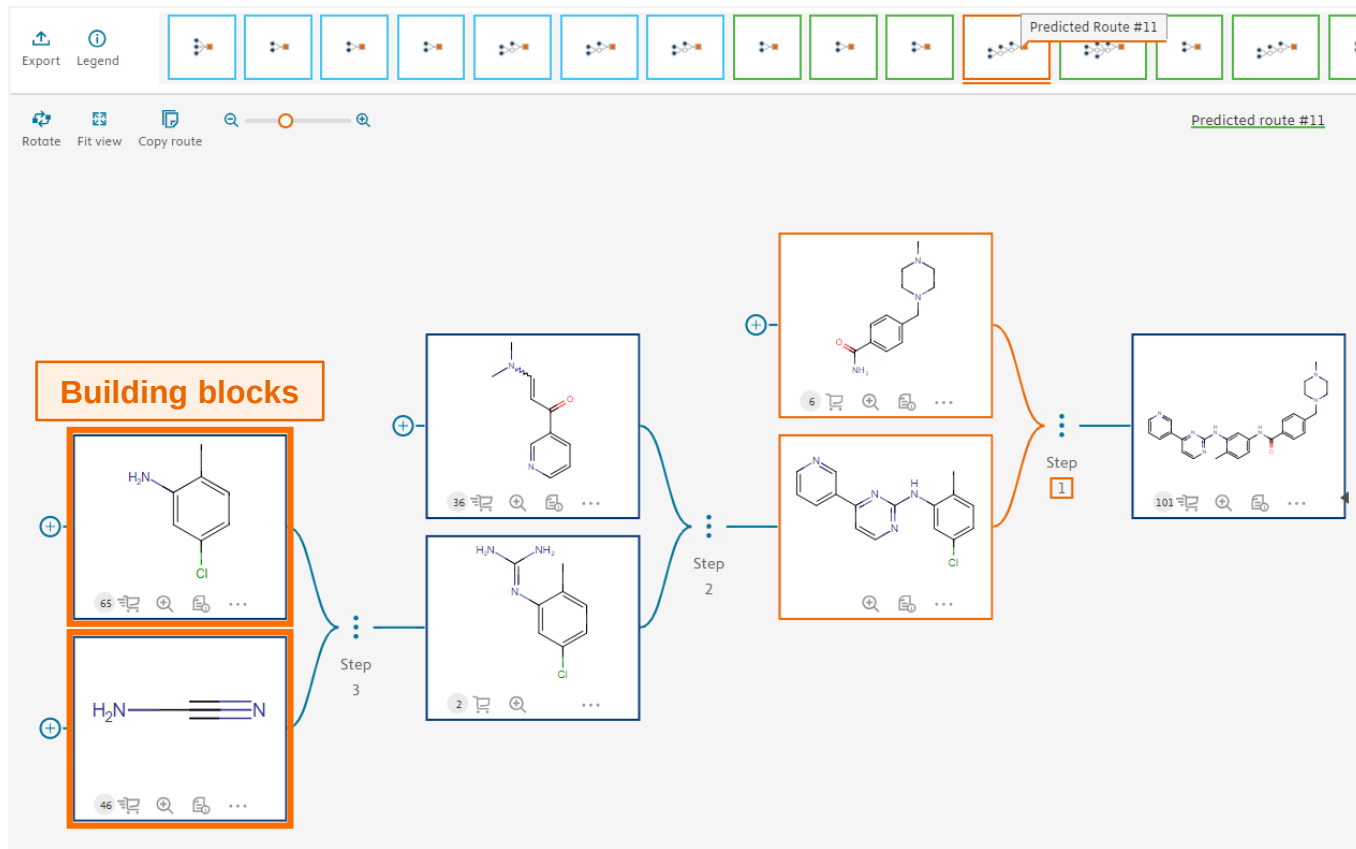
No.	Synthesis Date	Project name	No. of routes
Click to view a list of your retrosynthesis projects			
Draw Click to draw a target molecule for retrosynthesis			
☐	2307807	03 Oct 2024	Project #2307807
			Delete
			+ Draw new structure  101 Edit

