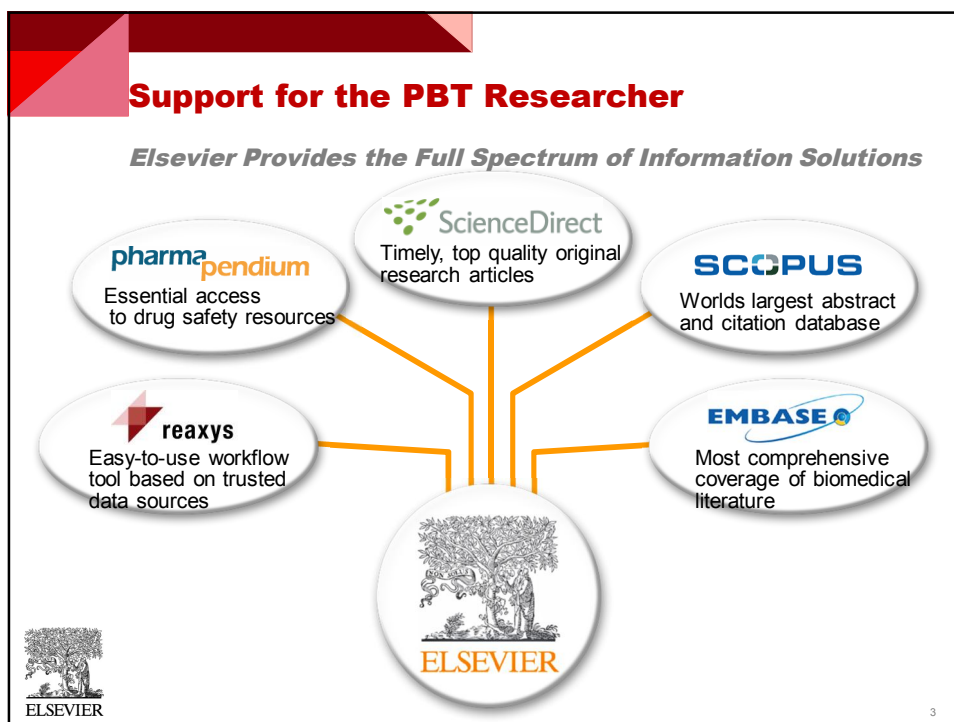




Agenda

- Reaxys 簡介
 - Elsevier PBT products
 - Contents
 - Advantages
- 工作流程和介面概述
 - Query page
 - Result page
 - Synthesis planner





What is Reaxys?

A workflow solution for researchers in **chemistry, drug discovery and related scientific areas**

Using Reaxys researchers can

- Easily access validated reaction and substance data, ranking and filtering for relevant results
- Source available chemicals
- Plan and optimize synthetic route
- Export and share results for immediate action in the lab

An extensive repository of reaction and substance property data, Reaxys includes:

- Organic, inorganic, organometallic chemistry from 400 journals
- Coverage from 1771 - present
- World Patent Office, European Patent Office and US English language patents from the major chemistry patent classes

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4

Reaxys Database Suite = Experimental data extracted from journals & patent documents

Databases	What?	For Whom?
	Reactions and experimental substance data from ...	
CrossFire	Organic Chemistry from key journals and patent documents (up to 1980)	Organic Chemists; LifeScientists (Pharma, Biotech, Agro)
Patent Chemistry Database	Organic Chemistry and Life Science from patents (WO, EP and US 1976-)	Organic Chemists; LifeScientists (Pharma, Biotech, Agro)
Gmelin	Inorganic and Organometallic Chemistry (1771 -) from key journals	Inorg./ Organometallic Chemists, Catalyst Researchers, Materials Scientists
PubChem	Provides information on the biological activities of small molecules Maintained by NCBI, released in 2004	Organic Chemists; LifeScientists (Pharma, Biotech, Agro)



5

What do chemists (you) want to know?

1. What is this?

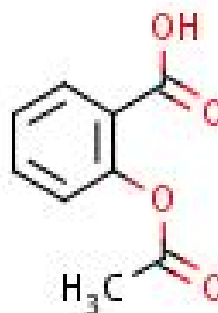
- > Is it novel? Patented?
- > What are its physical characteristics (weight, melting point, etc)?

2. What does it do?

- > Is it a reagent? Solvent?
- > What is its bioactivity? Pharmacology?
- > Is it toxic?

3. How can I make it?

- > How can I change it?
- > How can I make it better?



