Reaxys

Smarter search in chemistry to save your valuable time

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NARLabs 財團法人國家實驗研究院

科技政策研究與資訊中心

Science & Technology Policy Research and Information Center

ELSEVIER

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ELSEVIER LIFE SCIENCES

OUR SHARED PURPOSE

TO ACCELERATE SCIENCE TO IMPROVE HEALTH

A Knowledge & Information Analytics Company

OUR PROMISE

Partners in propelling research and innovation forward to transform the way you bring new medicines to the world

OUR KEY DIFFERENTIATORS

- Customer First Commitment
- Our Roots As A Knowledge Company
- Open Integrated Systems
- Accelerating Data-Driven Decisions
- Market-Leading Talent

140+

years of scientific knowledge curated as semantically rich content to enable tomorrow's medical breakthroughs

RELX

$1.4bn
on technology annually

~30,000
employees

Serving customers in
180+ countries

Partnering with
90%
of top Pharma companies

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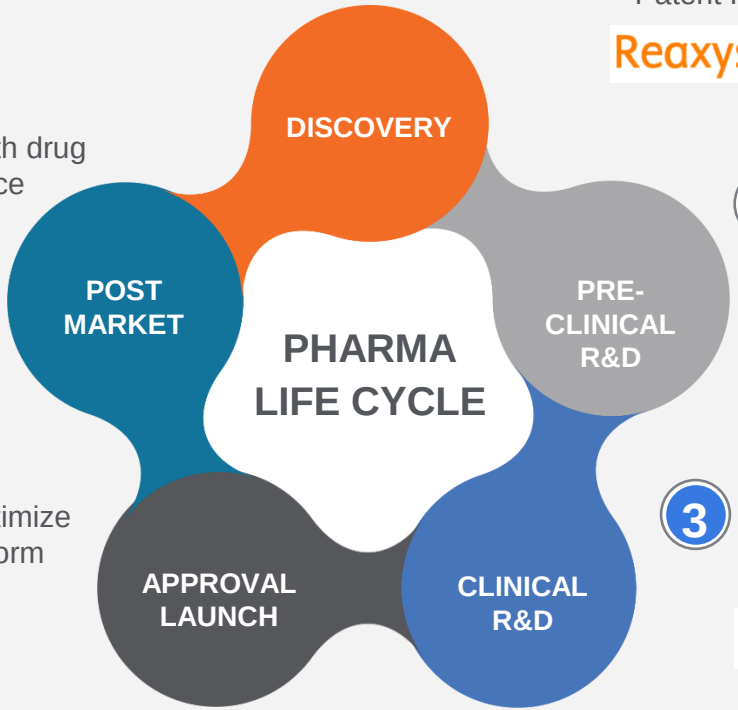
Elsevier 於科學文獻中摘錄實驗數據，提供新藥開發研發人員快速查詢整合資訊，輔助形成關鍵決策



1 DISCOVERY
- Pathways & Drug targets define
- Leads generation /Candidate optimization
- Patent FTO / Novelty research

Reaxys® Reaxys® Medicinal Chemistry

2 PRE-CLINICAL R&D Cull leads more quickly for safety & efficacy; Inform translational research

Reaxys® Medicinal Chemistry

PharmaPendium®

3 CLINICAL R&D Optimize clinical study design, primary endpoint for clinical trials

PharmaPendium®

4 APPROVAL LAUNCH Optimize supply chain efficiency; Inform HEOR and Market Access strategies

PharmaPendium®

5 POST MARKET Comply with drug safety and pharmacovigilance regulations; Adverse events monitoring and reporting

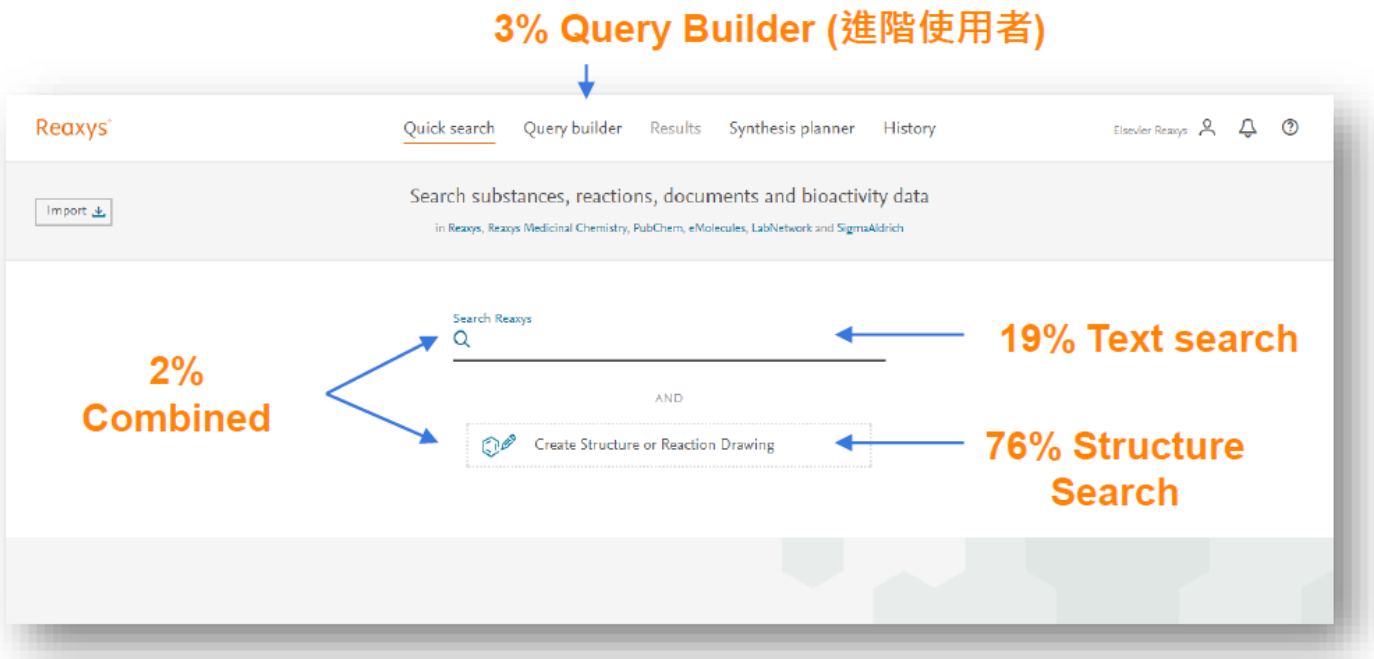
Quosa™

Embase®

ELSEVIER

Reaxys提供四種搜尋介面協助研究人員快速取得可應用的實驗資訊

- 搜尋介面統計

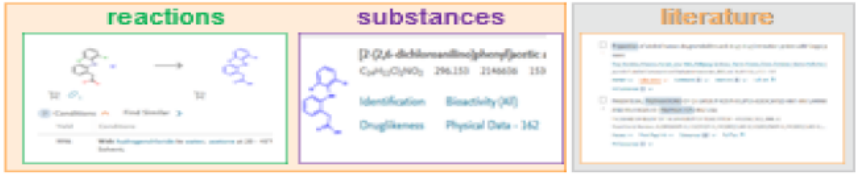


ELSEVIER

研究人員仰賴Reaxy提供實驗數據並直接應用於實驗中，而非花費大量時間搜尋、閱讀文獻

- 搜尋資料統計

實驗資料可直接進行應用



文獻資料仰賴人力閱讀

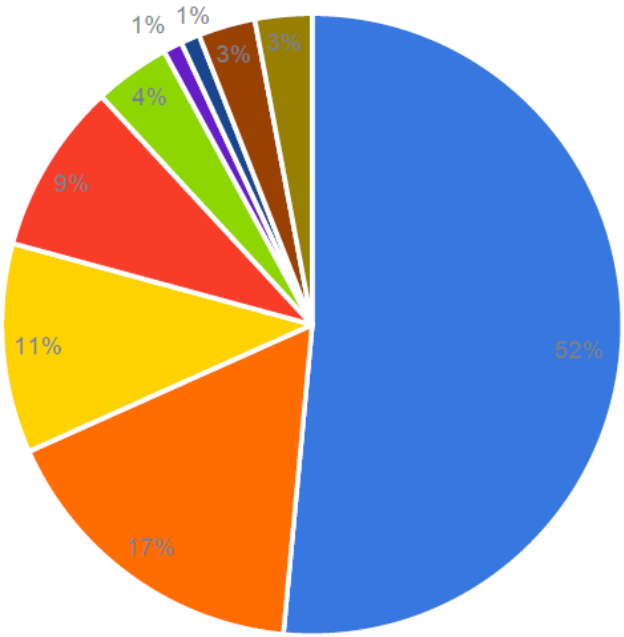
33%　61%　6%

台灣大學使用者94%搜尋專注於實驗數據

ELSEVIER

Reaxys 提供各類型資料類型資料，讓研究員把時間花在研究本身

台灣大學前三大資料類型:
1. 化學反應材料與方法
2. 光譜資料
3. 物理性質



- Experimental procedure and preparation data
- Spectra data
- Physical data
- Reaction data
- Document
- Other data
- Bioactivity data
- Druglikeness data
- Identification

Total clicks = 64,675

以其他方式取得 (實驗材料與方法, 物質光譜, 物理性質等資料) 將需要更大量的時間、人力與金錢成本

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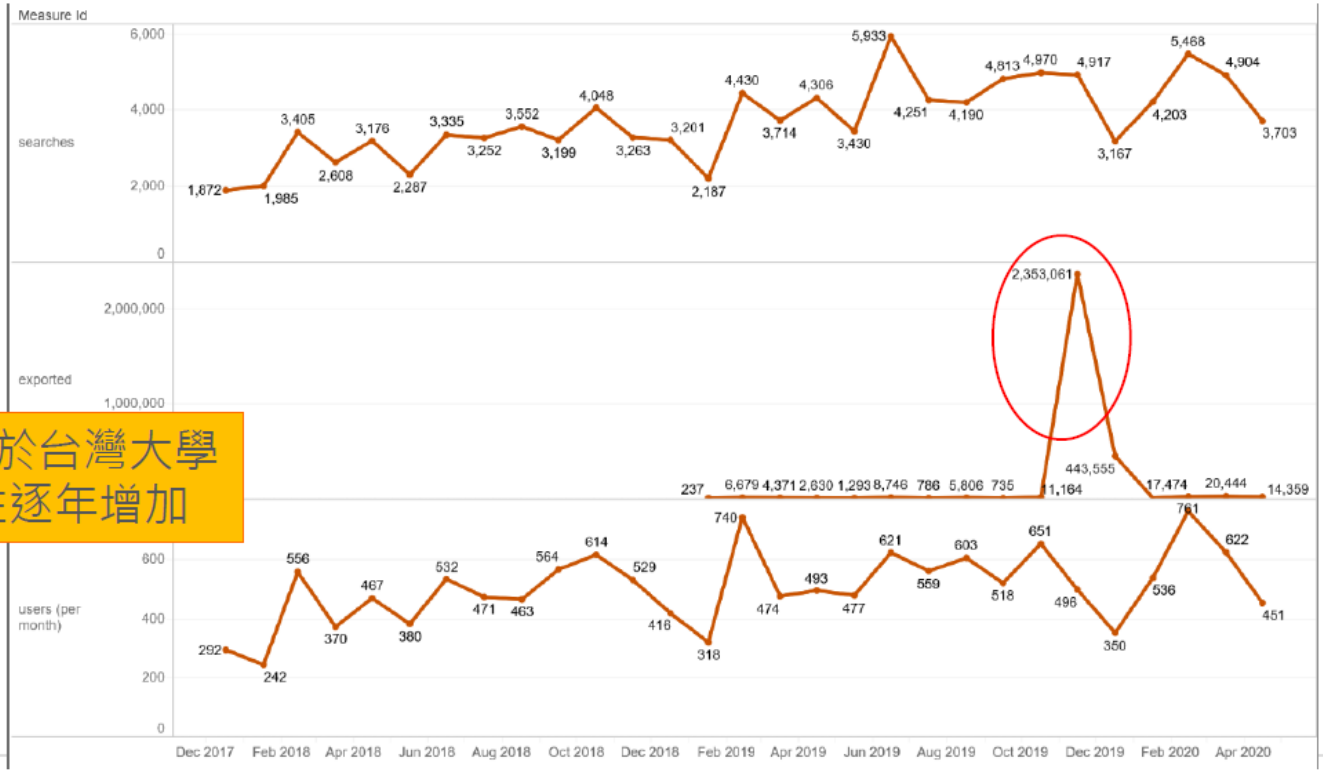
使用人數、搜尋次數、與資料輸出趨勢 (2018.1-2020.5)



