

Reaxys 更聰明的搜尋化學資料

Elsevier Life Science Solutions 2022.9





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TO ACCELERATE SCIENCE TO IMPROVE HEALTH

A Knowledge & Information Analytics Company



OUR PROMISE

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DIFFERENTIATORS

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OUR

KEY

years of scientific knowledge curated as semantically rich content to enable tomorrow's medical breakthroughs \$1.4bn on technology annually

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- 科技部科政中心贊助,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>
- Webinars網路會議分享化學研 究新知





今日教育訓練目標

- 1. Reaxys 化學資料庫的基本認識 有哪些資料? 基本搜尋方法?
- 2. 自我學習網路資源
- 3. 進階的操作技巧-業界搜尋範例

- 歡迎提問:將您的問題打在chat box,我會協助您找到答案。
- 網路資源、QR Code、網頁連結會後提供給圖書館



Reaxys是一個數據資料庫

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,更注重於縮短您搜尋文獻的時間,直在您的研究中使用數據



Reaxys與書目資料庫的差別





Reaxys涵蓋的範圍

學術論文

專家從大約460個期刊標題中手動提取實驗數據

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

此外,從16,000個期刊標題中機器提取結構和其他資訊

專利

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

2021年起, 覆盖範圍將擴大到105個專利局和所有化學品分類





>500 M Experimental data



>49 M Reactions



>54 M Journal articles & Patents



如何連上Reaxys

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





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進階搜尋 Query Builder





逆合成工具 Retrosynthesis









Quick Search 關鍵字查詢文獻





預覽畫面 – 選擇文獻Documents資料類型





文獻介面的重點提示①

Reaxys

ELSEVIER



Quick search Query builder Results Retrosynthesis History Alerts

文獻介面的重點提示② - Index & Substances



文獻介面的重點提示③

Reaxys			Quick search Query builder Results Retrosynthesis History Alerts	Ryan Huang 🗙 📀						
1.78 K	Filters 1, Limit to > Exclude >		1,779 Documents with 3,306 Substances, 345 Reactions, 5 Targets	ear \downarrow 🗸 🛛 Heatmap 🎛						
	Publication Year	\sim	Q Weed control by metabolites produced from Diaporthe schini							
	Document Type	\checkmark	Brun, Thiarles; Rabuske, Jéssica E.; Confortin, Tássia C.; Luft, Luciana; Todero, Izelmar; Fischer, Marnese, 2004, 100, 100, 100, 100, 100, 100, 100,	- I						
	Authors/Inventors	Abstract ∨ Index Terms ∨ Full Text ¬								
	Current Patent Assignee	\sim	Abstract hit: {Amaranthus viridis, Bidens pilosa, Echinocloa crusgalli, and Lollium multiflorum were performed. Fungal broth}	~						
	Patent Office	\checkmark	Index Terms hit: {article, Bidens pilosa, controlled study}	~						
	Journal Title Substance Classes Yang, Meng Medica 202		ictional and Mechanistic Studies of Two Anti-coccidial Herbs, Bidens pilosa and Artemisia indica							
			² Yang, Meng-Ting; Lin, Yi-Xian; Yang, Greta; Kuo, Tien-Fen; Liang, Yu-Chen; Lee, Tsung-Han; Chang, Cicero Lee-Tian; Yang, Wen-Chin [Planta Medica 2022 vol 88 # 3.4 n 282 - 291]							
	Reaction Classes	\sim	Abstract ∨ Index Terms ∨ Substances 3 ∨ Full Text 7							
	Index Terms (List)	\sim	Abstract hit: {composed of Bidens pilosa, Artemisia indica, and both used in combination. We found}	~						
	Index Terms (ReaxysTree)	\checkmark	Index Terms hit: {Asteraceae, Bidens pilosa, chicken}	~						
	Manually processed content only		Effects of applying Bidens species straw to Cd-contaminated soil on growth and cadmium accumulation of Ziziphus Acidojujuba seedlings							