Predicted 16

Published 7

View

Retrosynthesis: Paxlovid



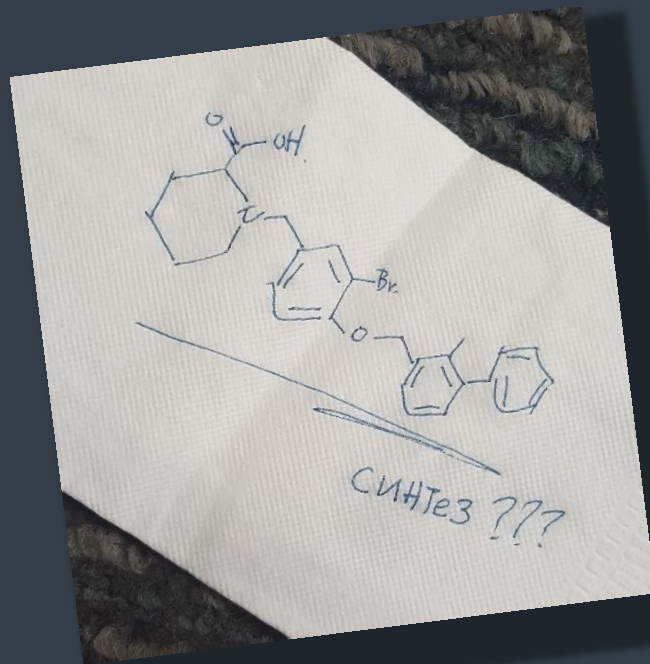
The screenshot displays the Reaxys Examples interface, showing a multi-step reaction route. The interface includes a top toolbar with icons for Export, Legend, and various view controls. A central workspace displays a reaction scheme with three steps. Step 1 involves the reaction of 4-chloroaniline with benzamide. Step 2 involves the reaction of the intermediate with 4-chloroaniline. Step 3 involves the reaction of the intermediate with 4-chloroaniline. A context menu is open over Step 2, showing options: Show Conditions/Reaxys Examples, Add reaction step (one step only), Delete prior step(s), and Copy reaction. The right sidebar shows the 'Predicted route #11' and a list of reaction examples, including the one shown in the workspace.



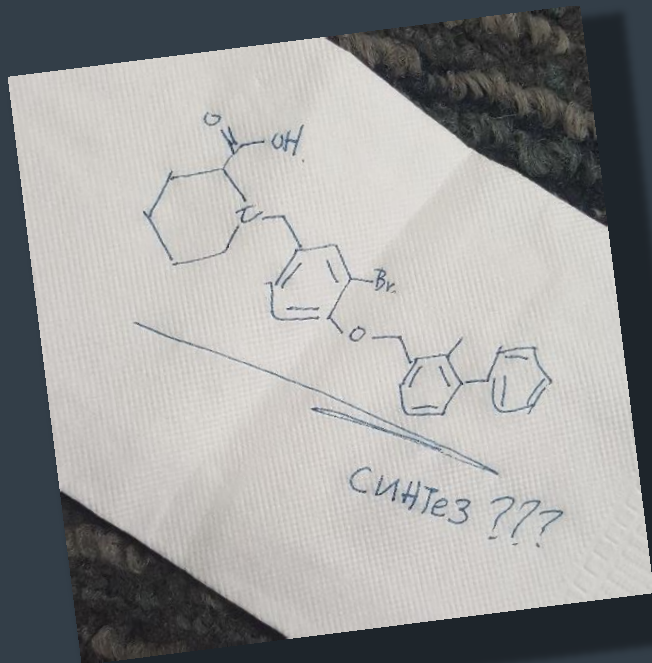
實際操作小遊戲

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



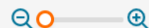
在餐巾紙上的化合物有哪些已知的應用方式：

- 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)

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

Reaxys - 1

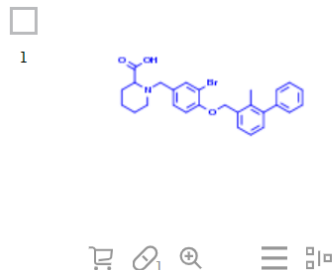
☐ 0 Limit To Exclude Export Preparations