Reaxys對於台灣大學的重要性逐年增加

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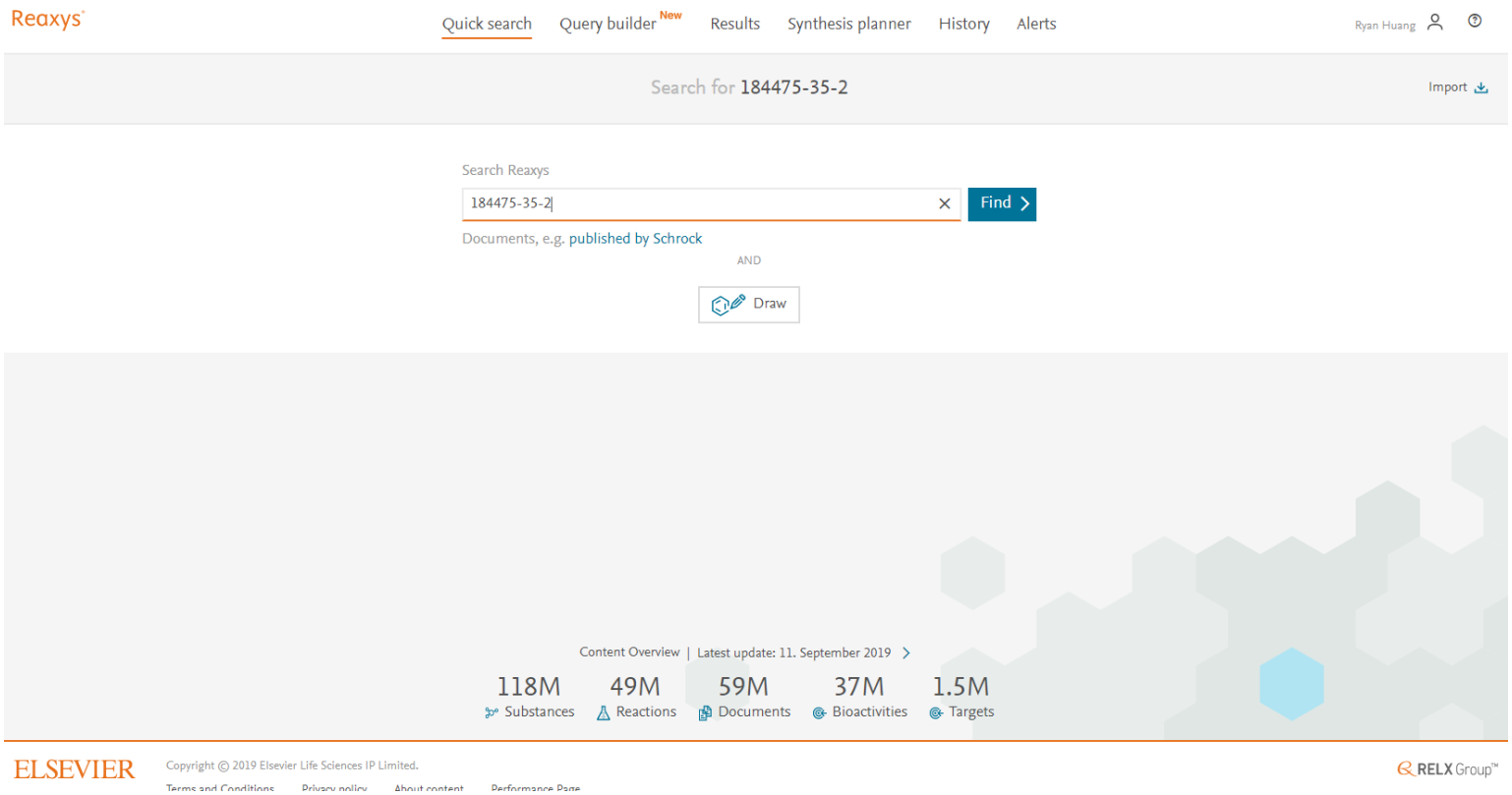
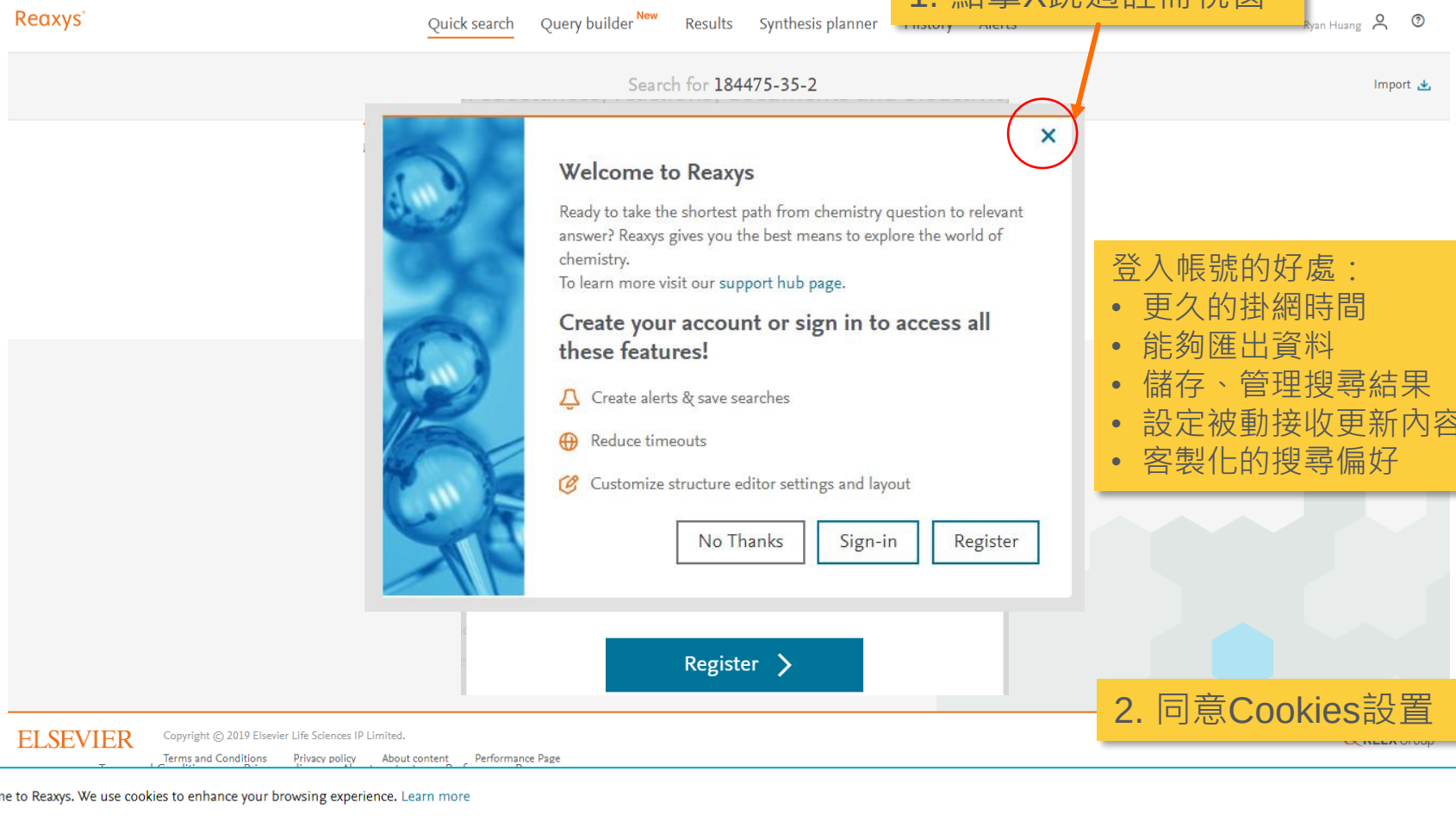
如何連上Reaxys

在學校IP範圍內，打開瀏覽器鍵入 http://reaxys.com

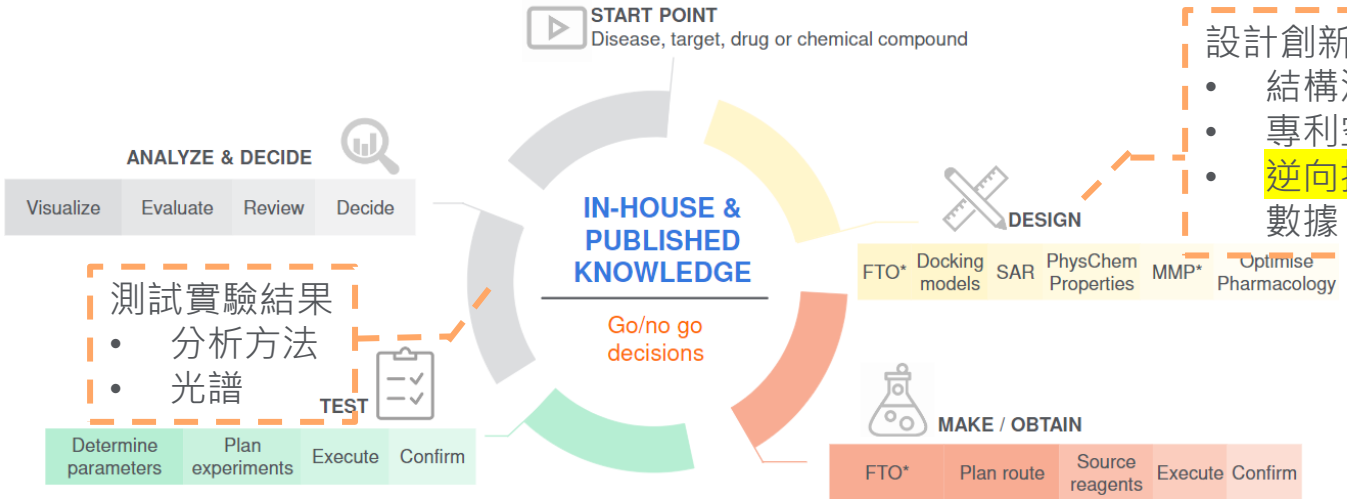


初次登入Reaxys –註冊免費帳號的好處



Reaxys在研發階段提供關鍵資料，節省人力、時間成本，加速專案進度

- 背景資料收集
- 競爭者資訊(專利、期刊文獻)



設計創新化合物
- 結構活性分析
- 專利空間研究
- 逆向搜尋物理性質等實驗數據

測試實驗結果
- 分析方法
- 光譜

創造新化合物、新材料
- 合成路徑規劃、產率優化、降低成本
- 純化、不純物分析

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範例1 請利用Quick search 欄位搜尋 “sglt2 inhibitor”

註 SGL2 (Sodium glucose co-transporters2) 與胰島素作用無關的新機轉第二型糖尿病藥物

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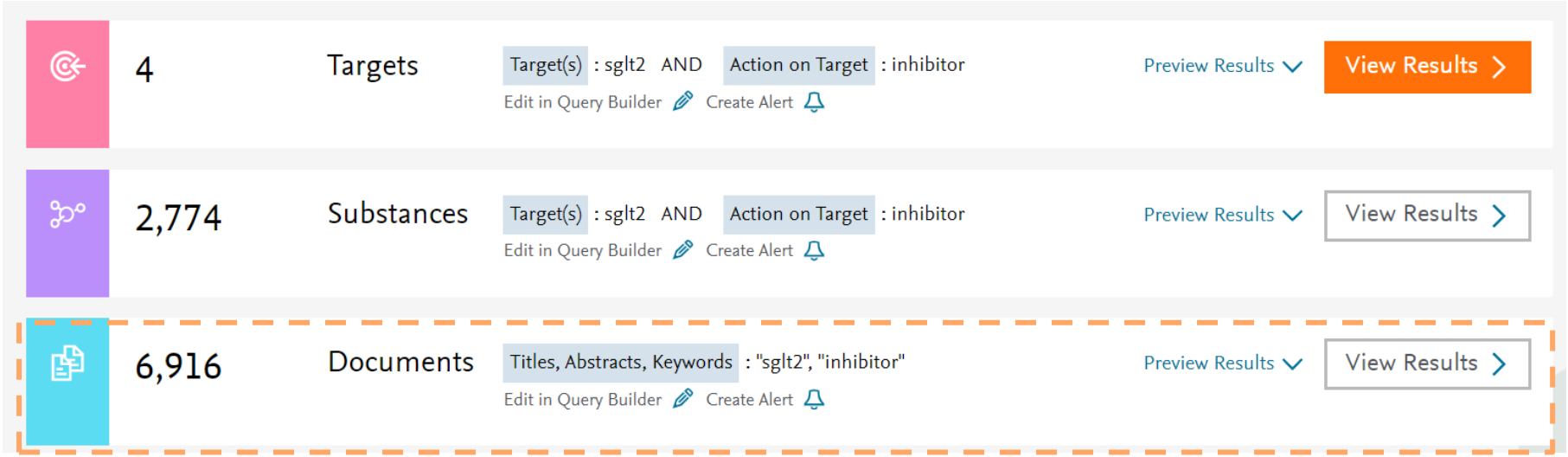
搜尋預覽頁面



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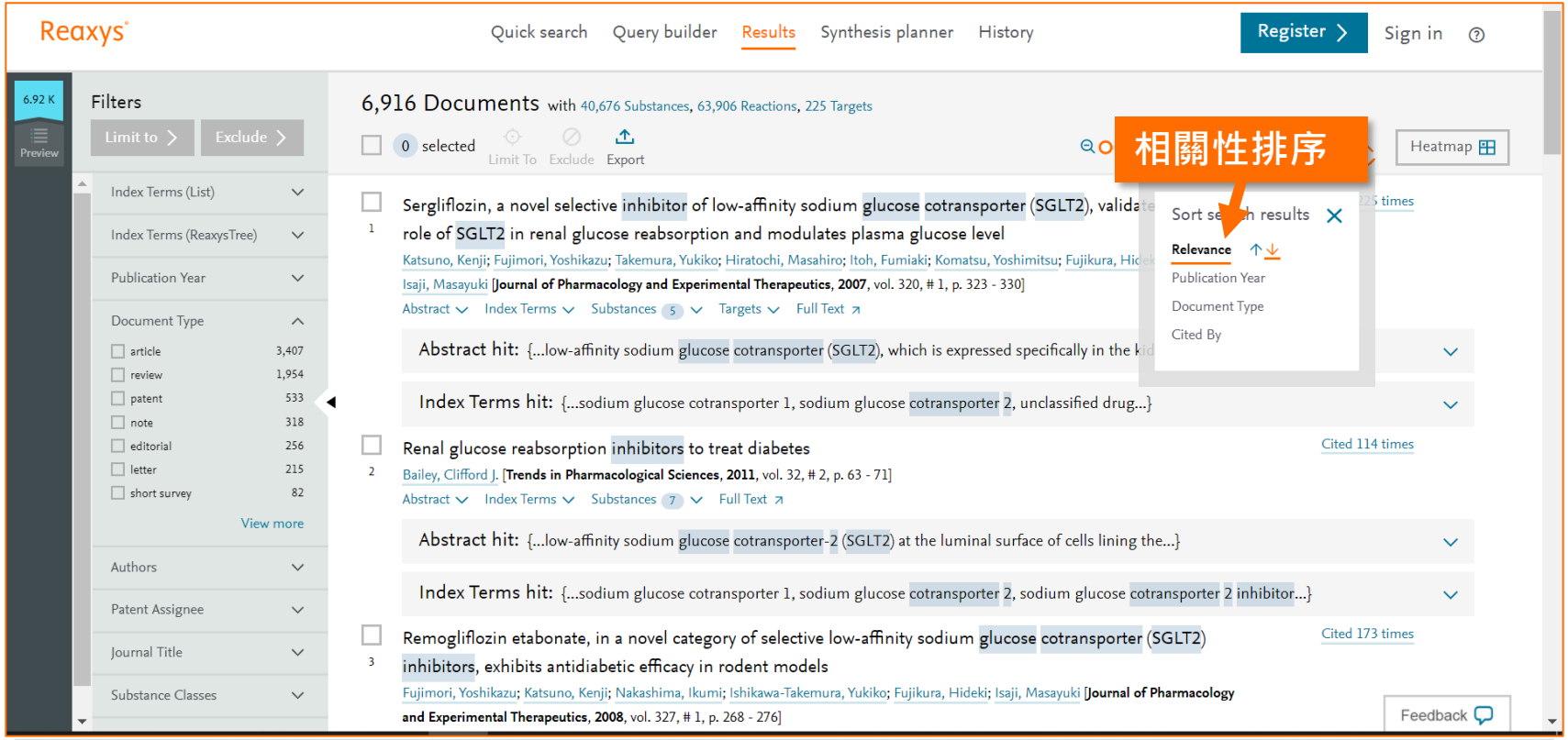
關鍵字搜尋 – 相關性排序 (Relevance ranking)



