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Reaxys

Smarter search in chemistry to save your valuable time

Ryan Huang 黃恪涵

Solution Sales Manger / Customer Consultant

Life Science Solutions – Elsevier

r.huang@elsevier.com



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Science & Technology Policy Research and Information Center





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OUR SHARED PURPOSE

TO ACCELERATE
SCIENCE TO
IMPROVE HEALTH

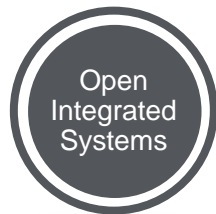
A Knowledge & Information
Analytics Company



OUR PROMISE

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

OUR KEY DIFFERENTIATORS



140+

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

RELX

\$1.4bn
on technology annually

~30,000
employees

Serving customers in
180+
countries

Partnering with

90%

of top Pharma
companies

Elsevier 於科學文獻中摘錄實驗數據，
提供新藥開發研發人員快速查詢整合資
訊，輔助形成關鍵決策

5 POST MARKET Comply with drug safety and pharmacovigilance regulations; Adverse events monitoring and reporting

Quosa™
Embase®

4 APPROVAL LAUNCH Optimize supply chain efficiency; Inform HEOR and Market Access strategies

PharmaPendium®

1

DISCOVERY - Pathways & Drug targets define
- Leads generation /Candidate optimization
- Patent FTO / Novelty research

Reaxys® Reaxys® Medicinal Chemistry

DISCOVERY

2

PRE-CLINICAL R&D Cull leads more quickly for safety & efficacy; Inform translational research

Reaxys® Medicinal Chemistry

PharmaPendium®

PRE-CLINICAL R&D

3

CLINICAL R&D Optimize clinical study design, primary endpoint for clinical trials

PharmaPendium®

CLINICAL R&D

APPROVAL LAUNCH

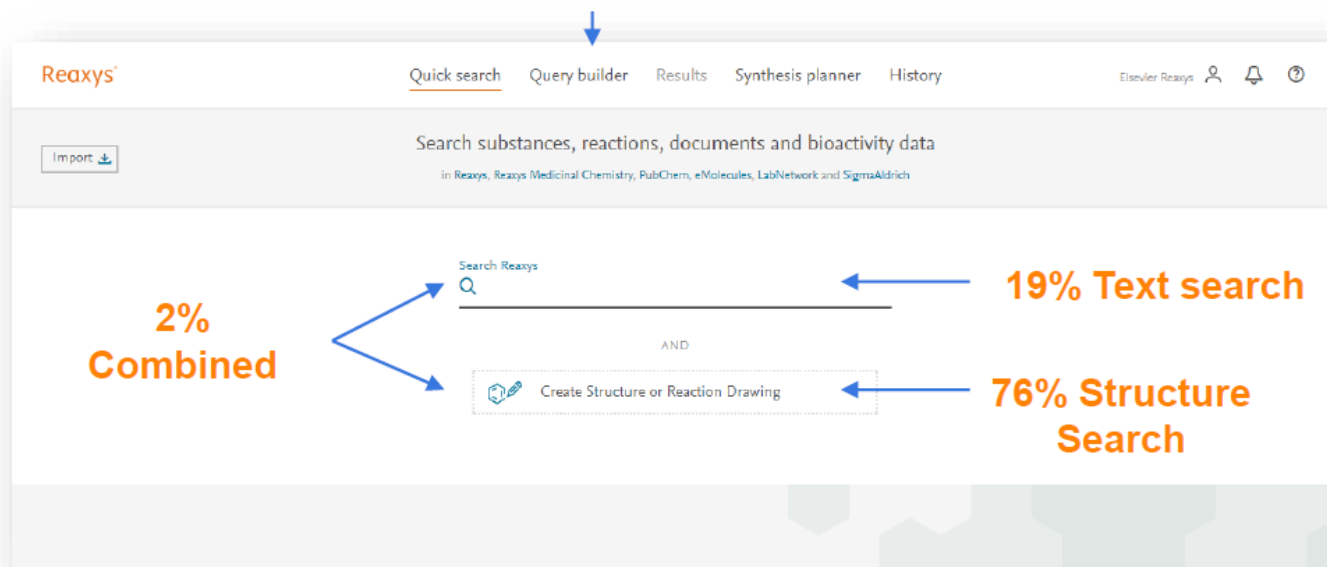
PHARMA LIFE CYCLE

POST MARKET

Reaxys提供四種搜尋介面協助研究人員快速取得可應用的實驗資訊

- 搜尋介面統計

3% Query Builder (進階使用者)

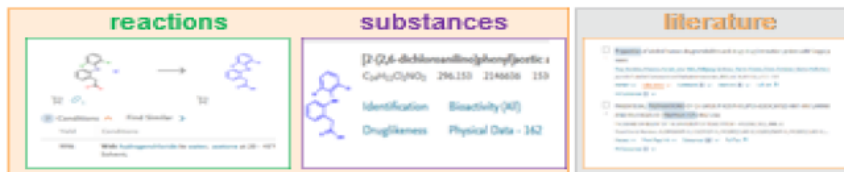


研究人員仰賴Reaxys提供實驗數據並直接應用於實驗中，而非花費大量時間搜尋、閱讀文獻

- 搜尋資料統計



實驗資料可直接進行應用



33%

61%

6%

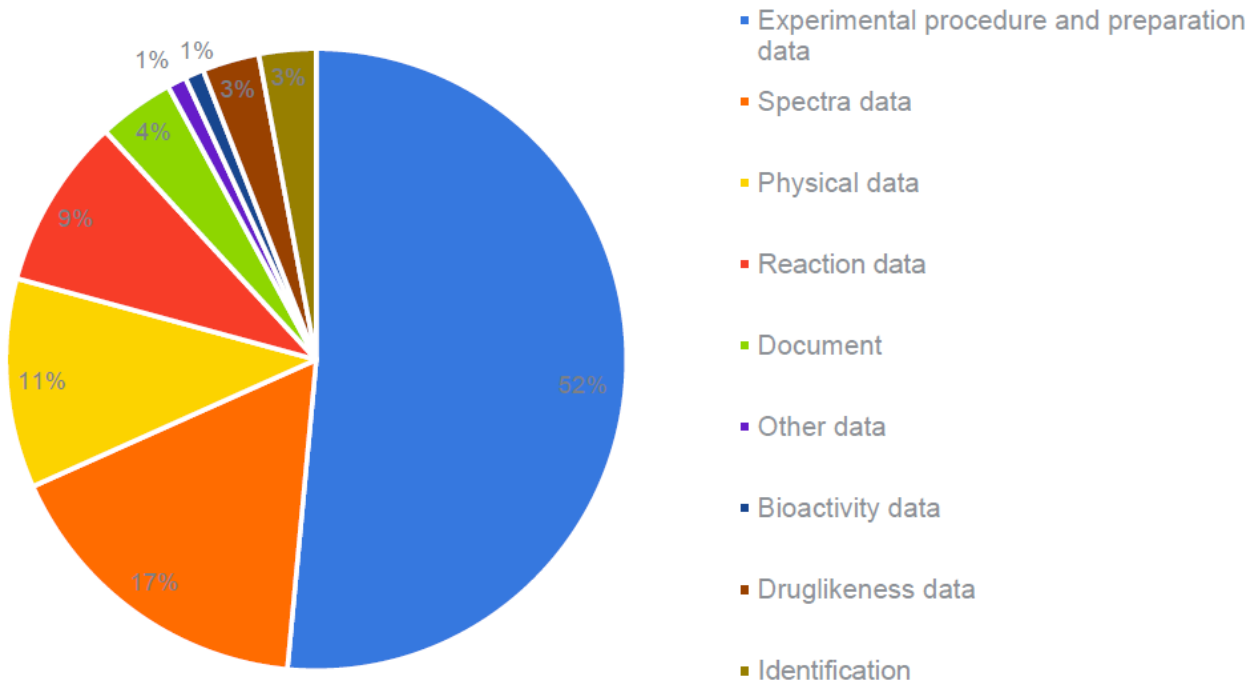
文獻資料仰賴人力閱讀

台灣大學使用者94%搜尋專注於實驗數據

Reaxys 提供各類型資料類型資料，讓研究員把時間花在研究本身

台灣大學前三大資料類型:

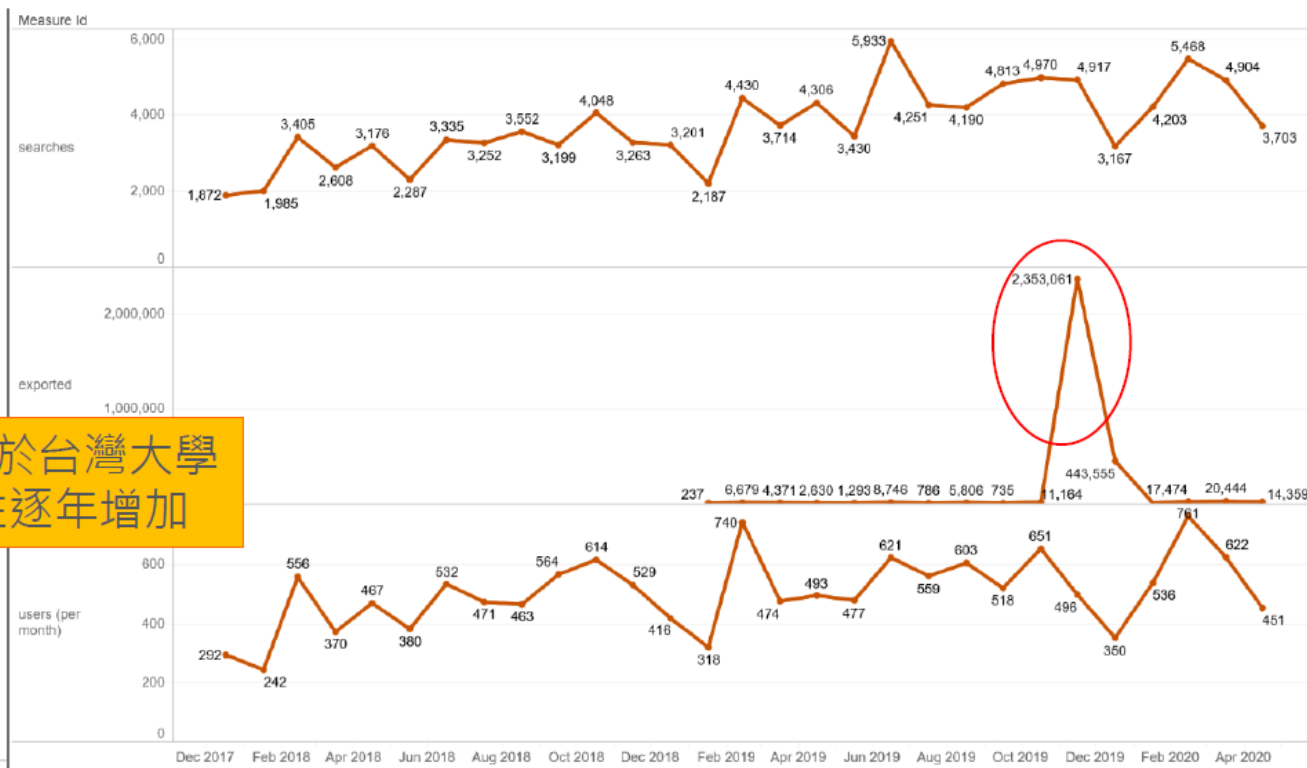
1. 化學反應材料與方法
2. 光譜資料
3. 物理性質



Total clicks = 64,675

以其他方式取得 (實驗材料與方法, 物質光譜, 物理性質等資料) 將需要更大量的時間、人力與金錢成本

使用人數、搜尋次數、與資料輸出趨勢 (2018.1-2020.5)



Reaxys對於台灣大學
的重要性逐年增加

如何連上Reaxys

在學校IP範圍內，打開瀏覽器鍵入 <http://reaxys.com>

Reaxys[®]

[Quick search](#)



[Query builder](#) ^{New}

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

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Search for 184475-35-2

Import 

Search Reaxys

184475-35-2

×

Find >


Documents, e.g. published by Schrock

AND

 Draw

Content Overview | Latest update: 11. September 2019 >


118M

 Substances


49M

 Reactions

59M

 Documents

37M

 Bioactivities

1.5M

 Targets

初次登入Reaxys – 註冊免費帳號的好處

Reaxys®

[Quick search](#)

[Query builder](#) ^{New}

[Results](#)

[Synthesis planner](#)

[History](#)

[Alerts](#)

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Search for 184475-35-2

Import

1. 點擊X跳過註冊視窗



Welcome to Reaxys

Ready to take the shortest path from chemistry question to relevant answer? Reaxys gives you the best means to explore the world of chemistry.

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Reduce timeouts

Customize structure editor settings and layout

No Thanks

Sign-in

Register

Register

登入帳號的好處：

- 更久的掛網時間
- 能夠匯出資料
- 儲存、管理搜尋結果
- 設定被動接收更新內容
- 客製化的搜尋偏好

2. 同意Cookies設置

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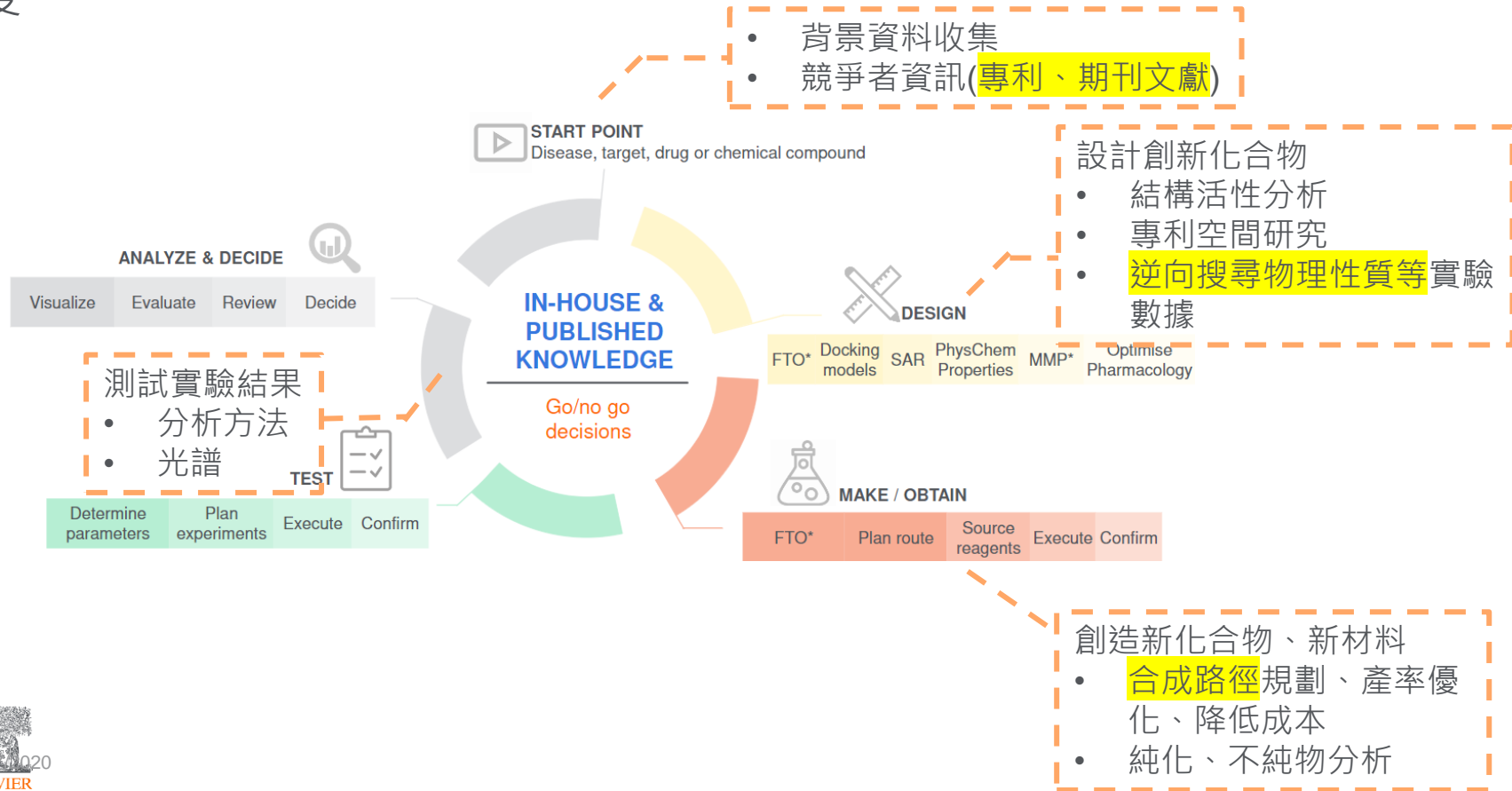
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Reaxys在研發階段提供關鍵資料，節省人力、時間成本，加速專案進度















範例1 請利用Quick search 欄位搜尋 “sglt2 inhibitor”

註 SGL2 (Sodium glucose co-transporters2) 與胰島素作用無關的新機轉第二型糖尿病藥物



搜尋預覽頁面

	4	Targets	Target(s) : sglT2 AND Action on Target : inhibitor Edit in Query Builder  Create Alert 	Preview Results 	View Results >
	2,774	Substances	Target(s) : sglT2 AND Action on Target : inhibitor Edit in Query Builder  Create Alert 	Preview Results 	View Results >
	6,916	Documents	Titles, Abstracts, Keywords : "sglt2", "inhibitor" Edit in Query Builder  Create Alert 	Preview Results 	View Results >

關鍵字搜尋 – 相關性排序 (Relevance ranking)

Reaxys® Quick search Query builder **Results** Synthesis planner History Register > Sign in

6.92 K Filters

Limit to > Exclude >

6,916 Documents with 40,676 Substances, 63,906 Reactions, 225 Targets

0 selected Limit To Exclude Export

Search 🔍 相關性排序 Heatmap

Sort search results ×

- Relevance ↑↓
- Publication Year
- Document Type
- Cited By

1 **Sergliflozin, a novel selective inhibitor of low-affinity sodium glucose cotransporter (SGLT2), validates the role of SGLT2 in renal glucose reabsorption and modulates plasma glucose level** Cited 225 times
Katsuno, Kenji; Fujimori, Yoshikazu; Takemura, Yukiko; Hiratochi, Masahiro; Itoh, Fumiaki; Komatsu, Yoshimitsu; Fujikura, Hideki; Isaji, Masayuki *Journal of Pharmacology and Experimental Therapeutics*, 2007, vol. 320, # 1, p. 323 - 330
Abstract Index Terms Substances (5) Targets Full Text

Abstract hit: {...low-affinity sodium glucose cotransporter (SGLT2), which is expressed specifically in the kidney...}

Index Terms hit: {...sodium glucose cotransporter 1, sodium glucose cotransporter 2, unclassified drug...}

2 **Renal glucose reabsorption inhibitors to treat diabetes** Cited 114 times
Bailey, Clifford J. [*Trends in Pharmacological Sciences*, 2011, vol. 32, # 2, p. 63 - 71]
Abstract Index Terms Substances (7) Full Text

Abstract hit: {...low-affinity sodium glucose cotransporter-2 (SGLT2) at the luminal surface of cells lining the...}

Index Terms hit: {...sodium glucose cotransporter 1, sodium glucose cotransporter 2, sodium glucose cotransporter 2 inhibitor...}

3 **Remogliflozin etabonate, in a novel category of selective low-affinity sodium glucose cotransporter (SGLT2) inhibitors, exhibits antidiabetic efficacy in rodent models** Cited 173 times
Fujimori, Yoshikazu; Katsuno, Kenji; Nakashima, Ikumi; Ishikawa-Takemura, Yukiko; Fujikura, Hideki; Isaji, Masayuki *Journal of Pharmacology and Experimental Therapeutics*, 2008, vol. 327, # 1, p. 268 - 276