文獻介面的重點提示④

Deenver

ELSEVIER

Reaxys					Quick search	Query builder Resu	Retrosynthesis	History Alerts			Ryan Huang 👌 🤇
1.85 K	Filters Limit to > Exclude	>	1,847	Documents with 3,45 selected O	0 Substances, 345 Reaction) <u>1</u> ude Export	ns, 5 Targets			ଷ୍ <mark>ଠ</mark> ଷ୍	Sort by Publication Year 🕹 🗸	Bioactivity Visualization
ľ	letter short survey View I	3 2 more	L W	/eed control by metab run, Thiarles; Rabuske, Jéssic nvironmental technology, 2 ostract v Index Terms v	olites produced from ca E.; Confortin, Tássia C.; 2022, vol. 43, # 1, p. 139 - 1 Full Text ㅋ	1 Diaporthe schini Luft, Luciana; Todero, Izelmar, 48]	Fischer, Matheus; Zabot, G	iovani L; Mazutti, Marcio A	Cited	5 times	
	Current Patent Assignee	~		Abstract hit: {Amara	inthus viridis, Bidens pi	losa, Echinocloa crusgalli,	and Lollium multiflorun	n were performed. Fung	al broth}		~
Patent Office V Index Terms hit: {article, Bidens pilosa, controlled study}							~				
Journal Title V P P P P P P P P P P P P P P P P P P				Powder containing biomolecules from Diaporthe schini for weed control Brun, Thiaries; Rabuske, Jéssica E.; Luft, Luciana; Confortin, Tássia C.; Todero, Izelmar; Alta, Bruno C.; Zabot, Giovani L.; Mazutti, Marcio A. [Environmental technology, 2022, vol. 43, # 14, p. 2135 - 2144] Abstract V Index Terms V Substances I V Full Text R							
	Index Terms (115)	~		Abstract hit: {contro	l of Bidens pilosa L., Ar	naranthus viridis L., Echin	ochloa crusgalli (L.) Beau	ıv., and}			~
	Index Terms (ReaxysTree)			Index Terms hit: {A	rticle, Bidens pilosa, cor	ntrolled study}					~
	physico chemical proper physico chemical analysi chemical transformations quantum chemical calcula	344 219 177 at 3	J Fu 3 Ya Ab	unctional and Med ang, Meng-Ting; Lin, Yi Indica, 2022, vol. 88, # : ostract 🗸 Index Term	Highligh 尋找特定	<mark>it:</mark> 旨的材料 [;]	<mark>性質、分</mark>	ca V <u>en-Chin</u> [Planta	1		
	View	more		Abstract hit: {co	析方法	,看這裡	^Γ Index				~
30	Manually processed content only			Index Terms hit:	Term (R	eaxys tr	ee)」				Feedback [

文獻介面的重點提示(5)

Reaxys

_							
	17 1.85 К	Filters					
	E Preview	Publication Year	~	位于19	<u> </u>		
		Document Type	\sim	的授	守紀木,王朳迭倖迥 日		
		Authors/Inventors	~	/忠			
		Current Patent Assignee	~		Author keyword: Artemisi		
		Current Patent Assignee	~		genic feed additive • phyt		
		Patent Office	\sim		EMTREE medical term: A		
					fection • bacterium • Bur		
		Journal Title	\sim		Lauraceae • Lythraceae • I		
					Piperaceae • plant • Poace		
		Substance Classes	\sim	•	 systematic review - Tax: 		
		Ponction Classes			Reaxys Index Terms: Pern		
		Reaction Classes	Ý		Review on Documented I		
		Index Terms (List)	\sim	2	Joshi, Bhuwan C.; Juyal, Vijay; Sa		
		Index Terms (ReaxysTree)	^		E111021197159, p. 2 - 158] Abstract 🗸 Index Terms 🗸		
2		chemical transformations physico chemical analysis meth.	16 8		Index Terms hit: {Bhe		







Quick Search 輸入Cas Number



如何進行新的Quick Search





Quick search 輸入Cas registry number

Quick search Query builder Results Retrosynthesis History Alerts Search for "50-00-0" Search Reaxys ["50-00-0"] x Find > Documents, e.g. Tetrahedron, 2014, 70, 2343 AND 100 Draw