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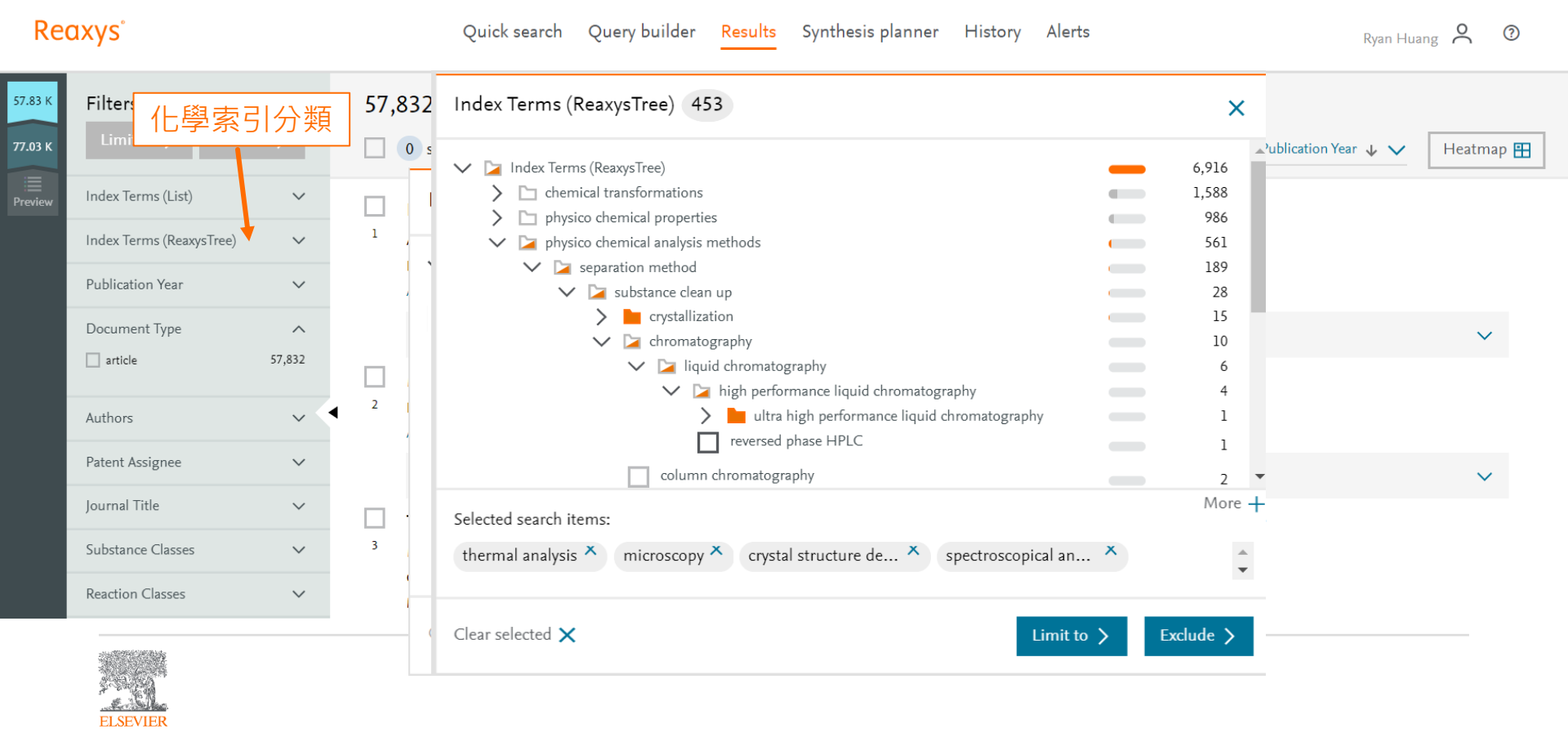
關鍵字搜尋 – 研究主題篩選器 (Index Terms)



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關鍵字搜尋 – 期刊資訊 (全文索引詞index terms 快速了解文獻內容相關性)

Reaxys

Quick search | Query builder | Results | Synthesis planner | History | Alerts

Ryan Huang

249
951
1.63 K
Preview

Filters

Limit to | Exclude

Index Terms (List)

Index Terms (ReaxysTree)

Publication Year

2020 114
2019 135

Filter by value

Document Type

Authors

Patent Assignee

Journal Title

Substance Classes

0 selected | Limit To | Exclude | Export | Sort by Relevance | Heatmap

Abstract hit: {...corroded and crude oil played a role of inhibitor, thus it influenced the...}

Index Terms hit: {...Corrosion products, Crude oil, X65 steel...}

8 Evaluation of the localized corrosion resistance of 316 L austenitic and 430Ti ferritic stainless steel in aqueous chloride/sulphate media for application in petrochemical crude distillation units

Cited 2 times

Loto, Roland Tolulope; Loto, Cleophas Akintoye [**Materials Research Express**, **2019**, vol. 6, # 8, art. no. 086516]

Abstract | Index Terms | Substances 2 | Full Text

Abstract hit: {...constituents of crude oil. Potentiodynamic polarization test, potentiostatic measurement, open circuit potential measurement...}

Index Terms

Author keyword: chloride, Corrosion, pitting, steel, sulfate

Engineering uncontrolled terms: chloride, Crude distillation units, Open circuit potential, Open circuit potential measurements, Potentiodynamic polarization tests, Potentiostatic measurements, sulfate, Surface deterioration

Engineering controlled terms: Austenite, Corrosion, Corrosion rate, Corrosion resistance, Crude oil, Deterioration, Distillation, Distillation equipment, Ferrite, Ferritic stainless steel, Morphology, Passivation, Petrochemicals, Pitting, Polarization, Sodium chloride, Steel, Steel corrosion, Sulfur compounds, Surface resistance, Titanium alloys

Reaxys Index Terms: Petroleum refining, chemical passivation, corrosion resistance, electrooxidation, open circuit potential

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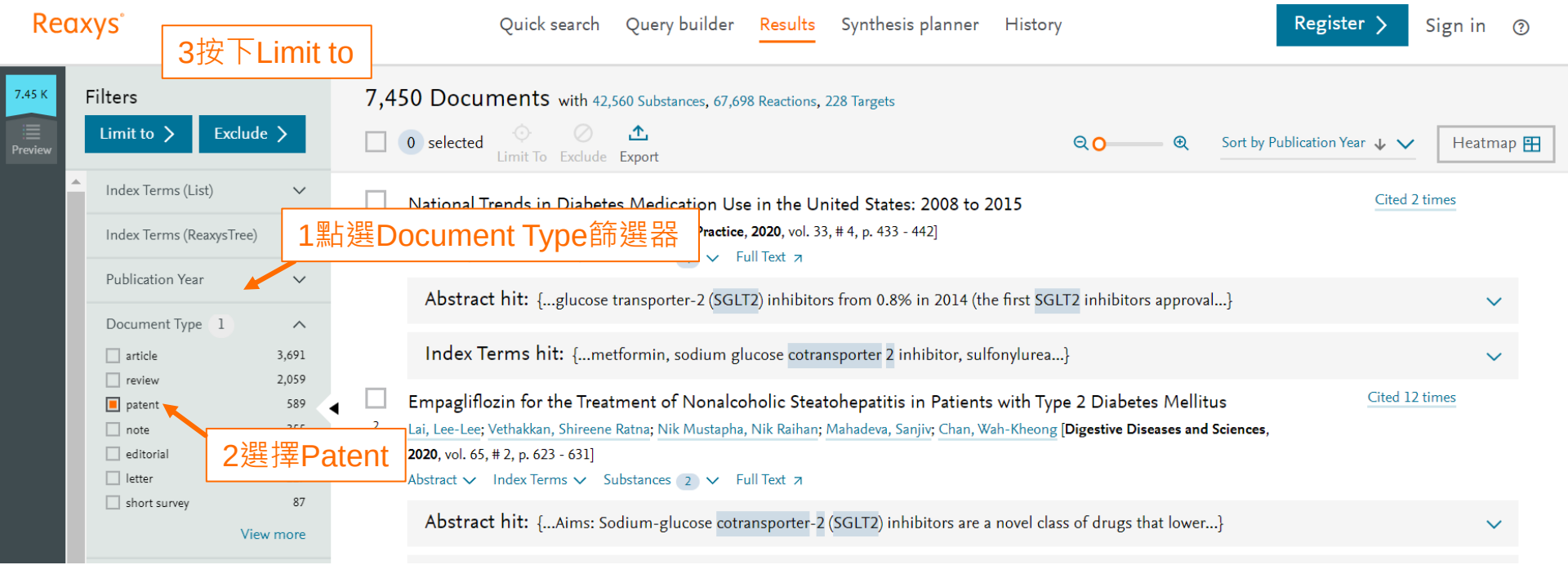
關鍵字搜尋 – 篩選專利文件 (2020預計專利擴增>100 patent offices)



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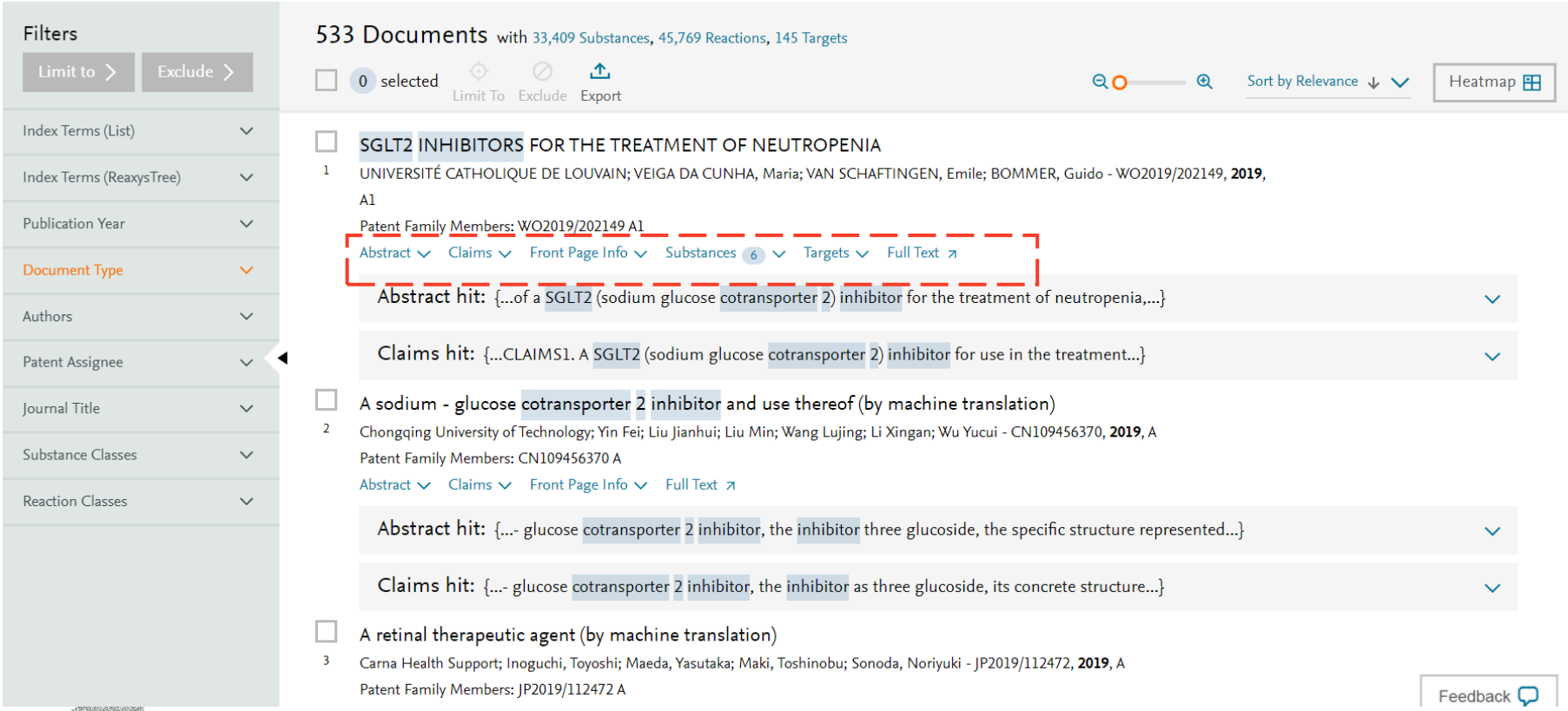
關鍵字搜尋 – 人工擷取(摘要、專利要求、專利家族、分類號、物質、反應及全文連結)



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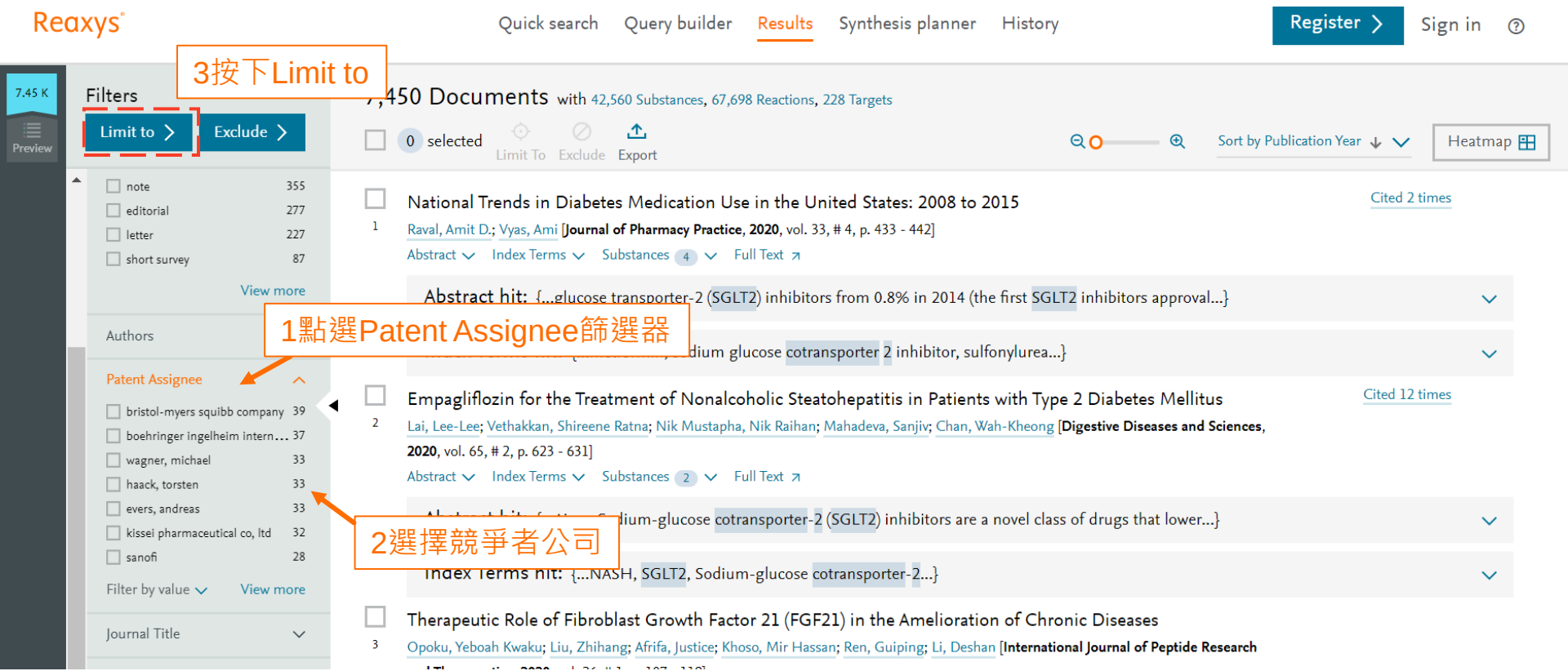
關鍵字搜尋 – 競爭者分析