Feedback

Filters:

- Index Terms (List)
- Index Terms (ReaxysTree)
- Publication Year
- Document Type
 - article 3,407
 - review 1,954
 - patent 533
 - note 318
 - editorial 256
 - letter 215
 - short survey 82
- Authors
- Patent Assignee
- Journal Title
- Substance Classes

View more

關鍵字搜尋 – 研究主題篩選器 (Index Terms)

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Quick search Query builder **Results** Synthesis planner History Alerts

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57.83 K
77.03 K
Preview

Filters 57,832

化學索引分類

- Limit 0 s
- Index Terms (List)
- Index Terms (ReaxysTree) 1
- Publication Year
- Document Type
- article 57,832
- Authors 2
- Patent Assignee
- Journal Title
- Substance Classes 3
- Reaction Classes

Index Terms (ReaxysTree) 453

- Index Terms (ReaxysTree) 6,916
 - chemical transformations 1,588
 - physico chemical properties 986
 - physico chemical analysis methods 561
 - separation method 189
 - substance clean up 28
 - crystallization 15
 - chromatography 10
 - liquid chromatography 6
 - high performance liquid chromatography 4
 - ultra high performance liquid chromatography 1
 - reversed phase HPLC 1
 - column chromatography 2

Publication Year Heatmap

Selected search items:

- thermal analysis
- microscopy
- crystal structure de...
- spectroscopical an...

Clear selected

Limit to >

Exclude >



關鍵字搜尋 – 期刊資訊 (全文索引詞index terms 快速了解文獻內容相關性)

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Quick search Query builder **Results** Synthesis planner History Alerts

Ryan Huang  

249
951
1.63 K
Preview

Filters

Limit to > Exclude >

Index Terms (List) v

Index Terms (ReaxysTree) v

Publication Year ^

2020 114

2019 135

Filter by value v




Document Type v




Authors v

Patent Assignee v

Journal Title v

Substance Classes v

0 selected    Limit To Exclude Export

  Sort by Relevance v Heatmap 

Abstract hit: {...corroded and crude oil played a role of inhibitor, thus it influenced the...} v


Index Terms hit: {...Corrosion products, Crude oil, X65 steel...} v

Evaluation of the localized corrosion resistance of 316 L austenitic and 430Ti ferritic stainless steel in aqueous chloride/sulphate media for application in petrochemical crude distillation units [Cited 2 times](#)

⁸ [Loto, Roland Tolulope; Loto, Cleophas Akintoye \[Materials Research Express, 2019, vol. 6, # 8, art. no. 086516\]](#)

[Abstract](#) v [Index Terms](#) ^ [Substances](#) 2 v [Full Text](#) ↗

Abstract hit: {...constituents of crude oil. Potentiodynamic polarization test, potentiostatic measurement, open circuit potential measurement...} v

Index Terms 

Author keyword: chloride, Corrosion, pitting, steel, sulfate

Engineering uncontrolled terms: chloride, Crude distillation units, Open circuit potential, Open circuit potential measurements, Potentiodynamic polarization tests, Potentiostatic measurements, sulfate, Surface deterioration

Engineering controlled terms: Austenite, Corrosion, Corrosion rate, Corrosion resistance, Crude oil, Deterioration, Distillation, Distillation equipment, Ferrite, Ferritic stainless steel, Morphology, Passivation, Petrochemicals, Pitting, Polarization, Sodium chloride, Steel, Steel corrosion, Sulfur compounds, Surface resistance, Titanium alloys

Reaxys Index Terms: Petroleum refining, chemical passivation, corrosion resistance, electrooxidation, open circuit potential



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關鍵字搜尋 – 篩選專利文件 (2020預計專利擴增>100 patent offices)

Reaxys®

Quick search Query builder **Results** Synthesis planner History

Register >

Sign in ?

3按下Limit to

7.45 K

Preview

Filters

Limit to >

Exclude >

0 selected

Limit To

Exclude

Export

🔍

🔍

Sort by Publication Year ↓

Heatmap

Index Terms (List) ↓

Index Terms (ReaxysTree)

Publication Year ↓

Document Type 1 ↑

article 3,691

review 2,059

patent 589

note 2

editorial

letter

short survey 87

[View more](#)

7,450 Documents with 42,560 Substances, 67,698 Reactions, 228 Targets

1點選Document Type篩選器

National Trends in Diabetes Medication Use in the United States: 2008 to 2015

[Cited 2 times](#)

[Practice](#), 2020, vol. 33, # 4, p. 433 - 442]

Full Text ↗

Abstract hit: {...glucose transporter-2 (SGLT2) inhibitors from 0.8% in 2014 (the first SGLT2 inhibitors approval...)} ↓

Index Terms hit: {...metformin, sodium glucose cotransporter 2 inhibitor, sulfonylurea...} ↓

Empagliflozin for the Treatment of Nonalcoholic Steatohepatitis in Patients with Type 2 Diabetes Mellitus

[Cited 12 times](#)

[Lai, Lee-Lee; Vethakkan, Shireene Ratna; Nik Mustapha, Nik Raihan; Mahadeva, Sanjiv; Chan, Wah-Kheong](#) [[Digestive Diseases and Sciences](#), 2020, vol. 65, # 2, p. 623 - 631]

Abstract ↓ Index Terms ↓ Substances 2 ↓ Full Text ↗

Abstract hit: {...Aims: Sodium-glucose cotransporter-2 (SGLT2) inhibitors are a novel class of drugs that lower...} ↓

2選擇Patent



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關鍵字搜尋 – 人工擷取(摘要、專利要求、專利家族、分類號、物質、反應及全文連結)

Filters

Limit to > Exclude >

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

Document Type ▾

Authors ▾

Patent Assignee ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

533 Documents with 33,409 Substances, 45,769 Reactions, 145 Targets

0 selected Limit To Exclude Export Search Sort by Relevance Heatmap

SGLT2 INHIBITORS FOR THE TREATMENT OF NEUTROPENIA

1 UNIVERSITÉ CATHOLIQUE DE LOUVAIN; VEIGA DA CUNHA, Maria; VAN SCHAFFINGEN, Emile; BOMMER, Guido - WO2019/202149, 2019, A1

Patent Family Members: WO2019/202149 A1

[Abstract](#) ▾ [Claims](#) ▾ [Front Page Info](#) ▾ [Substances](#) 6 ▾ [Targets](#) ▾ [Full Text](#) ↗

Abstract hit: {...of a SGLT2 (sodium glucose cotransporter 2) inhibitor for the treatment of neutropenia,...} ▾

Claims hit: {...CLAIMS1. A SGLT2 (sodium glucose cotransporter 2) inhibitor for use in the treatment...} ▾

A sodium - glucose cotransporter 2 inhibitor and use thereof (by machine translation)

2 Chongqing University of Technology; Yin Fei; Liu Jianhui; Liu Min; Wang Lujing; Li Xingan; Wu Yucui - CN109456370, 2019, A

Patent Family Members: CN109456370 A

[Abstract](#) ▾ [Claims](#) ▾ [Front Page Info](#) ▾ [Full Text](#) ↗

Abstract hit: {...- glucose cotransporter 2 inhibitor, the inhibitor three glucoside, the specific structure represented...} ▾

Claims hit: {...- glucose cotransporter 2 inhibitor, the inhibitor as three glucoside, its concrete structure...} ▾

A retinal therapeutic agent (by machine translation)

3 Carna Health Support; Inoguchi, Toyoshi; Maeda, Yasutaka; Maki, Toshinobu; Sonoda, Noriyuki - JP2019/112472, 2019, A

Patent Family Members: JP2019/112472 A

Feedback

關鍵字搜尋 – 競爭者分析

Reaxys®

Quick search Query builder Results Synthesis planner History

Register >

Sign in ⓘ

3 按下 Limit to

Filters

7,450 Documents with 42,560 Substances, 67,698 Reactions, 228 Targets

Limit to >

Exclude >

0 selected Limit To Exclude Export

Sort by Publication Year ↓ Heatmap

- note 355
- editorial 277
- letter 227
- short survey 87

View more

Authors

Patent Assignee

- bristol-myers squibb company 39
- boehringer ingelheim intern... 37
- wagner, michael 33
- haack, torsten 33
- evers, andreas 33
- kissei pharmaceutical co, ltd 32
- sanofi 28

Filter by value View more

Journal Title

1 點選 Patent Assignee 篩選器

2 選擇競爭者公司

National Trends in Diabetes Medication Use in the United States: 2008 to 2015 Cited 2 times

1 Raval, Amit D.; Vyas, Ami [Journal of Pharmacy Practice, 2020, vol. 33, # 4, p. 433 - 442]

Abstract Index Terms Substances 4 Full Text

Abstract hit: {...glucose transporter-2 (SGLT2) inhibitors from 0.8% in 2014 (the first SGLT2 inhibitors approval...)}

...medium glucose cotransporter 2 inhibitor, sulfonyleurea...}

Empagliflozin for the Treatment of Nonalcoholic Steatohepatitis in Patients with Type 2 Diabetes Mellitus Cited 12 times

2 Lai, Lee-Lee; Vethakkan, Shireene Ratna; Nik Mustapha, Nik Raihan; Mahadeva, Sanjiv; Chan, Wah-Kheong [Digestive Diseases and Sciences, 2020, vol. 65, # 2, p. 623 - 631]

Abstract Index Terms Substances 2 Full Text

Abstract hit: {...sodium-glucose cotransporter-2 (SGLT2) inhibitors are a novel class of drugs that lower...}

Index Terms hit: {...NASH, SGLT2, Sodium-glucose cotransporter-2...}













Therapeutic Role of Fibroblast Growth Factor 21 (FGF21) in the Amelioration of Chronic Diseases