找尋化學相關資訊 → 搜尋與閱讀 → 花時間

目的：找資料

方法：資料來源

擷取：資料抽出

Time

Time

101年11月20日星期二

Slide 7

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7

Why Reaxys?

What is known about this compound. How do I make it?

Process using a bibliographic chemical database

Read each individual article

Factual and actionable outcome with Reaxys!

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8

Reaxys extracts valuable chemical properties and reaction details from journals and patents.

The screenshot displays the Reaxys web interface. On the left, there is a sidebar with navigation options like 'Home', 'My Alerts', and 'My Settings'. The main area shows a chemical reaction scheme for the synthesis of a tetrahydroquinoline derivative. Below the reaction, there is a table with columns for 'Description', 'Nucleus', 'Solvents', 'Frequency', and 'Reference'. The table contains one entry: 'Spectrum 1H', 'CDCl3', '300MHz', and 'Fukuda, Tsutomu; Honda, Ryoichi; Inoue, Masamoto; Tetrahedron, 1999, vol. 55, # 30, p. 9151-9162'. To the right of the reaction, there is a '1H NMR 300 MHz' section with a chemical structure and a list of peaks. The background shows a blurred image of a journal page with the title 'TETRAHYDROQUINOLINE'.

Four good reasons to use Reaxys

1. The wealth of **experimentally validated data** which can be searched, filtered and ranked to find the most relevant answer to a specific question quickly.
2. Functionality beyond data searching: **synthesis planner**, results management, smart analysis tools for fast evaluation.
3. The **intuitive interface** and **online educational material** help reduce your training efforts.
4. **Interoperable**: linking to *SciVerse Scopus*, full-texts at publishers and patent offices. Access to your own library settings via OpenURL resolver is possible.



"The flat rate access is important for every moderate to large institution and the University of Leeds is no exception."

Professor Peter Johnson, University of Leeds

Full open library for searching and grouping. The available data "group" increases the entry limit to your interest.

100 "groups" of individual chemical reactions

107 citations found

工作流程和介面概述

Instantly view and analyze the results

This can filter by chemical type, e.g. natural products or publications year

Download to Excel, PDF or Full Text. All the data can be downloaded for further analysis

11

搜尋頁面-Substance and Properties

93 substances out of 372 citations

Query Results Synthesis

Substances (Grid) Substances (Table) Citations

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by: No of References

go to Page: Page 1 of 31

Reactions Substances and Properties

Generate structure from name

Double click this frame and

Properties (Form-based)

Substance Data

Bibliographic Data

Clear Query

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	N° ref
	<p>Chemical Name: (Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-((S)-E)-3-hydroxyoct-1-enyl]-cyclopentyl]hept-5-enoic acid</p> <p>Reaxys Registry Number: 2225571</p> <p>CAS Registry Number: 551-11-1</p> <p>Type of Substance: isocyclic</p> <p>Molecular Formula: C₂₇H₃₄O₅</p> <p>Linear Structure Formula: C₂₇H₃₄O₅</p> <p>Molecular Weight: 354.487</p> <p>InChI Key: PXGFLTODNUJGFL-YNPNMKQSA-N</p>	134 prep out of 179 reactions.	Identification Physical Data (45) Spectra (35) Bioactivity/ECotox (265) Use/Application (20) Natural Product (8)	23 Qry His
	<p>Chemical Name: iso-prostaglandin F_{2α} type III</p> <p>Reaxys Registry Number: 7170215</p> <p>CAS Registry Number: 27415-26-5</p> <p>Type of Substance: isocyclic</p> <p>Molecular Formula: C₂₇H₃₄O₅</p> <p>Linear Structure Formula: C₂₇H₃₄O₅</p> <p>Molecular Weight: 354.487</p> <p>InChI Key: PXGFLTODNUJGFL-NAPLMKITS-A-N</p>	19 prep out of 23 reactions.	Identification Physical Data (3) Spectra (15) Bioactivity/ECotox (71) Use/Application (2)	33 Qry His
	<p>Chemical Name: (+)-prostaglandin F_{2α}</p> <p>Reaxys Registry Number: 4153898</p> <p>CAS Registry Number: 23518-25-4</p> <p>Type of Substance: isocyclic</p> <p>Molecular Formula: C₂₇H₃₄O₅</p> <p>Linear Structure Formula: C₂₇H₃₄O₅</p> <p>Molecular Weight: 354.487</p> <p>InChI Key: PXGFLTODNUJGFL-FCINMCKXSA-N</p>	53 prep out of 54 reactions.	Identification Physical Data (5) Spectra (2)	18