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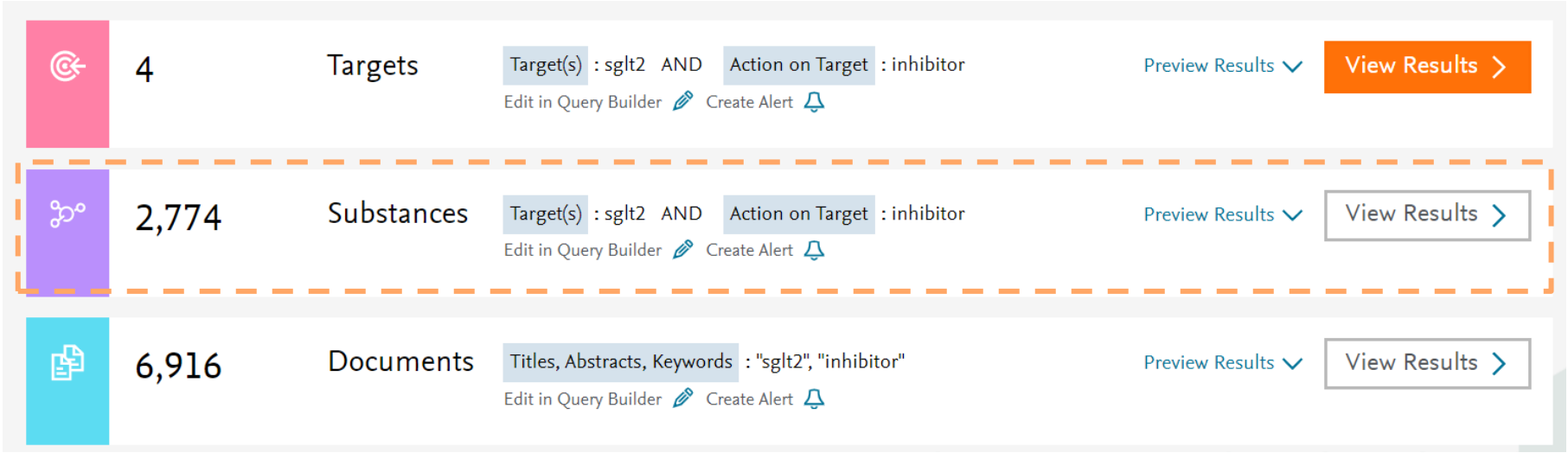
搜尋預覽頁面



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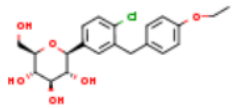
Reaxys資料結構-十大類資訊



dapagliflozin

$C_{21}H_{25}ClO_6$ 408.879 11966426 461432-26-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 53

Spectra - 57

物理性質

光譜

Other Data - 351

合成方法

製備反應

所有反應

Preparations - 85

Reactions - 403

Targets - 24

Documents - 220

期刊文獻、專利文件

RMC 藥物化學模組

類藥性數據

生物活性

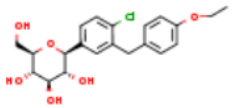
生物靶點蛋白

逆合成計畫推導快速鍵

供應商資訊

ELSEVIER

Reaxys資料結構-十大類資訊



dapagliflozin

$C_{21}H_{25}ClO_6$ 408.879 11966426 461432-26-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 53

Spectra - 57

Other Data - 351

Preparations - 85

Reactions - 403

Targets - 24

Documents - 220

其他資料

化合物用途
天然萃取化合物
環境暴露/汙染
生物降解

View related Markush

專利式空間檢索

分子量/分子式
CAS號 /Reaxys號
專利出處
專利相關名稱
純化方法

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問題2　請找出

治療C型肝炎病毒口服藥

Sofosbuvir

相關專利資料，最早由那家公司申請了專利?

A. GILEAD SCIENCES

B. ELIAN LLC

C. PHARMASSET, INC.

D. Favilavir

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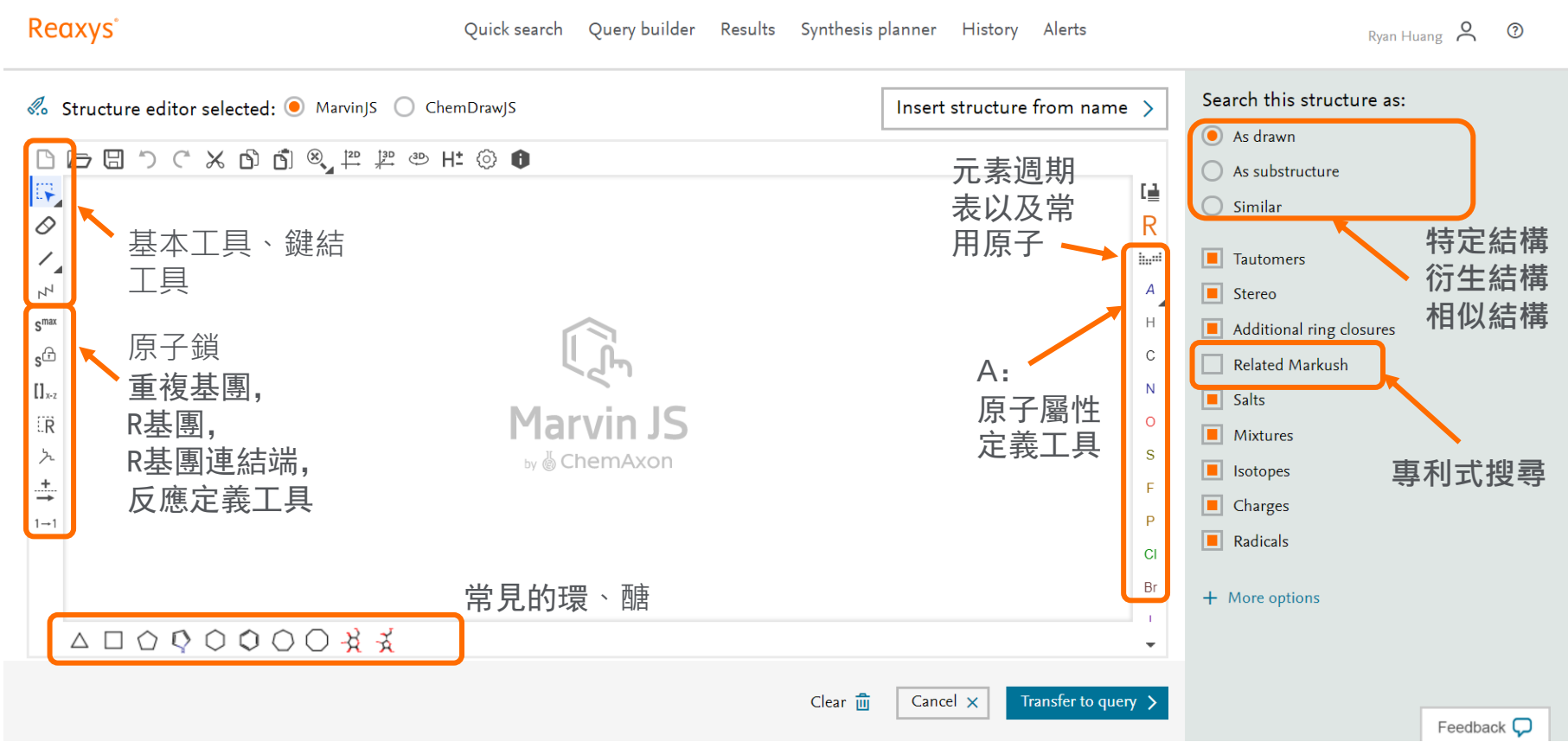
結構搜尋 –MarvinJS 結構編輯器

中文自我學習資源
(2020)

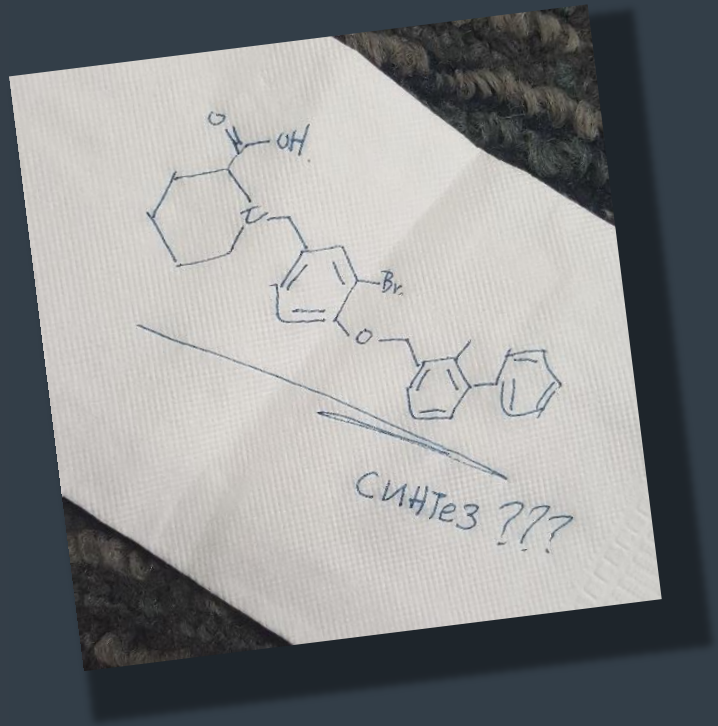
Reaxys實用功能簡介



問題3　昏暗的酒館與神秘的科學家

一個身穿實驗衣的科學家醉醺醺的從你身邊踉蹌的走出酒吧，
地上遺落了一張明顯是他遺落的餐巾紙，上面似乎寫了甚麼?

你拾起並追出門口，卻已不見科學家人影，你突然想到似乎可
以用Reaxys查查有沒有更多的線索?



請問該物質已知用途是?

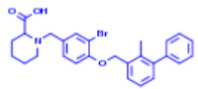
A. 航太研發部的耐高溫塗料　B. 醫藥研發部的抗癌藥物　C. 健康食品研發部的新抗氧化萃取物　D. 犯罪調查科的新毒品跡證

1 Substances out of 4 Documents, containing 6 Reactions, 2 Targets

Reaxys - 1

0 Limit To Exclude Export Preparations No of References Grid Heatmap

1



1-({3-bromo-4-[(2-methyl-3-phenyl-phenyl)methoxy]phenyl}methyl)piperidine-2-carboxylic acid

$C_{27}H_{28}BrNO_3$ 494.428 27956541

Identification | Physical Data - 5 | Preparations - 6

Druglikeness | Spectra - 10 | Reactions - 6

Bioactivity (All) | Targets - 2

Documents - 4

4 Documents with 535 Substances, 668 Reactions, 3 Targets

Reaxys - 4

0 Limit To Exclude Export Publication Year Heatmap

1 Novel multitarget inhibitors with antiangiogenic and immunomodulator properties

Cited 2 times

Conesa-Milián, Laura; Falomir, Eva; Murga, Juan; Carda, Miguel; Marco, J. Alberto [**European Journal of Medicinal Chemistry, 2019**, vol. 170, p. 87 - 98]