3 Opoku, Yeboah Kwaku; Liu, Zhihang; Afrifa, Justice; Khoso, Mir Hassan; Ren, Guiping; Li, Deshan [International Journal of Peptide Research

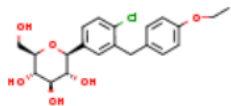


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搜尋預覽頁面

	4	Targets	Target(s) : sglT2 AND Action on Target : inhibitor Edit in Query Builder  Create Alert 	Preview Results 	View Results >
	2,774	Substances	Target(s) : sglT2 AND Action on Target : inhibitor Edit in Query Builder  Create Alert 	Preview Results 	View Results >
	6,916	Documents	Titles, Abstracts, Keywords : "sglt2", "inhibitor" Edit in Query Builder  Create Alert 	Preview Results 	View Results >

Reaxys資料結構-十大類資訊



dapagliflozin

C₂₁H₂₅ClO₆ 408.879 11966426 461432-26-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 53

Spectra - 57

物理性質

光譜

Other Data - 351

合成方法

製備反應

所有反應

Preparations - 85 >

Reactions - 403 >

Targets - 24 >

Documents - 220 >

期刊文獻、專利文件



供
應
商
資
訊

逆合成計畫推導快速鍵

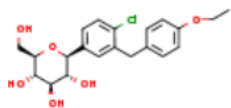
RMC 藥物化學模組

類藥性數據

生物活性

生物靶點蛋白

Reaxys資料結構-十大類資訊



dapagliflozin

C₂₁H₂₅ClO₆ 408.879 11966426 461432-26-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 53

Spectra - 57

Other Data - 351

其他資料

化合物用途
天然萃取化合物
環境暴露/汙染
生物降解

Preparations - 85 >

Reactions - 403 >

Targets - 24 >

Documents - 220 >



> [View related Markush](#)

專利式空間檢索

分子量/分子式
CAS號 /Reaxys號
專利出處
專利相關名稱
純化方法

問題2 請找出

治療C型肝炎病毒口服藥

Sofosbuvir

相關專利資料，最早由那家公司
申請了專利？

- A. GILEAD SCIENCES
- B. ELIAN LLC
- C. PHARMASSET, INC.
- D. Favilavir



結構搜尋 – MarvinJS 結構編輯器

中文自我學習資源
(2020)



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Quick search Query builder Results Synthesis planner History Alerts

Ryan Huang

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >



基本工具、鍵結工具

原子鎖
重複基團,
R基團,
R基團連結端,
反應定義工具



常見的環、醜

元素週期表以及常用原子

A:
原子屬性
定義工具



Search this structure as:

- As drawn
- As substructure
- Similar

特定結構
衍生結構
相似結構

- Tautomers
- Stereo
- Additional ring closures

Related Markush

專利式搜尋

- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

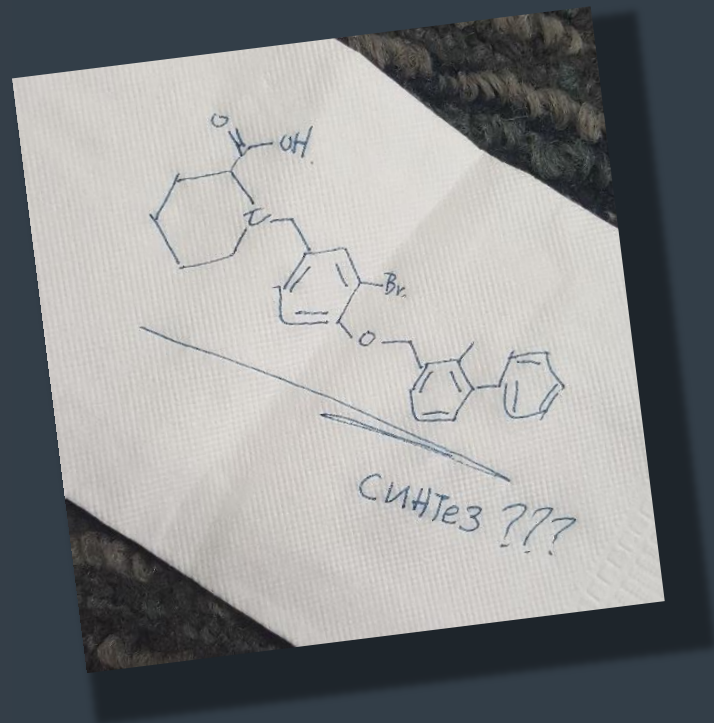
Clear Cancel Transfer to query >

Feedback

問題3 昏暗的酒館與神秘的科學家

一個身穿實驗衣的科學家醉醺醺的從你身邊踉蹌的走出酒吧，地上遺落了一張明顯是他遺落的餐巾紙，上面似乎寫了甚麼？

你拾起並追出門口，卻已不見科學家人影，你突然想到似乎可以用Reaxys查查有沒有更多的線索？



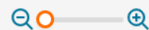
請問該物質已知用途是？

- A. 航太研發部的耐高溫塗料 B. 醫藥研發部的抗癌藥物 C. 健康食品研發部的新抗氧化萃取物 D. 犯罪調查科的新毒品跡證

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

Reaxys - 1

0 Limit To Exclude Export Preparations



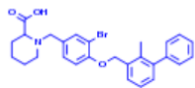
No of References ↓

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

Druglikeness

Bioactivity (All)

Physical Data - 5

Spectra - 10

Preparations - 6 >

Reactions - 6 >

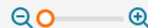
Targets - 2 >

Documents - 4 >

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](#) [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

Case2: 如何利用Reaxys/RMC快速篩選對”冠狀病毒”有活性的化合物

- 獲取文獻中報導對”RNA dependent RNA Polymerase” 有活性報導的化合物
- 希望化合物的IC50在 μM 級別

The screenshot displays the Reaxys Query Builder interface. The top navigation bar includes "Quick search", "Query builder" (highlighted), "Results", "Synthesis planner", "History", and "Alerts". The user "Ryan Huang" is logged in. The search criteria are defined as follows:

- Search in: **Substances** (highlighted)
- Target Name: is rdrp
- Group 1 (AND):
 - Measurement pX: \geq 6
 - Measurement Parameter: contains IC50

On the right, the "Search fields" dropdown is open, showing "measurement" selected. Below it, "Measurement pX" and "Measurement Parameter" are listed as available fields.

利用Query Builder組合
想要的搜尋條件

1. 靶點
2. 參數 (IC50)
3. 參數範圍 (低於 μM)

Reaxys中的結果

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Alerts Ryan Huang

1,21 K Query

Filters

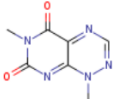


Limit to > Exclude >

0 selected Limit To Exclude Export Preparations

Sort by No of References ↓

Grid Heatmap

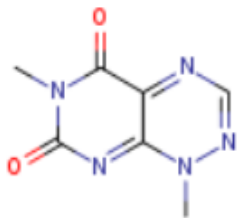
1,205 Substances out of 34 Documents, containing 2,897 Reactions, 6 Targets

<input type="checkbox"/>		toxflovin C ₇ H ₇ N ₅ O ₂ 193.165 21014 84-82-2	Identification	Bioactivity (All)	Other Data - 3	Preparations - 19 >
			Druglikeness	Physical Data - 22		Reactions - 23 >
			Bioactivity (Hit Data)	Spectra - 29		Targets - 27 >
						Documents - 136 >
<input type="checkbox"/>		3'-deoxycytidine C ₉ H ₁₃ N ₃ O ₄ 227.22 616742 7057-33-2	Identification	Bioactivity (Hit Data)	Physical Data - 15	Preparations - 54 >
			Druglikeness	Bioactivity (All)	Spectra - 31	Reactions - 92 >
						Targets - 10 >
						Documents - 44 >
<input type="checkbox"/>		3'-deoxyguanosine C ₁₀ H ₁₃ N ₅ O ₄ 267.244 561508 3608-58-0				

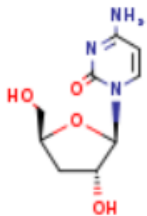
Feedback

Reaxys直接
給出符合條件的化合物，
大量節省閱讀“34篇”文獻，
查找數據的時間，
點擊Hit Data查看
數據出處

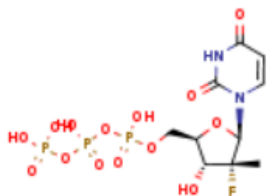
Reaxys中的結果



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	Reference
6.22	IC50	=	0.6	μM	Hepatitis C virus	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Other compound: ATP; Radioligand: [3H]UTP;	Middleton; Lim; Montgomery; Rockway; Liu; Klein; Qin; Harlan; Kati; Molla [Letters in drug design and discovery , 2007, vol. 4, # 1, p. 1 - 8] Full Text ↗ Cited 3 times ↗ Details > Abstract >



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	Reference
7.1	IC50		0.08 - 1.2	μM	Hepatitis C virus		RNA-dependent RNA polymerase [Hepatitis C virus]:Wild			Mayhoub, Abdelrahman S. [Bioorganic and Medicinal Chemistry , 2012, vol. 20, # 10, p. 3150 - 3161] Full Text ↗ Cited 35 times ↗ Details > Abstract >



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	1...	Reference
7.1	IC50		0.079	μM	Hepatitis C virus subtype 1b	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild				Alexandre, François-René; Badaroux, Eric; Bilello, John I Bot, Stéphanie; Bouisset, Tony; Brandt, Guillaume; Cappelle, Sylvie; (...) Surleraux, Dominique; Dousson, Cyril B. [Bioorganic and Medicinal Chemistry Letters , 2017, vol. 27, # 18, p. 4323 - 4330] Full Text ↗ Cited 11 times ↗ Details > Abstract >

利用Heatmap看結構與靶點關係

Reaxys Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

1,205 Substances out of 34 Documents, containing 2,897 Reactions, 6 Targets

selected Limit To Exclude Export Preparations

Sort by No of References Grid Heatmap

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases Available Data Document Type Publication Year

toxoflavin
C7H7N3O2 193.165 21014 84-82-2

Identification Bioactivity (All) Other Data - 3 Preparations - 19 >
Druglikeness Physical Data - 22 Reactions - 23 >
Bioactivity (Hit Data) Spectra - 29 Targets - 27 >
Documents - 136 >

