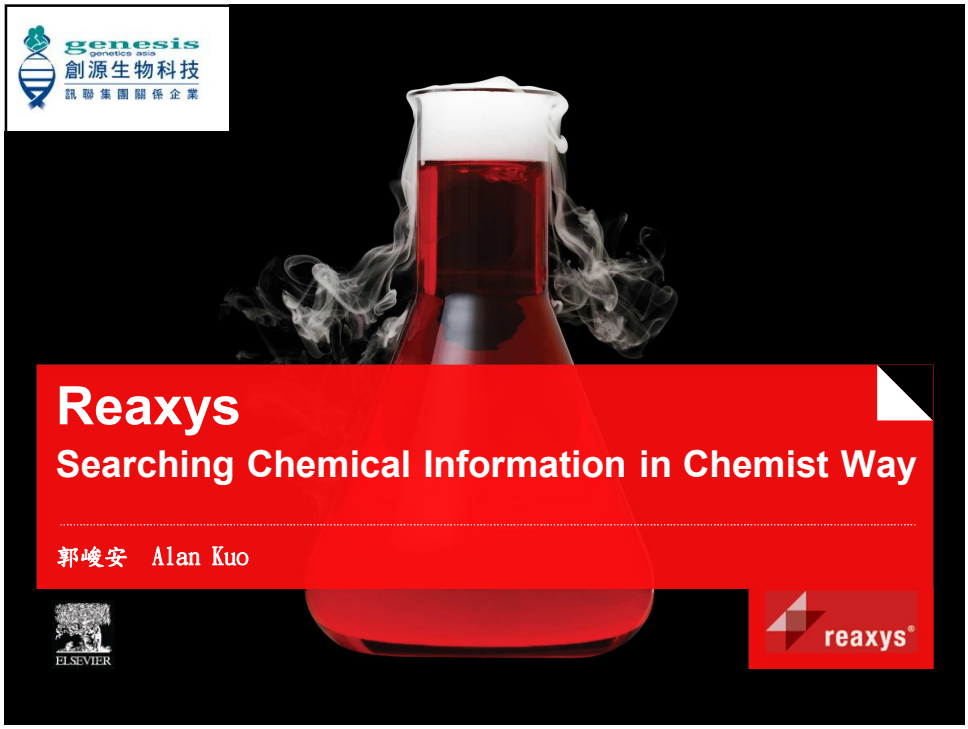


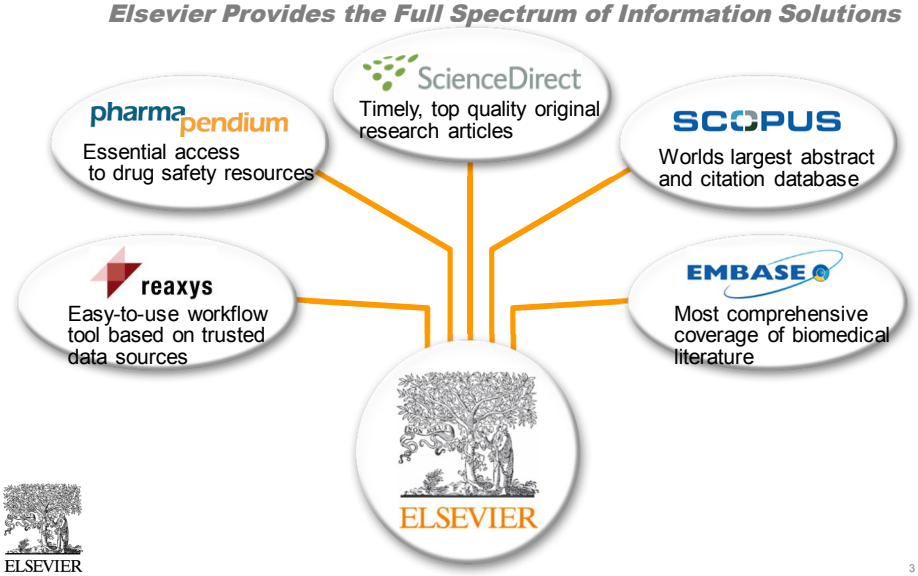
Agenda

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

ELSEVIER reaxys®

Support for the PBT Researcher

Elsevier Provides the Full Spectrum of Information Solutions



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3

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)

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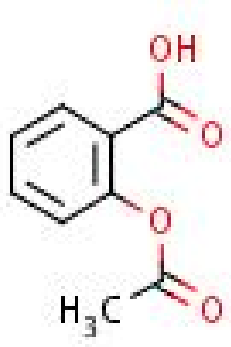
5

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?



