



使用Reaxys精準搜尋關鍵數據, 節省查找時間





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- 2. Reaxys查詢頁面介紹
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- 5. Quick Search: 化合物、物性查詢
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 - 多條件查詢 (天然物、抗菌活性、分子式)
 - 排除雜訊
 - 多條件查詢(用途)



Reaxys介紹



What in Reaxys?

- 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」



What in Reaxys?

從研究人員最常關注450種期刊、專利,萃取實用的實驗數據

- 有機化學 1771年~
- 無機化學·有機金屬 1772年~

來自超過15,000種期刊的全文資料,使用自然語言處理技術抽出資料

- 化合物名稱
- 反應分類(氧化、還原、縮合....)
- 人名反應、物性...

收錄專利報告相關內容



Reaxys的資料結構

- 從多個資料來源將化合物及反應彙整到1筆紀錄
- 並且保留資料來源的連結



Reaxys 為使用者設計最簡明的搜尋入口

Quick Search



Reaxys 為使用者顯示最相關的查詢結果



Reaxys 提供進階的查詢方式



Reaxys 透過單筆查詢紀錄提供大量數據

顯示文章相關化合物



Reaxys 提供篩選條件快速縮小查詢範圍

142	Filters and Analysis	Apply	*	142	2	Filters and Analysis	Apply	≽	
queries 420	Index Terms (List) 1		^	quer 420	ies 0	Index Terms (List) 1		^	
1.21	stereoselectivity	—	44			stereoselectivity	—	44	
1,21 mm	enantioselectivity		24	1,21	mii	enantioselectivity	-	24	
984.003	total synthesis	-	18	984.0	003	total synthesis	-	18	
231	oxidation reaction	-	18	23	1	oxidation reaction	-	18	
589	enantiomer excess	-	11	58	9	enantiomer excess	-	11	
612	catalysed reaction	-	11	61	,	catalysed reaction	-	11	
	catalyst	-	10			catalyst	-	10	
142	+ More			142	2	+ More			
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	Publication Year		~			Publication Year		~	
	1998	-	3			Desument			
	2006	-	2			Document Type		~	
	2009	-	2			Authors		~	
	1994	-	1			weinreb, steven m	_	2	
	2008	-	1			nakata, tadashi	-	1	
	2015		0			kroutil, wolfgang		0	
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	+ More					oishi, takeshi		0	
	Document Type		~			nakamura, kaoru		0	





Reaxys查詢頁面介紹



Reaxys – Quick search page

JRL: <u>www.rea</u>	<u>xys.com</u>	
← → C ■ 安全 https	://new.reaxys.com/#/search/quick	07 ☆
Reaxys	Quick search Query builder Results Synthesis planner () History	^ Ţ Ø
Import 坐	Search for esterification of benzoic acid	Find >
關鍵字輸入	Search Reaxys Q esterification of benzoic acid X	
結構、反應 繪製	AND	
ELSEVIER	© 2018 RELX Intellectual Properties SA. Terms and Conditions Privacy policy Performance Page	≪ RELX Group™
4	Cookies are used by this site. To decline or learn more, visit our Cookies page	Feedback 💭

- Quick search: 關鍵字查詢、結構查詢
- **②** Query builder:多條件組合查詢
- ③ Results:查詢結果顯示,優先顯示最相關結果。
- **④** Synthesis planner: 逆合成分析。
- **⑤** History: 歷史紀錄查詢。

Reaxys – Query builder page





Quick Search: 反應查詢



反應條件設定(1/3)

検索例:Esomeprazole之衍生物合成方式查詢

Esomeprazole為一種稱為「氫離子幫浦阻斷劑」類的藥物。此類藥物具有顯著及長效、降低「胃酸分泌」的作用。

① 點擊「Create Structure or Reaction Drawing」,移至繪圖畫面



反應條件設定(2/3)

Create structure ten	nplate from name			×
is is tratewith	Enter a chemical name, CAS-RN, InChiKey or SMILES	Q		
ends with contains	Marvin JS		O S F	Stereo Additional r Related Mar



名稱輸入畫面:

輸入"esomeprazole"→點擊放大鏡圖案 Q

- 還可選擇以下條件
 - 完全一致(is)
 - 前方一致(starts with)
 - 後方一致(ends with)
 - 部分一致(contains)
- 可能同時有多種名稱可供選擇