12

搜尋頁面- Reactions

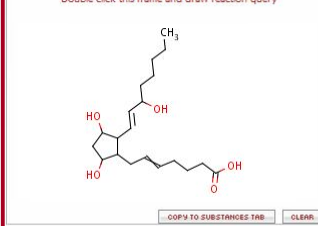
592 reactions out of 115 citations

Query Results Synthesis Plans History My Alerts My S

Reactions Substances and Properties Literature

Generate structure from name

Double click this frame and draw reaction query



Search: Prod Star Any Rea Sub Sim

Conditions (Form-based) Conditions (Advanced)

Reaction Data Bibliographic Data

Clear Query Load Query/Batch Save Query

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Reactions Citations

Line to Exclude Output Print Zoom in Zoom out Hide

Sort by Reaxys-Ranking

Yield Conditions References

1

55% With potassium hexamethylsilazane in tetrahydrofuran; toluene T=20°C; 2 h; Wittig olefination; Rx-ID: 2266602 Find similar reactions

2

54% With potassium hexamethylsilazane in tetrahydrofuran 1.5 h; Rx-ID: 2790002 Find similar reactions

3

90% With water in tert-butyl methyl ether T=35°C; 18 h; Enzymatic reaction; base hydrolysis; Yield given; Rx-ID: 4308445 Find similar reactions

93% With potassium hydroxide; oxalic acid 0.366667 h; Ambient temperature; Rx-ID: 4308445 Find similar reactions

78% With lithium hydroxide monohydrate in tetrahydrofuran; water T=20°C; 3 h; Rx-ID: 4308445 Find similar reactions

Quan, Long Guo; Cha, Jin Kun Journal of the American Chemical Society, 2002, vol. 124, # 42, p. 12424-12425 Title/Abstract Full Text View citing articles Show Details

Lerock, Richard C.; Lee, Nam Ho Journal of the American Chemical Society, 1991, vol. 113, # 20, p. 7815-7816 Title/Abstract Full Text View citing articles Show Details

Zanoni, Giuseppe; Valli, Matteo; Bendjeddo, Lyamine; Porta, Alessio; Bruno, Paolo; Vidari, Giovanni Journal of Organic Chemistry, 2010, vol. 75, # 23, p. 8311-8314 Title/Abstract Full Text View citing articles Show Details

Cai, Zuyun; Nassium, Bahman; Crabbe, Pierre Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1983, # 7, p. 1573-1576 Title/Abstract Full Text View citing articles Show Details

Hwang, Seong Woo; Aiyaman, Mustafa; Khanapure, Subhash; Schio, Laurent; Rokach, Joshua Journal of the American Chemical Society, 1994, vol. 116, # 23, p. 10829-10830 Title/Abstract Full Text View citing articles Show Details

Oger, Camille; Brinkmann, Yasmine; Bouazzaoui, Samira; Durand, Thierry; Galsbol, Jean-Marie Organic Letters, 2008, vol. 39, # 21, p. 5087-5090 Title/Abstract Full Text View citing articles Show Details

13

搜尋頁面- Literature

Query Results Synthesis Plans History My Alerts My Settings Help

Reactions Substances and Properties Literature

Form-based Advanced

Quick Search: e.g. Stereoselective A

Author(s) Assignee(s): Gupta, Mon e.g. Snyder, Peter A.

Journal Title: e.g. Journal of Organ

Patent Number: e.g. US12345678

Publication Year: 2005 e.g. 2005, e.g. 2000-

Clear Query Load Query/E

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Gupta, Monika; Paul, Satya; Gupta, Rajive; Loupy, Andre Tetrahedron Letters, 2005, vol. 46, # 30, p. 4957-4960

go to Page Page 1 of 1

Line to Exclude Output Print Zoom in Zoom out Hide

Sort by Publication Year

Title of the Document	Authors	Year	Source	Times cited
1 A Simple and Efficient Method for Selective Single Aldol Condensation Between Arylaldehydes and Acetone	Paul, Satya; Gupta, Monika	2005	Synthetic Communications, 2005, vol. 35, # 2, p. 213-222 Full Text View citing articles	11
2 A Mild, Efficient, and Green Procedure for Michael Addition of Active Methylene Compounds to Chalcones Under Microwave Irradiation	Paul, Satya; Gupta, Monika; Singh, Parvinder Pal; Gupta, Rajive; Loupy, Andre	2005	Synthetic Communications, 2005, vol. 35, # 2, p. 325-332 Full Text View citing articles	9
3 ZnO: a versatile agent for benzylic oxidations	Gupta, Monika; Paul, Satya; Gupta, Rajive; Loupy, Andre	2005	Tetrahedron Letters, 2005, vol. 46, # 30, p. 4957-4960 Full Text View citing articles	30

