



Reaxys全國學術版 台灣大學化學系

Elsevier Life Science Solutions 黃恪涵 Ryan Huang 2023.9



Reaxys 全國學術版2023

- 國研院科政中心訂閱,授權設 有化學、應化、藥學等大專院 校限研究、教學使用
- 免費教育推廣、技術支援、<u>網路自學資源</u>(歡迎圖書館、系所、PI、 老師來信)
- Webinars網路會議分享化學研 究新知





Reaxys為化學家設計 - 專注於實驗數據

ELSEVIER	Nonderine states 12 (2012) eth Mil Generate law analtaka di Schwarz Samoudreas Tetrahedron Letters Journal homepage: www.alawsiar.aam/locate/peties	n	
An efficient and Emiliano Marzo *, Ma Inter el Ostro Brendenico, Ol A ETICLE INFO Marte Barrow (2011) Restar de Ostro Barrow (2011)	A A Decide definition of DOCUMENT A DECIDENT A DECIDE	CH ₃ O O OH	Structures
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讓Reaxys伴隨你的學習與職涯歷程



Learning Undergraduates



Research

Laboratories, Research institutes



Career

Pharmaceutical company, R&D of chemical company

今日目標

- Reaxys 化學資料庫的基本認識 有哪些資料? 化學檢索介面?
- 有機分子結構檢索、天然化合物探索生物活性應用作為示範。
- 分子式檢索、實驗數據檢索。
- 自我學習網路資源。
- 進階的操作技巧-業界搜尋範例。

Swiss Champ



Image adopted from https://www.victorinox.com/tw/en/Products/Swiss-Army-Knives/Medium-Pocket-Knives/Swiss-Champ/p/1.6795

Reaxys資料庫涵蓋的範圍



Gmelin's Handbook of Inorganic Chemistry

Every substance/reaction discovered between 1772 and 1995, with extensive properties information

First edition 1817

(1788-1853)



Beilstein's Handbook of Organic Chemistry

Collection of experimentally validated data (structures, properties, reactions) on known organic substances from 1771 onward

First edition 1881



Reaxys資料庫擷取的資料種類



學術論文

專家從大約460個期刊標題中手動提取實驗數據

- ・ 有機化学
 1771年~
- 無機化学·有機金屬錯合物 1772年~

此外,從16,000個期刊標題中機器提取結構和其他資訊

專利

目前七個專利局手動提取,主要為有機化合物(WO,US,EP,JP,CN,KR,TW)

2021年起,覆盖範圍將擴大到105個專利局和所有化學品分類



>500 M Experimental data



>60 M
Reactions



>101 M Journal articles & Patents



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在授權IP範圍內,打開瀏覽器鍵入<u>http://www.reaxys.com</u>

Welcome to Reaxys Welcome to Reaxys Ready to take the shorts path from chemistry question to relevant arker Reaxys gives you the best means to explore the world of chemistry. To learn more visit our support hub page. Create your account or sign in to access all these features! Reduce timeouts Customize structure editor settings and layout. No Thanks Sign-in	Reaxys' Quick see	rch Query builder ^{New} Result	不用註冊!關閉]	直接體驗 _{kyan Huang Ջ ●}
these features! Create alerts & save searches Reduce timeouts Customize structure editor settings and layout No Thanks Sign-in Register		Search for 1844 Welcome to Reaxy Ready to take the shortest p answer? Reaxys gives you th chemistry. To learn more visit our sup Create your accourt	A475-35-2 TS path from chemistry question to relevant he best means to explore the world of poort hub page. Int or sign in to access all	Import 🛓
Content Overview Latest update: 11. September 2019 >		these features! Create alerts & save se Reduce timeouts Customize structure ed No Th Content Overview Latest update: 18M 49M 59M	earches ditor settings and layout hanks Sign-in Register a: 11. September 2019 > 37 M 1 5 M	



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Starter













- 從結構出發
- 天然萃取物 文獻與物質整理
- 分子式檢索電極材料
- 實驗數據檢索
- 觸媒研究檢索

- 反應式搜尋
- 逆合成面板
- Reaxys Academy
- 線上資源







我有一個實驗室感興趣的藥物結構,是沒有人發表過的,如何從有<mark>相似</mark> 化學結構的文獻中,找尋可以參考應用、關鍵的實驗數據。



CN1CCC(CC1)=C1C2=C(CCC3=C1C(C)=CC=C3)C(Br)=C(Br)C=N2





MarvinJS 結構編輯器





補充-你應該認識的Reaxys結構編輯器 ①



- Reaxys內建 ChemDrawJS 剪貼插件



1. 如果你有ChemOffice,需要「複製」把繪製於ChemDraw裡面的結構 「貼上」到 Reaxys裡面去檢索,安裝剪貼插件!