編輯構造式:

依名稱自動產生結構

為了以esomeprazole的主結構進行查詢,透過 Structure editor進行編輯,將環上的取代基全 部刪除

反應條件設定(3/3)



傳送結構至查詢頁面

- ① 選擇 As Substructure
- 點擊「Transfer to query」進入查詢 頁面



開始進行查詢

當結構顯示在畫面上後,點擊「Find」 開始查詢





①結構查詢選項

- As Drawn:完全相同
- As Substructure:衍生物查詢
 - on all atoms:所有原子取代
 - on heteroatoms: 雜原子取代
- Similarity:相似性查詢

2 其他查詢選項

- Tautomers
- Stereo
- Additional ring closure
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges



Reaxys會先顯示分類結果,如以結構查詢,會同時顯示化合物結果及反應結果。

為了查詢Esomeprazole及其衍生物的合成方法,點擊Reaction之中的「View Results」按鈕



查詢結果畫面(1/7)

Esomeprazole及其衍生物合成方法的搜索結果,可使用各種篩選條件縮小查詢範圍,並可從 搜索結果中連結全文頁面及還檢視引用情形。



查詢結果畫面(2/7)

③實驗步驟



⑥切換結果排序方式



排序類型

- Reaxys ranking
- No of references
- Reactant availability
- Product availability
- MW of product
- Yield
- Publication year

反應查詢之篩選條件

4篩選條件

3,487	Filters and Analysis			
	By Structure	\sim	← 結構	使用篩選功能,除了縮小查詢結果
	Yield	\sim	← 產率	範圍外,還可以作為瞭解趨勢的簡 留丁目
	Reagent/Catalyst	\sim	← 試劑、催化劑	
	Solvent	\sim	← 溶劑	
	Catalyst Classes	\sim	← 催化劑分類	
	Solvent Classes	\sim	← 溶劑分類	
	Product Availability	~	← 作為產物的可用性	
	Reactant Availability	\sim	← 作為反應物的可用性	
	Reaction Classes	\sim	← 反應類型	
	Document Type	\sim	← 文獻類型	
	Publication Year	\sim	← 出版年	
	Single step reactions only		← 1步反應	

查詢結果畫面(4/7)

第1筆紀錄的詳細內容:

- Experimental Procedure
 - 實驗步驟詳細顯示
- Show Reference
 - 文獻來源顯示



2.2. Standard procedure for small-scale catalytic sulfoxidation

General procedure: Sulfide (OMS or LPS, 100 mol) and the Ti-salalen catalyst(1.1 mol) were dissolved in the solvent (typically: EtOAc, 6.0 mL),the mixture was thermostatted at desired temperature (typically 0 °C, or -20 to +20 °C for variable-temperature measurements),and 30percent aqueous hydrogen peroxide (0.105 mmol of H_2O_2) was then introduced in one portion. Stirring (500 rpm) was continued at that temperature (typically 24 h). For low-temperature experiments, the reaction times were about 30 h at -10 °C and up to 10 days at -20 °C. To analyze the reaction outcome, 20 L aliquots of the reaction mixture were taken to a vial and immediately carefully evaporated to dryness with a stream of compressed air during ca. 15–20 s. The remaining solid was dissolved in 0.20 mL of 1percent Et₃N solution in isopropyl alcohol, and the contents of residual sulfide, (R)- and(S)-sulfoxide, and sulfone, were analyzed by chiral HPLC as noted above.





查詢結果畫面(6/7)

點擊Details後,會顯示文獻的Abstract、Index Term,另外點擊Substance及Reactions會顯示文獻中所有相關的化合物及反應,而Full Text則是文獻出處連結。



查詢結果畫面(7/7)



點擊作者名稱時,可連結至**Scopus**顯示該作者的相關著作及引用情形。

Scopus是什麼

Scopus是Elsevier所建構全球 最大的書目和引用信息數據庫 可以檢視Reaxys中文獻的被引 用情形



Synthesis Planner



建構合成路徑(1/3)