Title/Abstract Show All Reactions (21) Show All Substances (43)

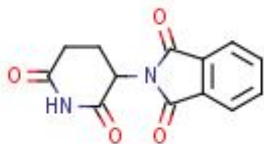
Title/Abstract Show All Reactions (12) Show All Substances (19)

Title/Abstract Show All Reactions (12) Show All Substances (20)

14

反應搜尋範例 - Thalidomide

> Thalidomide是最早上市的非處方鎮定劑，很多國家曾用於懷孕婦女的噁心、嘔吐症狀，卻也造成在1960年代上千位畸形兒的產生，因此而聲名狼藉...



最近幾年讓一些研究學者更感興趣的是 Thalidomide的：

1. 抗發炎作用(anti-inflammatory)
2. 免疫調節(Immunomodulatory)
3. 抑制血管增生(anti-angiogenic)

抗血管新生作用(Anti-angiogenesis Activity)

- (1) 血液腫瘤
 - (2) 多發性骨髓瘤(Multiple Myeloma)
 - (3) 肝癌 (Hepatocellular Carcinoma, H.C.C.)
- 不良反應
- (1) 致畸胎
 - (2) 週邊神經病變
 - (3) 副作用：嗜睡，暈眩等

參考網站：<http://www.tmn.idv.tw/cchtumor/drug/drug07.htm>



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Bioactivity/ Ecotox

Pharmacological Data (264)

4 of 264

Effect	ocular irritation; effect on
Species or Test-System	New Zealand albino rabbit
Route of Application	ocular
Concentration	1 µg
Further Details	hyperemia incidence related to: eye
Type	hyperemia incidence
Value of Type	100 percent
Reference	Feng, Zixia; Hellberg, Mark R.; Sharif, Najam A.; Williams, Gary W.; McLaughlin, Marsha A.; Scott, Daniel; Wallace, Tony Bioorganic and Medicinal Chemistry, 2009, vol. 17, # 2 p. 576 - 584 Title/Abstract Full Text View citing articles Show Details

Molecular Weight: 354.487
InChI Key: FXGLTODNUGFL-YNPMKQSA-N

Chemical Names and Use/Application

(Z)-7-[[1R,2R,3R,5S)-PG F2α, Prostalmon F

Use (20)

Use Pattern	Location	Reference
Ocular hypotensive agent		TECHFIELDS BIOCHEM CO. LTD; YU, Chongxi Patent: WO2008/41054 A1, 2008; Title/Abstract Full Text Show Details

Natural Product

Isolation from Natural Product (8)

Isolation from Natural Product	Reference
prostaglandins extracts from thermophilic cyanobacteria of the taxa Oscillatoria and Microcystidaceae.	Kafanova, T. V.; Busarova, N. G.; Isai, S. V.; Zvyagintseva, T. Ya. Chemistry of Natural Compounds, 1996, vol. 32, # 6 p. 861 - 865 Khimiya Prirodnikh Soedinenii, 1996, # 6 p. 869 - 874 Title/Abstract Full Text View citing articles Show Details
freshly removed, skin-free horns of the spotted deer (Cervus nippon)	Isai, S. V.; Ivankina, N. F.; Kafanova, T. V.; Elyakov, G. B. Pharmaceutical Chemistry Journal, 1994, vol. 28, # 7 p. 521 - 525 Khimko-Farmatsevticheski Zhurnal, 1994, vol. 28, # 7 p. 60 - 63 Title/Abstract Full Text View citing articles Show Details

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◆ 購買化學藥品
 ◆ 提供2D跟3D結構
 ◆ Synthesize Plans

從 eMolecules 找可購買之化學藥品

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42 reactions out of 5 classes go to Page 1 of 14

Yield Conditions References

55% With potassium hexamethylsilazane in tetrahydrofuran; toluene T=20°C; 2 h; Wittig olefination; Rx-ID: 2246969