2. 安裝好之後,快捷鍵是「複製」 Ctrl+C、「貼上」 Ctrl+V



補充-你應該認識的Reaxys獨特功能①



- Marvin JS 是官方推薦且最靈活的結構編輯器



MarvinJS 小技巧① - 從名稱繪製結構





MarvinJS 小技巧① - 從名稱繪製結構







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Reaxys三種結構搜尋與怎麼用







補充- Similar Search的定義



X

Query Structure —

Database	Position/Stereo Isomers 🕜	Near 🕐	Medium 🕐	Wide 🕐	Widest 🕐
Reaxys	1	5	171	205	1,249

Near

Near: includes structures containing the same ring and chain systems (possibly multiple) with the original relative positions of substituents and extended by further simple substituents such as hydrocarbons

Medium

X

Medium: includes structures with a wider range of rings and substituents: the degree of unsaturation, form and substitution patterns of rings is extended

X

Wide

Widest

X

Wide: includes a still wider range of substituents, but retaining to some extent the influence of the relative positions of substituents

Widest: as for Wide but without any restrictions on the relative positions of substituents



MarvinJS 結構編輯器-自我學習的管道





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https://www.youtube.com/pl aylist?list=PLBSTWvuNnJAI 4laTo5zNkqaJ9va-LUtj0





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學名 Bidens Pilosa

圖片取自中文維基百科 https://zh.wikipedia.org/wiki/%E 9%AC%BC%E9%92%88%E8% 8D%89 Question: 探索藥用植物萃取物的生物活性應用,已發表文獻中有哪些substances紀錄,如何

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」





輸入學名「Bidens pilosa」,選擇搜尋文獻

Reaxys	Quick search Query builder Results Retrosynthesis History
	Search for bidens
	Search Reaxys bidens Find > Concepts bidens bidens pilosus bidens pilosus

找到~1,800 文獻紀錄,點擊「View Results」

Result	s for "biden	s pilosa"		New 🔿 Edit 🖉
₿	1,872	Documents	Titles, Abstracts, Keywords ∶"bidens pilosa" Edit in Query Builder 🔗 Create Alert 🗘	Preview Results View Results >

天然萃取物檢索②





天然萃取物檢索③





天然萃取物檢索④



1. 繪製感興趣的核心結構



2. 選擇As substructure



3. Transfer to filter



4. Limit to









1. 繪製感興趣的四環結構







4. Transfer to filter 5. 按下Limit to









~利用進階天然萃取物檢索工具「Isolated from natural source」~



- 1. 進階搜尋Query builder
- 2. 輸入「Isolated from natural source」
- 3. 左鍵點擊「Isolated from natural source」工具
- 4. 點擊Show fields 開啟欄位 Show fields ✓ 輸入鬼針草屬「Bidens」
- 5. 點擊Substances



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358 Substances out of 425,560 Documents, containing 132,795 Reactions, 3,941 Targets 土 A 0 selected Sort by No of References ↓ ∨ Grid 🔜 Bioactivity Visualization 🖽 QO Limit To Exclude Export Preparations quercetol (HO)2C₆H₃C₉H₂O(O)(OH)3 302.24 317313 117-39-5 Preparations - 190 Hit Data - 2 Bioactivity (All) Other Data - 4.863 Reactions - 1.424 > Identification Physical Data - 1,190 Targets - 1,353 Druglikeness Spectra - 1.644 > . . . Documents - 51,604 > 小提示! 利用天然物萃取工具找 Hit Data - 2 ~ 到的substances記錄較少,但會 Isolated from Natural Source - 2 hits out of 1549 保留文獻出處,且不會有一般實 驗試劑 (water, ethanol)等雜訊。 Isolated from Natural Source Reference aerial parts of Bidens tripartita; Uysal, Sengul; Ugurlu, Asli; Zengin, Gokhan; Baloglu, Mehmet Cengiz; Altunoglu, Yasemin Celik; Mollica, Adriano; Custodio, Luisa; Neng, Nuno R.; collected from Afyon Nogueira, José M.F.; Mahomoodally, M. Fawzi [Food and Chemical Toxicology, 2018, vol. 111, p. 525 - 536] Full Text 7 Cited 28 times 7 Details > Abstract > whole plant of Bidens parviflora Willd. Li, Yu-Lan; Li, Jun; Wang, Nai-Li; Yao, Xin-Sheng[Molecules, 2008, vol. 13, # 8, p. 1931 - 1941] collected in Liaoning province, China Full Text 7 Cited 159 times 7 Details > Abstract >