Synthesis Planner: 可透過逆合成分析建構合成路徑

- 畫面上可同時提供多種合成方式,便利比較評估
- 也可於化合物查詢結果頁面進入Synthesis Planner

<u> 查詢範例:Omeprazole的合成</u>

從反應查詢結果進入Synthesis Planner。

- ① 點擊 🖫 ,將該化合物作為起始點
- ② 可選擇使用Manually或Autoplan 啟動Synthesis Planner
 - Manually:手動逐步建立合成路徑
 - Autoplan:顯示Reaxys建議合成路徑



Weiwei Cheng 👌 🛴

⊙

] 문 Ø1

Full Text 🛪 Details > Abstract >

RATIOPHARM GMBH - US2008/319195, 2008, A1 en en sou parte de la composición de la

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Q ---- Q

£ Ξ

×

Synthesis Planner Plan 1 Edit 🧬 ≏ 坐 Autoplan 1 5 🔨 Import Save Export Plan 1 2 Plan 2 3 Plan 3 \odot 8 <u>=</u> 4 Plan 4 Plan 5 93.5% $\mathbf{P} \mathcal{O}_1$ 80 (i) Show conditions × 🚫 Hide preparation + Add preparations Conditions 💼 Remove preparation Preparation - 1 Yield Conditions Reference 93.5% With C68H72N4O10Ti2; dihydrogen peroxide In water; ethyl Talsi, Evgenii P.; Bryliakov, Konstantin P. - Catalysis Today, 2017, acetate at 0°C; for 24h; Reagent/catalyst; enantioselective vol. 279, p. 84 - 89 reaction; Full Text 7 Cited 1 times 7 Details > Experimental Procedure 🗸 Abstract > 86% With N-methyl-6-aza-5β,6β-epoxy-cholestane-3β-tert-Zhou, Guobin; Guan, Yueqing - Heterocyclic Communications, butyldiphenylsilyloxy tetrafluoroborate In dichloromethane at 2016, vol. 22, # 1, p. 17 - 19 -70 - 20°C; for 3h; Inert atmosphere; enantioselective reaction;

93 % ee

Reaxys

Quick search Query builder Results Synthesis planner History

With tert.-butylhydroperoxide In water; toluene at -20°C; for

Autoplan

- •自動規劃5種合成路徑
- •反應產率顯示於路徑上,點擊可顯 示實驗步驟

建構合成路徑(2/3)

建構合成路徑(3/3)

Manually

•選擇要加入的反應,按下**Syn-Plan** •反應直接加入於合成路徑





Quick Search: 化合物、物性查詢





検索例: Gefitinib (吉非替尼)之溶解度查詢

Gefitinib為表皮生長因子接受體(epidermal growth factor receptor, EGFR) 酪胺酸激酶酵素 (tyrosine kinase)之專一性抑制劑,通常表現於上皮細胞源頭之人類實體腫瘤。抑制EGFR 酪胺酸激酶酵素之活性,便抑制了腫瘤之生長、轉移及血管增生,並促進癌細胞之脫離。

在畫面中央輸入Solubility of geftinib,再按下左上角的Find。

Reaxys	Quick search Query builder Results Synthesis planner	History	Sam Yu 🎗	Ŷ	?
Import 🕹	Search for solubility of gefitinib			Fine	4 >
	Search Reaxys Q solubility of gefitinib	×			
	Create Structure or Reaction Drawing				



查詢結果分類:Substances、Documents



查詢結果畫面(1/5)

Hit Data直接給出具體的實驗資料、實驗條件及全文連結



查詢結果畫面(2/5)

Reaxys直接將物性分類,並直接顯示相關數據



查詢結果畫面(3/5)

Reaxys直接摘錄原文中的NMR圖譜描述,並標註原文中的位置



查詢結果畫面(4/5)

Reaxys的文獻整理·讓閱讀文獻更加快速



查詢結果畫面(5/5)

Reaxys通過Index Term Reaxys Tree的方式,將文獻進行分類,幫助大家快速查找所需文獻。

chemical transformations
physico chemical properties
physico chemical analysis methods
quantum chemical calculation methods





查詢結果的輸出、儲存及通知



輸出查詢結果(1/3)

查詢結果可以導出的格式包含PDF、XML、Word、Excel。



輸出查詢結果(2/3)