54% With potassium hexamethylsilazane in tetrahydrofuran 1.5 h; Rx-ID: 530713

84% With acetic acid in tetrahydrofuran; water T=20°C; 48 h; Hydrolysis; Rx-ID: 146423

Multi-step reaction with 10 steps
 1.1: 27 percent / DIBAL-H / toluene / 3.5 h / -78 °C
 2.1: 95 percent / DMAP; Et₃N / CH₂Cl₂ / 11 h / 20 °C
 3.1: 55 percent / DMAP; [PtCl₂(PPh)₂] / benzene / 6.5 h / heating
 4.1: 48 percent / NaBH₄ / methanol / 6.5 h / 0 - 20 °C
 5.1: DMAP; triethylamine / CH₂Cl₂ / 4 h / 20 °C
 6.1: 91 percent / DIBAL-H / toluene / 0 - 20 °C
 7.1: 94800 / tetrahydrofuran / 0 - 20 °C
 7.2: 85 percent / aq. NaOH; aq. H₂O₂ / tetrahydrofuran / 0 - 20 °C
 8.1: TEMPO; NCS; TBAC / CH₂Cl₂; H₂O / 1.2 h / 20 °C / pH 8.6
 9.1: TEMPS / tetrahydrofuran / 3.5 h / 20 °C
 10.1: 3.0 mg / TBAC / tetrahydrofuran / 19 h / 20 °C
 View Scheme

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◆ 反應有關檔案
◆ 全文瀏覽
◆ 引用紀錄
◆ SCOPUS

連結至SCOPUS查看引用文獻之全文

Title of the Document	Authors	Year	Source	Times cited
1 Beyond prostaglandins - Chemistry and biology of cyclic oxygenated metabolites formed by free-radical pathways from polyunsaturated fatty acids	Jahn, U.; Galano, J.-M.; Durand, T.	2008	Angewandte Chemie - International Edition, 2008, vol. 47, p. 5894-5955 View citing articles Full Text	48
2 Quantification of F-ring isoprostane-like compounds (F4-neuroprostanes) derived from docosahexaenoic acid in vivo in humans by a stable isotope dilution mass spectrometric assay	Musiek, E.S.; Cha, J.K.; Yin, H.; Zackert, W.E.; Terry, E.S.; Porter, N.A.; Montine, T.J.; Morrow, J.D.	2004	Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2004, vol. 799, p. 95-102 View citing articles Full Text	43
3 Regiochemistry of neuroprostanes generated from the peroxidation of docosahexaenoic acid in vitro and in vivo	Yin, H.; Musiek, E.S.; Gao, L.; Porter, N.A.; Morrow, J.D.	2005	Journal of Biological Chemistry, 2005, vol. 280, p. 26600-26611 View citing articles Full Text	36
4 Radical cyclization of haloacetals: The Ueno-Stork reaction	Salom-Roig, X.J.; Dénès, F.; Renaud, P.	2004	Synthesis, 2004, vol. , p. 1903-1928 View citing articles Full Text	28
5 Total synthesis of isoprostanes: Discovery and quantitation in biological systems	Rokach, J.; Kim, S.; Bellone, S.; Lawson, J.A.; Praticó, D.; Powell, W.S.; FitzGerald, G.A.	2004	Chemistry and Physics of Lipids, 2004, vol. 128, p. 35-56 View citing articles Full Text	27

查看該反應被引用的紀錄

◆ 過濾資訊
◆ 合成方法以及反應數
◆ 數據輸出

reaxys®

Reaxys ID 2225571 [View in Reaxys](#) 1/1

CAS Registry Number: 551-11-1
Chemical Name: (2S,7R,2R,5S)-3,5-dihydroxy-2-((S)-(E)-3-hydroxyoct-1-en-1-yl)cyclopentylhept-5-enoic acid, prostaglandin F2 α , PGF $_{2\alpha}$, PGF $_{2\alpha}$, Dinoprost(R), PG F2 α , Prostalon F



Linear Structure Formula: C₂₀H₃₄O₆
Molecular Formula: C₂₀H₃₄O₆
Molecular Weight: 354.487
Type of Substance: isocyclic
InChI Key: PXGLTODNUVJGFLYNNPMVQKSA-N
Note:

Substance Label (25)