分子式檢索



Question: "鈷是很常見的電極材料,然而因為社會經濟、環境 與安全性的考量,實驗室希望設計不含鈷的鋰電池電極材料。"

利用進階搜尋工具「Molecular Formula」

分子式檢索①





分子式檢索(2)











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」





1. 以關鍵字搜尋Sublimation





















觸媒研究檢索①











其他值得探索的實驗數據檢索工具



Physical Properties	Autoignition	😂 Enthalpy of Combustion	
🛇 Melting Point	🛇 Azeotropes	😂 Enthalpy of Formation	😂 Heat Capacity Cp
😂 Boiling Point	🔗 Boundary Surface Phenomena	Enthalpy of Fusion	🔅 Heat Capacity Cp0
😔 Sublimation	😣 Chromatographic Data	😂 Enthalpy of Hydrogenation	📚 Heat Capacity Cv
Pofractive Index	Pulk Viscosity	Enthalmu of Sublimation	😔 Henry Constant
			Interatomic Distances and Angles
🛇 Density	Circular Dichroism	Enthalpy of Vaporization	➢ Ionization Potential
℅ Adsorption	😂 Complex Phase Equilibria	Explosion Limits	Soelectric Point pH
℅ Association	Compressibility	😂 Flash Point	Skinematic Viscosity

Latent heat of fusion

ELSEVIER



Latent heat of vaporization



 P. 1069 - 1079]
 Full Text ar Gited 60 times ar Details > Abstract >

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 Verexkin, Sergey P.[Journal of Chemical Thermodynamics, 1998, vol. 30, # 9, p. 1069 - 1079]

 Full Text ar Coll (Application of Chemical Thermodynamics, 1998, vol. 30, # 9, p. 1069 - 1079]
 Full Text ar Coll (Application of Chemical Thermodynamics, 1998, vol. 30, # 9, p. 1069 - 1079]





Reactions Search 反應式查詢



Reaxys尋找反應式的方法



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





Reaxys尋找反應式的方法



~已知物質的製備方式~





Reaxys尋找反應式的方法 ~ 關鍵字檢索①~













Reaxys尋找反應式的方法 ~繪製反應式①~

Reaxys	Quick search	Query builder	Results	Synthesis planner	History	Alerts	
🐔 Structure editor selected: 🖲 MarvinJS 🔇) ChemDrawJS			Insert	structure	from name >	>
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S ^{max} H ₃ C						н	н
s ^{fr}		ЛН				C	0
	> H					N	N
		CH3				0	C
入 +						5	5
						-	-
1 加入反應箭頭	音						2
						в	Br
						-	-
				Clear 💼 🛛 Cano	el 🗙 🛛 T	ransfer to query	>



Reaxys尋找反應式的方法





箭頭在左 產物



[] ℓ € € = 10 [2] ②] ④ 邑 ⊟ 10

9 Conditions 🔨 Find Similar 🔪 Reaction ID: 29521413 🐢

Yield Reference

@ 🗟 🗄 🕪

92%

B 0.