3'-deoxycytidine
C8H13N3O4 227.22 616742 7057-33-2

Identification Bioactivity (Hit Data) Physical Data - 15 Preparations - 54 >
Druglikeness Bioactivity (All) Spectra - 31 Reactions - 92 >
Targets - 10 >
Documents - 44 >

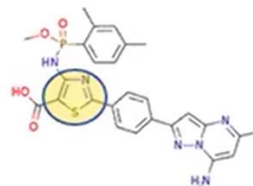
3'-deoxyguanosine
C10H13N4O4 267.244 561508 3608-58-0



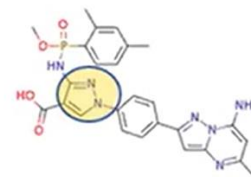
利用Reaxys中的Heat Map，直接觀察結構、靶點、活性數據之間的關係，並且可以把活性從高排到低

找出有意思的結構

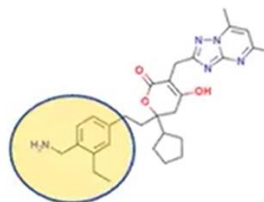
		Targets
		RNA-dependent RNA polymerase
		...
		●
Substances (i)		
5-thiazolecar... ylamine]	●	9.5
(E)-N-(4-(3-t... fonamide	●	9.5
IDX17119	●	9.4
20673525	●	9.3
5-thiazolecarb...l-amine]	●	9.1
20673509	●	9.1
20673487	●	9.1
29885944	●	9
27259279	●	9
6-cyclopentyl...an-2-one	●	9
(6R)-6-cyclop...an-2-one	●	9
6-cyclopentyl...an-2-one ...	●	9



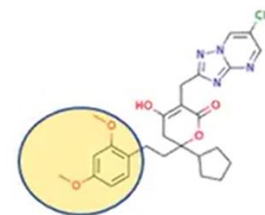
PX=9.5



PX=9.4



PX=8.0



PX=7.7

進階搜尋(Advanced search)

- 結合結構、實驗資料、關鍵字或任何你想搜尋的欄位

Reaxys

Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

搜尋要件蒐尋器

Find search fields and forms

Fields Forms History

Reaxys ^

Topics and Keywords

Identification

Physical Properties

Spectra

MedChem

Reactions

排列組合想要的搜尋條件

Drag & Drop to build a new



超過100種搜尋條件

進階搜尋範例

- 搜尋天然萃取物質，分子式至少含有30個碳並有文獻報導具有抗菌效果 (anti-microbiotic effect)
- 鑑定未知天然萃取物質，已知的分子量(M.W.173)，並以一組NMR實驗數據進行排除
- 搜尋Rufinamide的合成反應，結合flow reactor關鍵字進行反應條件搜尋

Query Builder – search Natural Compounds plus Applications

Example 1

Search for compounds isolated from natural source, have 30 carbons and reported antimicrobial effect.

Isolated from natural products

Molecular Formula

Use

Query Builder – search Natural Compounds and Applications

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation tabs for 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History' are in the center. On the right, the user name 'Ryan Huang' and notification icons are visible. Below the navigation, a 'Search in:' section contains buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar below this includes 'Import', 'Save', 'Reset form', and 'Delete all' on the left, and 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW' on the right. The main search area shows a search block: 'Isolated from Natural...' with a 'Find any' checkbox and a 'Show fields' dropdown menu (circled with a red '3'). A search results panel on the right shows a search for 'natural' (circled with a red '1') and a list of results, with 'Isolated from Natural Source' selected (circled with a red '2').

1. Type in “natural” to search for “Isolated from Natural Source” search block
2. Select by left click
3. Most of the search block require fill in values. Click show fields.

Query Builder – search Natural Compounds and Applications

Reaxys®

Quick search

Query builder

Results

Synthesis planner

History

Ryan Huang



Search in:

Reactions >

Targets >

Substances >

Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Find search fields and forms

Q natural



Reaxys ^

◇ Isolated from Natural... Find any Show fields (Isolated from Natural Source) X

◇ Molecular Formula is C30* X

1. Select Molecular Formula
2. Typing C30*



Query Builder – search Natural Compounds and Applications

Reaxys®

Quick search

Query builder

Results

Synthesis planner

History

Ryan Huang



Search in:

Reactions >

Targets >

Substances >

Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Isolated from Natural... Find any Show fields (Isolated from Natural Source) X

AND

◇ Molecular Formula is C30* X

AND

◇ Use Find any Hide fields X

is Laboratory Use and Handling X

is antimicrobio* X

1 Find search fields and forms use X

2 Use X



ELSEVIER

活動4 請利用Query builder搜尋
萃取自紅藜屬 (Chenopodium)的萃
取物質中，有多少被報導可溶於水中？

台灣藜

植物



台灣藜為莧科藜亞科藜屬之台灣原生種植物。傳統稱為紅藜，於2008年12月正名為台灣藜，是台灣原住民耕作百年以上的傳統作物，布農語稱為mukun，排灣語稱為djulis或tjulis，卑南語稱為duli，魯凱語稱為baae或ba'e，阿美語稱為kowal。 [維基百科](#)

學名： **Chenopodium** formosanum

上一層分類： 藜屬

界： 植物界 Plantae

分類階層： 物種

科： 莧科 **Amaranthaceae**



ELSEVIER

Reaxys Reaction Search

反應式查詢



Reaction Search

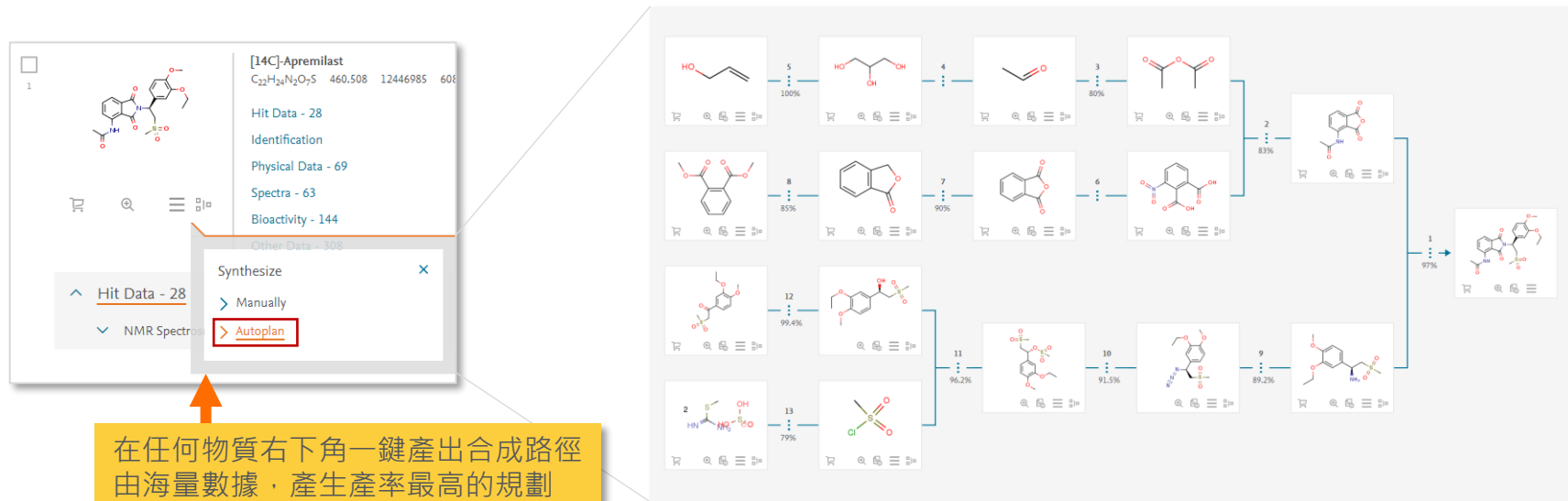
1. (逆)合成路徑規劃
2. 由物質資訊連結到製備方式
3. 由結構搜尋反應式
4. 由關鍵字搜尋反應式



兩鍵逆合成規劃

Reactions of interest can be curated and stored in the **Synthesis Planner**.

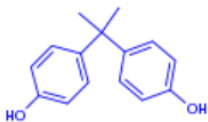
Autoplan facilitates synthetic blueprinting of substances of interest based on reactions with literature precedence



由物質資訊連結到製備方式

□

1



BPA

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

Identification

Druglikeness

Bioactivity (All)

Physical Data - 346

Spectra - 139

Other Data - 470

Preparations - 98 >

Reactions - 1,366 >

Targets - 157 >

Documents - 13,432 >

只出現在產物

可出現在產物或起始物

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

Reaxys - 99

□

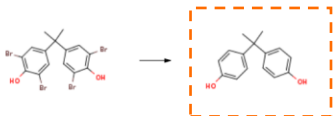
0 selected

Limit To Exclude Export Syn-Plan Show Conditions

Sort by Reaxys Ranking

□

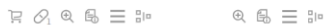
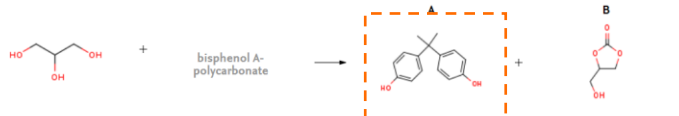
1



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

Reaxys - 1,402

□

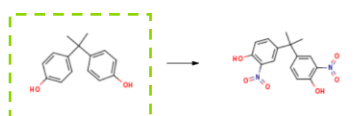
0 selected

Limit To Exclude Export Syn-Plan Show Conditions

Sort by Reaxys Ranking

□

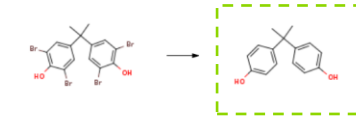
1



8 Conditions Find Similar Reaction ID: 70732

□

2




4 Conditions Find Similar Reaction ID: 46083924

畫結構搜尋反應式

Reaxys

[Quick search](#) [Query builder](#) ^{New} [Results](#) [Synthesis planner](#) [History](#) [Alerts](#)

