

新版 Reaxys 化學資料庫

收錄內容更多、操作更直覺

www.reaxys.com
new.reaxys.com

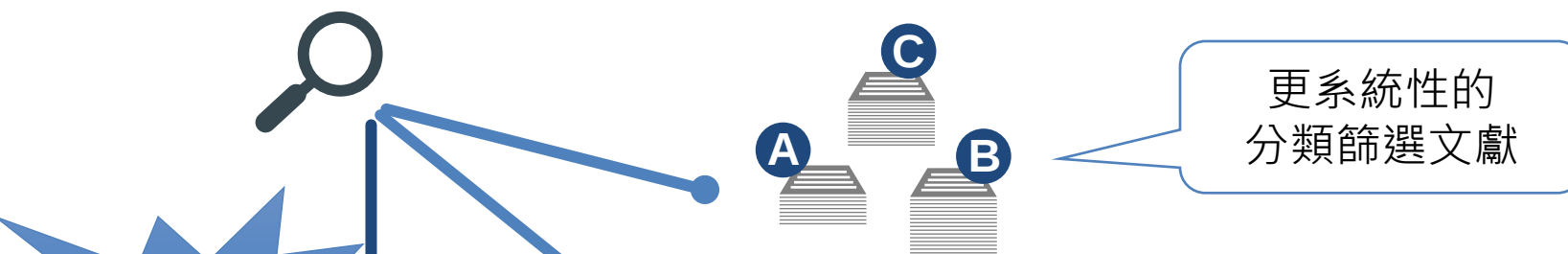
Elsevier 生命科學解決方案經理 梁成芝

2017

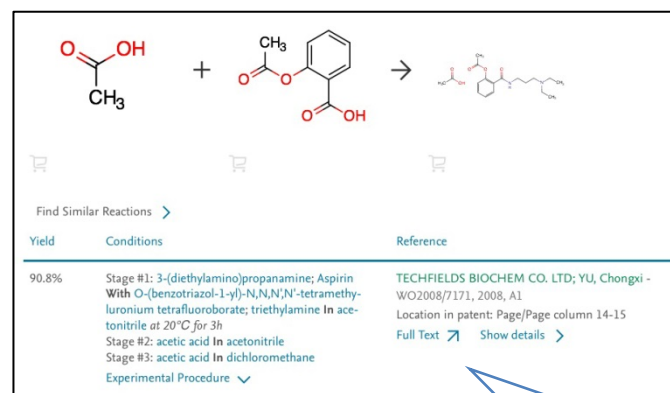
Reaxys 化學資料庫如何開啟?

- **Reaxys 化學資料庫**
 - IP 開放，免帳號密碼
 - www.reaxys.com
 - 新介面 <https://new.reaxys.com>
- 可使用 proxy 或 VPN 遠端連線或加購遠端連線帳號