Preview page各種資料類型



Recap <文獻搜尋>

- 如何進行關鍵字搜尋
- 區分科學文獻與專利
- 找討論分析方法與材料性質的文章: Index Term Reaxys Tree
- 從眾多文獻中整理所有相關的化合物 (天然物、藥物文獻)
- Quick Search 提供各種資料類型 挑選正確的資料類型







Quick Search 結構搜尋



Quick Search 結構搜尋









MarvinJS 結構編輯器





絕對結構搜尋 As drawn





相似結構搜尋 As substructure





相似結構搜尋 Slock & Smax

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Ryan Huang 👌 🕐





(151) Reaxys 結構編輯器 - 相似結構搜尋 原子鎖工具 - YouTube

不定位鍵的使用



(151) Reaxys 結構編輯器 - 不定位鍵 - YouTube



更多關於結構編輯器的進階技巧

(151) Reaxys 結構編輯器 - 縮寫官能基團 - YouTube

(151) Reaxys 結構編輯器 - 原子屬性列表 - YouTube

<u>(151) Reaxys 結構編輯器 - G 任意官能基工具定義 - YouTube</u>

(151) Reaxys 結構編輯器 - R 基團與末端定義工具 - YouTube

<u>(151) Reaxys</u> 結構編輯器 - 原子列表與原子列表非 - YouTube

(151) Reaxys 結構編輯器 - 鹽類與同位素 - YouTube





訂閱Elsevier Taiwan 自學線上資源



https://www.youtube.com/playlist?list=PLBSTWv uNnJAl4laTo5zNkqaJ9va-LUtj0



應用案例-新穎性搜尋Novelty Search









ELSE

Solubility, g∙l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					water, soluble III	[אמנוסוווסובנעומו מוסגנבוונב, צעד, יטו. בד, ה בב, ף. בסטר בסטט]
					organic solvents	Full Text 7 Cited 27 times 7 Details > Abstract >
6.73904	in pure solvent		aq. phosphate buffer	supporting information		Chung, Sanny S. W.; Cuellar, Rebecca A. D.; Wang, Xiangyuan; Reczek, Peter R. ; Georg, Gunda I.; Wolgemuth, Debra J.[ACS Medicinal Chemistry Letters, 2013, vol. 4, # 5, p. 446 - 450] Full Text a Cited 8 times a Details > Abstract >
15	in solution	25	aq. phosphate buffer			Ambike, Anshuman A.; Mahac 提供原始文獻連結 2005, vol. 22, # 6, p. 990 - 998] Full Text ㅋ Cited 149 times ㅋ Details > Abstract >
7.3E-05	in pure solvent	25	H2O			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002 , vol. 25, # 3, p. 346 - 350] Full Text 🤉 Details > Abstract >
79.55	in pure solvent	25	propan-2- ol			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and pharmaceutical bulletin, 2002 , vol. 25, # 3, p. 346 - 350] Full Text a Details > Abstract >
19.09	in pure solvent	25	diethyl ether			Matsuyama, Kenji; Nakagawa, Kimiko; Nakai, Aki; Konishi, Yuriko; Nishikata, Mayumi; Tanaka, Hiromi; Uchida, Takahiro[Biological and














Recap <結構搜尋>

- ChemDraw 複製 Ctrl+Alt+C 貼上Ctrl+V
- 原子鎖與開放工具
- 不定位鍵的使用
- 進階搜尋的Youtube短片合輯







Reactions Search





您可以用各種方式搜尋Reaction

1. 從物質資訊頁面連結到製備方式

 關鍵字搜尋、命名反應搜尋 (例如 Suzuki coupling)