Abstract Index Terms Substances 56 Reactions 110 Targets Full Text

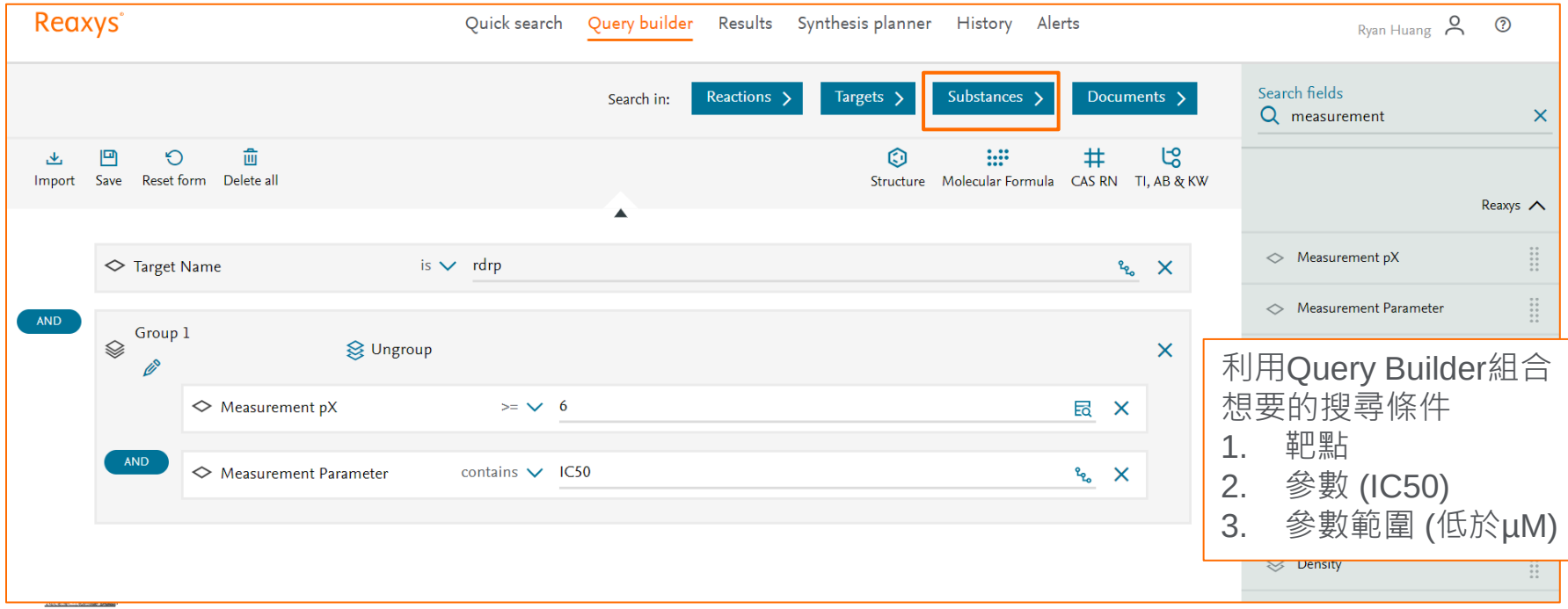
Hit Substances 1

Abstract

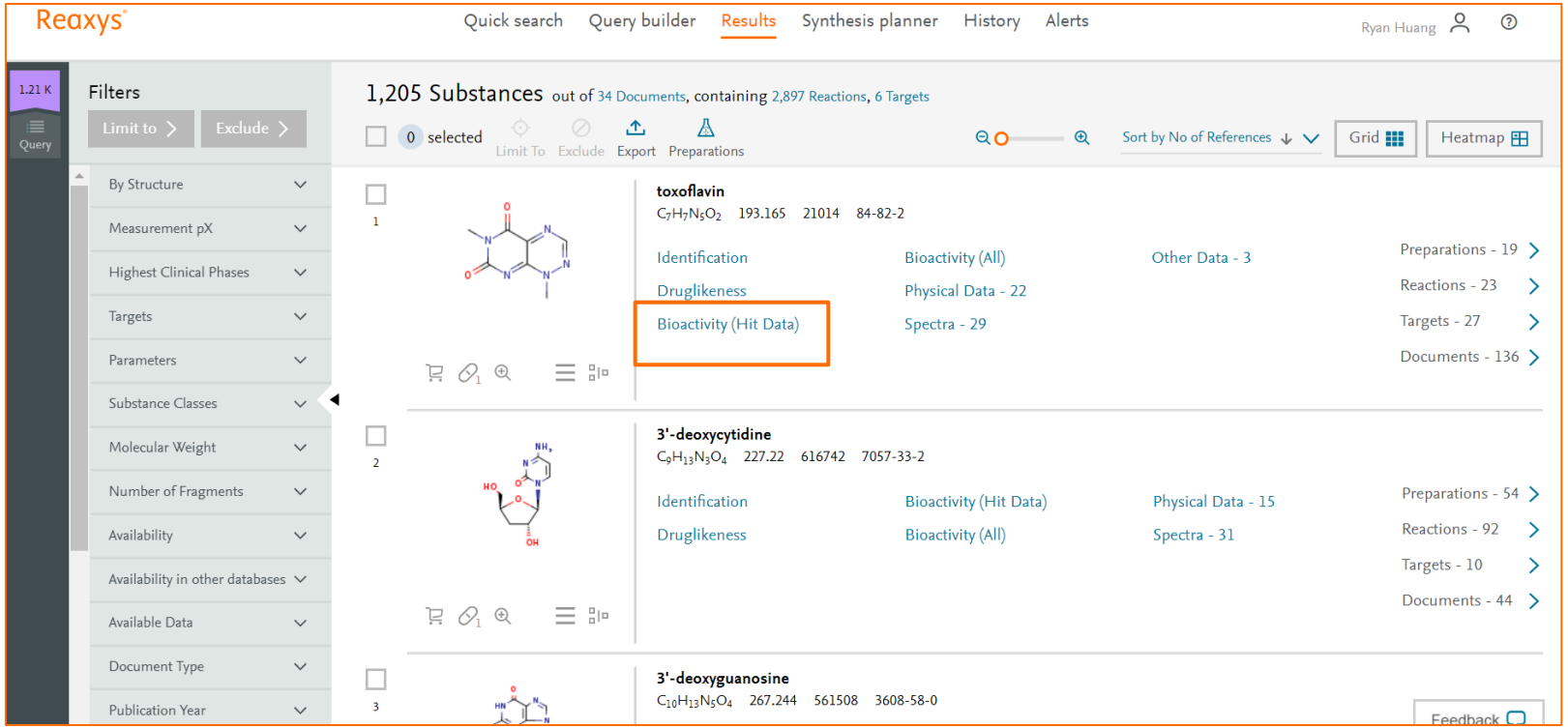
By means of docking studies, seventeen compounds T.1-T17 have been designed and evaluated as multitarget inhibitors of VEGFR-2 and PD-L1 proteins in order to overcome resistance phenomena offered by cancer. All these designed molecules display a urea moiety as a common structural feature and eight of them (T.1-T8) further contain a 1,2,3-triazol moiety. The antiproliferative activity of these molecules on several tumor cell lines (HT-29, MCF-7, HeLa, A549, HL-60), on the endothelial cell line HMEC-1 and on the

Case2: 如何利用Reaxys/RMC快速篩選對”冠狀病毒”有活性的化合物

- 獲取文獻中報導對”RNA dependent RNA Polymerase” 有活性報導的化合物
- 希望化合物的IC50在μM級別

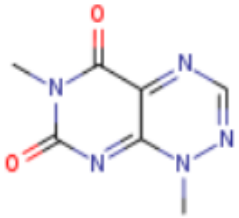


Reaxys中的結果

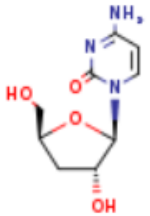


Reaxys直接給出符合條件的化合物，大量節省閱讀”34篇”文獻，查找數據的時間，點擊Hit Data查看數據出處

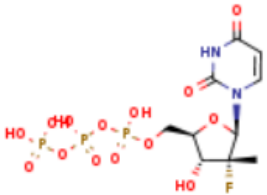
Reaxys中的結果



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	Reference
6.22	IC50	=	0.6	μM	Hepatitis C virus	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Other compound: ATP; Radioligand: [3H]UTP;	Middleton; Lim; Montgomery; Rockway; Liu; Klein; Qin; Harlan; Kati; Molla[**Letters in drug design and discovery, 2007**, vol. 4, # 1, p. 1 - 8] Full Text ↗ Cited 3 times ↗ Details › Abstract ›

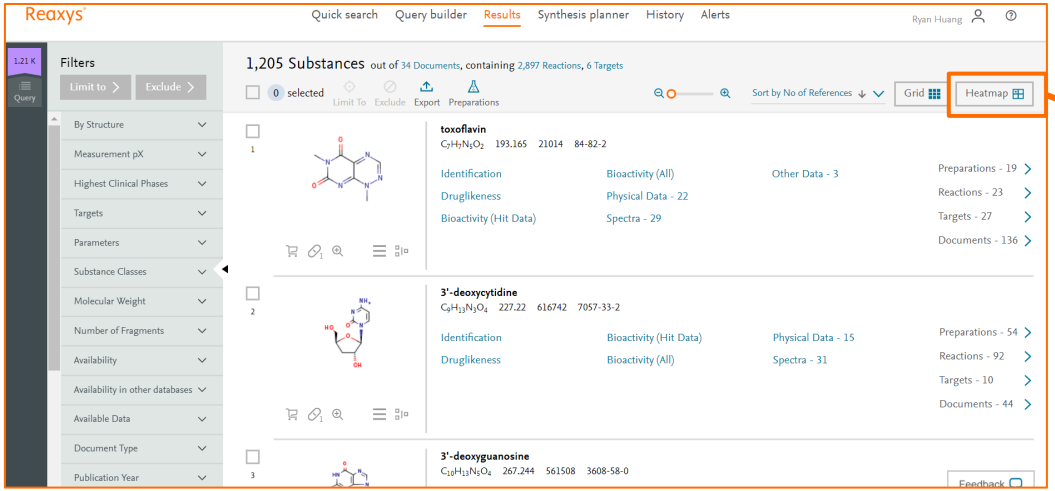


pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	Reference
7.1	IC50		0.08 - 1.2	μM	Hepatitis C virus		RNA-dependent RNA polymerase [Hepatitis C virus]:Wild			Mayhoub, Abdelrahman S.[**Bioorganic and Medicinal Chemistry, 2012**, vol. 20, # 10, p. 3150 - 3161] Full Text ↗ Cited 35 times ↗ Details › Abstract ›



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Concomitants	1...	Reference
7.1	IC50		0.079	μM	Hepatitis C virus subtype 1b	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild				Alexandre, François-René; Badaroux, Eric; Bilello, John F; Bot, Stéphanie; Bouisset, Tony; Brandt, Guillaume; Cappelle, Sylvie; (...) Surleraux, Dominique; Dousson, Cyril B.[**Bioorganic and Medicinal Chemistry Letters, 2017**, vol. 27, # 18, p. 4323 - 4330] Full Text ↗ Cited 11 times ↗ Details › Abstract

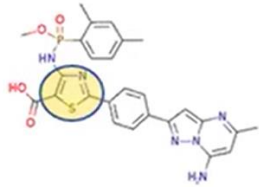
利用Heatmap看結構與靶點關係



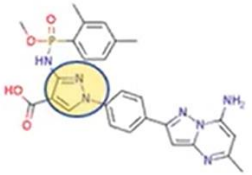
利用Reaxys中的Heat Map，直接觀察結構、靶點、活性數據之間的關係，並且可以把活性從高排到低

找出有意思的結構

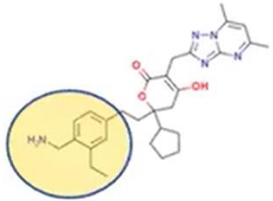
Substances	RNA-dependent RNA polymerase
5-thiazolecar... ylamine]	9.5
(E)-N-(4-(3-t... fonamide	9.5
IDX17119	9.4
20673525	9.3
5-thiazolecarb...l-amine]	9.1
20673509	9.1
20673487	9.1
29885944	9
27259279	9
6-cyclopentyl...an-2-one	9
(6R)-6-cyclop...an-2-one	9
6-cyclopentyl...an-2-one	9



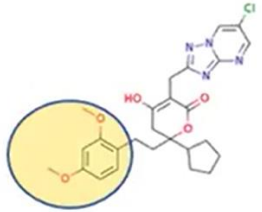
PX=9.5



PX=9.4



PX=8.0

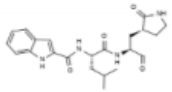
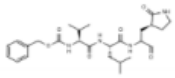
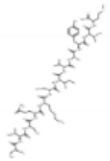


PX=7.7

393 substances that interact with 25 targets related to 6 target species

(SARS coronavirus, Middle East respiratory syndrome coronavirus, human Middle East respiratory syndrome coronavirus, Human coronavirus 229E, Coronaviridae and Coronavirinae, with normalized affinity value > 6)

Reaxys® Medicinal Chemistry

Structure	SMILES	Reaxys Registry Number	Link to Reaxys	pX	CAS Registry Number	Chemical Name	Molecular Formula	Molecular Weight	InChI Key	LogP	Lipinski Number	Veber Number	Target Name	Target Species	Substance Action on Target	Bioassay Details	Measured Parameter	Unit	Qualitative value	Quantitative value
	CC(C)C[C@H](NC(=O)C1=CC2=CC=CC=C2N1)C(=O)N[C@@H](C[C@@H]1CCNC1=O)C=O	1.3E+07	1.3E+07	10.7		N-((S)-1-((S)-1-formyl-2-((S)-2-oxopyrrolidin-3-yl)ethylcarbamoyl)-3-methylbutyl)-1H-indole-2-carboxamide	C22H28N4O4	412.489	HXJZYYCIL	2.331	4	1	Sars Cov 3C-Like Protease (Coronaviridae)	Coronaviridae	Inhibitor	Inhibitory; IC50	nM	=	0.02
	CC(C)C[C@H](NC(=O)[C@@H](NC(=O)OCC1=CC=CC=C1)C(C)C)C(=O)N[C@@H](CCNC1=O)C=O	1.5E+07	1.5E+07	10.2		N-[(benzyloxy)carbonyl]-L-valyl-N1-[1-formyl-2-[(3S)-2-oxopyrrolidin-3-yl]ethyl]-L-leucinamide	C26H38N4O6	502.611	RUHYGYHI	2.682	3	0	Sars Cov 3C-Like Protease (Coronaviridae)	Coronaviridae	Inhibitor	Inhibitory; IC50	nM	=	0.06
	CC[C@H](C)[C@H](NC(=O)[C@H](CO)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CC(N)=O)NC(=O)[C@H](CO)NC(=O)[C@@H](N)CO)[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](CC1=CC=C(O)C=C1)C(=O)N[C@@H](C[C@@H]1C(O)C(=O)N[C@@H](CCSC)C(O)=O	2.5E+07	2.5E+07	8.73			C56H94N14	1315.51	RBLTWUZI	-8.375	1	0	Spike glycoprotein (SARS coronavirus)	SARS coronavirus	Inhibitor	Concentral	IC50	nM	=	1.88

https://www.elsevier.com/connect/coronavirus-information-center

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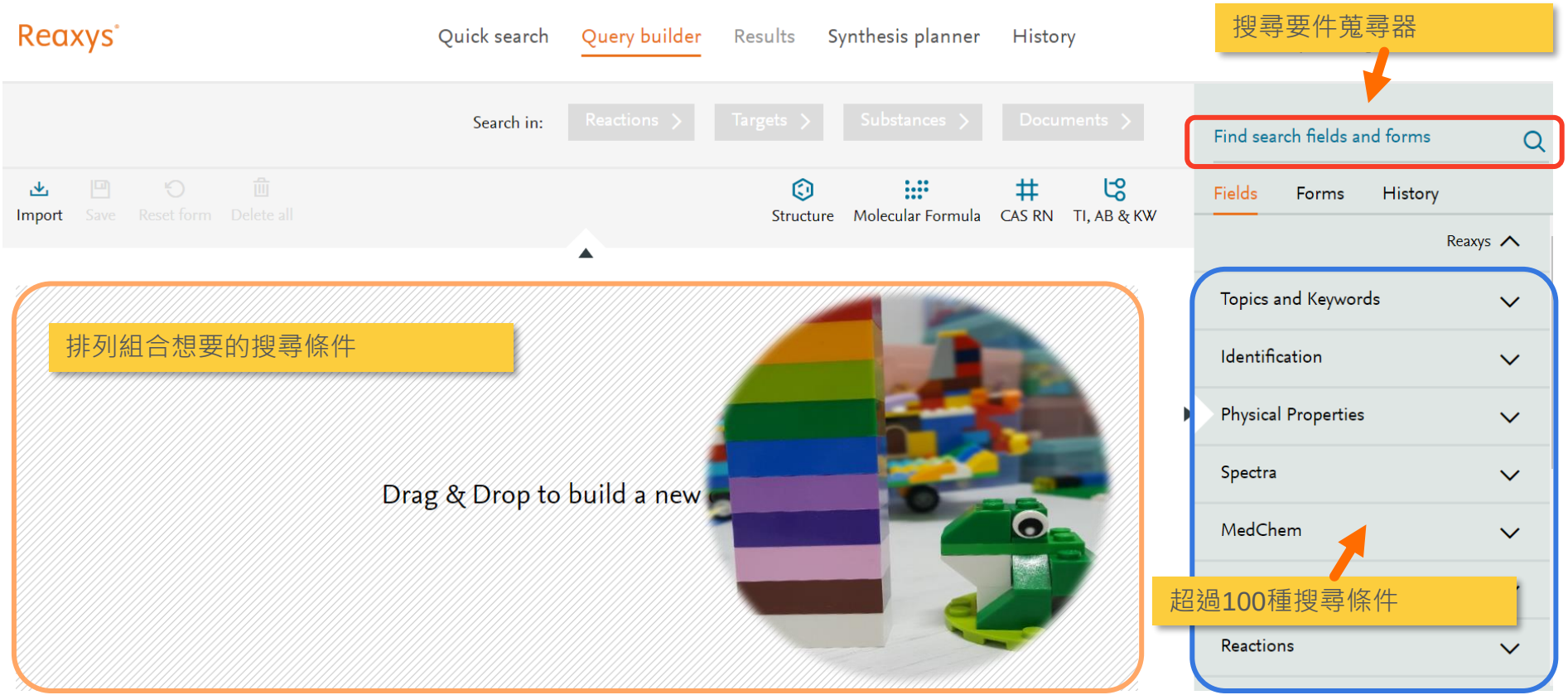
進階搜尋(Advanced search)

- 結合結構、實驗資料、關鍵字或任何你想搜尋的欄位



進階搜尋範例

- 搜尋天然萃取物質，分子式至少含有30個碳並有文獻報導具有抗菌效果 (anti-microbiotic effect)
- 鑑定未知天然萃取物質，已知的分子量(M.W.173)，並以一組NMR實驗數據進行排除
- 搜尋Rufinamide的合成反應，結合flow reactor關鍵字進行反應條件搜尋

Query Builder – search Natural Compounds plus Applications

Example 1

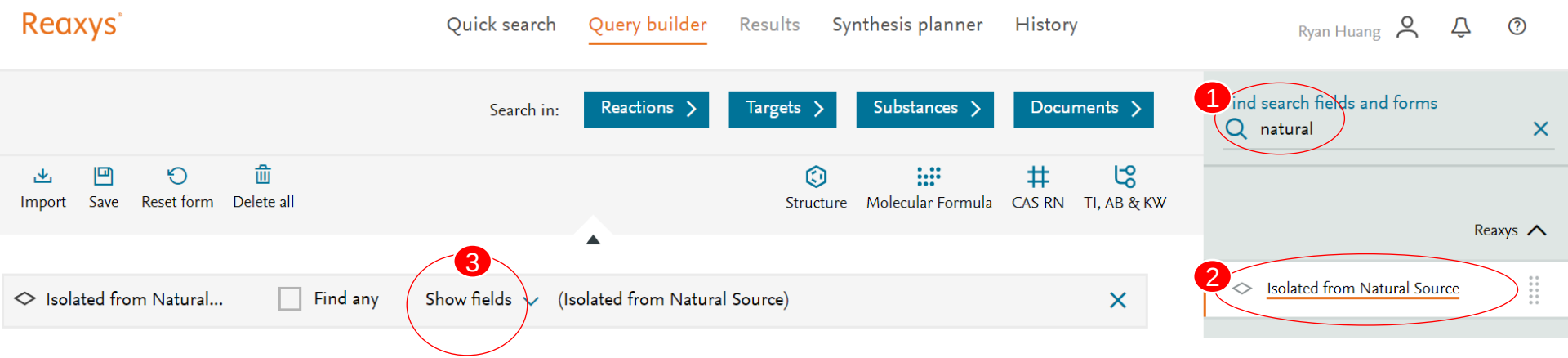
Search for compounds isolated from natural source, have 30 carbons and reported antimicrobial effect.