Export會顯示目前的導出狀態,

完成後會顯示Download,點擊即可儲存,

下載完成後,點擊Cancel已關閉畫面,

如果沒有關閉下載畫面,無法開始下一次 的輸出。







輸出查詢結果(3/3)

輸出詳細設定說明:

Choose a format:格式選擇

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Electronic Lab Netbook
- RD File
- SD/Molfile
- Smiles

Range:結果輸出範圍選擇

- 上限為5,000筆數據

Export:輸出數據類型選擇

- All available data
- Identification data only
- Hit data only
- Choose sepcific data

Additional option:

- Include structure
- Include a description in the document

Export substances	Reaxys	
Choose a format:	PDF/Print	~
Range:	All results - 66	×
Export:	 All available data 	
	O Identification data only	
	◯ Hit data only	
	O Choose specific data	
Additional options:	Include structures	
	Include a description in the docu	ument
		E



每次使用完**Reaxys**後,查詢紀錄會自動清除,但登入帳號可以儲存查詢紀錄,下 次可以再度回顧先前查詢紀錄,

點擊畫面上方的History,

	Quick search Q	uery builder	Results	Synthesis planner	History	
-	Recent Saved					
	918 Substances	Today 18:46	Quick Search:	9		Edit Query C Save W Jert C View >

在**Recent**頁面中,確認要儲存的查詢紀錄, 按下**「Save」**,

在跳出的視窗輸入自訂名稱,再按下 Save,即完成儲存,

下次登入時,進入**History-Saved**頁面, 即可檢視上次儲存的查詢紀錄



Alert功能

Alert需於登入後才能使用,透過設定查詢結果,Reaxys會自動通知是否有最新研究

- 獲取相同查詢條件的反應及化合物最新資訊
- 可選定通知時間(Monthly / after each update)
- 訊息將會發送到註冊的e-mail,也可以寄送給其他人

Alert功能設定:

- ① 進入History頁面,將滑鼠移至要設定Alert的查詢紀錄,
- ② 點擊畫面右方出現的Alert,即可進入設定畫面。

Reaxys	Quick	search Query bui	lder <u>Results</u> Synthe	esis planner History & Q @		
876 Filters and Analysis		876 Substance	es out of 8,918 Documents, conta	ining 8,308 Reactions, 482 Targets 00 - 9 b		
By Structure	\sim	Limit To E	⊘ <u>↑</u> «dude Export	Reaxys' uick search Query builder Results Synthesis planner History	ς Ĵ	?
Measurement pX	\sim		Oleanolic acid	History		
Highest Clinical Phases	\sim	1	нс ан. C ₃₀ H ₄₈ O ₃ 456.	709 Recent Saved		
Targets	~		Druglikeness			
Parameters	~	▲ <u></u>	Bioactivity (All)	Reaxys		ſ
Substance Classes Molecular Weight	~		ursolic acid	876 Substances 🛛 Today 14:25 Query Builder: in substances - Molecular Formula "C30*" AND Subs Edit Query 🕞 Save 🖭 🔬	View)	>
		2	а, С ₃₀ Н48О3 450.	8 308 Reactions Today 14/24 Query Builder in reactions - Molecular Formula "C30*" AND Substance Basic Index "antimicrobi*"	View	la "C30*" ANI
				Opport reactions roughther query burden in reactions - Morecular Formula Col Airo bussance basic fluex antimicroor	view ,	
				8,308 Reactions Today 14:24 Query Builder: in reactions - Molecular Formula "C30*" AND Substance Basic Index "antimicrobi*"	View 🕽	>

Alert功能的設定及管理

Alert的設定:

Create Alert	
Query:	Query Builder: in substances - Molecular Formula "C30*" AND Substance Basic Index "antimicrobi*"
Alert name:	Choose a name
	Please enter a value
Send alerts to:	Email address
Frequency:	After each update
From databases:	PubChem LabNetwork
	eMolecules SigmaAldrich
	Reaxys

- Alert name: 名稱
- Send alerts to: 可同時輸入多組e-mail
- Frequency: 通知頻率
 - After each update
 - Monthly
 - Deactivate
- From databases: 來源資料庫選擇

點擊「Create Alert」即可完成設定。

Alert的管理:





Quick Search:文字查詢





検索例: Xylitol的熔點(melting point of xylitol)





<u>検索例:Benzoic acid(苯甲香酸)的酯化反應(esterification of benzoic acid)</u>





<u>検索例:Glutamine的HPLC分析結果(hplc glutamine)</u>



^	Hit Data - 2		
	 Chromatogr 	aphic Data - 2	2 hits out of 3 Show/Hide columns ↓
	Chromatographic data	Location	Reference
	HPLC (High performance liquid chromatography)		Han, Ningning; Li, Longlong; Peng, Mengling; Ma, Haitian - Phytotherapy Research, 2016, p. 1316 - 1329 Full Text 7 Cited 1 times 7 Details > Abstract >
	HPLC (High performance liquid chromatography)	supporting information	Taglang, Céline; Martínez-Prieto, Luis Miguel; Del Rosal, Iker; Maron, Laurent; Poteau, Romuald; Philippot, Karine; Chaudret, Bruno; () Rousseau, Bernard; Pieters, Grégory - Angewandte Chemie - International Edition, 2015 , vol. 54, # 36, p. 10474 - 10477, Angew. Chem., 2015 , vol. 127, # 36, p. 10620 - 10623,4 Full Text



Query Builder



Query Builder(1/2)

點擊上方Query Builder即可進入進階查詢頁面

Reaxys	Quick search Query builder Results Synthesis planner (1) History	Û ()
▲ 🖻 🌖 💼 Import Save Reset form Delete all	Search > Search > Find search fields and forms Structure Molecular Formula CAS RN Doc. Index Fields Forms History	Q
		Reaxys 🔨
	Basic Indexes	\sim
	Identification	\sim
	Physical Properties	~
Dra	ag & Drop to build a new query Spectra	~
	MedChem	\sim
	Other	\sim
	Reactions	\sim

- ① 查詢條件顯示區域
- ② 查詢條件(結構、分子式、CAS registry number、Document Basic Index)
- ③ 查詢條件(物性、光譜、反應條件、等)

Query Builder(2/2)

可以在右方清單找尋需要的查詢條件,或直接以文字在Find search and fields and forms 搜尋所需查詢條件。

Reaxys	Quick search Query bu	ilder Results Synthesis planner	History Sign in	0
날 🕑 🌖 Import Save Reset form De	dete all Stru	Search > Search > # 5 cture Molecular Formula CAS RN Doc. Inde	Find search fields and forms Q sped	Find search fields and forms
			Rea:	Fields Forms History Reaxys 🔨
			Patent Specific Data exists/any	Recent
IXYS Quick search	Query builder Results Synthesis planner	History 1 Sign in 3	℅ NMR Spectroscopy	950 Substances
lon s) 音	Search > ∨	Find search fields and forms	► 😣 IR Spectroscopy	Compound (substructure search), isot
ort Save Reset form Delete all	Structure Molecular Formula CAS RN Doc. Index	Field: Forms History	Mass Spectrometry	158 Substances
Physical Data	×	Documents		Compound (substructure search), isot
♦ Melting Point Find any	Show fields 🗸 🗙	Natural Product	Raman Spectroscopy	
◇ Boiling Point ☐ Find any	Show fields \checkmark X	Physical Data Reactions	SESR Spectroscopy	·····································
AND ◇ Density □ Find any AND	Show fields \checkmark X	● spei ● sub ● sub ● Sub	入物性或天然	·····································
Dissociation Exponent Fine	d any Show fields \checkmark X	Reaxys M /生 1/汀 II ゾ J ゾ 只 山又 目 II.		⊂ ,
Dynamic Viscosity Find any	y Show fields ∨ ×			



Query Builder: 查詢範例

- ① 多條件查詢(天然物、抗菌活性、分子式)
- ② 排除雜訊
- ③ 多條件查詢(用途)



Query Builder查詢範例1(1/4)

查詢範例:

是從天然物中萃取出來的化合物,分子式帶有30個碳並具有抗菌效果

• Molecular formular/Natural product/Substance basic index

내 🖾 <table-cell> 🗓 Import Save Reset form Delete</table-cell>		Structure Molecular Formula CAS RN Doc. Index	Search properties Fields Forms History	Q
				Reaxys 🔨
Molecular Formula		×	Basic Indexes	~
is	Molecular Formula	… 民	Identification	^
ends with			♦ Chemical Name	= ii
contains			Element Symbols	
starts with			🗢 Molecular Formula	
			◇ Molecular Weight	