3. 畫出反應式搜尋





方法一、由物質頁面連結到製備方式 Preparation





方法二、直接輸入反應關鍵字或是命名反應













ELSEVIER







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Conditions	Yield	Reference		
With tris(dibenzylideneacetone)dipalladium ⁽⁹⁾ chloroform complex; 2,2'-bis-(diphenylphosphino)-1,1'- binaphthyl; sodium t-butanolate In 5,5-dimethyl-1,3-cyclohexadiene at 140°C; for Sh; Temperature;	92%	Kang, Julie; Lee, Jun Young; Park, Jeong-Hoon; Chang, Dong-Jo [Journal of labelled compounds and radiopharmaceuticals, 2020, vol 63, #4, p. 174 - 182] Full Text z Details > Abstract >		
Conditions A 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 🛩		KRKA, D. D., NOVO MESTO; BENKIC Primoz; TIHI Jaroslav; PECAVAR Anica; CERMAN Tamara; VRECER Franc; VAJS Anamarija SKRABANJA Vda WO2011/157450, 2011 , A1 Location in patent: Page/Page column 19 Full Text a Details > Abstract >		
	100%	METHYLGENE INC.		
With dihydrogen peroxide; methyltrioxorhenium(VII) In dichloromethane; water at 15°C; for 5h; Experimental Procedure 🗸	10076	WO2005/92899, 2005 , A1 Location in patent: Page/Page column 73 Full Text > Details > Abstract >		





箭頭在下 <mark>催化劑</mark> 或溶劑



方法三、結構編輯器畫反應式

- 指定反應中心





- 記得探索左邊的反應過濾器

Reaxys Quick search Query builder Results Retrosynthesis History Alerts Ryan Huang 🕺 📀 11.49 K Filters 11,489 Reactions out of 6,833 Documents, containing 12,995 Substances, 2,202 Targets ⊥ 0 0 selected Q O Sort by No of References 🚽 🗸 Limit To Exclude Export Show Conditions 隱藏實驗條件 By Structure \sim Yield \sim Reagent/Catalyst \sim Solvent E 🖉 🕀 🖶 … 🗳 분 Ø, Q B ··· ऄ Catalyst Classes 究主題有 ar > Reaction ID: 601797 Solvent Classes 興趣的催化劑/溶 劑/反應類型 oduct Availability Reactant Availability \sim Reaction Classes ᇆ Ø, @ B ··· ऄ ₽ 0, 0, 8 ... 3 Document Type \sim Publication 511 Conditions V Find Similar > Reaction ID: 608056 Single step reactions only 篩襈有曺驗材料 mental procedu 方法的反應式 _ (152) Reaxys 反應式搜尋 - 基本過濾工具 - YouTube ELSEVIER





Query Search 進階查詢



進階搜尋的使用時機







進階搜尋 – 結合反應式+實驗細節關鍵字





更多進階搜尋範例



Elsevier 簡介 產品與解決方案 服務 購物與探索 搜尋 Q

- 🗸 Reaxys API Case Study
- ↓ Reaxys 快速參考指南
- Facebook 粉絲專業 「Reaxys」的研究迷俱樂部 ↗
- Reaxys User Day 2022 線上研討會

搜尋範例與技巧

- ↓ 如何尋找商用大量的合成原料
- ↓ 如何搜尋不含鈷的電極材料資訊
- ↓ 如何鑑定副產物
- ↓ 汽車催化劑領域
- ↓ 尋找攝氏 6o 度昇華的特定結構有機材料
- ↓ 農藥領域
- ↓ 電子材料領域
- ↓ 電池領域材料
- ↓碳材料領域
- ↓ 顔料領域



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化學資料和文獻 - Reaxys | Elsevier







Retrosynthesis 逆合成面板



在Reaxys的任何位置點及燒瓶圖示即可搜尋全合成計畫





Retrosynthesis 逆合成工具



Retrosynthesis 逆合成工具



ELSEVIER

Reaxys Retrosynthesi AI

-結合 高品質的Reaxys reactions資料 與 神經網路 (Neural Network) 3N-MCTS 科技



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





Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler^{1,2}, Mike Preuss² & Mark P. Waller⁴