Elsevier R&D Solution 致力於更快找到答案

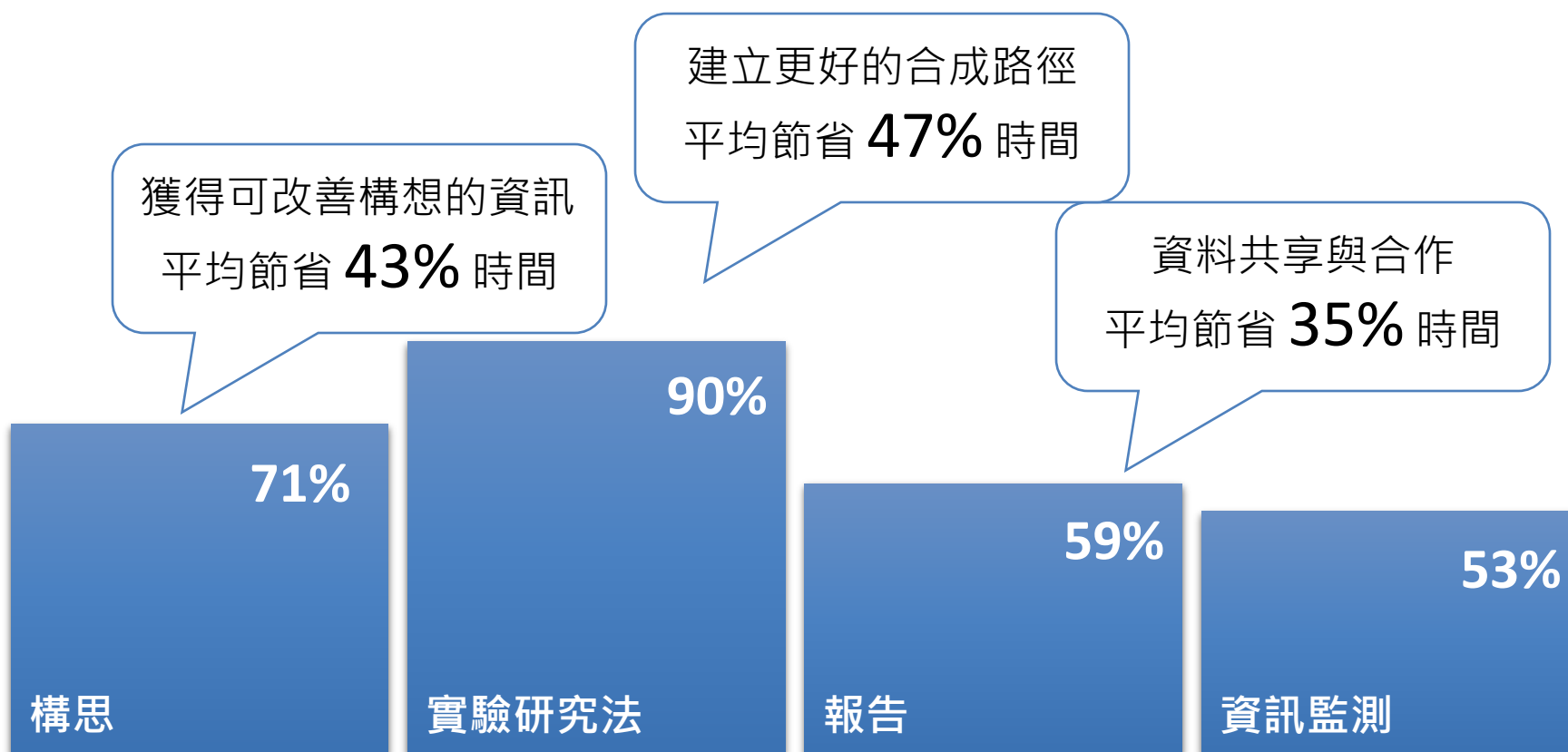


當其他資料庫的目標是提供更多
與關鍵字相關的文獻列表



直接摘錄重要資訊

Reaxys 可有效提升研究效率，平均省下 35 - 47% 時間

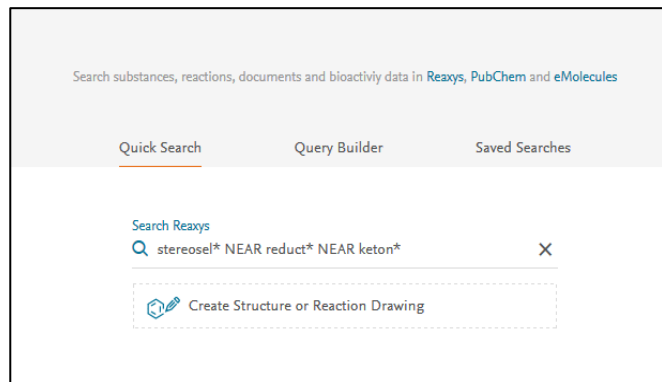


新版 Reaxys 三大變化



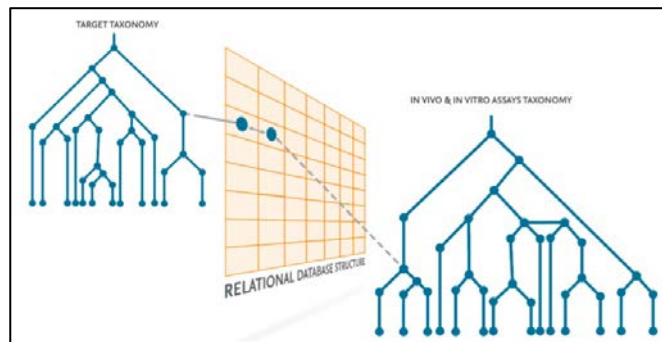
擴充收錄內容

- 16,000種期刊與主要專利局
- 5億筆實驗數據摘錄
- 281本期刊及專利**化學反應**全文材料方法摘錄



使用者介面

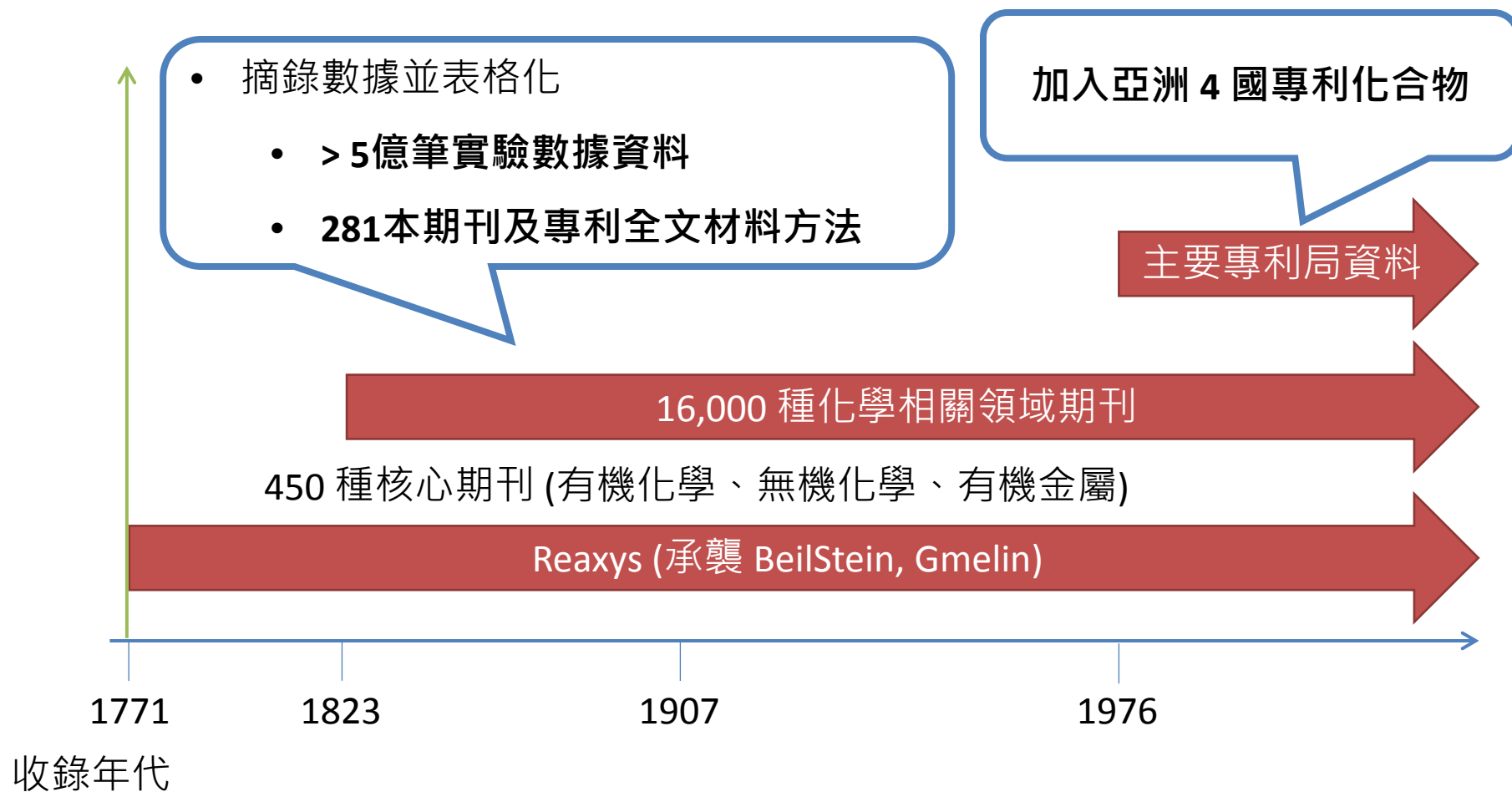
依據實際使用頻率設計
常用功能一目了然



自動索引技術與資料庫架構

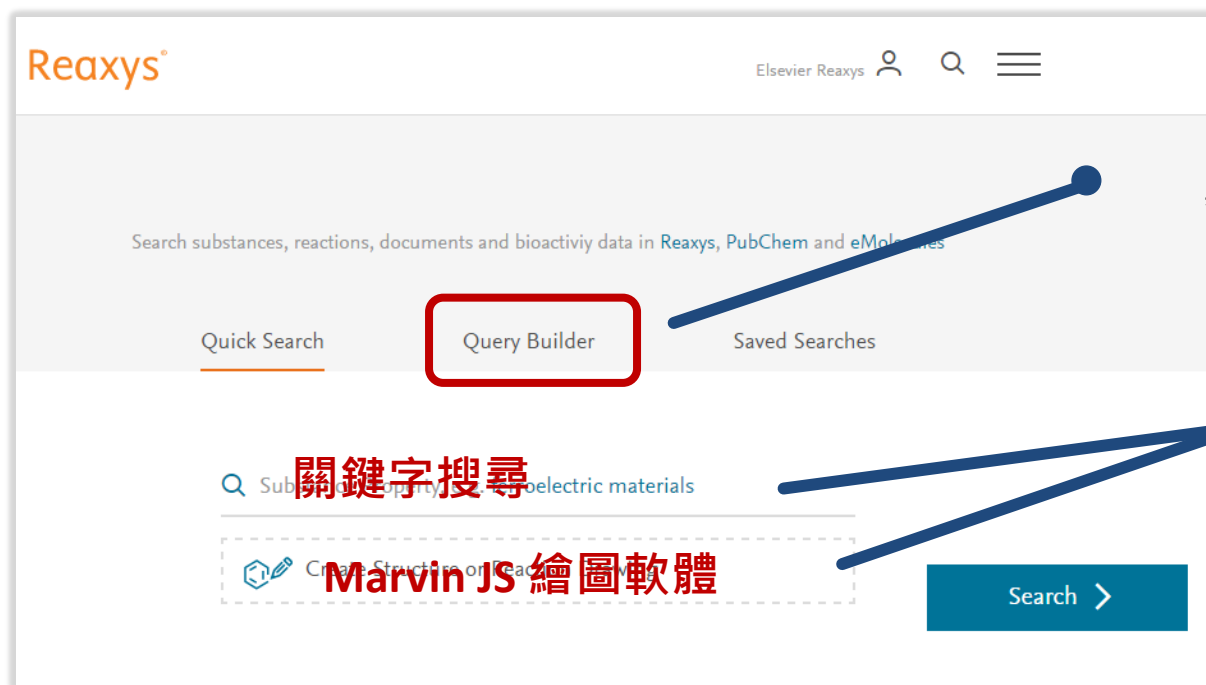
- 先進的全文自動索引技術
- 多元搜尋工具，如結構、實驗數值....更多
- 表格化整理與超連結串連

Reaxys 收錄內容



使用者介面

依據實際使用頻率設計，常用功能一目了然



進階搜尋

彙整 > 400 種搜尋欄位

> 95% 使用者

最常使用

關鍵字 + 結構搜尋

智慧辨識與預覽功能

自動辨識關鍵字，推薦相關結果，供您預覽及挑選

Search Reaxys
Q esterification of benzoic acid X

Create Structure or Reaction Drawing

關鍵字搜尋
支援 AND OR NOT * 等指令

自動辨識提供
化學反應搜尋結果

自動推薦其他相關結果

82	Reactions	benzoic acid starting (exact search) AND Reaction Type : esterification; esterifications OR Other Conditions : esterification; esterifications	Preview Results View Results
399	Documents	Titles, Abstracts and Keywords : Document Basic Index : "esterification"; "esterifications" AND Document Basic Index : benzoic acid	Preview Results View Results
21316	Documents	Titles, Abstracts and Keywords : Document Basic Index : benzoic acid	Preview Results View Results
48655	Documents	Titles, Abstracts and Keywords : Document Basic Index : "esterification"; "esterifications"	Preview Results View Results

預覽搜尋結果
是否符合需求

多元搜尋工具 – Query Builder

The screenshot displays the Reaxys Query Builder interface. The top toolbar includes 'Import', 'Save', 'Reset form', and 'Delete' buttons, along with tabs for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. A 'Search' button with a dropdown arrow is also present.