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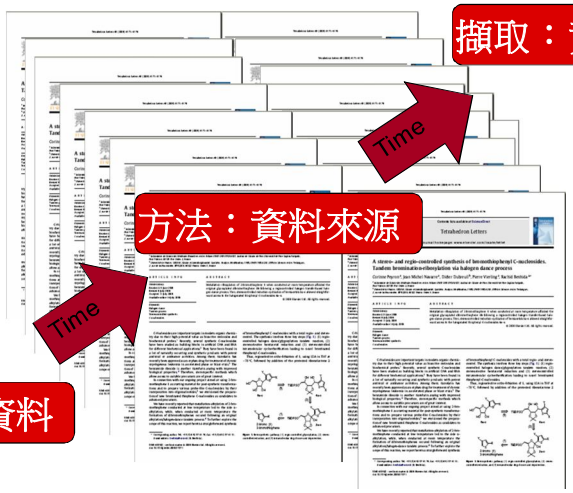
找尋化學相關資訊 → 搜尋與閱讀 → 花時間

擷取：資料抽出



目的：找資料

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101年11月20日星期二 Slide 7

7

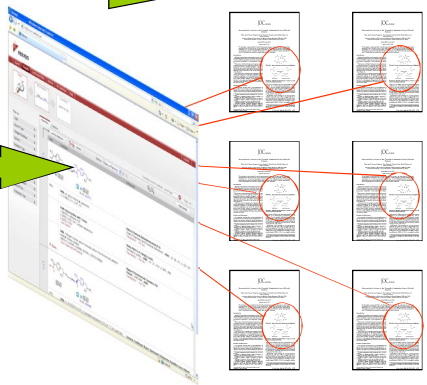
Why Reaxys?

Process using a bibliographic chemical database

Read each individual article

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

Factual and actionable outcome with Reaxys!



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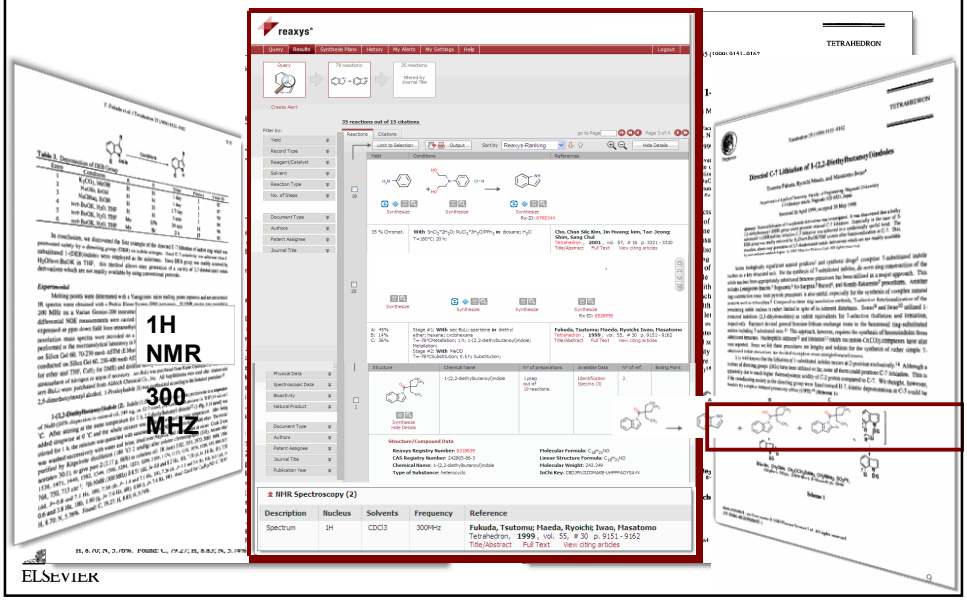
8