3N-MCTS : 3 layers Neural Network - Monte-Carlo-Tree-Search



簡單的介面,只要10分鐘的預測時間 -只要畫出目標分子, Reaxys 15M的反應式做後盾





簡單的介面,只要10分鐘的預測時間 -只要畫出目標分子, Reaxys 15M的反應式做後盾

Reaxys	Quick search Query b	uilder	Results	Retrosynthesis History Petervan Stroaten 🐣 🧟 🕐
Baste Lecurt		toon _o o		Hale Econoples Fallsacen Tells view Too very
Predicated 15 Project 10	Predicted routes #1	Step 1	Stup 2 Stup D Score VA	p 1 Stup 4 P D X
ille, Sochuch Vegedz Grav		*of23 1 6	0,89	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ \hline \Pi & \mathcal{O}_1 & \oplus & \oplus \\ & & \\ & & \\ \hline \Pi & \mathcal{O}_1 & \oplus & \oplus \\ & & \\ & & \\ \hline \Pi & \mathcal{O}_1 & \oplus & \oplus \\ & & \\ \hline \Pi & \mathcal{O}_1 & \oplus \\ & & \\ \hline \Pi & \Pi & \\ \Pi & \Pi & \\ \hline \Pi & \Pi & \\ \Pi & \Pi & \\ \hline \Pi & \Pi & \\ \Pi & \Pi & \\ \hline \Pi & \Pi & \\ \hline \Pi & \Pi & \\ \Pi & \Pi &$
	Sup 2 Sup 3		•	Continuos Vield Beforece Vield Continuos Vield Control Contro
		2	6.89	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & & $
				With pyridinium toflumasentite at 110°C; fir 50% Chen, Xianfong, Lin, Suit; Xu, Yuan; Zou, Gang Tetrahadran, 2022, vol. 64, ii. 24, p. 4813 - 4810 Superimental Procedure ∨ Full Test ≠ Cited 20 times ≠ Details 5 -

自動搜尋呈現文獻中"相似"的反應,畫 面(左側)呈現預測路徑,(右側)呈現 Reference路徑,讓您輕鬆判斷可行性

提供完整的實驗材料方法
 Experimental Procedure讓您參考
 如何規劃實驗細節





How chemists evaluate Reaxys AI Retrosynthesis Tool

- Pilot trial in ETH Zurich, Professor Carreira Research Group





Moritz Classen of the Carreira Research Group, ETH Zurich

- > 30 molecules tested with 7 groups (PhD students, postdoc)
- Manual & AI routes were separately generated and compared
- If AI were innovative enough to find novel structure disonnects?



Image acquired from webinar: Development of Reaxys retrosynthesis, its use and adoption by chemist <u>https://www.youtube.com/watch?v=7DZgX8do5wM</u>

An online Taiwan webinar to share with academic community

- You can now test Reaxys AI retrosynthesis!

人工智慧在藥物合成設計中的應用 -Reaxys 預測逆合成工具為你解密 Development of Reaxys[®] Predictive Retrosynthesis, its use and adoption by chemists





ETH Zurich 蘇黎世聯邦理工學院

Moritz Hansen 在蘇黎世聯邦理工學院獲得學士和碩士學位,在此之前他在大學時期跟著 Bode 教授、Schlüter 教授和 Rivera-Fuentes 教授的團隊進行研究。 2019 年,他加入了 Carreira 教授*的研究小組,繼續他的博士研究,主要研究工作是從人類微生物組中提取複 雜天然產品的合成。查看英文簡歷 View English bio +

Moritz Classen

ETH Zurich 蘇黎世聯邦理工學院

Moritz Classen 於 2012 年在德國路德維希 - 馬克西米利安 - 慕尼黑大學開始他的化學研究。 在跟著 Trauner 教授和 Aggarwal 教授的研究小組後,他加入了 Erick. M. Carreira 教授^{*} 在蘇 黎世聯邦理工學院的研究小組,於 2017 年發表碩士論文,2018 年發表博士論文。他的研究 重點是從甘遂 (Euphorbia kansui)中分離出的複雜二萜類化合物的合成。查看英文簡歷 View English bio⁺

Dr. Abhinav Kumar

Elsevier

Abhinav 是 Reaxys 產品研發團隊的一員,主要負責將創新產品推向市場。在加入 Reaxys 團隊 之前, Abhinav 在德勤工作,主要負責生命科學領域的客戶諮詢工作,涉及策略和運營,專 注於研發職能,並為研發和商業的資深領導團隊提供服務。Abhinav 在倫敦國王學院獲得了 製藥科學的博士學位。Abhinav 已經發表了 10 多篇論文,指導了 2 名博士生和 10 多名碩士 生的論文,並獲得了多項獎補助和獎項,包括 2014 年 Pat Burnell 肺部藥物輸送新研究者 獎。查看英文簡歷 View English bio +