The main workspace contains three search criteria:

- Structure**: Labeled '結構搜尋' (Structure Search). It includes a 'Create Structure / Reaction Drawing' button. A callout bubble points to this area, listing features: '支援 ChemDraw 複製貼上' (Supports ChemDraw copy-paste), '強大衍生物搜尋功能' (Powerful derivative search function), and 'Marvin JS 免安裝 JAVA' (Marvin JS, no Java installation required).
- Optical Rotatory Power**: Labeled '物質特性、實驗數據種類及其數值範圍' (Substance properties, experimental data types, and their numerical ranges). It includes an 'Exist' dropdown.
- Document Basic Index**: Labeled '進階關鍵字搜尋' (Advanced keyword search). It includes a 'Document Basic Index' dropdown.

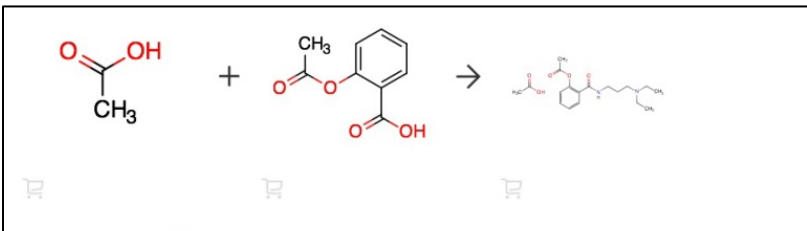
Between the criteria, logical operators 'AND' are visible. A callout bubble points to these operators, stating: '布林邏輯自由結合搜尋條件 (AND OR NOT Proximity)' (Boolean logic freely combines search conditions (AND OR NOT Proximity)).

On the right side, a sidebar titled 'Search properties' is shown. It has a search bar and tabs for 'Fields', 'Forms', and 'History'. A callout bubble points to the 'Forms' tab, stating: 'Forms 常用欄位組合' (Forms commonly used field combinations). Another callout bubble points to the 'History' tab, stating: 'History 歷史搜尋結果' (History search results). The sidebar lists various properties such as 'Basic Index', 'Document Basic Index', 'Identification', 'Physical Properties', 'Melting Point', 'Boiling Point', and 'Sublimation'. A 'Feedback' button is at the bottom.

At the top right, a callout bubble states: '超過 400 種搜尋欄位' (Over 400 search fields).

資料表格化

直接比較數據資料，節省全文閱讀的時間與經費



Find Similar Reactions

Yield	Condition
90.8%	Stage #1: With O-(b-luronium tonitrile at Stage #2: Stage #3: Experiment

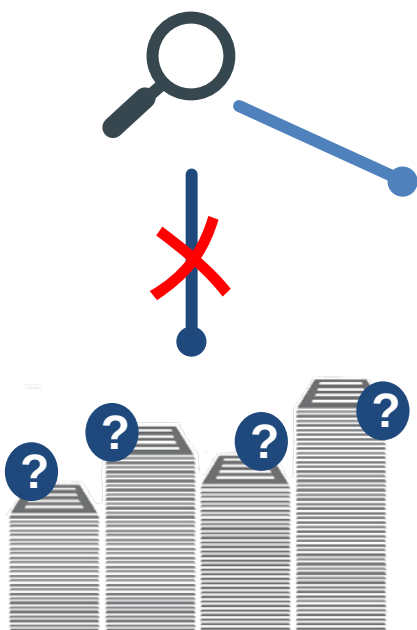
Dissociation Exponent - 27						
Dissociation Exponent (pK)	Dissociation Group	Temperature (Dissociation Exponent), °C	Solvent (Dissociation Exponent)	Method (Dissociation Exponent)	Type (Dissociation Exponent)	Reference
3.48	RCOO-H	25	dimethylsulfoxide, H2O	spectrophotometric	a1/apparent	Article, 2003 Citation Journals: Analytical Chemistry, 4, 75, 2003, 883 - 892
3.47		25	dimethylsulfoxide, H2O		a1/thermodynamic	Article, 2002 Citation Journals: Journal of Pharmaceutical Sciences, 4, 91, 2002, 933 - 942
3.55	COOH	37	H2O		a1/apparent	Article, 1995 Citation Journals: Biological and Pharmaceutical Bulletin, 2, 18, 1995, 310 - 314
3.6	COOH	25			a1/apparent	Article, 1993 Citation Journals: Chemical and Pharmaceutical Bulletin, 6, 41, 1993, 1137 - 1143

- 表格中的文字皆可篩選
- 沒有購買全文也可以獲得
 - 5 億筆實驗數據資料
 - 281 種期刊及專利的合成材料方法

450 → 12,000 本期刊

開始使用 Reaxys

- ✓ 找到**答案**而非堆積如山的待唸文獻
- ✓ 摘錄更多數據資料、合成方法
- ✓ 搜尋方法更多元彈性



Chemical reaction scheme showing the synthesis of aspirin (acetylsalicylic acid) from salicylic acid and acetic anhydride.

Physical Data - 532

Dissociation Exponent - 27

Yield	Conditions
90.8%	Stage #1: 3-(diethylamino) With O-(benzotriazol-1-yl)uronium tetrafluoroborate in acetonitrile at 20°C for 3h Stage #2: acetic acid In acetonitrile Stage #3: acetic acid In dichloromethane Experimental Procedure

Find Similar Reactions >

Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs [Cited 1 times](#)
Lin, Lee-Shuan; Kayasuga, Yuko; Shimohata, Nobuyuki; +6 others - Journal of Veterinary Medical Science, 2012, vol. 74, # 11, p. 1511 - 1516
[Abstract](#) [Index Terms](#) [Full Text](#)

Incidence of aspirin resistance in the patient group of a university hospital in Korea [Cited 6 times](#)
Lee, Young Kyung; Kim, Han-Sung; Park, Ji-Young; +1 other - Korean Journal of Laboratory Medicine, 2008, vol. 28, # 4, p. 251 - 257
[Abstract](#) [Index Terms](#) [Full Text](#)

Increased platelet expression of glycoprotein IIIa following aspirin treatment in aspirin-resistant but not aspirin-sensitive subjects [Cited 3 times](#)
Floyd, Christopher N.; Goodman, Timothy; Becker, Silke; +7 others - British Journal of Clinical Pharmacology, 2014, vol. 78, # 2, p. 320 - 328
[Abstract](#) [Index Terms](#) [Full Text](#)

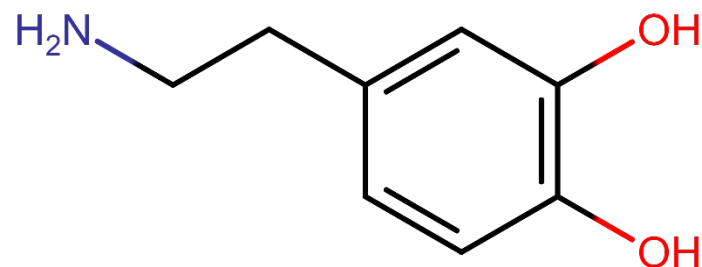
Reaxys 搜尋實例與技巧

Presented By

Date

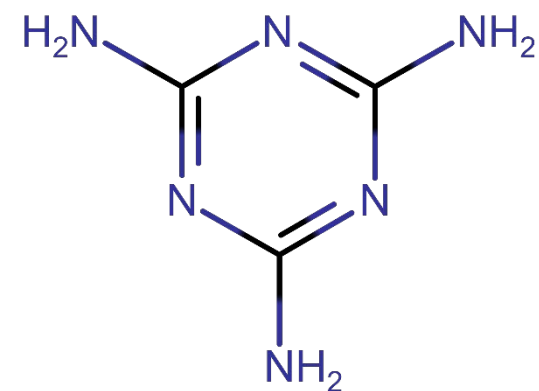
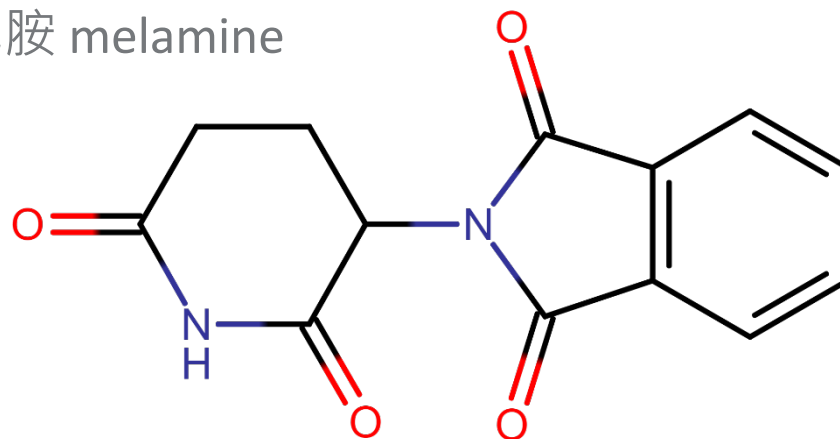
結構繪製與搜尋技巧