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



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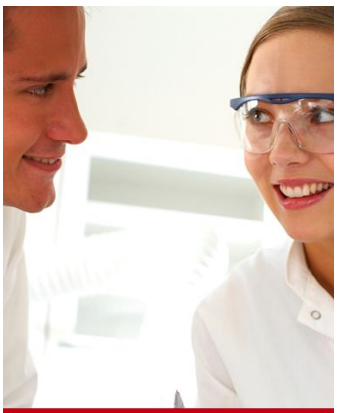
Four good reasons to use Reaxys

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

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10


工作流程和介面概述
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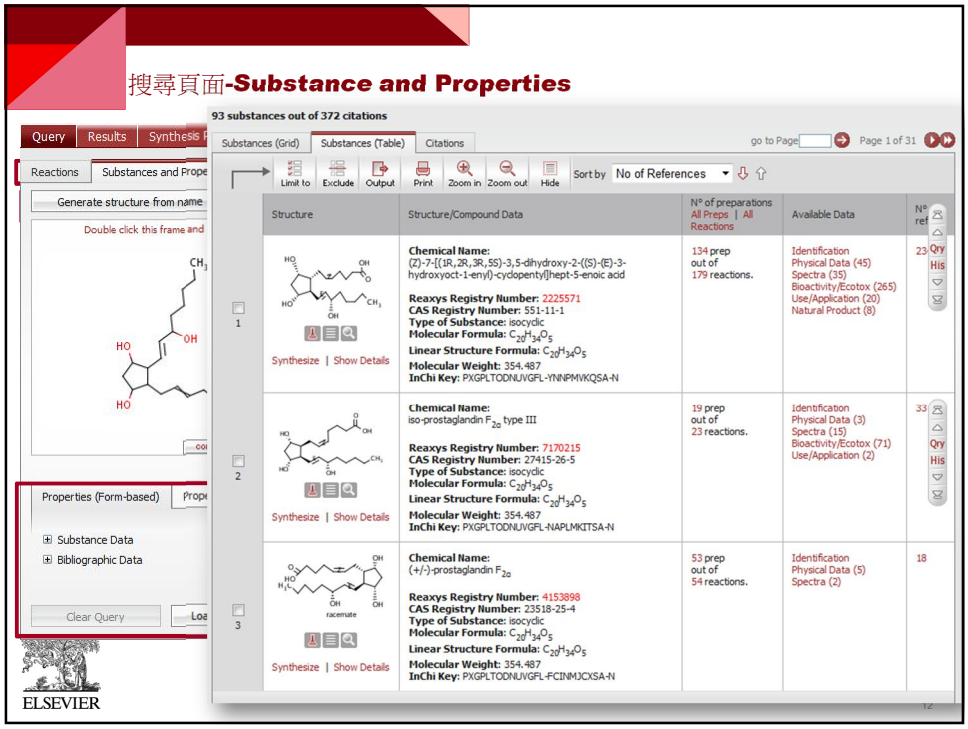
11