Isolated from natural products

Molecular Formula

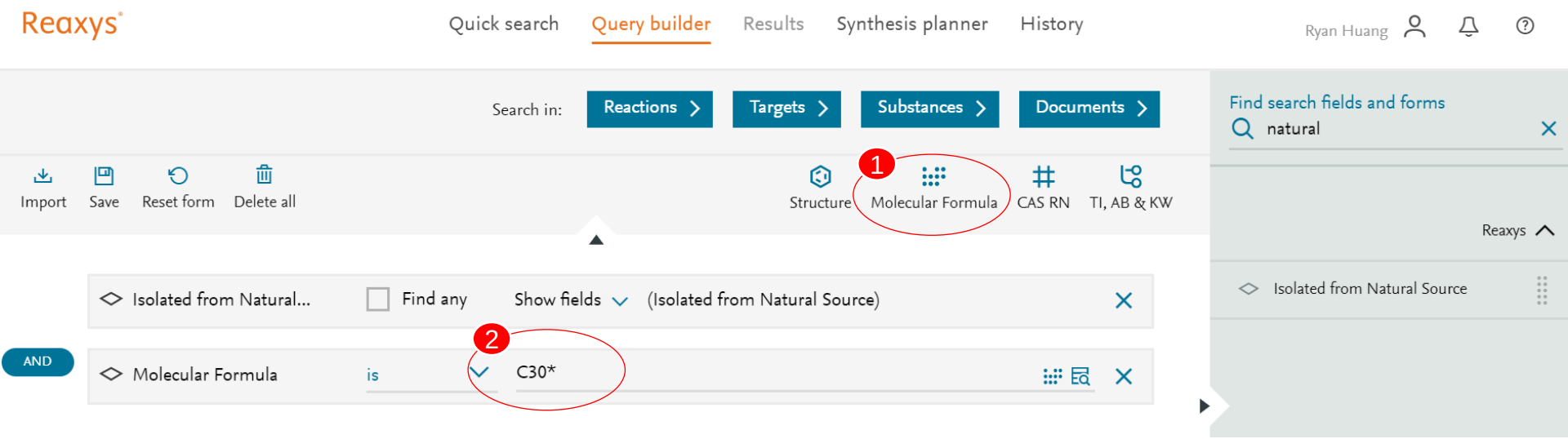
Use

Query Builder – search Natural Compounds and Applications



1. Type in “natural” to search for “Isolated from Natural Source” search block
2. Select by left click
3. Most of the search block require fill in values. Click show fields.

Query Builder – search Natural Compounds and Applications



1. Select Molecular Formula
2. Typing C30*

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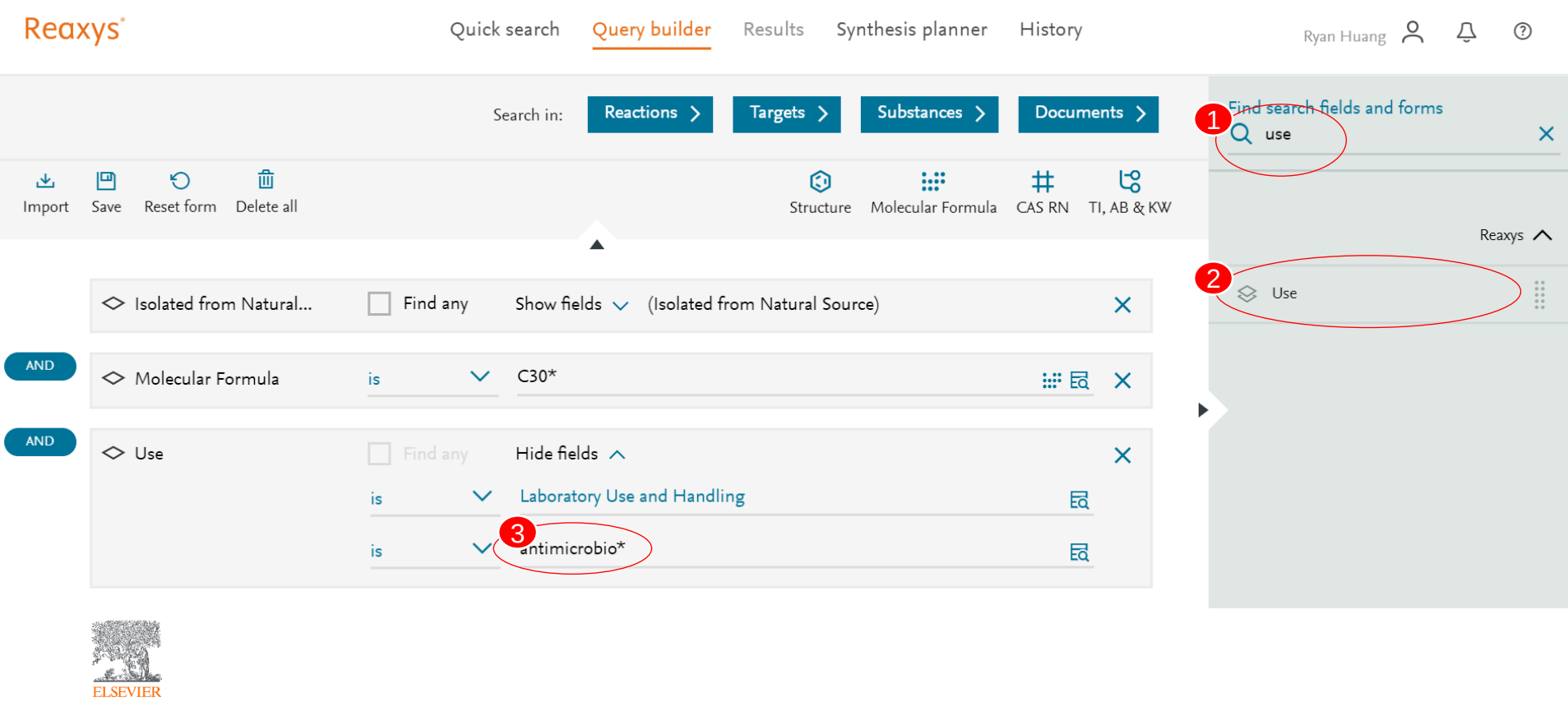
Query Builder – search Natural Compounds and Applications



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活動4 請利用Query builder搜尋
萃取自紅藜屬 (Chenopodium)的萃
取物質中，有多少被報導可溶於水中?

台灣藜

植物

台灣藜為莧科藜亞科藜屬之台灣原生種植物。傳統稱為紅藜，於2008年12月正名為台灣藜，是台灣原住民耕作百年以上的傳統作物，布農語稱為mukun，排灣語稱為djulis或tjulis，卑南語稱為duli，魯凱語稱為baae或ba'e，阿美語稱為kowal。 維基百科

學名： Chenopodium formosanum

上一層分類： 藜屬

界： 植物界 Plantae

分類階層： 物種

科： 莧科 Amaranthaceae

Reaxys Reaction Search

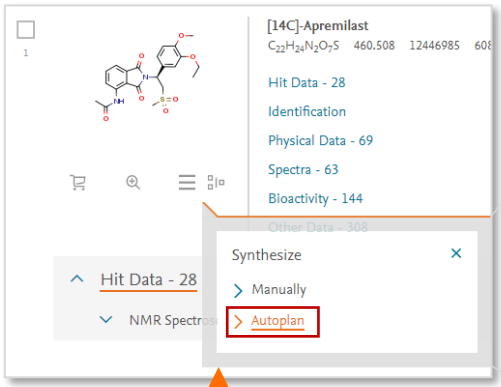
反應式查詢

Reaction Search

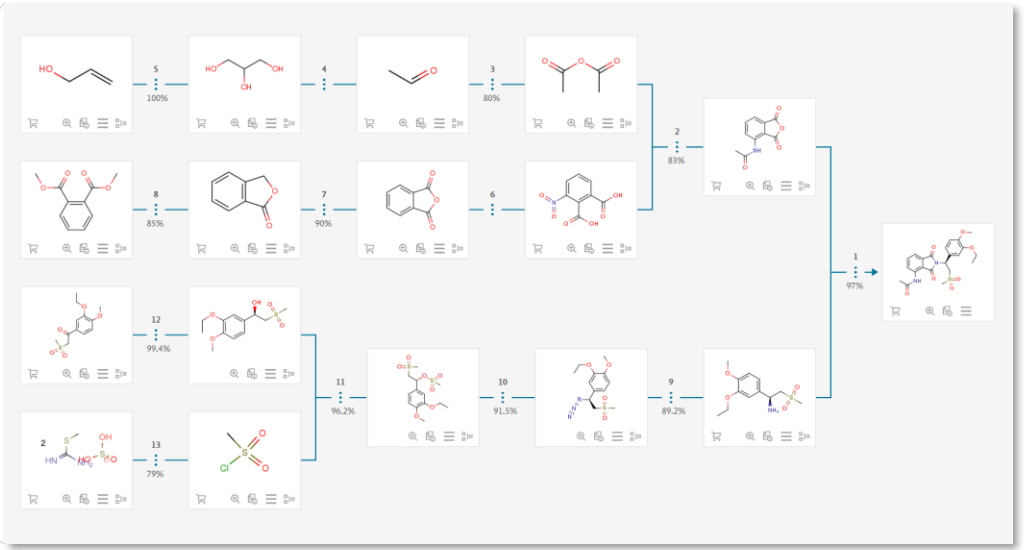
1. (逆)合成路徑規劃
2. 由物質資訊連結到製備方式
3. 由結構搜尋反應式
4. 由關鍵字搜尋反應式

兩鍵逆合成規劃

Reactions of interest can be curated and stored in the **Synthesis Planner**.
Autoplan facilitates synthetic blueprinting of substances of interest based on reactions with literature precedence