- 多巴胺 dopamine



- 其他範例

- 沙利竇邁 thalidomide
- 三聚氰胺 melamine

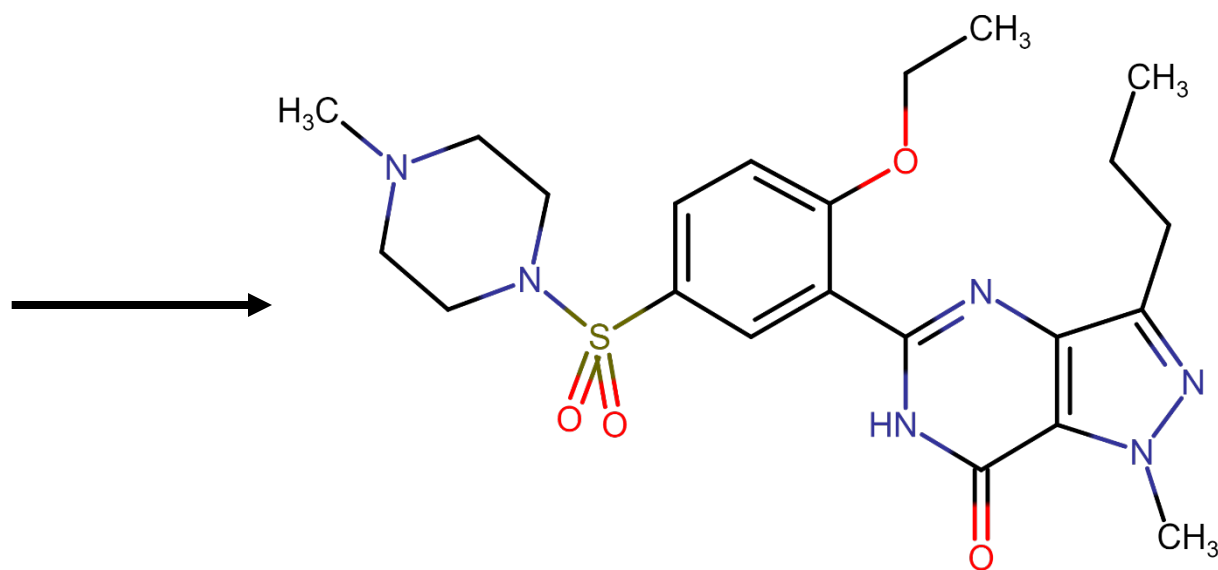


關鍵字搜尋化合物 & 實驗數據

- 神經傳導物質 多巴胺 Dopamine
- 其他範例
 - Tamiflu 克流感
 - Melamine 三聚氰胺
 - Melting point 熔點
 - Boiling point 沸點
 - HPLC 液相層析數據

化學反應搜尋

- 多巴胺合成 dopamine synthesis
- 其他範例
 - 苯佐卡因合成 Benzocaine Synthesis



關鍵字搜尋

- 化合物名稱、分子式
 - 多巴胺 Dopamine, 三聚氰胺 Melamine
- 化學反應
 - Esterification, 合成 synthesis, 製備 preparation
 - 起始物 to 產物
- 實驗數據或物化特性名稱
 - 物化特性 melting point, boiling point, solubility, log POW
 - 光譜 HPLC, NMR, IR
- 其他關鍵字
 - 藥物劑型 Drug formulation
 - 掌性異構物分離 Chiral separations

多元搜尋工具 – Query Builder

- 超過 400 種搜尋欄位
- Forms: 預設常用欄位
- History: 搜尋歷史紀錄

The screenshot displays the Reaxys Query Builder interface. At the top, there is a toolbar with icons for Import, Save, Reset form, and Delete. Below this, a search bar is visible with a 'Search' button and a dropdown arrow. The main workspace is divided into three sections: Structure, Optical Rotatory Power, and Document Basic Index. The Structure section contains a 'Create Structure / Reaction Drawing' button. The Optical Rotatory Power section shows a search condition 'Optical Rotatory Power is ...'. The Document Basic Index section shows a search condition 'Document Basic Index is ...'. A sidebar on the right lists search properties: Basic Indexes (Substance Basic Index, Reaction Basic Index, Document Basic Index), Identification, Physical Properties (Melting Point, Boiling Point, Sublimation), and a Feedback button. Callouts provide additional information: one points to the 'Create Structure / Reaction Drawing' button, another points to the 'AND' operator, and a third points to the 'is' operator.

Structure

結構搜尋

Create Structure / Reaction Drawing

AND

Optical Rotatory Power

物質特性、實驗數據種類及其數值範圍

AND

Document Basic Index

is

Document Basic Index

進階關鍵字搜尋

- 支援 ChemDraw 複製貼上
- 強大衍生物搜尋功能
- Marvin JS 免安裝 JAVA

布林邏輯自由結合搜尋條件 (AND OR NOT Proximity)

Search properties

Fields Forms History

Basic Indexes

- ◇ Substance Basic Index
- ◇ Reaction Basic Index
- ◇ Document Basic Index

Identification

Physical Properties

- ◇ Melting Point
- ◇ Boiling Point
- ◇ Sublimation

Feedback

Query Builder 進階搜尋

搜尋包含34個碳，旋光度=18.2的所有化合物

Molecular Formula

is



Molecular Formula
C34*

搭配分子式搜尋
C34* 表示此分子含有34個碳，其餘未知

AND

Isolation from Natural Product



Find any

Show fields



化合物來源為天然物

AND

Optical Rotatory Power



Find any

Hide fields



is



Type (Optical Rotatory Power)

is



Solvent (Optical Rotatory Power)

=

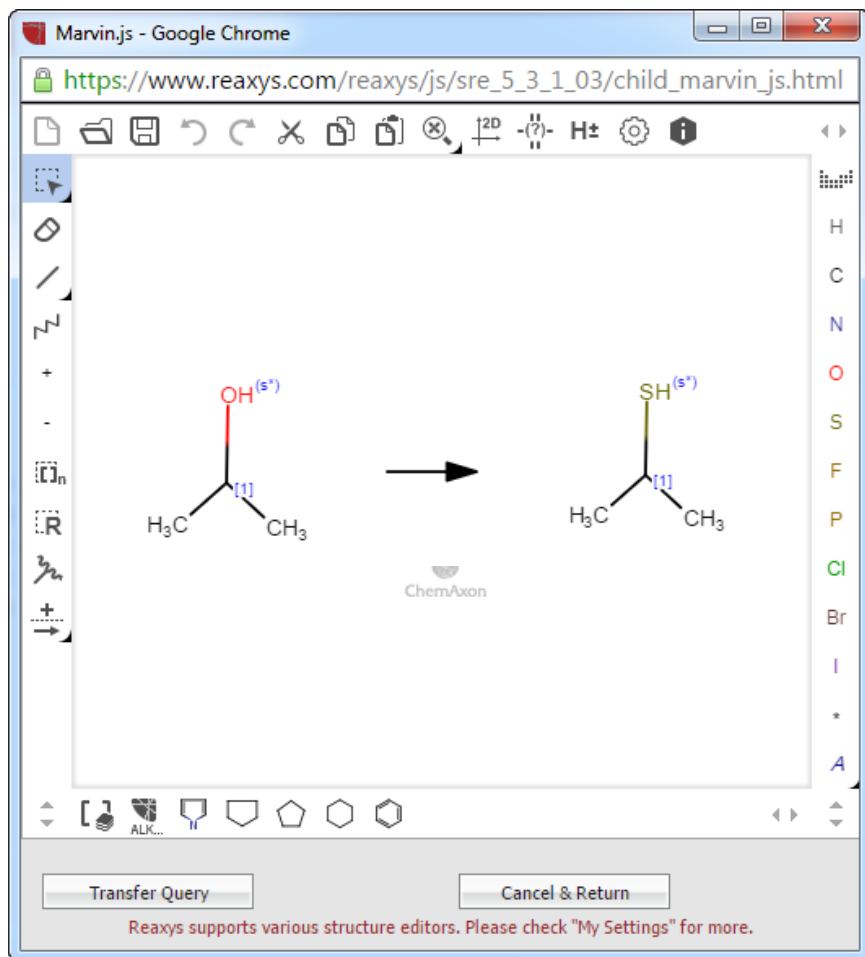


Optical Rotatory Power, deg
18.2

選擇旋光度
optical rotatory power (deg)
選擇 = 輸入 18.2

繪圖軟體 – Marvin JS

Reaxys 支援新版 Marvin JS 種繪圖軟體



- 無須安裝 JAVA
- 可從 ChemDraw 複製貼上
- 衍生物搜尋功能
 - 限定特定位置的鍵結、原子、或官能基種類，並具備多種彈性選項
 - R-group 及 R-logic 功能
 - Substitution 限定特定原子是否接上官能基或接上鍵結的數量
 - Position variation bond 限定指定鍵結或官能基可能連接的多個位置
- 繪製完畢的結構可存成透明背景圖檔，並可調整檔案解析度