搜尋頁面-Substance and Properties
93 substances out of 372 citations
Query
Results
Reactions
Substances and Prope
Generate structure from name
Double click this frame and
Properties (Form-based)
Substance Data
Bibliographic Data
Clear Query
Substances (Grid)
Substances (Table)
Citations
Limit to
Exclude
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Print
Zoom in
Zoom out
Hide
Sort by
No of References
Structure
Structure/Compound Data
N° of preparations
All Preps | All Reactions
Available Data
Synthesize | Show Details
Chemical Name:
(Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-((S)-(E)-3-hydroxyoct-1-enyl)-cyclopentyl]hept-5-enoic acid
Reaxys Registry Number: 2225571
CAS Registry Number: 551-11-1
Type of Substance: isocyclic
Molecular Formula: C20H34O5
Linear Structure Formula: C20H34O5
Molecular Weight: 354.487
InChi Key: PXGPLTODNUVGFL-YNNPMVKQSA-N
134 prep out of 179 reactions.
Identification
Physical Data (45)
Spectra (35)
Bioactivity/Ecotox (265)
Use/Application (20)
Natural Product (8)
Chemical Name:
iso-prostaglandin F2α type III
Reaxys Registry Number: 7170215
CAS Registry Number: 27415-26-5
Type of Substance: isocyclic
Molecular Formula: C20H34O5
Linear Structure Formula: C20H34O5
Molecular Weight: 354.487
InChi Key: PXGPLTODNUVGFL-NAPLMKITSA-N
19 prep out of 23 reactions.
Identification
Physical Data (3)
Spectra (15)
Bioactivity/Ecotox (71)
Use/Application (2)
Chemical Name:
(+/-)-prostaglandin F2α
Reaxys Registry Number: 4153898
CAS Registry Number: 23518-25-4
Type of Substance: isocyclic
Molecular Formula: C20H34O5
Linear Structure Formula: C20H34O5
Molecular Weight: 354.487
InChi Key: PXGPLTODNUVGFL-FCINMJCXSA-N
53 prep out of 54 reactions.
Identification
Physical Data (5)
Spectra (2)
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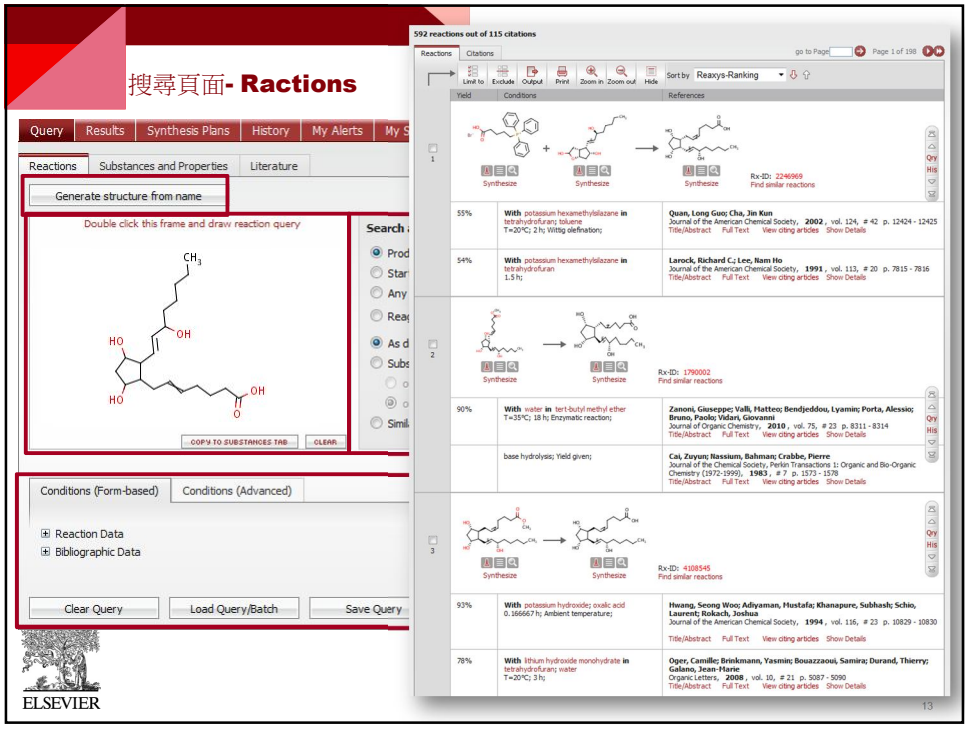
搜尋頁面- Ractions
Query
Results
Synthesis Plans
History
My Alerts
Reactions
Substances and Properties
Literature
Generate structure from name
Double click this frame and draw reaction query
COPY TO SUBSTANCES TAB
CLEAR
Conditions (Form-based)
Conditions (Advanced)
Reaction Data
Bibliographic Data
Clear Query
Load Query/Batch
Save Query
592 reactions out of 115 citations
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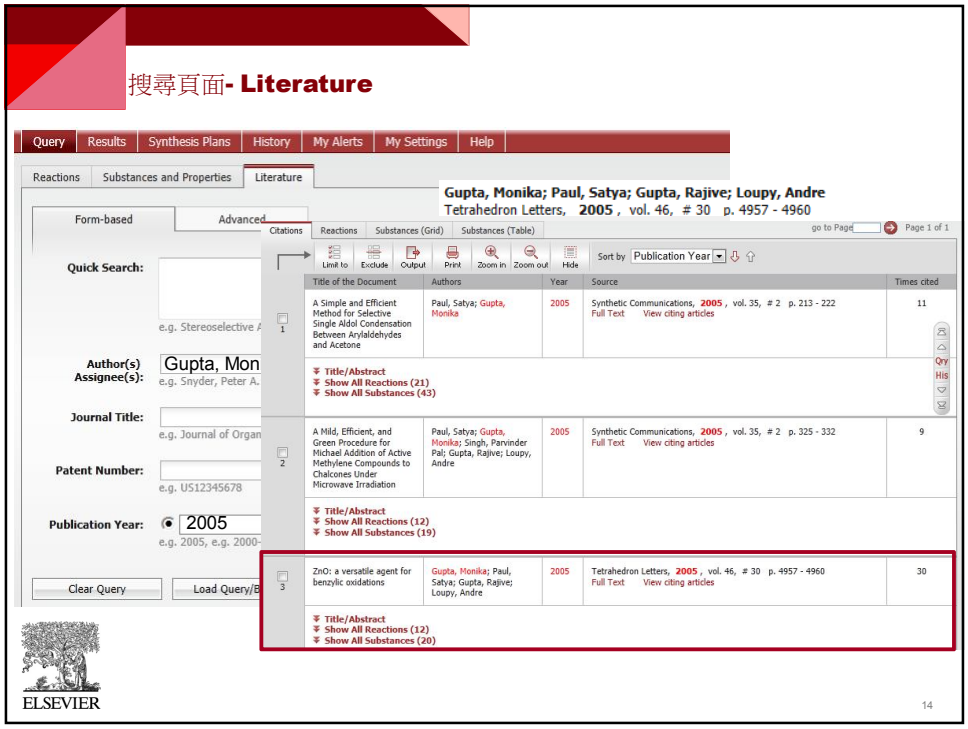
搜尋頁面- Literature
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Results
Synthesis Plans
History
My Alerts
My Settings
Help
Reactions
Substances and Properties
Literature
Form-based
Advanced
Quick Search:
Author(s) Assignee(s):
Journal Title:
Patent Number:
Publication Year:
Clear Query
Load Query/B
Gupta, Monika; Paul, Satya; Gupta, Rajive; Loupy, Andre
Tetrahedron Letters, 2005, vol. 46, # 30 p. 4957 - 4960
Citations
Reactions
Substances (Grid)
Substances (Table)
Sort by Publication Year
Title of the Document
Authors
Year
Source
Times cited
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
11
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
9
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
30
Title/Abstract
Show All Reactions (21)
Show All Substances (43)
Show All Reactions (12)
Show All Substances (19)
Show All Reactions (12)
Show All Substances (20)
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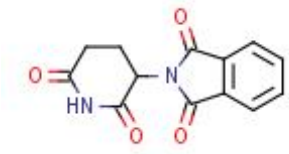
反應搜尋範例 - **Thalidomide**