Ryan Huang  

Search for 184475-35-2

Import 

Search Reaxys

184475-35-2

×

Find >

Documents, e.g. published by Schrock






AND



結構編輯器



Content Overview | Latest update: 11. September 2019 >

118M 49M 59M 37M 1.5M
 Substances  Reactions  Documents  Bioactivities  Targets



ELSEVIER

畫結構搜尋反應式

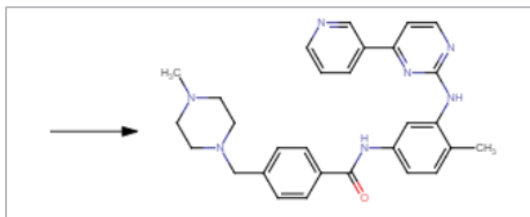
Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >

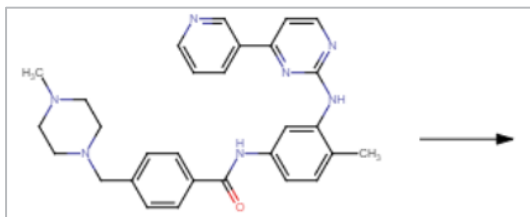
Reaction arrow icon (反應箭頭)

Clear Cancel Transfer to query >

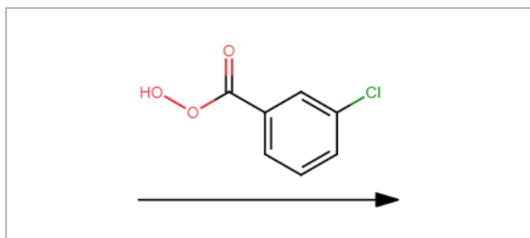
畫結構搜尋反應式



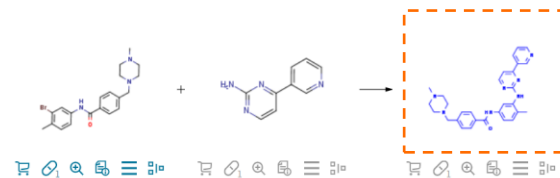
箭頭在左
產物



箭頭在右
起始物



箭頭在下
催化劑或溶劑



Conditions Find Similar Reaction ID: 29521413

Conditions	Yield	Reference
With tris(dibenzylideneacetone)dipalladium ⁰ chloroform complex; 2,2'-bis-(diphenylphosphino)-1,1'-binaphthyl; sodium t-butanol 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 <i>Journal of labelled compounds and radiopharmaceuticals</i> , 2020, vol. 63, # 4, p. 174 - 182 Full Text Details Abstract



1 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; Experimental Procedure	93%	KRKA, D. D., NOVO MESTO; BENKIC Primož; TIHI Jaroslav; PECAVAR Anica; GERMAN Tamara; VREČER Franc; VAJS Anamarija; SKRABANJA Vida WO2011/157450, 2011, A1 Location in patent: Page/Page column 19 Full Text Details Abstract

With dihydrogen peroxide; methyltrioxorhenium(VII) In dichloromethane; water at 15°C; for 5h; Experimental Procedure	100%	METHYLGENE INC. WO2005/92899, 2005, A1 Location in patent: Page/Page column 73 Full Text Details Abstract
---	------	--

With 3-chloro-benzenecarboxylic acid In dichloromethane at 20°C; Inert atmosphere;	100%	Roudestly, Fares; Veiros, Luis F.; Oble, Julie; Poli, Giovanni <i>Organic Letters</i> , 2018, vol. 20, # 8, p. 2346 - 2350 Full Text Cited 19 times Details Abstract
--	------	--

畫結構搜尋反應式

The image displays two overlapping screenshots of the Reaxys software interface. The left screenshot shows the 'Structure editor' with 'MarvinJS' selected. A chemical structure of a piperazine derivative with a methyl group and a vinyl group is shown. The right screenshot shows the 'Quick search' window. The search bar is empty, and the 'Find >' button is circled in orange. Below the search bar, the target name 'Polo-like kinase 1' is entered, and the search results show a chemical structure of a complex molecule with a piperazine ring and a benzimidazole moiety. The search results are displayed as 'As drawn'.

Reaxys® Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

As drawn

As substructure

Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

Search for

Search Reaxys

Find >

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

AND

As drawn

Content Overview | Latest update: 31. August 2020 >

118M 49M 59M 37M

Substances Reactions Documents Bioactivities



Feedback
















07.10.2020

ELSEVIER

畫結構搜尋反應式

Reaxys® [Quick search](#) Query builder Results Synthesis planner History Alerts Ryan Huang  

Results for  New  Edit 

	170	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results  View Results >
	499	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 >

畫結構搜尋反應式

Reaxys

Quick search Query builder Results Synthesis planner History Alerts

Ryan Huang  

Filters

Limit to > Exclude >

56
170
Preview

- Reagent/Catalyst
- Solvent
- Catalyst Classes
- Solvent Classes
- Product Availability 1
 - all prods for purchase 114
 - all prods prep known 56
- Reactant Availability
- Reaction Classes
- Document Type
- Publication Year
- Single step reactions only
- Experimental procedure only



170 Reactions out of 122 Documents containing 175 Substances, 1,977 Targets

0 selected

Limit To Exclude Export Syn-Plan



 Hide Conditions

隱藏實驗條件

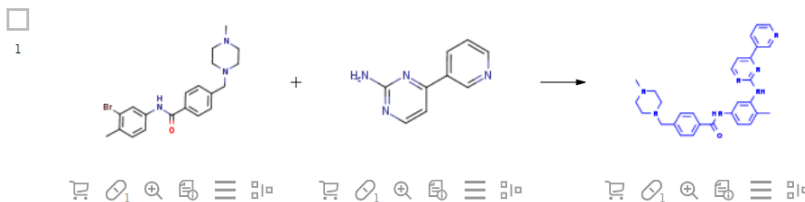
 

Sort by Reaxys Ranking 

Sort search results 

Reaxys Ranking  

- No of References
- Reactant Availability
- Product Availability
- MW of product
- Yield
- Publication Year



9 Conditions Find Similar > Reaction ID: 29521413

Conditions

Yield

Reference

With tris(dibenzylideneacetone)dipalladium⁽⁰⁾ 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, [Journal of labelled compounds a 63, # 4, p. 174 - 182]
[Full Text](#) [Details](#) [Abstract](#) >

Stage #1: N-(3-bromo-4-methylphenyl)-4-((4-methylpiperazin-1-yl)-methyl)benzamide; 4-pyridin-3-ylpyrimidin-2-ylamine In ethanol at 60°C; for 3h; Inert atmosphere;

91%

Yangzhou University; Yu Lei; Deng Xin
CN108164505, 2018, A
Location in patent: Paragraph 0015-0019; 0032

Stage #2: With sodium hydroxide In water pH=8.7; Reagent/catalyst;

[Experimental Procedure](#) 

1 Example 1

Under nitrogen protection, 40 mg of N,N'-diisopropylselenourea was uniformly mixed with 10 g of chitosan. It was placed in a tubular reactor and calcined at 500 °C for 5 hours under nitrogen to obtain selenium and nitrogen-doped nano-carbon fibers with selenium promoting large specific surface area. The material was immersed in 0.05 mol/L copper chloride aqueous solution for 18 hours. Filtration, washing with water, drying to obtain a catalyst. The above catalyst is determined by ICP, wherein the mass ratio of selenium is 0.01%, and the mass ratio of copper is 0.12%. The specific surface area is 28 cc/g. 20 mg of the above catalyst with 1.72 g of 4-(3-pyridyl)-2-aminopyrimidine (see I in the following reaction formula) and 4.02 g of 4-(N-methylpiperazine)methylbenzoyl (3-bromo-4-methylphenyl)amine (see II in the following reaction formula) were mixed in 20 mL of ethanol under nitrogen protection. Heat at 60 °C for 3 hours. The catalyst is recovered by centrifugation. Concentrate the supernatant to within 5 mL, that is, a large amount of crystals are precipitated, filtered, and washed with petroleum ether. Imadinib hydrobromide was obtained in a yield of 96%. Dissolve the salt in 20 mL of water, adjust the pH to 8.7 with 0.2 mol/L NaOH, and extract with ethyl acetate. (3 extractions per 20 mL). The organic phases were combined and dried over anhydrous sodium sulfate. After filtering, the solvent is evaporated. That is, free imatinib was obtained, and the yield was 91%. ICP analysis indicated that the copper residue in the product was less than 0.03 ppm.