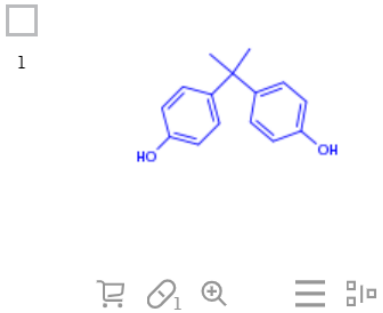


在任何物質右下角一鍵產出合成路徑
由海量數據，產生產率最高的規劃

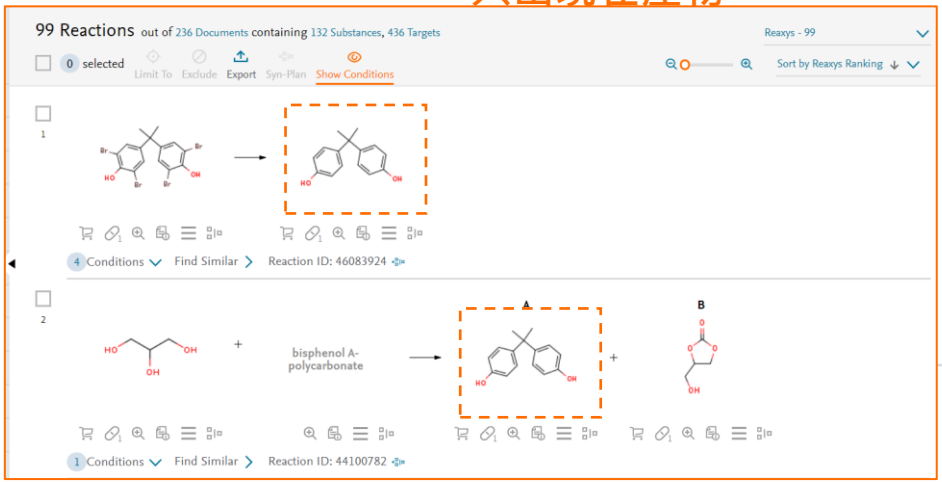


ELSEVIER

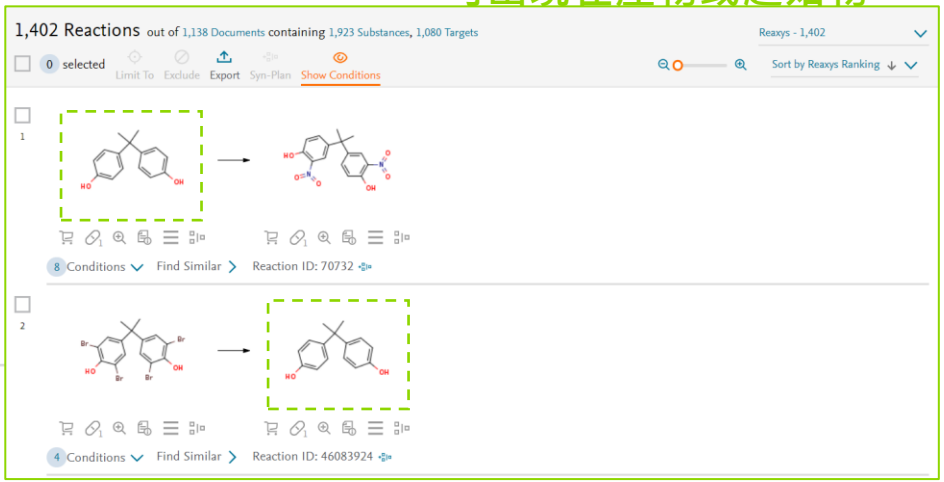
由物質資訊連結到製備方式



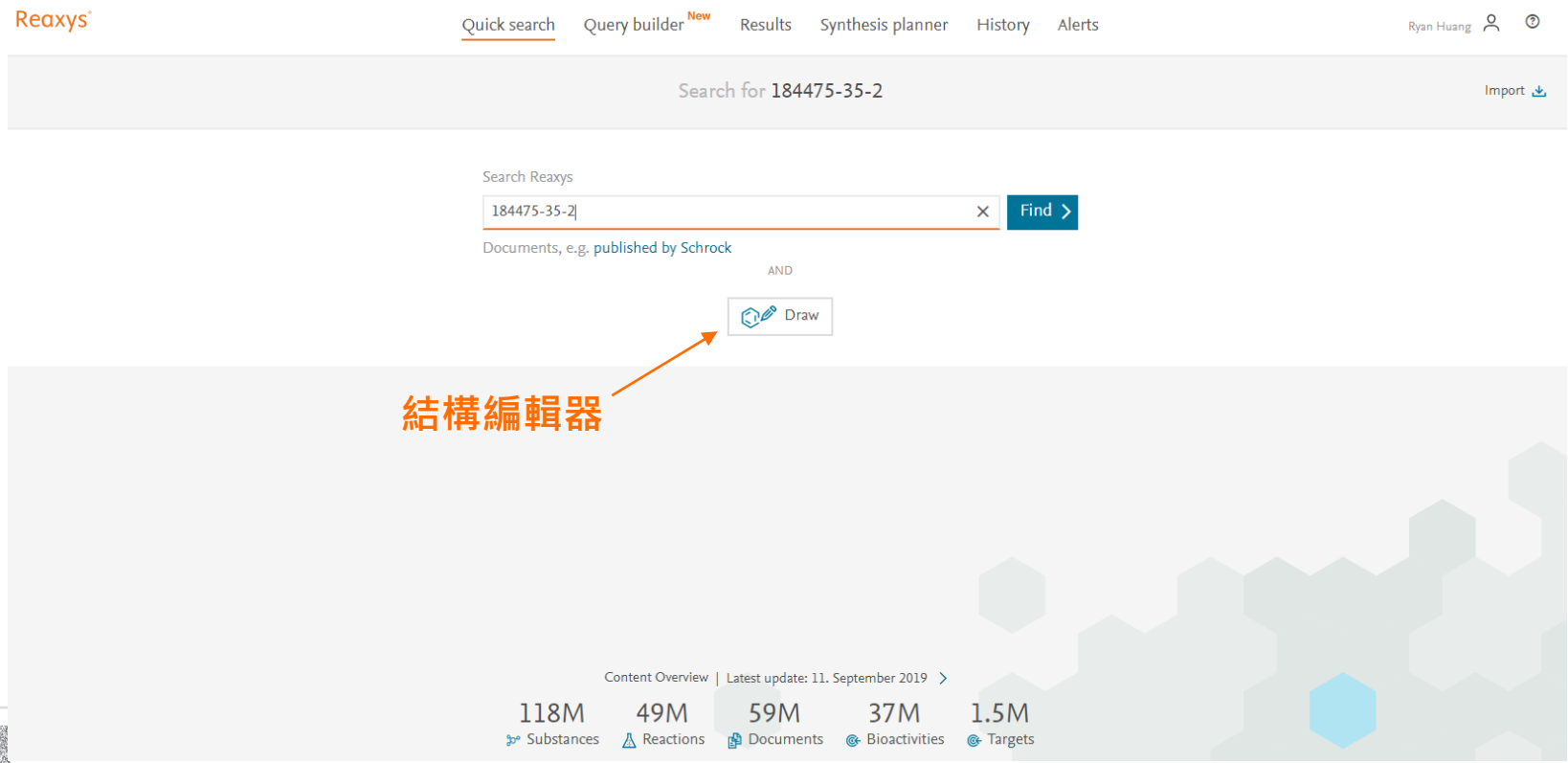
只出現在產物



可出現在產物或起始物



畫結構搜尋反應式



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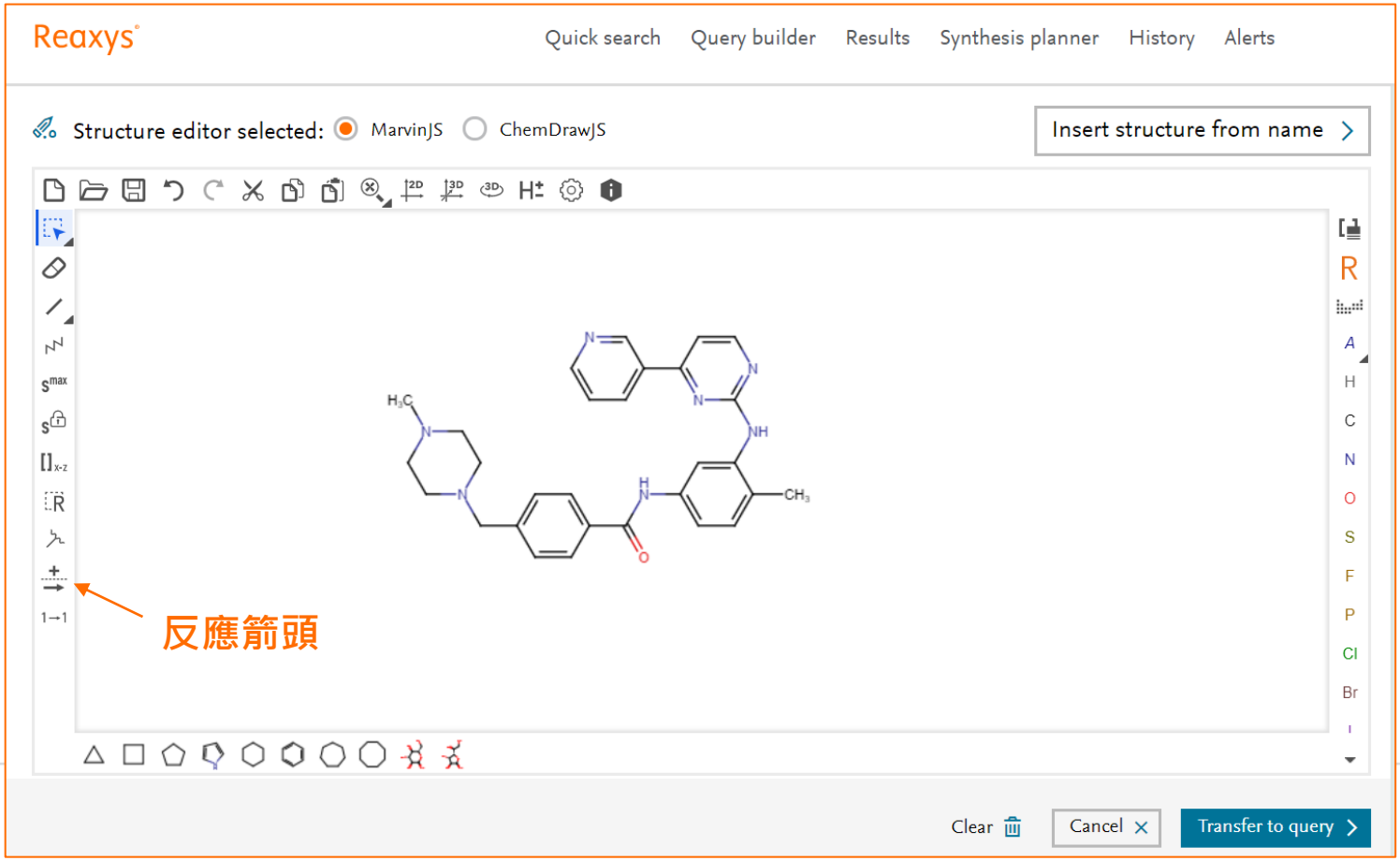
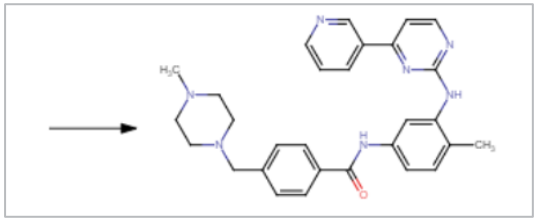
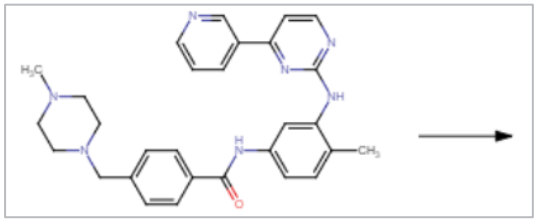
畫結構搜尋反應式


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Structure editor selected:
MarvinJS
ChemDrawJS
Insert structure from name
反應箭頭
Clear
Cancel
Transfer to query