> 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-inflamatory)
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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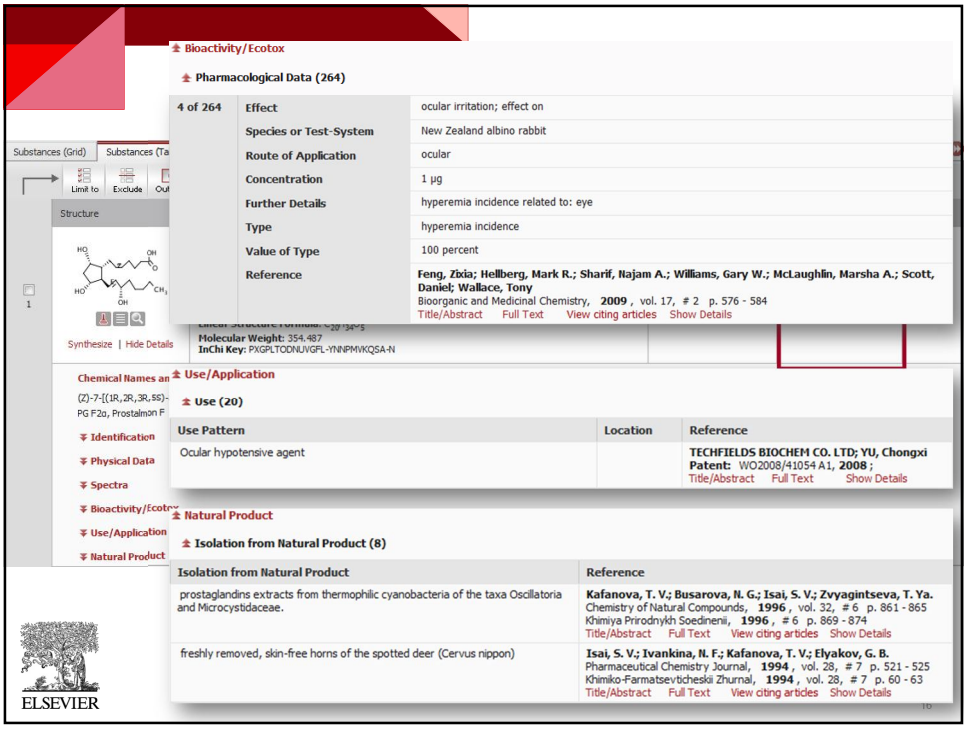
15