歷史紀錄

逆合成路徑規劃

Reaxys®

Quick search Query builder **Results** Synthesis planner History Alerts

Ryan Huang  

15
170
Preview

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

1 selected

Limit To Exclude Export Syn-Plan Hide Conditions

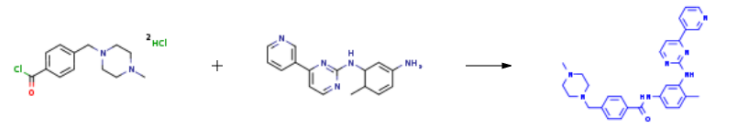
Experimental Procedure >

加入合成計畫

SKRABANJA Vida
WO2011/157450, 2011, A1
Location in patent: Page/Page column 19
Full Text > Details > Abstract >

1 out of 1


7



1 Conditions > Find Similar > Reaction ID: 32644292

Conditions	Yield	Reference
With sodium hydroxide In water at 0 - 55°C; pH=9 - 9.5; Experimental Procedure >	99.26%	MUSTAFA NEVZAT İLAÇ SANAYU A.Ş.; GÜNDÜZİ Halit; ÖZLÜ Yusuf; YALÇIN, Serkan WO2012/26897, 2012, A1 Location in patent: Page/Page column 15 Full Text > Details > Abstract >

1 out of 1

Feedback 



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逆合成路徑規劃

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Synthesis Planner 






Synthesis plan 1

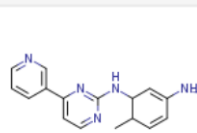
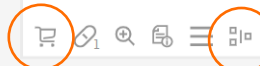
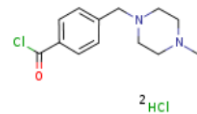
  
Import Save Export


Synthesis plan 1

Synthesis plan 2

Substance Availability 

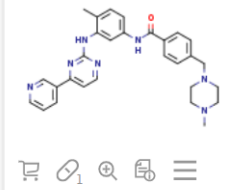
-  Accelrys' ACD [↗](#)
-  CambridgeSoft ACX [↗](#)
-  Labnetwork [↗](#)
-  Sigma Aldrich [↗](#)
-  eMolecules [↗](#)



Synthesize 

- [Manually](#)
- [Autoplan](#)

1
⋮
99.26%



Conditions


With sodium hydroxide In water at 0 - 55°C; pH=9 - 9.5;
Experimental Procedure [^](#)

99.26%

MUSTAFA NEVZAT İLAÇ SANAYU A.Ş.; GÜNDÜZ1 Halit; ÖZLÜ Yusuf;
YALÇIN, Serkan
WO2012/26897, 2012, A1
Location in patent: Page/Page column 15
[Full Text](#) [Details](#) [Abstract](#) [>](#)

Feedback 


+ Create new
07.10.2020


    

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Synthesis Planner 

Edit 


Synthesis plan 1

 Import  Save  Export

Synthesis plan 1

Synthesis plan 2

Export reactions

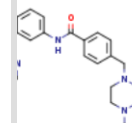
Export documents 

Choose a format:

PDF/Print  


Additional options:

- Include structures
- Include experimental procedure
- Include a description in the document




Conditions

With sodium hydroxide In water
Experimental Procedure 

Export 

+ Create new
07.10.2020

STAFANEVZAT İLAÇ SANAYU A.Ş.; GÜNDÜZ1 Halit; ÖZLÜ Yusuf;
ÇİN, Serkan
2012/26897, 2012, A1
ation in patent: Page/Page column 15
[Full Text](#) [Details](#) [Abstract](#) 

由關鍵字搜尋反應式

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Search for "radical cyclization"

Import 

Search Reaxys

"radical cyclization"



Find >

Reactions, e.g. [Suzuki coupling](#)


AND




Draw

[Content Overview](#) | Latest update: 31. August 2020 >


118M

 Substances


49M

 Reactions

59M

 Documents

37M

 Bioactivities

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Ryan Huang



Results for "radical cyclization"

New Edit

	75	Reactions	Condition : radical cyclization Edit in Query Builder Create Alert	Preview Results	View Results >
	6,113	Documents	Titles, Abstracts, Keywords : "radical cyclization" Edit in Query Builder Create Alert	Preview Results	View Results >



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Quick search Query builder **Results** Synthesis planner History Alerts

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75 **Filters**

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, 40 Targets


0 selected

1 Hits **9** Conditions Find 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 <input type="button" value="↗"/> Cited 62 times <input type="button" value="↗"/> Details <input type="button" value=">"/> Abstract <input type="button" value=">"/>

1 hit out of 1

2





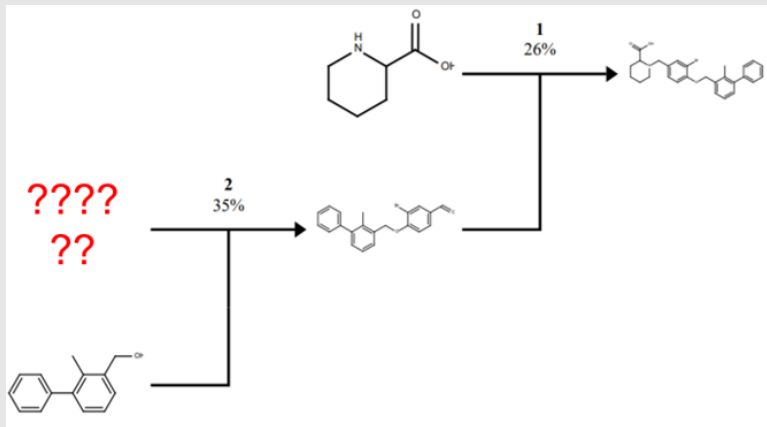
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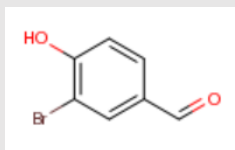
問題5

循著線索追到附近的實驗室大樓，遠遠看到酒吧撞見的科學家在大廳咆嘯，臉色發青似乎酒醒了一半。

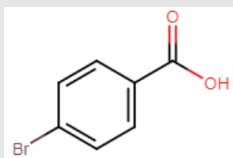
上前遞還他遺落的餐巾紙後，他感激的邀請你到他的實驗室，並央求你協助填入該物質合成計畫中消失的環節？



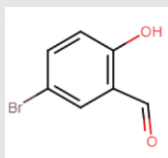
A.



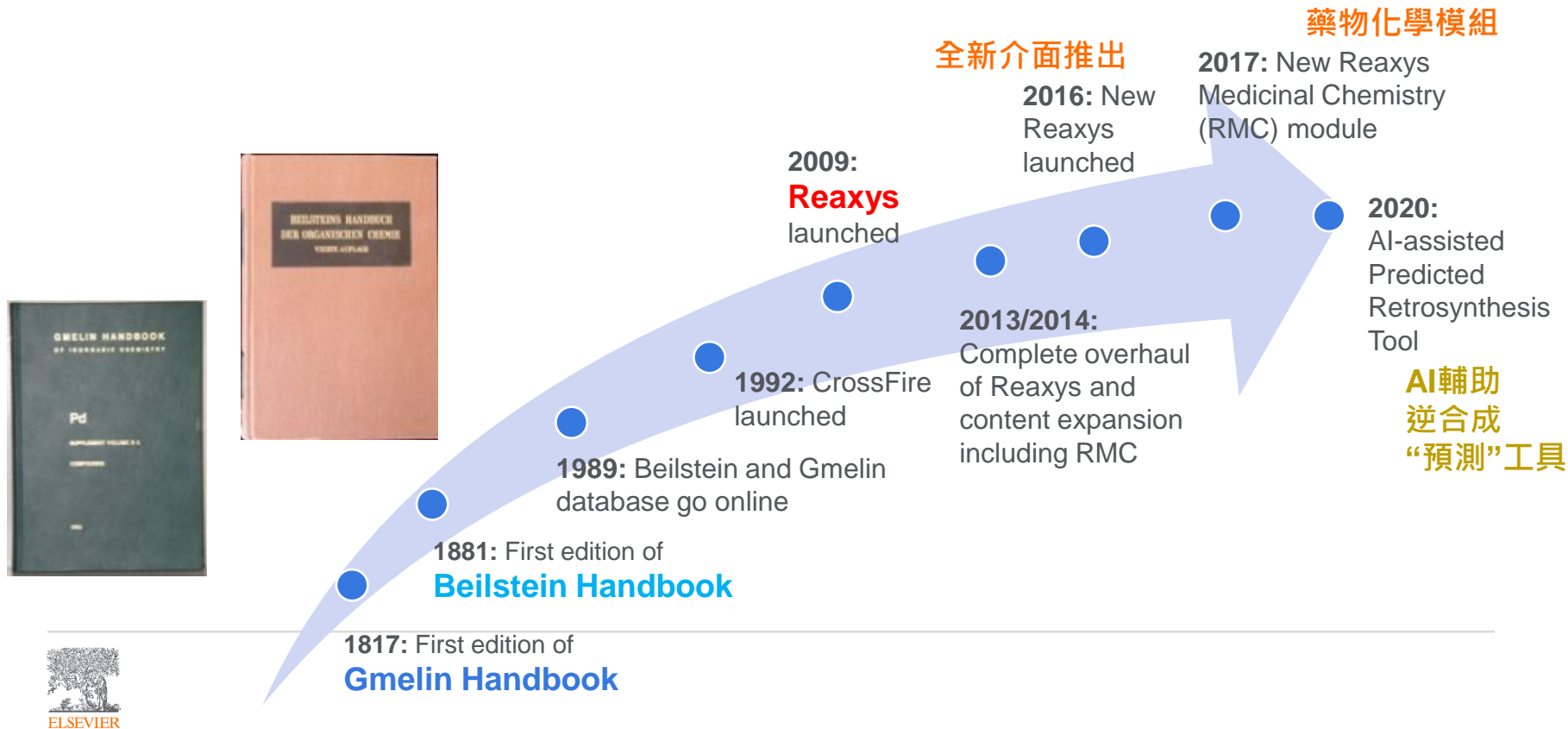
B.



C.



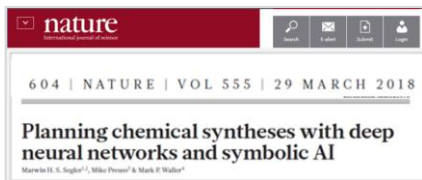
Reaxys具有長遠的歷史，提供創新所需的資訊



Reaxys predictive retrosynthesis solution combines unparalleled Reaxys content with AI & ML technologies

One of the most cited works in the fields of predictive retrosynthesis has been enabled by a partnership between Elsevier, Dr. Marwin Segler and Prof. Dr. Mark Waller

Reaxys predictive retrosynthesis tool in news



NEWS

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

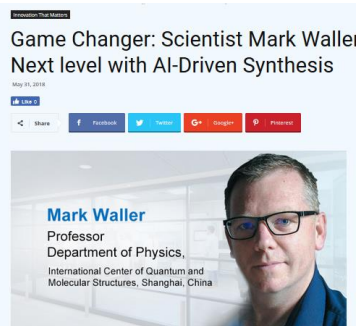
Robert F. Service
* See all authors and affiliations
Science 07 Jul 2017
Vol. 357, Issue 6346, pp. 27
DOI: 10.1126/science.357.6346.27







NEWS · 28 MARCH 2018

Need to make a molecule? Ask this AI for instructions





Artificial-intelligence tool that has digested nearly every reaction ever performed could transform chemistry.