No of References ↓

Grid

Heatmap



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

C₂₇H₂₈BrNO₃ 494.428 27956541

Identification

Druglikeness

Bioactivity (All)

Physical Data - 5

Spectra - 10

Preparations - 6

Reactions - 6

Targets - 2

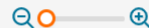
Documents - 4

答案: B

4 Documents with 535 Substances, 668 Reactions, 3 Targets

Reaxys - 4

☐ 0 Limit To Exclude Export



Publication Year ↓

Heatmap

Novel multitarget inhibitors with antiangiogenic and immunomodulator properties

Cited 2 times

- 1 [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 v Substances 56 v Reactions 110 v Targets v Full Text ↗

Hit Substances 1 v

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

Filters

Publication Year

Document Type

☐ patent 47

Authors/Inventors

Current Patent Assignee

Patent Office

Journal Title

Substance Classes

Reaction Classes

Index Terms (List)

Index Terms (ReaxysTree)

☐ Manually processed content only

47 Documents with 1,477 Substances, 767 Reactions, 3 Targets

☐ 0 selected

☐ 1

COMPOUNDS USEFUL AS IMMUNOMODULATORS

Current Patent Assignee: BRISTOL-MYERS SQUIBB CO - WO2015/34820, 2015, A1

Patent Family Members: AU2014315457 A1; AU2014315457 B2; BR112016004194 A8; BRPI1604194 A2; CA2923184 A1; ...

Abstract Index Terms Claims Bibliographic Info Substances 391 Reactions 423 Targets Full Text

Hit Substances 1

☐ 2

COMPOUNDS USEFUL AS IMMUNOMODULATORS

Current Patent Assignee: BRISTOL-MYERS SQUIBB CO - CA2923184, 2015, A1

Patent Family Members: AU2014315457 A1; AU2014315457 B2; BR112016004194 A8; BRPI1604194 A2; CA2923184 A1; ...

Abstract Index Terms Bibliographic Info Substances 260 Full Text

Hit Substances 1

☐ 3

Compounds useful as immunomodulators

Current Patent Assignee: BRISTOL-MYERS SQUIBB CO - CN105705489, 2016, A

Patent Family Members: AU2014315457 A1; AU2014315457 B2; BR112016004194 A8; BRPI1604194 A2; CA2923184 A1; ...

Abstract Index Terms Claims Bibliographic Info Substances 382 Full Text

Hit Substances 1

☐ 4

COMPOUNDS USEFUL AS IMMUNOMODULATORS

Current Patent Assignee: BRISTOL-MYERS SQUIBB CO - US2016/194307, 2016, A1

Patent Family Members: AU2014315457 A1; AU2014315457 B2; BR112016004194 A8; BRPI1604194 A2; CA2923184 A1; ...