*更多Marvin JS 技巧請參考 Facebook 粉絲團
<https://www.facebook.com/ReaxysClub>

Reaction 搜尋結果

找到 1205 筆反應

Reactions (1205) Substances (1918) Citations (474) go to Page Page 1 of 134

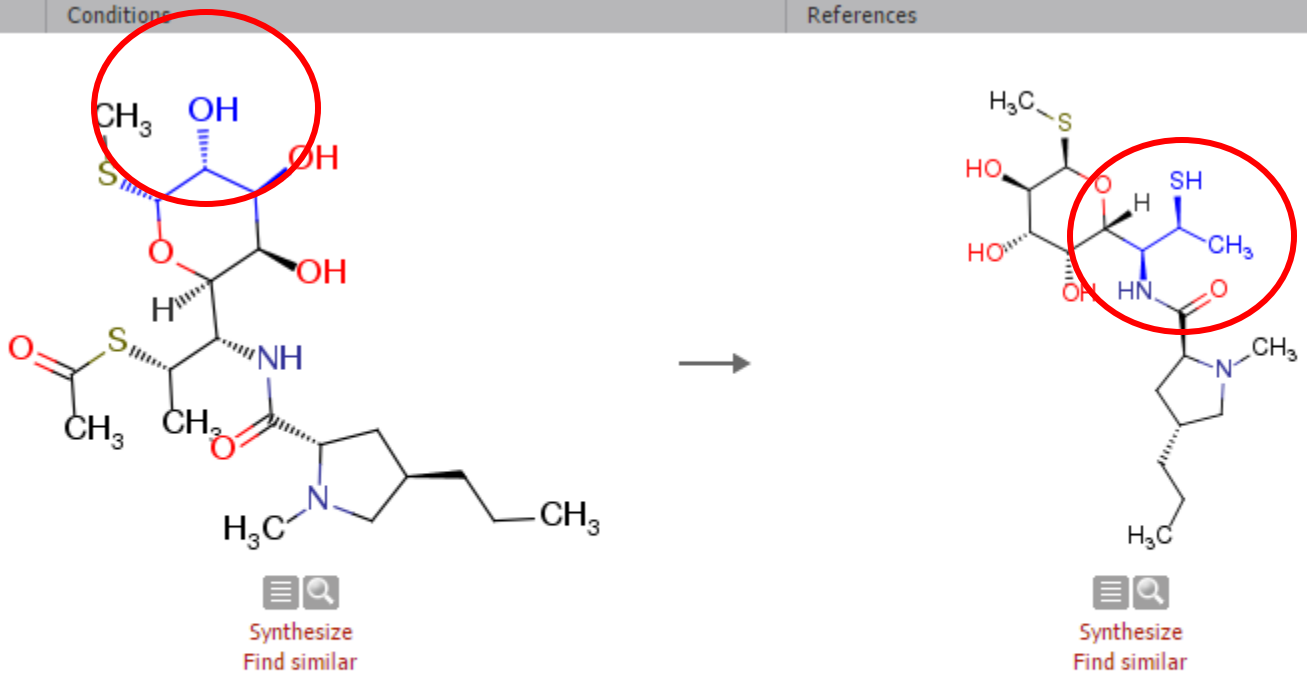
Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
 Synthesize Find similar Synthesize Find similar Rx-ID: 1786437 Find similar reactions		
94%	With Lawessons reagent in toluene 0.5 h; Heating;	Nishio, Takehiko Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1993 , # 10 p. 1113 - 1118 Title/Abstract Full Text View citing articles Show Details
94%	With Lawessons reagent in toluene 0.5 h; Heating;	Nishio, Takehiko Journal of the Chemical Society, Chemical Communications, 1989 , # 4 p. 205 - 206 Title/Abstract Full Text View citing articles Show Details
94%	With Lawessons reagent; water in toluene T=50°C;	Ohno, Michihiro; Miyamoto, Mitsuko; Hoshi, Kazuhiro; Takeda, Takahiro; Yamada, Naohiro; Ohtake, Atsushi Journal of Medicinal Chemistry, 2005 , vol. 48, # 16 p. 5279 - 5294 Title/Abstract Full Text View citing articles Show Details

Show All Remaining Details (4)

若不使用 atom mapping

找到 3158 個反應，但官能基的位置可能不同

Yield	Conditions	References
  Synthesize Find similar	With methanol; sodium methylate T=20°C; 0.333333 h; Show Experimental Procedure	Meiji Seika Kaisha, Ltd. Patent: EP1970377 A1, 2008 ; Location in patent: Page/Page column 48 ; Title/Abstract Full Text Show Details  Synthesize Find similar Rx-ID: 27887377 Find similar reactions
94%		

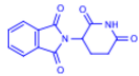
快速搜尋 – Ask Reaxys

Ask Reaxys **Search**

Smart searching with Ask Reaxys. [See examples >](#)

Reactions (130) Substances (90) Citations (470) go to Page Page 1 of 10

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	N° of ref.
 Synthesize Hide Details Find similar	Chemical Name: THALIDOMIDE Reaxys Registry Number: 30233 CAS Registry Number: 50-35-1 Type of Substance: heterocyclic Molecular Formula: C ₁₃ H ₁₀ N ₂ O ₄ Linear Structure Formula: C ₁₃ H ₁₀ N ₂ O ₄ Molecular Weight: 258.233 InChI Key: UEJHQNACJXSKW-UHFFFAOYSA-N	26 prep out of 76 reactions.	Identification Physical Data (68) Spectra (29) Bioactivity (485) Ecological Data (2) Use/Application (1511)	437

Chemical Names and Synonyms
THALIDOMIDE, thalidomide

- Identification
- Physical Data
- Spectra
- Bioactivity
- Pharmacological Data (482)
- Ecotoxicology (3)
- Ecological Data
- Use/Application

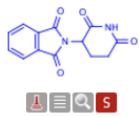
紅色字皆為超連結

瀏覽物化特性、光譜、生物活性、用途、天然物等相關數據

Bioactivity (Reaxys only)

Reactions (130) Substances (90) Citations (470) go to Page Page 1 of 10

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	N° of ref.
 Synthesize Hide Details Find similar	Chemical Name: THALIDOMIDE Reaxys Registry Number: 30233 CAS Registry Number: 50-35-1 Type of Substance: heterocyclic Molecular Formula: C ₁₃ H ₁₀ N ₂ O ₄ Linear Structure Formula: C ₁₃ H ₁₀ N ₂ O ₄ Molecular Weight: 258.233 InChI Key: UEJHQACIXKW-UHFFFAOYSA-N	26 prep out of 76 reactions	Identification Physical Data (68) Spectra (29) Bioactivity (485) Ecological Data (2) Use/Application (1511)	437
Chemical Names and Synonyms THALIDOMIDE, thalidomide Identification Physical Data Spectra Bioactivity Pharmacological Data (482) Ecotoxicology (3) Ecological Data Use/Application	25 of 482 Effect (Pharmacological Data) Species or Test-System (Pharmacological Data) Method (Pharmacological Data) Type (Pharmacological Data) Value of Type (Pharmacological Data) Reference	VEGF production; inhibition of lung adenocarcinoma A549 cells of human name of assay/method: ELISA VEGF level Ca. 1350 - 1600 pg/ml Lue, Wen-Wen; Gao, Yun-Jia; Su, Ming-Zhi; Luo, Zhou; Zhang, Wei; Shi, Guo-Bing; Zhao, Qing-Chun Helvetica Chimica Acta, 2013 , vol. 96, # 1 p. 109 - 113 Title/Abstract Full Text View citing articles Show Details		
	26 of 482 Comment (Pharmacological Data) Reference	physiological behaviour discussed Burkhard, Johannes A.; Wuitschik, Georg; Plancher, Jean-Marc; Rogers-Evans, Mark; Carreira, Erick M. Organic Letters, 2013 , vol. 15, # 17 p. 4312 - 4315 Title/Abstract Full Text View citing articles Show Details		
1 of 3	Effect (Ecotoxicology) Species or Test-System (Ecotoxicology) Concentration (Ecotoxicology) Kind of Dosing (Ecotoxicology) Method (Ecotoxicology) Comment (Ecotoxicology) Reference	angiogenesis; inhibition of white Leghorn embryos 1 µg/disc applied to CAM of individual embryos in 0.5 percent carboxymethylcellulose disc chick chorioallantoic membrane (CAM) assay; embryos with intact yolk from 3-day-old fertilized eggs; 3 percent CO ₂ ; 37 deg C; incubated for 48 h; developing vasculature observed by stereomicroscope No effect Perino, Sandrine; Contino-Pepin, Christiane; Satchi-Fainaro, Ronit; Butterfield, Catherine; Pucci, Bernard Bioorganic and Medicinal Chemistry Letters, 2004 , vol. 14, # 2 p. 421 - 425 Title/Abstract Full Text View citing articles Show Details		