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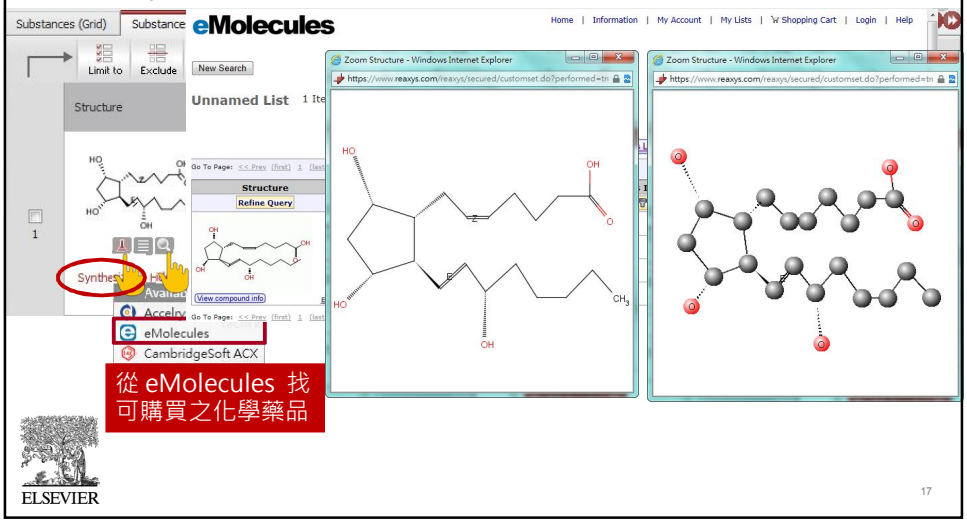
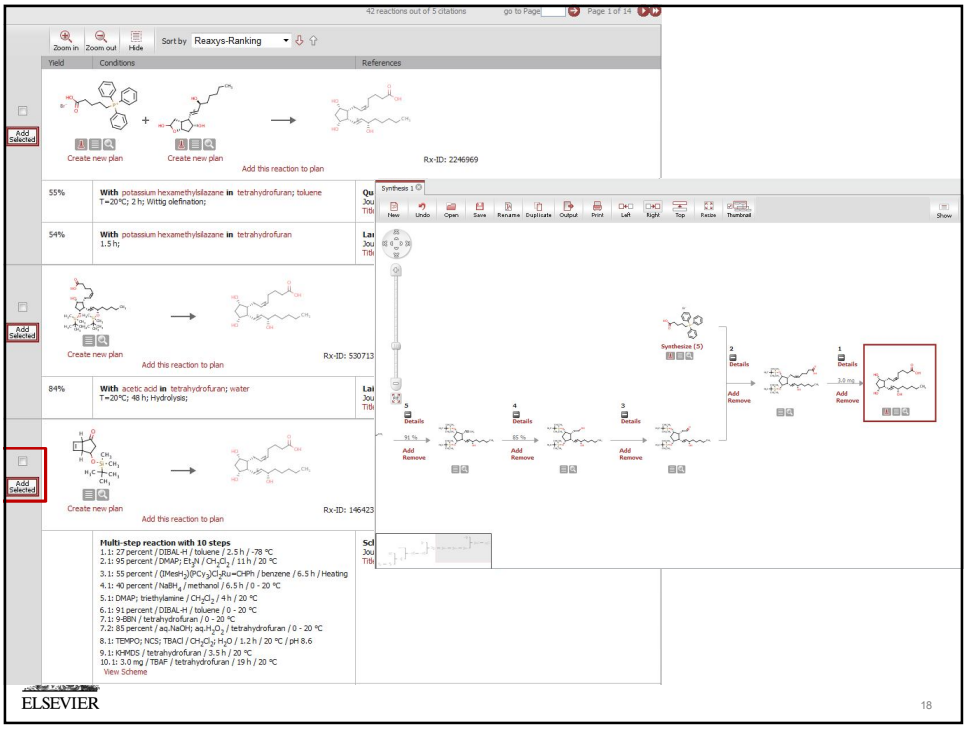
- 購買化學藥品
- 提供2D跟3D結構
- Synthesize Plans