Label	References
J	Patent; TECHFIELDS BIOCHEM CO. LTD; YU, Chongxi; WO2008/41054; (2008); (A1) English, View in Reaxys
PGF2 α	DiFranco, Elso; Subbanagounder, Ganesamoorthy; Kim, Seokchan; Muthi, Krishnakumar; Taneda, Shinji; et al., Chemical Research in Toxicology, vol. 8, no. 1, (1995), p. 61 - 67, View in Reaxys ; Simko, F.; Martinka, P.; Brassanova, J.; Klimes, J.; Kyselovic, J., Pharmazie, vol. 54, no. 8, (1999), p. 632 - 631, View in Reaxys ; Woodward, David F.; Nieves, Amelia L.; Friedlaender, Mitchell H., Journal of Pharmacology and Experimental Therapeutics, vol. 278, no. 1, (1996), p. 137 - 142, View in Reaxys ; Yagami, Tatsuro; Ueda, Keiichi; Asakura, Kenji; Hata, Satoshi; Kuroda, Takayuki; Sakaeda, Toshiyuki; Takasa, Nobuo; Tanaka, Kazushige; Takefumi, Gamba; Hori, Yoza, Molecular Pharmacology, vol. 61, no. 1, (2002), p. 114 - 126, View in Reaxys ; Yamane, Naoto; Tozuka, Zenzaburo; Okada, Yasuyo; Honda, Chie; Nishi, Yuki; Tanimoto, Toshihiko, Bioscience, Biotechnology, and Biochemistry, vol. 72, no. 8, (2008), p. 2164 - 2169, View in Reaxys
Table 1 (x = 2)	Viljo, Ly; Danilas, Kady; Metsala, Andrus; Kreen, Malle; Valtikivi, Imre; Viija, Siije; Pehk, Tonis; Saso, Luciano; Parve, Omar, Journal of Organic Chemistry, vol. 72, no. 15, (2007), p. 5813 - 5816, View in Reaxys
PGF82 α %	Uneyama, Hisayuki; Tanaka, Yoshio; Iwata, Seinosuke; Ishiguro, Tsuneo; Nakayama, Koichi; Biological & Pharmaceutical Bulletin, vol. 18, no. 4, (1995), p. 501 - 506, View in Reaxys ; Aikawa, Jo; Fukazawa, Masayuki; Ishikawa, Michiro; Moroi, Masao; Hamaki, Atsushi; et al., Journal of Cardiovascular Pharmacology, vol. 27, no. 1, (1996), p. 33 - 36, View in Reaxys ; Robertson, Tom F.; Aronson, Philip L.; Ward, Jeremy P. T., American Journal of Physiology, vol. 268/37, no. 1, (1995), p. H301 - H307, View in Reaxys ; Okamura, Tomio; Ide, Shoichiro; Toda, Noboru, Pharmacology, vol. 50, no. 8, (1995), p. 370 - 379, View in Reaxys

1. 在歷史紀錄中，可以組合的方式進行查詢。
2. 透過選擇性儲存，讓歷史紀錄更精簡，增加回顧效率。
3. 點擊檢索結果頁或歷史紀錄中的”Create Alert”，可以利用email獲取該主題最新消息。

The screenshot displays the Reaxys interface. At the top, a navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'My Alerts', 'My Settings', 'Help', 'Forum', and 'Info'. Below this, a dialog box titled 'Select how you want to combine the hitsets' offers four options: 'Merge 4 with 2', 'Overlap 4 with 2', 'Exclude 4 from 2', and 'Exclude 2 from 4'. A red box highlights these options. Below the dialog, a search results table is visible. A red box labeled '1' highlights the 'Combine Hitsets' button. A red box labeled '2' highlights the 'Store' button in the table. A red box labeled '3' highlights the 'Create Alert' button. The table contains two rows of search results, each with a chemical structure, a description, and a date.

Query	Temporary result description	View	Store	Date
	157 substances Substances: As drawn 538 citations	View	Store	2011-05-18 23:55
	648 substances Substances: As drawn 9200 citations	View	Store	2011-05-18 23:32

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Supporting your Excellence in R&D

- > **Reaxys reduces time getting to the relevant results.**
Easy-to-use interface, powerful search and specialist content focused on synthetic chemistry (an extensive repository of chemical properties and reaction data presented with chemistry as the organizing principle)
- > **High quality answers you can use with confidence.**
Experimental data drawn from trusted sources.
- > **Designed around synthetic chemists workflow to improve efficiency.**
Functionality which goes beyond data searching with results management, analysis tools and new workflow features (synthesis planner, export tools).



Use Reaxys and see for yourself how it can improve your Research.

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For more information please contact...

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