無法量化的數據摘錄重點

Bioactivity (RMC 藥物化學資料庫)

In Vitro: Efficacy、In Vivo: Animal Model、Metabolism

Bioactivities (1798) Reactions (130) **Substances (90)** Targets (89) Citations (470)

go to Page Page 1 of 10

Limit to Exclude Export Print Zoom In Zoom Out Hide

Sort by No of References Display as

Structure

Structure/Compound Data

Chemical Name: THALIDOMIDE

Reaxys Registry Number: 30233
CAS Registry Number: 50-35-1

Quantitative Results

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on Target	Target	Target subunit	Target Species	Tissue/Organ	Cell	Bioassay	Dose	Effect	Reference (expand all/collapse all)
3.55	% Inhibition	#	26	%						HUVEC	Angiogenesis	100 µM		Bioorganic and Medicinal... Title/Abstract Full Text View citing articles Show Details
7.37	% Inhibition		70	%						LN-CAP	Flux release	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text View citing articles Show Details
3.74	EC50		183	µM							Flux release			Patent: EP1867649 A1, ... Title/Abstract Full Text Show Details
3.74	EC50		183	µM							Flux release			Patent: EP1867649 A1, ... Title/Abstract Full Text Show Details
3.74	IC50		183	µM							In Vitro (others)			Patent: EP1964842 A1, ... Title/Abstract Full Text Show Details

Quantitative Results

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on Target	Animal Model	Biological Species	Route of administration	Dose	Dosing regimen	Effect	Reference (expand all/collapse all)
	% Inhibition		36	%			Angiogenesis	rabbit	intragastric administration	200 mg/kg	Repeated	Patent: US6228879 B1, ... Title/Abstract Full Text Show Details
	MRT	=	8.23	hour			human	oral administration				... Full Text Show Details
	Concentration	=	793	pg/mL			mouse	subcutaneous administration			Antiinflammatory	Patent: WO2000/42071 A... Title/Abstract Full Text Show Details

Quantitative Results

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on Target	Target	Target Species	Tissue/Organ	Cell	Cell fraction	Substrate /Carried Molecule	Dose	Reference (expand all/collapse all)
1	IC50	>	100	µM		Cytochrome P450 1A2	human			Microsome	Ethoxyresorufin	0.100000 µM	Drug Metabolism Letters, ... Title/Abstract Full Text View citing articles Show Details
1	IC50	>	100	µM		Cytochrome P450 1A2	human		AHH-1 TK+/-	Microsome	Ethoxyresorufin	0.100000 µM	Drug Metabolism Letters, ... Title/Abstract Full Text View citing articles Show Details
1	IC50	>	100	µM		Cytochrome P450 2C9	human			Microsome	7-Methoxy-4-trifluoromethylcoumarin-3-Acetic acid	0.100000 µM	Drug Metabolism Letters, ... Title/Abstract Full Text View citing articles Show Details

Chemical Names and Synonyms
THALIDOMIDE, thalidomide

Druglikeness

Bioactivity

In vitro: Efficacy (701)

In vivo: Animal Model (104)

Metabolism (242)

Pharmacokinetic (622)

Toxicity/Safety Pharmacology (73)

Identification

Physical Data

Spectra

Ecological Data

Use/Application

Synthesize | Hide Details
Find similar

Target

Show Targets

N° of ref. 437

Physical Data (100)
Spectra (29)

藥物化學模組提供更完整生物活性資料

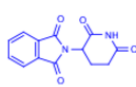
Bioactivity (RMC 藥物化學資料庫)

Pharmacokinetic、Toxicity/Safety Pharmacology

Bioactivities (1798) Reactions (130) Substances (90) Targets (89) Citations (470) go to Page Page 1 of 10

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as Exclude GOSTAR data

Structure



Synthesize | Hide Details
Find similar

Chemical Names and Synonyms
THALIDOMIDE, thalidomide

Druglikeness

Bioactivity

- In vitro: Efficacy (701)
- In vivo: Animal Model (104)
- Metabolism (242)
- Pharmacokinetic (622)
- Toxicity/Safety Pharmacology (73)

Identification

Physical Data

Spectra

Ecological Data

Use/Application

Quantitative Results											
pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Route of administration	Dose	Dosing regimen	Population	Reference (expand all/collapse all)	
	t1/2 abs		3.5	hour	human	oral administration	400 mg	Single	Lepromatous Leprosy	Clinical pharmacology an... Title/Abstract Full Text	Show Details
	Cmax		3.4	µg/mL	human	oral administration	400 mg	Single	Lepromatous Leprosy	Clinical pharmacology an... Title/Abstract Full Text	Show Details
	Tmax		5.7	hour	human	oral administration	400 mg	Single	Lepromatous Leprosy	Clinical pharmacology an... Title/Abstract Full Text	Show Details
	t1/2 el		5.8	hour	human	oral administration	400 mg	Single	Lepromatous Leprosy	Clinical pharmacology an... Title/Abstract Full Text	Show Details
	Vd ss		97	L	human					Clinical pharmacology an... Title/Abstract Full Text	Show Details
	Cl/F		11	L/h	human					Clinical pharmacology an... Title/Abstract Full Text	Show Details

可量化的數據摘錄重點並轉換為可互相比較的pX 值

Quantitative Results															
pX	Parameter	Value (qual)	Value (quant)	Unit	Action on Target	Target	Target subunit	Target Species	Tissue	Cell	Bioassay	Dose	Effect	Reference (expand all/collapse all)	
1	IC50	>	300	µM						HMEC	Cell/tumor cell: proliferation/viability/growth	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text	View citing articles Show Details
1	IC50	>	300	µM						HMEC	Cell/tumor cell: proliferation/viability/growth	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text	View citing articles Show Details
1	IC50	>	300	µM						PC-3	Cell/tumor cell: proliferation/viability/growth	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text	View citing articles Show Details
1	IC50	>	300	µM						DU 145	Cell/tumor cell: proliferation/viability/growth	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text	View citing articles Show Details
4.6	IC50		25.3	µM						LN-CAP	Cell/tumor cell: proliferation/viability/growth	0.100000 µM		Bioorganic and Medicinal... Title/Abstract Full Text	View citing articles Show Details
5.83	% Inhibition		87 - 94	%						FRT-Jurkat TNF	Cell/tumor cell: proliferation/viability/growth	10 µM		MedChemComm, 2011, vol... Title/Abstract Full Text	View citing articles Show Details
4.28	IC50		52.9	µM						Hep G 2	Cell/tumor cell: proliferation/viability/growth	1.00000E-08 M	Cytotoxic	Chemistry and Biodiversi... Title/Abstract Full Text	View citing articles Show Details
4.48	IC50		33.4	µM						PC-3	Cell/tumor cell: proliferation/viability/growth	1.00000E-08 M	Cytotoxic	Chemistry and Biodiversi... Title/Abstract Full Text	View citing articles Show Details
4.32	IC50		47.5	µM						A 549	Cell/tumor cell: proliferation/viability/growth	1.00000E-08 M	Cytotoxic	Chemistry and Biodiversi... Title/Abstract Full Text	View citing articles Show Details
1	% Inhibition		1.5	%						RPME 7951	Cell/tumor cell: proliferation/viability/growth	20 µM		Patent: US2002/19382 A... Title/Abstract Full Text	Show Details
1	% Inhibition	NA								RPME 7951	Cell/tumor cell: proliferation/viability/growth	5 µM		Patent: US2002/19382 A... Title/Abstract Full Text	Show Details

HeatMap 協助篩選生物活性資料

預設 THALIDOMIDE 與結合的標靶蛋白質

切換 XY 軸座標

Heatmap interface showing a grid of data points (pX values) for various targets and substances. The X-axis is labeled "Targets" and the Y-axis is labeled "Substances". The color scale ranges from 0 (blue) to 15.0 (red).