- ① 點擊右方的Identification>Molecular Formula
- ② 因為不知道其他成分,選擇"is",再輸入「C30*」

Query Builder查詢範例1(2/4)

・ Marken Marken Marken Marken Marken Mar	Search > Search > Structure Molecular Formula CAS RN Doc. Index	Search properties Q Natural
Molecular Formula is V C30*	× ₩ 6	Reaxys Isolation from Natural Product Natural Product
OR AND NOT PROXIMITY AND Isolation from Natural Product	Hide fields ^ X	

*可使用關鍵字查詢篩選條件

- ③ 在右上方Find search and fields and form 輸入"Natural",點擊「Isolation from Natural Product」
- ④ 在左方的運算子選擇AND,內容可不輸入

Query Builder查詢範例1(3/4)

▶ 🖳 🌍 前 Import Save Reset form Delete	Structure Molecular Formula Reactions	Search properties Q Fields Forms History
	Substances	Reaxys 🔨
Molecular Formula		Basic Indexes
is C30*	… 民	Substance Basic Index
AND		
Isolation from Natural Product Find any	Hide fields 🔨 🗙	◇ Document Basic Index
is V Isolation from Natural Product	民	Identification 🗸
AND		Physical Properties 🗸 🗸
Substance Basic Index	×	Spectra 🗸
is Substance Basic Index	R	Pharmacological Data 🗸 🗸 🗸
	EQ	Ecotoxicology 🗸 🗸

- ⑤ 點擊右方Basic Indexes>「Substance Basic Index」
- ⑥ 輸入"antimicrobi*"
- ⑦ 因為要找化合物,所以在右上的Search選擇Substance

Query Builder查詢範例1(4/4)

Rea	xys	Quick se	earch	Query builder	Results	Synthesis planner	History		Sign in	?
876	Filters and Analysis		< E	Back to Query Buil	der			Database:	Reaxys - 876	~
	By Structure	\sim	876	Substand	Ces out of	8,094 Documents con	taining 7,885 Reaction	ons		
	Substances Classes	\sim) selected: Optic	ons 🗸	0 (o @	No of R	eferences 🗸 🗸	$\wedge \downarrow$
	Molecular Weight	\sim			Ť		- ·			· <u>·</u>
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	Available Data	\sim	1	, (PL)		Hit Data - 27			Preparations - 17	1 >
	Document Type	~ ~			ä	Identification			Reactions - 1,45	1 >
	Publication Year	\sim		Ĩ		Physical Data - 319 Spectra - 234		I	Documents - 2,06	5 >
						Bioactivity - 1,148				
						Other Data - 869				
				✓ Hit Data	a - 27					

查詢結果畫面:

分子式,化學名,測試項目,合成方法,衍生物的合成方法等都可以得到確認,

如果有其他條件,可透過左方的篩選功能縮小範圍。

Query Builder查詢範例2(1/3)

查詢範例: (去除不需要資訊的查詢方式) 查詢以Isoquinoline作為主結構及產物的反應,但需 去除以Isoquinoline做為反應物的反應。

• History

先從Quick search開始,

- ① 將Isoquinoline作為主結構及產物進行反應查詢
- ② 將Isoquinoline作為反應物進行反應查詢
 * 查詢的過程中,須選擇As substructure
- 查詢結果出現後,點擊「View Result」進入查 詢結果畫面





Query Builder查詢範例2(2/3)

完成2個反應查詢後,回到Query Builder並開啟右側的「History」 History會顯示2次的查詢紀錄

① Isoquinoline作為主結構的產物的反應

② Isoquinoline作為主結構的反應物的反應

Reaxys	Quick search Query buil	der Results	Synthesis	planner	History	Sign	in 🕐
➡ 🖻 🕤 🛅 Import Save Reset form Delete		© Structure Mole	cular Formula	Search # CAS RN	Doc. Index	Search properties Fields Forms History	Q)
							Reaxys 🔨
						Recent	^
						78,474 Reactions Reagent (SubstrL Ring Closed)	sures 2
					•	159,838 Reactions Product (SubstrL Ring Close)	sures 1
Drag	; & Drop to build a ne	w query					