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;







With ammonia In water; isopropyl alcohol at 20°C; for 4h; pH=7.6 - 8.5;

Experimental Procedure V

With dihydrogen peroxide; methyltrioxorhei Experimental Procedure 🗸

With 3-chloro-benzenecarboperoxoic acid

Kang, Julie; Lee, Jun Young; Park, Jeong-Hoon; Chang, Dong-Jo Journal of labelled compounds and radiopharmaceuticals, 2020, vol. 63, #4, p. 174 - 182] Full Text > Details > Abstract >

Yield	Reference
93%	KRKA, D. D., NOVO MESTO; BENKIC Primoz; TIHI Jaroslav; PECAVAR Anica; GERMAN Tamara; VRECER Franc; VAJS Anamarija; SKRABANJA Vida WO2011/157450; 2011 , A1 Location in patent: Page/Page column 19
	Full Text 7 Details > Abstract >
100%	METHYLGENE INC.

nium(VII) In dichloromethane; water at 15°C; for Sh;	100%	METHYLGENE INC. WO2005/92899, 2005 , A1 Location in patent: Page/Page column 73 Full Text > Details > Abstract >
n dichloromethane at 20°C; Inert atmosphere;	100%	Roudesly, Fares; Veiros, Luis F.; Oble, Julie; Poli, Giovanni [Organic Letters, 2018, vol. 20, # 8, p. 2346 - 2350] Full Text a Cited 19 times a Details > Abstract >









欄位名稱: fulltext of reaction

詳細實驗步驟(文獻原文移植) 資訊量最豐富,包含詳細步驟、分析方法、數值



欄位名稱: fulltext of reaction

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



Reaxys進階反應式檢索 ~利用Query builder進一步「加工」搜尋條件~







Reaxys進階反應式檢索 ~利用Query builder進一步「加工」搜尋條件~







Reaxys進階反應式檢索 ~利用Query builder進一步「加工」搜尋條件~







Retrosynthesis 逆合成規劃



Retrosynthesis介面 ~逆合成的使用時機~

ELSEVIER



Retrosynthesis介面 ~逆合成的使用時機 —以Paxlovid為例~





Retrosynthesis介面 ~比較、增加、刪除並匯出~





找不到合成方法的分子 ~逆合成AI工具在有機分子合成中的應用~



CC1=NC=C(C=C1)C(=O)NC1NC(C2=CC=CO2)=C(S1)C(=O)C1CCOCC1





找不到合成方法的有機分子-讓逆合成AI工具給一點提示





AI針對每一步驟尋找相似反應的references

Reaxys 逆合成AI與機器學習研討會演講





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首頁 > 所有解決方案 > Reaxys > Reaxys AI 於中研院化學與機器學習研討會演講影片放送

Reaxys AI 於中研院化學與機器學習研討會演講影片放送

Reaxys 逆合成 AI 預測工具(Reaxys Predictive Retrosynthesis, 簡稱 Reaxys pRT)在臺灣如火如荼的展開一系列活 動與試用,希望讓研究人員體驗 Reaxys 逆合成 AI 預測工具所帶來全新的合成路徑設計思路。



原子與分子科學研究所在今(2023)年6月舉辦 Chen 內外研究人員分享人工智慧(AI)或機器學習(ML) 這場盛會,分享 Reaxys 逆合成 AI 預測工具,這場 30: **Q Reaxys 團隊合作發展了一個深度學習的電腦演算法,** 現劃逆合成藍圖,也就是現在的 Reaxys 逆合成 AI 預測 理, 且與 Elsevier 生命科學產品管理總監 Dr. Jurgen Sv



Reaxys學院 - 線上學習與認證平台



Reaxys Academy

students and educators

Reaxys Academy

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



Reaxys Academy (elsevier.com)





Introduction to Reaxys

● Welcome to Reaxys ↗

Conducting textual searches

- Literature Search: How to retrieve documents for a topic of interest 🛪
- Search for Reaction by text terms 🛪

Searching by structure

- An introduction to searching for compounds by structure in Reaxys
- How to create a structure drawing from a substance name in Reaxys **a**
- How to create a structure drawing from scratch in Reaxys
 Reaxys
- How to copy and paste a structure drawing from an external editor into Reaxys >

Using Query builder

- An introduction to searching with Query Builder in Reaxys a
- How to build a search using Query Builder in Reaxys aturnov Reaxys = Re
- How to refine a search using Query Builder in Reaxys ↗

Receive your certificate for *Reaxys Academy: Reaxys* 101

Take the quiz ゝ

讓Reaxys伴隨你的化學旅程





歡迎來信留下您對Reaxys的建議與問題~r.huang@elsevier.com



Thank you

歡迎來信留下您的問題與寶貴建議 <u>r.huang@elsevier.com</u>