Annotations:

- 點擊查看詳細資訊 (Click to view detailed information)
- 依照 pX 值遞減排序 (Sort by pX value in descending order)

Heatmap Cell Details for Substance 1 of 1 (THALIDOMIDE):

Structure/Compound Data:

- Chemical Name: THALIDOMIDE
- Reaxys Registry Number: 30233
- CAS Registry Number: 50-35-1
- Type of Substance: heterocyclic
- Molecular Formula: $C_{13}H_{10}N_2O_4$
- Linear Structure Formula: $C_{13}H_{10}N_2O_4$
- Molecular Weight: 258.233
- InChI Key: UEJHQNACXSKW-UHFFFAOYSA-N
- Highest Clinical Phase: Withdrawn

Chemical Names and Synonyms:

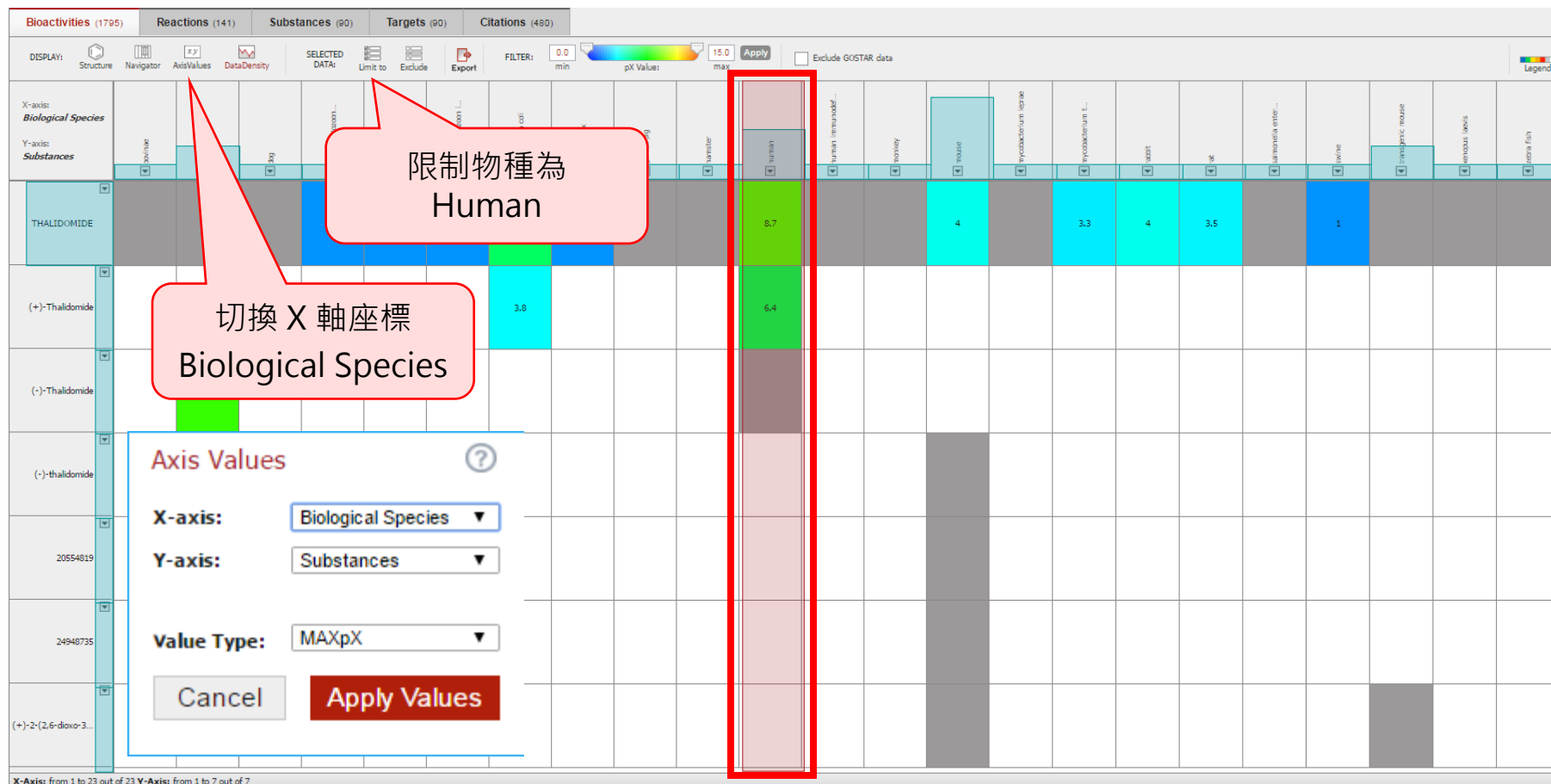
THALIDOMIDE, thalidomide

Druglikeness:

Lipinski rules component	
Molecular Weight	258.233
logP	0.257
HBA	6
HBD	1
Matching Lipinski Rules	4

Veber rules component	
Polar surface Area (PSA)	83.55
Rotatable bond count	1
Matching Veber rules	2

THALIDOMIDE 人類試驗數據



Reaxys 中文學習平台

taiwan.elsevier.com/reaxyshelp

FB 不定期更新
搜尋小技巧

Reaxys 線上學習平台



[首頁](#) | [線上學習](#) | [線上研討會](#) | [考試認證](#) | [聯絡我們](#)



Reaxys 期刊、專利資料庫

查找化學反應式、文獻、化合物及其特性與實驗數據
國研院科資中心免費提供全國大專院校使用

○ ○ ○ ●

學習影片 Learning Video

利用學習影片自我學習如何有效使用Reaxys，一步一步教學，讓資訊檢索變得更簡單。



文件下載 Document Download

快速上手Reaxys，並用實例介紹如何使用Reaxys功能，您可快速找到答案，讓學習變得更有興趣。



線上研討會 Webinar

邀請專家分享使用Reaxys技巧和實例演練操作，讓您從學習中了解如何與資訊互動。



連線問題 Connection Issues

了解常見連線問題，並提供解決之道與聯絡方式。





Thank You!

附錄

Marvin JS 搜尋小技巧

由 ChemDraw 複製結構到 MarvinJS

Reaxys 結構搜尋 – 匯入與匯出 – 1



Edit → Copy as → SMILES

Ctrl + V 貼上

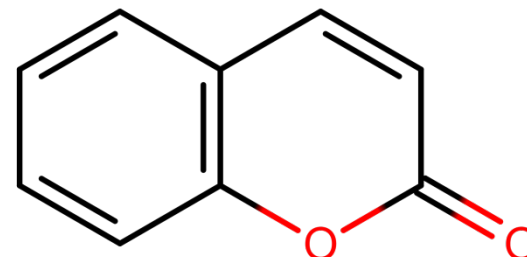
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由化合物名稱產生結構

Reaxys 結構搜尋 – 匯入與匯出 – 2

化合物名稱
Coumarin



Create structure template from name >

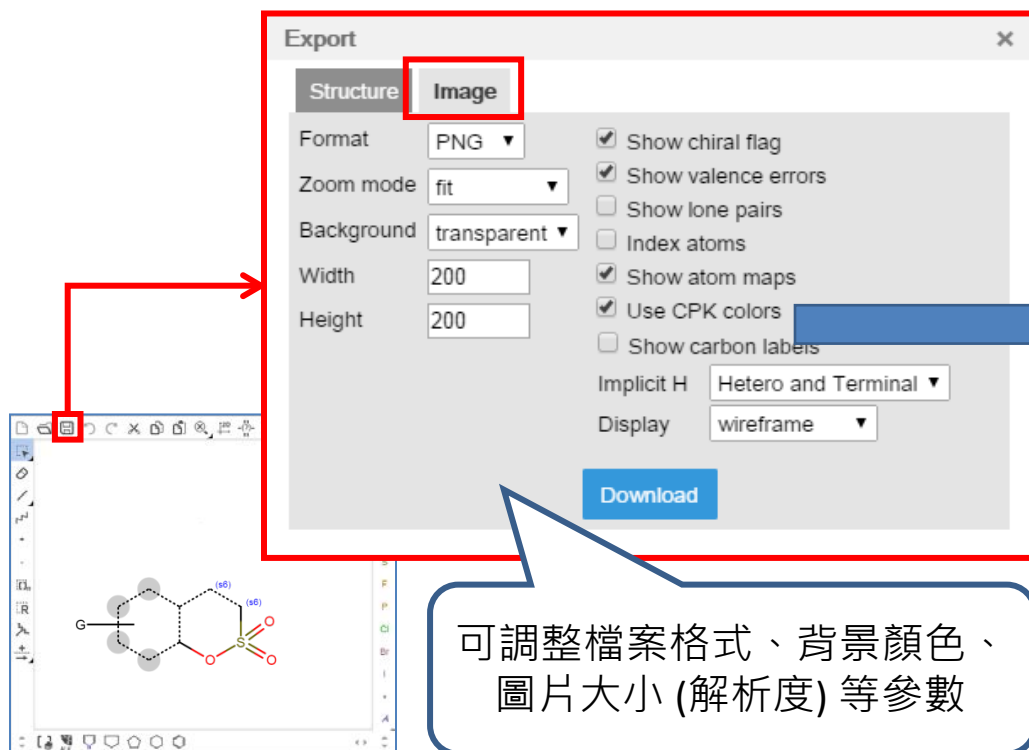
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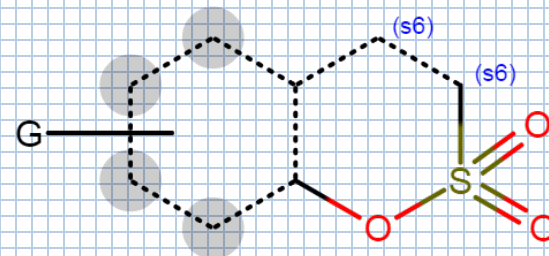
<https://youtu.be/Y2sBPt4o>