*雖然也可以直接查詢lsoquinoline的製備,但其中將會包含許多取代反應,透過加入其他搜尋條件或查詢紀錄的比對, 就可以減少查詢,差到所需要的資料。

Query Builder查詢範例2(3/3)

- ① 先選擇以Isoquinoline作為主結構及產物進行反應的查詢紀錄
- ② 再選擇以Isoquinoline作為主結構及反應物進行反應的查詢紀錄
- ③ 將運算子設定為NOT
- ④ 在右上角選擇Reaction,然後點擊Search即可進行以Isoquinoline作為主結構及產物但不包含以 Isoquinoline作為主結構及反應物為條件的查詢。

Reaxys	Quick	search Query builder	r Results Synthes	is planner History	Sign in	
내 Parker Import Save	Reset form Delete	St	()	Search > Reactions	Search properties Q Fields Forms History	
 159, 159, 78,4 3 	838 Reactions Product (SubstrL Ring Closures 74 Reactions Reagent (SubstrL Ring Closures			Substances Documents	Reaxys A Recent A 78,474 Reactions Compared Reagent (SubstrL Ring Closures 159,838 Reactions Compared Product (SubstrL Ring Closures	
結果例		, , , , , , , , , , , , , , , , , , ,) НС 		$\begin{array}{c} & & \\ & & \\ & & \\ & & \\ & \\ & \\ & \\ & $	

Query Builder查詢範例3

查詢範例:可做為食物及補充劑的化合物(Food、Supplement)

• Use

Reaxys	Quick search	Query builder	Results	Synthesis	planner	History	S	ign in	and for Use Pa	m 輸入""Us uttren中輸/	se",再分別於 \Food及
소 凹 🕤 Import Save Reset form	<mark>윤</mark> Delete all	Structure Mole	Search S	Gubstances) CAS RN D	Co. Index	Find search Q use	fields and forms	×	Supple 運算子 最後在	ment [,] 選擇AND [,] 右上方點擊	≩ ^۲ Search
								Reaxys 🔨	Substa	nces」即可	完成。
♦ Use 🔳 R	nd any ✓ Laboratory Use a	nd Handling	Hide field	s ^		q C	uercetol 5 ₁₅ H ₁₀ O ₇ 302.24 3	17313 117-39-5			
contains	Vuse Pattern food				P:		lit Data - 20 dentification	Physi Spec	ical Data - 935 tra - 1,149	Bioactivity - 5,981 Other Data - 3,250	Preparations - 168 > Reactions - 982 > Documents - 12,439 >
♦ Use II FI			Hide field	s 🔨	^ <u>H</u>	it Data - 20					
is	✓ Laboratory Use a	nd Handling			^	Use - 20 hits out o	f 2,053				Show/Hide columns 🗸
contains	可應用於	《食物及礼	哺充劑	J	U:	e Pattern od/food additives	Location Paragraph 2	Reference Xie, Lingjun; War Full Text 7 D	ng, Nuan - CN106474454, 20 Details > Abstract >	D17, A	
			~	_	fo	od product	Paragraph 2	Xie, Lingjun; Wa Full Text ⊅ D	ng, Nuan - CN106474454, 20 Details > Abstract >	017, A	
					ne pr	w natural resource <mark>foor</mark> oduct	Paragraph 2	Xie, Lingjun; Wa Full Text ⊿ D	ng, Nuan - CN106474454, 20 Details > Abstract >	017, A	
					Fo	od/food additives	Page/Page column title page; 17-20	MYCOTOX SOLU A1 Full Text 7 C	JTIONS INC.; MARQUARDT, Details > Abstract >	, Ronald R.; MADHYASTHA, Sri	nivasa - WO2017/83964, 2017 ,
					fo	od allergies	Page/Page column 8	NEXIRA INTERN	IATIONAL; DAGUET, David - Details > Abstract >	US2015/306162, 2015 , A1	
					Di	etary supplement		Udell, Ronald G. Full Text 7 D	- US2005/249803, 2005, A1 Details > Abstract >		

在右上方Find search and fields



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