- 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

Print | Sort by Times Cited

	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.; Praticò, 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

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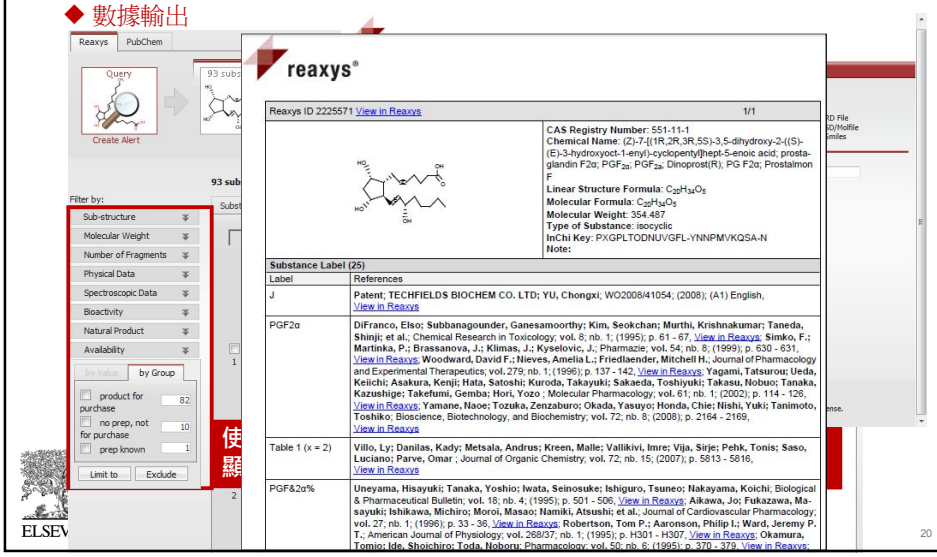
- 過濾資訊
- 合成方法以及反應數
- 數據輸出



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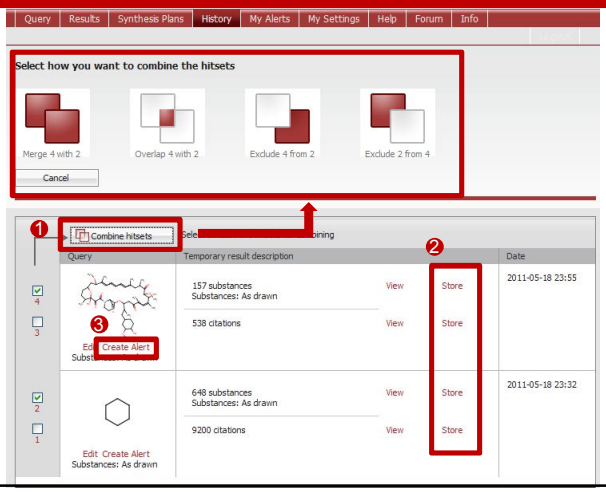
1.在歷史紀錄中，可以組合的方式進行查詢。

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。



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21

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...

ELSEVIER 台灣區總代理

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E-Mail: MSC-Support@gga.asia
www.gga.asia