將化學結構存成透明背景的圖檔

Reaxys 結構搜尋 – 匯入與匯出 – 3



背景透明的結構圖檔
可在 ppt 或海報使用



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儲存可編輯的結構檔 .mrv

Reaxys 結構搜尋 – 匯入與匯出 – 4

The diagram illustrates the workflow for saving and importing MRV files in Reaxys. It features three main components: a chemical structure editor, an export dialog, and a Marvin JS viewer.

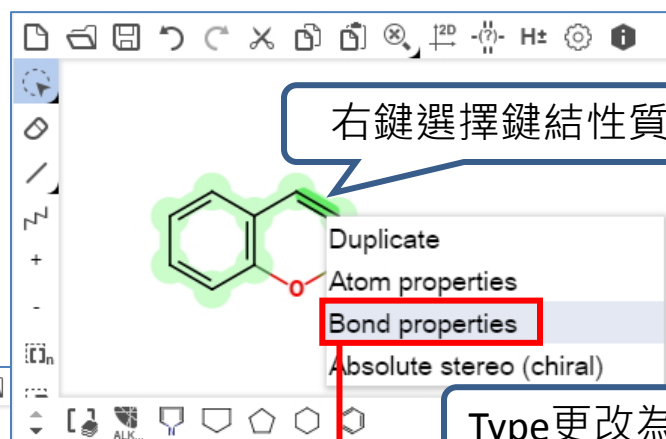
- 儲存檔案 (Save File):** A callout points to the 'Save' icon in the Reaxys editor toolbar.
- Export Dialog:** A red-bordered window titled 'Export' with tabs for 'Structure' and 'Image'. The 'Structure' tab is active, showing the 'Format' dropdown set to 'ChemAxon Marvin Document (MRV)'. The text area contains XML-like MRV code. A 'Download' button is at the bottom.
- 讀取檔案 (Load File):** A callout points to the 'Open' icon in the Marvin JS viewer toolbar.
- 匯入舊檔 (Import Old File):** A callout points to the 'Open' icon in the Reaxys editor toolbar.
- 支援多種檔案格式，也可匯入其他繪圖軟體的檔案 (Supports multiple file formats, can also import files from other drawing software):** A callout points to the Marvin JS viewer, which displays a chemical structure.

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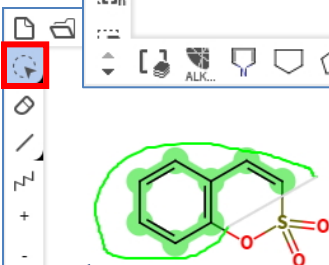
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不確定鍵結種類，該如何搜尋？

Reaxys 結構搜尋 – 衍生物搜尋 – bond property



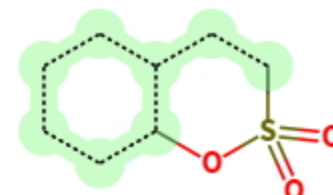
不確定鍵結種類時，可以用虛線表示任意鍵結 (如單鍵、雙鍵、其他)，可以一次找到所有符合條件的化合物



Bond properties

Type	any
Topology	undefined
Reacting center	undefined

Ok

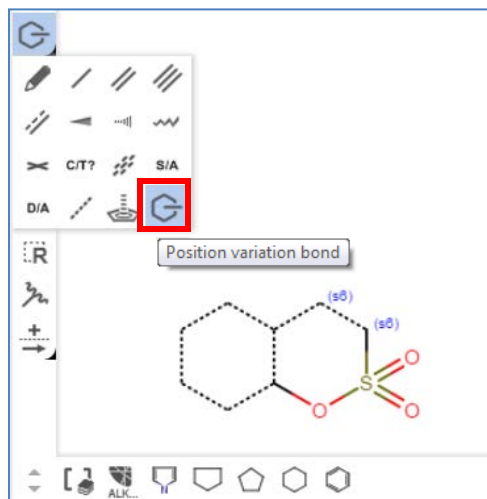


NewReaxys new.reaxys.com

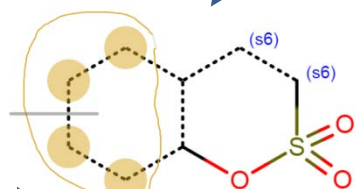
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不確定鍵結位置，該如何搜尋？

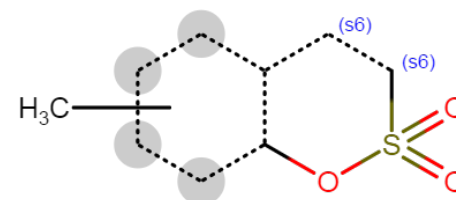
Reaxys 結構搜尋 – 衍生物搜尋 – position variation bond



圈選可能接上
取代基的原子



鍵結與官能基種類
可以再調整



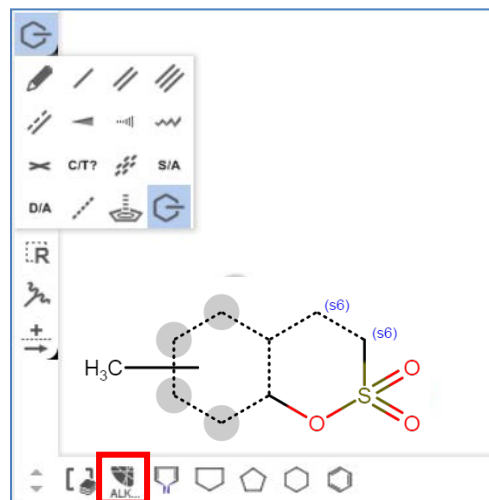
4 個灰色標記的原子
任 1 個接上甲基
就會被搜尋到

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在指定位置，搜尋任意官能基

Reaxys 結構搜尋 – 衍生物搜尋 – G 代表 any functional group



Search this structure as:

- ☒ As drawn
- ☐ As substructure
- ☐ Similar

選擇精準搜尋
As drawn

Reaxys Group Generics

Acyclic Cyclic

ACY ACH

Carb Hetero

ABC ABH AHC AHH

Alkynyl Alkoxy

AYL AYH AOX AOH

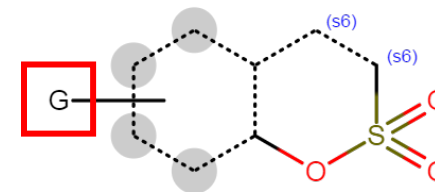
Alkyl

ALK ALH

Alkenyl

AEL AEH

G GH G* GH* Pol



搜尋結果中 G 的位置
可能接上任意官能基

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允許取代基

Reaxys 結構搜尋 – 衍生物搜尋 – Substitution 最高數量

在綠色原子上
按右鍵

Duplicate
+ R-group attachment
- R-group attachment
Atom properties
Absolute stereo (chiral)

設定取代基最高數量
最大 = 6

Atom properties

Change to: Element

Basic	Advanced
Total H (H)	
Implicit H (h)	
Bond orders (v)	
Connections (X)	
Ring count (R)	<not set>
Smallest ring size (r)	
Ring bond (rb)	<not set>
Substitutions (s)	exactly 6
Unsaturated (u)	<not set>
Aromaticity (a/A)	as drawn

Ok

搭配精準搜尋 As drawn
可以在指定位置，
指定取代基的最高數量

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