Learn more about Reaxys AI retrosynthesis in 20 minutes

- 20 minutes highlights with Chinese subtitles



戰看宗教:5次2022年6月19日 Elsevier 台灣線上研討會,邀請解發世聯邦理工學院 Carreira 教授 研究團隊成員,分享團隊到試 Reaxys Predictive Retrosynthesis 橫絕的反體 這個 viceo為研訂會對購購等 上 Monitz Classen (第二位講者)分享團隊如何比較人工與AI預則路 徑,並舒興地發現AI能協助創新的合成想法



✓ Scan QR ✓ Save ✓ Contact us

活動精華 + 中文字幕 "現階段的逆合成AI能做些甚麼?"



讓Reaxys伴隨你的化學旅程





其他自學線上資源

▶ YouTube [™]



RxED Learning Chemistry with Reaxys (English)



(152) RxED: Learning Chemistry with Reaxys - YouTube





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歡迎來信留下您對Reaxys的所有問題~ <u>r.huang@elsevier.com</u>





Reaxys Commercial Substances

供應商物質資料庫



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

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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

ELSEVIER


Reaxys Commercial Substances 為每一筆物質提供詳細的供應商列表(A)包括 純度、價格、包裝及到貨時間。您可利用篩選工具(B)加速挑選過程,並點擊供 應商品頁面連結(C)造訪供應商網頁。

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Interview	By Structure	~		Supplier	Product	Purity	Packag	e size & price	Availability	
	Molecular Weight	~		Enamine - USA (I) USA	186519-92-6 EN300-152527 7		mg		Lier Lime: Lier Z Last updated: 2020-06-01	
	Number of Fragments	~		eMolecules	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid	95%	500	159 USD	Shipment time: 2-10 days	
	Availability in other databases	~		Enamine - USA 🕕 USA	186519-92-6 EN300-152527 7		mg		Tier Time: Tier 2 Last updated: 2020-06-01	
	Supplier	~		eMolecules Manchester Organics Ltd. (0)	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid		1 g	994 USD	Shipment time: 12 weeks	
	Supplier Geolocation	~ <	1	USA	F45799 7				Last updated: 2020-06-01	
	Usage Classification	~		eMolecules Oakwood Chemicals	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6	95%	250	134 USD	Shipment time: 1-5 days Tier Time: Tier 1	
	Package Size	~	(B)	USA	076916 7		0		Last updated: 2020-06-01	
	Price	~		eMolecules Oakwood Chemicals ①	4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6	95%	lg	241 USD	Shipment time: 1-5 days Tier Time: Tier 1	
	Purity	~		USA					Last updated: 2020-06-01	
	Stock Availability	~		eMolecules Pharmablock ① USA	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid 186519-92-6 PB02420 7		10 g	670 USD	Shipment time: 4 weeks Tier Time: Tier 3 Last updated: 2020-06-01	
	Shipment Time	~		eMolecules	4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-car		50 g	2241 USD	Shipment time: 4 weeks	
	Shipment Country	~		Pharmablock 🕕 USA	186519-92-6 PB02420 7		5		Tier Time: Tier 3 Last updated: 20 Feedbac	ck 🖓



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如何管理搜尋結果 儲存、比較、Email提醒與資料匯 出



如何管理搜尋結果

需要申請(免費)個人帳號

- 儲存 搜尋結果隔日繼續
- 比較兩筆不同的搜尋結果
- Email提醒 –利用Reaxys主動通知符合搜尋條件的新文章
- 資料輸出 & 限制



如何儲存搜尋結果並於日後繼續使用 (1/3)





如何儲存搜尋結果並於日後繼續使用(2/3)

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如何儲存搜尋結果並於日後繼續使用 (3/3)





比較 兩筆不同的搜尋結果

 有時候我們會用不同的關鍵字、或搜尋策略來涵蓋同一個主題,如 何有效地排除相同的(文章、物質),節省時間?