Advantages of Reaxys RT over other RTs

-  Not reliant on extracting and encoding rules by hand (manually)
-  Integrate own custom building block libraries or proprietary reaction data
-  System solves retrosynthesis for almost twice as many molecules
-  Thirty times faster than the traditional computer-aided methods

Value of predictive retrosynthesis

-  New idea generation: find routes to make novel compounds
-  Time saving: reduce time and effort in developing synthesis routes
-  R&D cost reduction: improve synthesis success
-  Knowledge augmentation: a digital assistant to help chemists navigate route designs

Reaxys predictive retrosynthesis augments your expertise & helps drive innovation

Start your search

Retrosynthetic Route Designer Powered by Reaxys and Pending AI

My Synthesis Projects Draw a Target Logout

Draw a target substance

Intuitive and easy to use interface for drawing molecules

Flexibility to obtain full synthesis route or last step only

Option to obtain the most diverse route or route with highest probability

Multiple building blocks from Reaxys and various commercial suppliers

Ability to integrate your own building blocks

Retrosynthesis Parameters

- Length and depth of synthesis plans
 - Full synthesis plan (max 10)
 - Last step only (max 100)
- Diversity of synthesis plans
 - No filtering
 - Diversity filter on
- Select Building Block Libraries
 - Reaxys known substances (RCS)
 - Sigma Aldrich
 - LabNetworks
 - emolecules
 - Big Pharma AG

Clear Cancel X Synthesis >

Project summary

My Synthesis Projects Update automatically

Show 10 entries

No.	Date/Time	Structure	Parameters	No. of Routes
2	24 October 2019 10:55		TypeOfPlans: FullRoute Diversity: High Used building blocks: SIAL, LN, RX, EM	8
1	24 October 2019 09:01		TypeOfPlans: FullRoute Diversity: low Used building blocks: SIAL, LN, RX, EM	2

Showing 1 to 2 of 2 entries

Previous 1 Next

4. Click view results

- View result >
- Edit # Delete #

- Provides a summary of molecules searched for
- Summary of retrosynthesis parameters
- Summary of number of routes predicted

Routes summary

My Synthesis Projects > Project #2

Routes

Route no.	Building blocks to target	Score	No. of steps
Route 1		0.711	3
Route 7		0.71	3
Route 5		0.595	5
Route 3		0.575	5
Route 4		0.533	6

View route

5. Click Tree or Table view

- Table View >
- Tree View >

Confidence score generated based on literature evidence

Summary of building blocks needed to make the target molecule

Number of steps in predicted route

Detailed route view

Tree View Table View

Target molecule

Step 3

Step 2

Step 1

6. Click on any step number to go to Reaxys examples

Show Reaxys Examples

ntial

Reaxys predictive retrosynthesis – our USP

- 1. AI and ML training dataset:** Predicted algorithm trained on largest (>15m) chemistry reaction dataset, with ~400,000 rules auto-extracted
 - a) Reaxys data is powering the world's leading AI and ML development in predictive chemistry including MIT, SRI, Univ. of Cambridge and AstraZeneca
 - b) Training dataset also included 100 million negative chemical reactions (virtual) to enable scientifically robust predictions
- 2. Technology:** The only retrosynthesis solution based on auto-extracted rules and deep learning algorithm (3 neural networks coupled with Monte-Carlo tree search) i.e. similar technology that powered AlphaGo
 - a) This technology also enables the ability to easily update the model so that predictions keep pace with innovation in chemistry published
- 3. Scientifically robust:** Predictions have been tested using three approaches:
 - a) The false positive rate of the filter (that is, incorrect reactions passing the filter) is 1.5% indicating very good performance
 - b) Time split validation (basically we are trying to predict the future and by doing this we can get a good feeling about how well our model is performing) indicated that the model performed quite well when we analysed many drug molecules and the nice feature is that not only is the accuracy quite good but also that these deep neural networks are very fast
 - c) 'Chemical Turing Test' – double blinded test with organic chemists (45 PhDs and Post-docs) indicated high quality and robustness of predicted routes
- 4. Augmentable and customizable:** Ability to customize by adding your own building block library and augmentable by adding your own chemistry reactions data

Need to make a molecule? Ask this AI for instructions

Artificial-intelligence tool that has digested nearly every reaction ever performed could transform chemistry.



<https://www.nature.com/articles/d41586-018-03977-w>

An artificial-intelligence tool could help scientists plan multi-step chemical reactions. Credit: Roger Mayne Archive/Mary Evans Picture Library

Article | Published: 29 March 2018

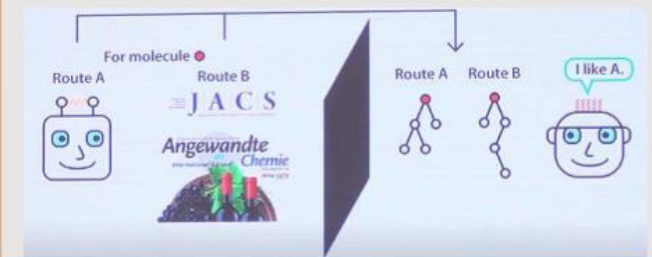
Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler , Mike Preuss & Mark P. Waller *Nature* 555, 604–610(2018) | [Cite this article](#)22k Accesses | 241 Citations | 574 Altmetric | [Metrics](#)

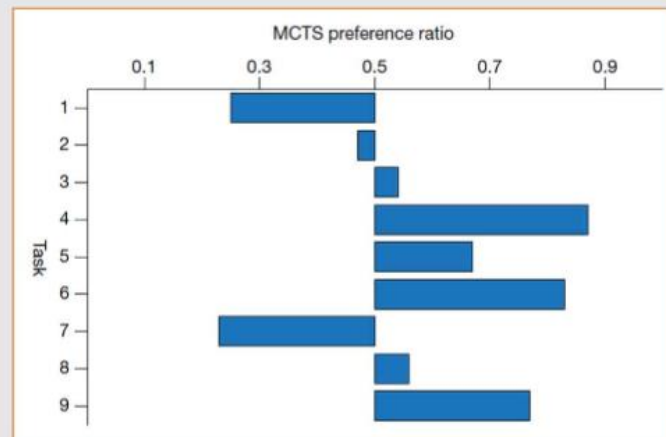
Abstract

To plan the syntheses of small organic molecules, chemists use retrosynthesis, a problem-solving technique in which target molecules are recursively transformed into increasingly simpler precursors. Computer-aided retrosynthesis would be a valuable tool but at present it is slow and provides results of unsatisfactory quality. Here we use Monte Carlo tree search and symbolic artificial intelligence (AI) to discover retrosynthetic routes. We combined Monte Carlo tree search with an

Qualitative evaluation 'Chemical Turing Test' methodology:



Qualitative evaluation result: No significant difference in expert choice

Expert choose Reaxys predictive retrosynthesis route (57%) versus literature route (43%) $p=0.26$



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新增分類"Commercial Substances"於預視頁面

- Quick Search輸入CAS#，或畫結構搜尋您要購買的物質

Reaxys®

Quick search


Query builder

Results

Synthesis planner

History












Alerts

Ryan Huang 



Results for "186519-92-6"

New  Edit 

	1	Substances CAS# : 186519-92-6 Edit in Query Builder  Create Alert 	Preview Results  View Results >
	0	Documents Titles, Abstracts, Keywords : "186519-92-6" Edit in Query Builder  Create Alert 	
	2	Commercial Substances CAS# : 186519-92-6 Edit in Query Builder  Create Alert 	Preview Results  View Results >



07.10.2020

物質頁面購物車新增分類”Commercial Substances”

- 或點擊右上方切換資料庫為Commercial Substances

Reaxys® Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

1 Substances out of 5 Documents, containing 11 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References

Grid Heatmap

Reaxys - 1

Reaxys - 1

- Reaxys - 1
- Commercial Substances - 2
- eMolecules - 2
- LabNetwork - 0
- PubChem - 1
- SigmaAldrich - 1

4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid
C₇H₄ClN₃O₂ 197.581 14006617 186519-92-6

Identification
Druglikeness
Physical Data - 1
Spectra - 2

Substance Availability

- [Commercial Substances](#)
- [Accelrys' ACD](#)
- [CambridgeSoft ACX](#)
- [Sigma Aldrich](#)
- [eMolecules](#)

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Reaxys[®] Quick search Query builder Results Synthesis planner History Alerts Ryan Huang

0 selected Limit To Exclude Export Sort by Commercial Substance ID ↑ Grid

Please take a moment to check individual supplier websites for the most up-to-date information on pricing and availability

Supplier (A)	Product	Purity	Package size & price		Availability
Enamine - USA USA	186519-92-6 EN300-152527 ↗		mg		Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Enamine - USA USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 EN300-152527 ↗	95%	500 mg	159 USD	Shipment time: 2-10 days Tier Time: Tier 2 Last updated: 2020-06-01
eMolecules Manchester Organics Ltd USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 F45799 ↗		1 g	994 USD	Shipment time: 12 weeks Tier Time: Tier 4 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	250 mg	134 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Oakwood Chemicals USA	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 076916 ↗	95%	1 g	241 USD	Shipment time: 1-5 days Tier Time: Tier 1 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		10 g	670 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01
eMolecules Pharmablock USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 ↗		50 g	2241 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01

Show Less ^

Feedback

(B)

(C)

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- 化學研究不可缺少之「數據」資料庫
- 從化學相關論文及專利萃取有用取必要的「數據」

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溶劑、催化劑及產
率等)

>54 M 文獻記錄
>16,000 期刊，專利
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>33 M 生物活性資料點
結構活性關係資料
動物活體細胞研究
細胞外療效
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Thank you

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