Abstract Index Terms Claims Bibliographic Info Substances 401 Full Text

Hit Substances 1

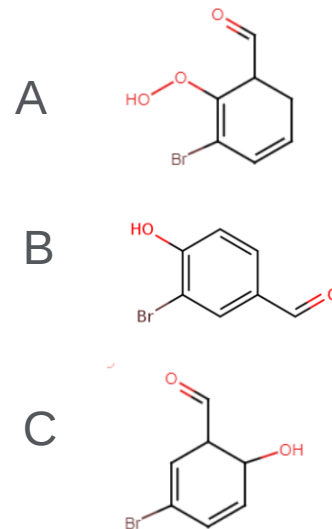
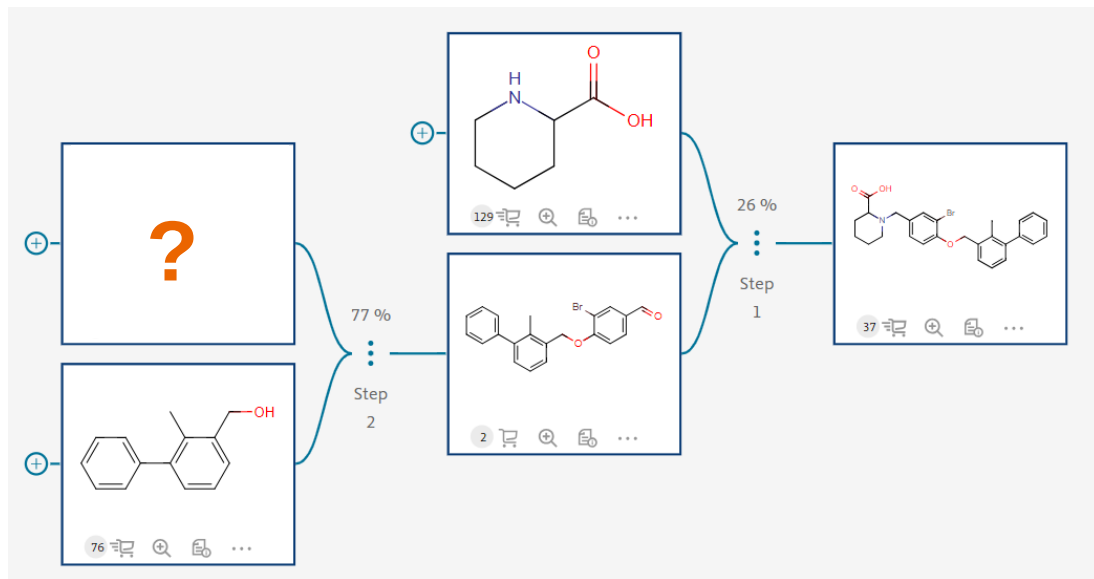
☐ 5

A compound useful as an immunomodulator

Current Patent Assignee: BRISTOL-MYERS SQUIBB CO - JP2016/536333, 2016, A

Patent Family Members: AU2014315457 A1; AU2014315457 B2; BR112016004194 A8; BRPI1604194 A2; CA2923184 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。



BMS-8

$C_{27}H_{28}BrNO_3$ 494.428 27956541  Retrieve CAS RN

Identification

Bioactivity (All)

Spectra - 12

Preparations - 8 >

Druglikeness

Physical Data - 6

Reactions - 20 >

Targets - 6 >

Documents - 79 >

37    ...



Synthesize



> Find preparations

> Create retrosynthesis plans

答案: B

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

Published route #1

Export Legend

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, Ricardo; 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	26%	Current Patent Assignee: UNIVERSITY OF GRONINGEN - WO2017/118762, 2017, A1 Location in patent: Page/Page column 44 Full Text  Details >
☐ Stage #1: 3-bromo-4-((2-methyl-1,1'-biphenyl)-3-ylmethoxy)benzoic acid; Dioxane		Current Patent Assignee: SOUTHERN MEDICAL UNIVERSITY  Feedback 



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。

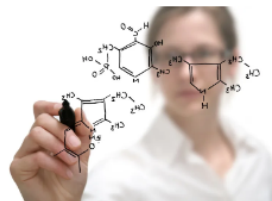


開始測驗

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。

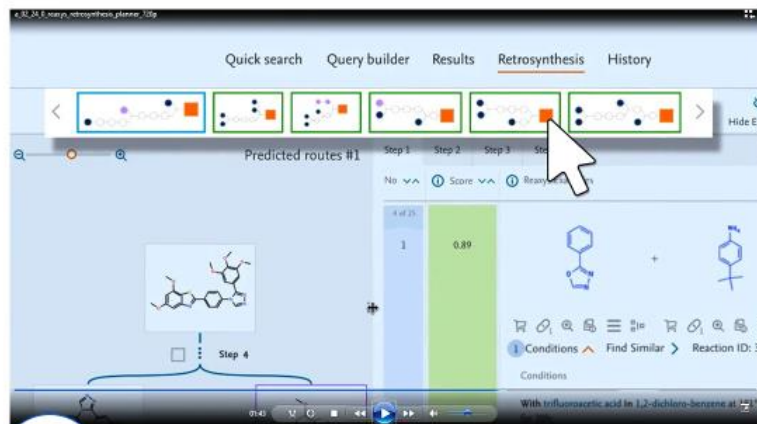


開始測驗

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。

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](#)

Reaxys®
Quick reference guide

[Bioactivity Visualization](#)

Reaxys® Medicinal Chemistry



Thank you