例如於兩天用兩組不同的關鍵字搜尋

(周一) Surface treatment + Boron nitride = 458 documents

(周二) Surface treatment + BN = 349 documents













Documents; substances; patents

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資料輸出 & 限制









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更多關於結構編輯器的進階技巧

(151) Reaxys 結構編輯器 - 縮寫官能基團 - YouTube

(151) Reaxys 結構編輯器 - 原子屬性列表 - YouTube

<u>(151) Reaxys 結構編輯器 - G 任意官能基工具定義 - YouTube</u>

(151) Reaxys 結構編輯器 - R 基團與末端定義工具 - YouTube

<u>(151) Reaxys</u> 結構編輯器 - 原子列表與原子列表非 - YouTube

(151) Reaxys 結構編輯器 - 鹽類與同位素 - YouTube





訂閱Elsevier Taiwan 自學線上資源



https://www.youtube.com/playlist?list=PLBSTWv uNnJAl4IaTo5zNkgaJ9va-LUtj0



Reaxys User Day

形式:網路研討會 日期:6 April 時間:台灣時間17:00-20:00

> Reaxys Vision and product roadmap How Reaxys help you



Customer presentations

How Reaxys helps me

KOL round table discussion:

Authoritativeness in Chem. R&D

Reaxys

A day of sharing with the global Reaxys community

The Reaxys User Day is a global event where experienced scientists from around the world will share how they're finding ways to gain faster and more reliable access to the information they need—and you're invited. It's a unique opportunity to update yourself on the newest developments in discovery technology, and participate in breakout sessions with our expert customer consultants where you can ask questions and learn how to make the most of Reaxys.

User presentations on successful approaches to key challenges:







Optimizing drug-target interactions with bioactivity and pharmacological data for effective compound design



Driving efficiencies in synthetic chemistry with AI-enhanced technology



Agenda

- 1. Reaxys簡易介紹
- 2. (示範) 結構搜尋
- 3. (示範) 進階關鍵字搜尋
- 4. 帳號、資料管理
- 5. 結構編輯器線上資源



6. Reaxys User Day 邀請



如何連上Reaxys

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



Got it

Reaxys 正在打造與製藥、化學研究領域最快速、完整的專利收集



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提供自2000~最新完整的藥物、化學專利收錄、提供藥物靶點、化合物索引

特色 (I) Reaxys 提供非英語專利高品質英文譯本

105 offices, 170 IPC, non-English language patents translated prior to processing by our supplier 🥢





	s; mTOR inhibitors; TGF-	b signaling agents; TGF-b red	ceptor agonists; histone deace	tylase inhibitors; corticoster	roids;}
ront page info					
Assignees			Inventors (Authors)		
THE REGENTS OF THE U	UNIVERSITY OF MICHIGAN		MOON, James J.; SCHV	VENDEMAN, Anna A.; NAJAFAI	BADI, Sayed Alireza Hassa
Patent No	Kind Code	Publ. Date	Application No	Filing Date	Indexed Patent
WO2021/16082	A1	2021/01/28		2020/07/17	yes
	~1	2023/03/26		2020/07/27	yes

COMPOSITIONS AND METHODS FOR TREATING AUTOMAMUNE DISORDER

Bibliographic excerption includes: Patent number, title, assignee and inventor, abstract, claims, IPC class, kind code, filing and publication dates and patent family members.



特色 (II) 靶點蛋白索引與搜尋

- 克服基因、蛋白名稱混亂,同義詞雜等搜尋障礙
- 以機器學習系統辨識相關性



Target indexing for 12 priority offices and 7 IPC classes



Primary target indexing over full patent document



Indexed terms highlight target name and searched synonyms





快速自動索引化學結構

- 深入內文、表格與圖片
- 以機器學習系統辨識相關性



Enrichment for 12 priority offices and 170 IPC classes

Substances names and structures (excl. Markush) excerpted from full patent document

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Substances discoverable via name or structure search and visible per patent record

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- 2. I2S技術搜尋化合物結構圖片、索引收錄物質資料庫。



自動索引系統確保即時性、人工索引系統兼顧深度與正確性





Primary Market PO: WO, EP, US, CN, JP, KR, TW

11 IPC including: Drugs, Dyes, Agrochemistry and Organic chemistry

人工索引系統 -索引內容





Substances

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Description

Chemical

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