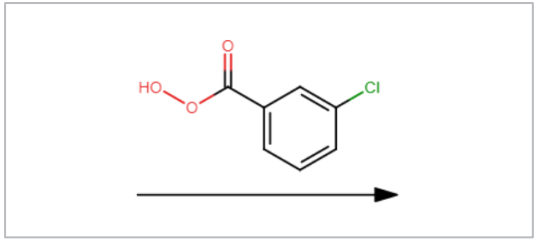
畫結構搜尋反應式



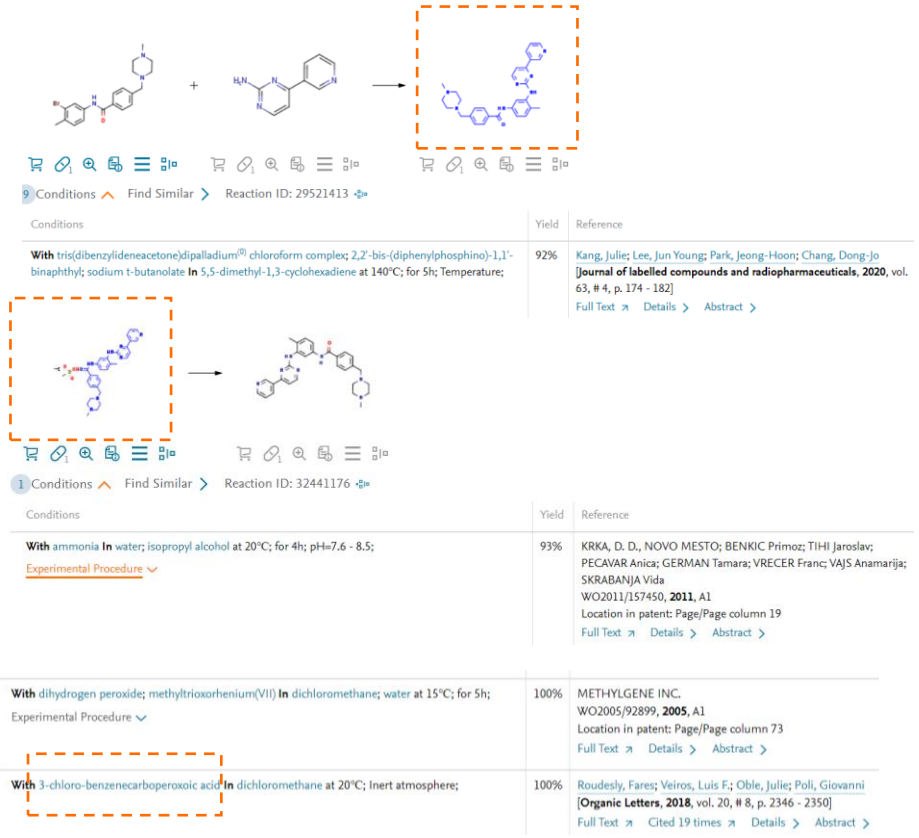
箭頭在左
產物



箭頭在右
起始物

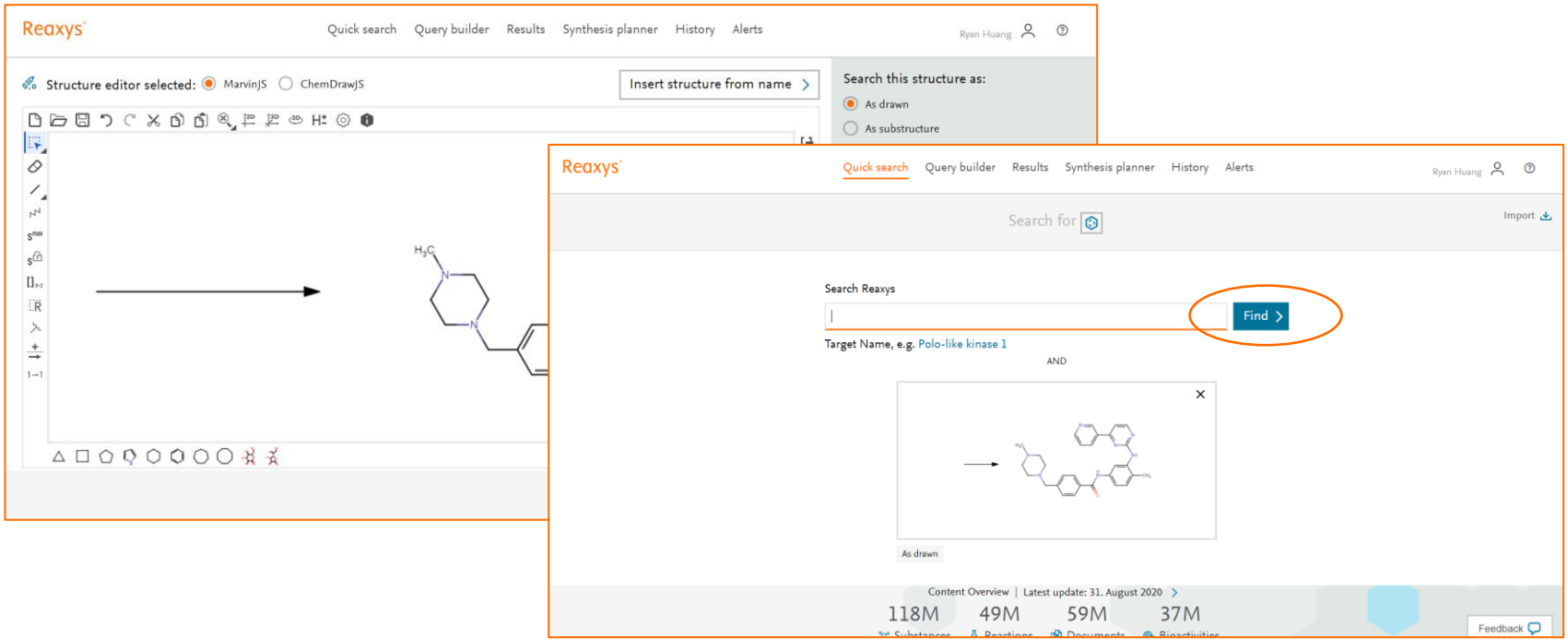


箭頭在下
催化劑或溶劑

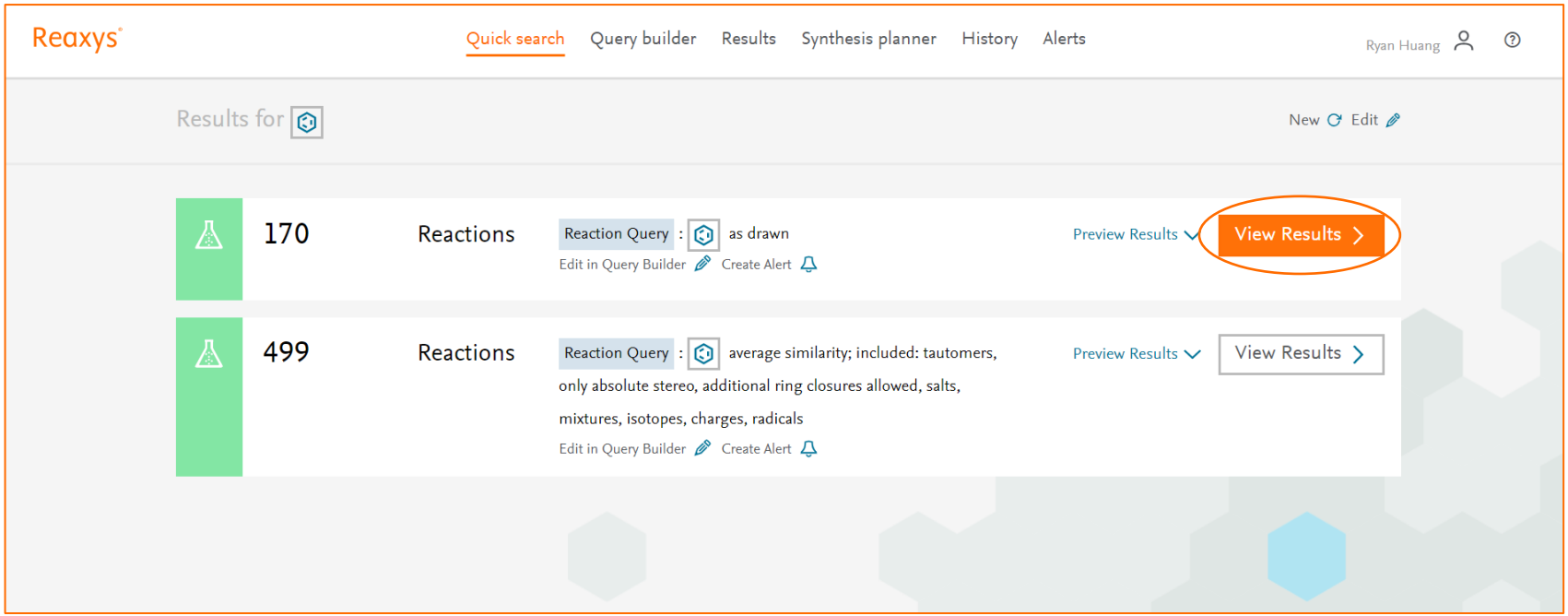


ELSEVIER

畫結構搜尋反應式


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Structure editor selected:
MarvinJS
ChemDrawJS
Insert structure from name
Search this structure as:
As drawn
As substructure
Search for
Import
Search Reaxys
Find
Target Name, e.g. Polo-like kinase 1
AND
As drawn
Content Overview | Latest update: 31. August 2020
118M
49M
59M
37M
Feedback

畫結構搜尋反應式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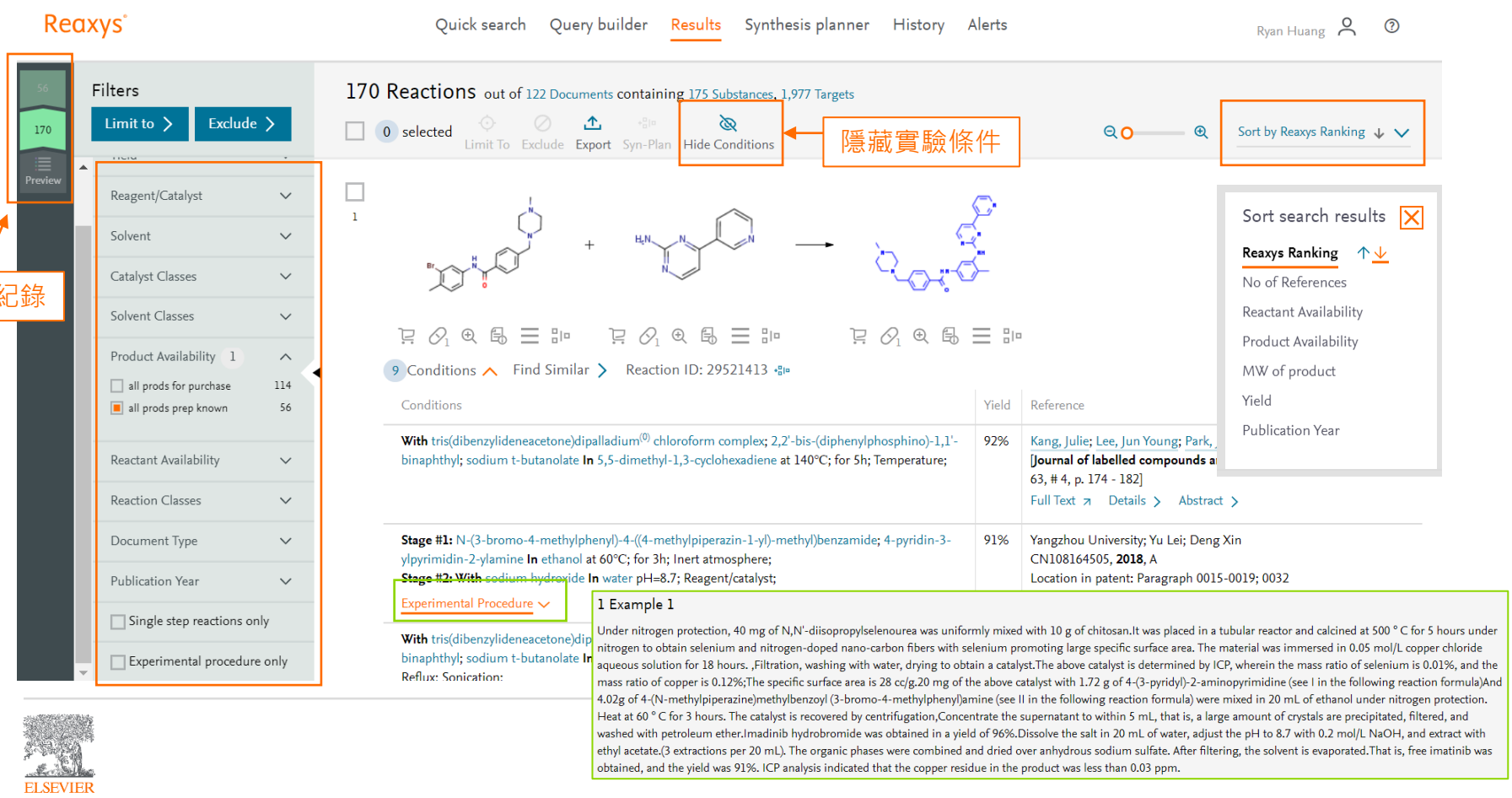
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Results for
New
Edit
170
Reactions
Reaction Query : as drawn
Edit in Query Builder
Create Alert
Preview Results
View Results
499
Reactions
Reaction Query : average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals
Edit in Query Builder
Create Alert
Preview Results
View Results

畫結構搜尋反應式



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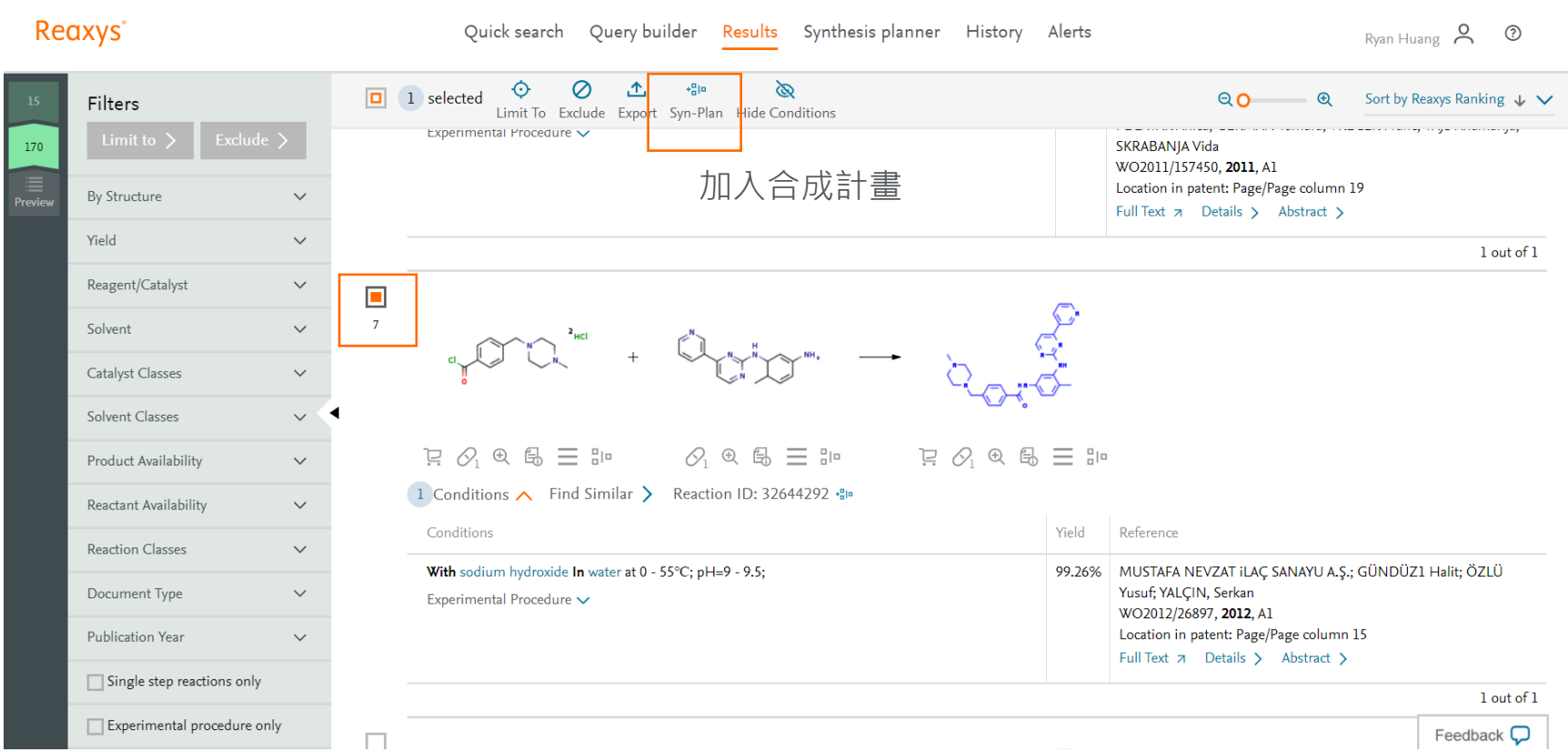
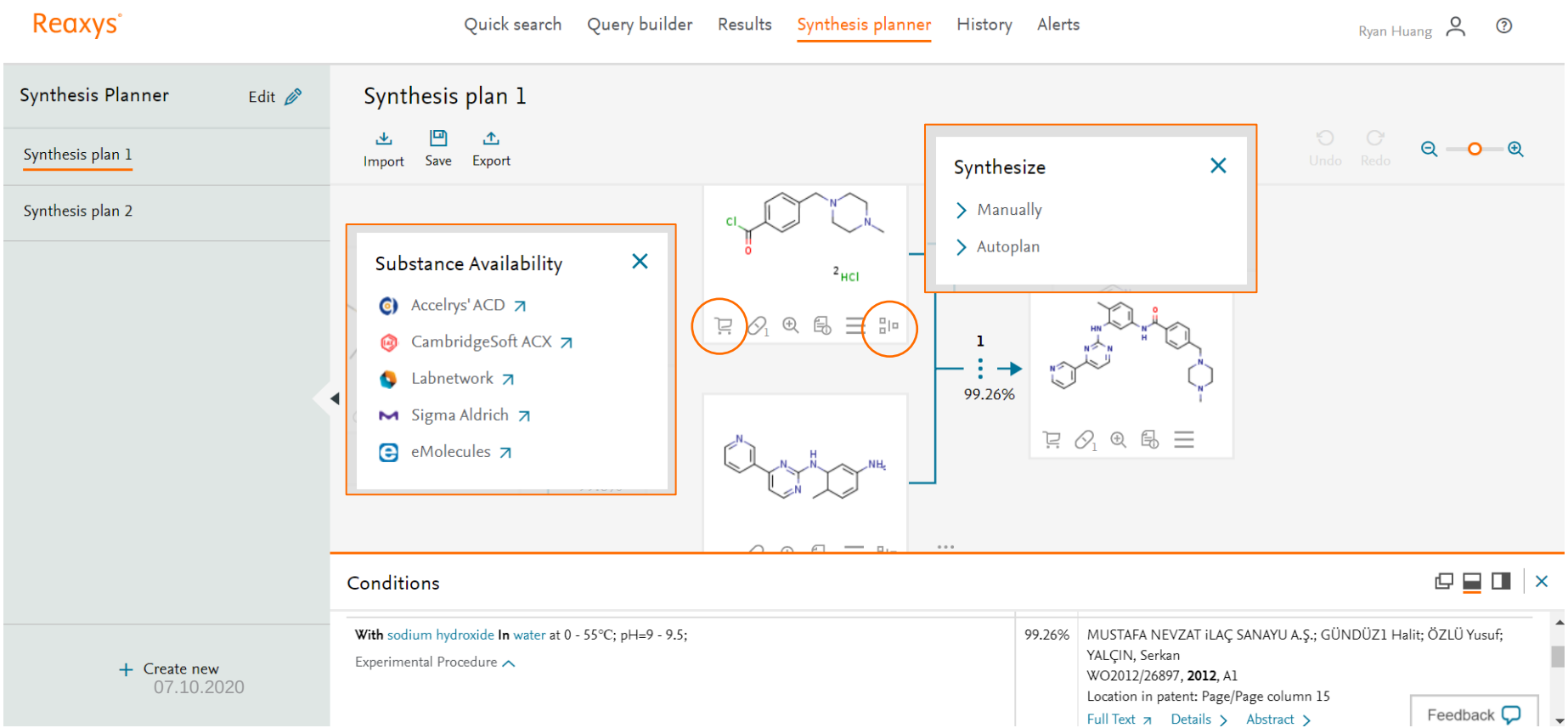
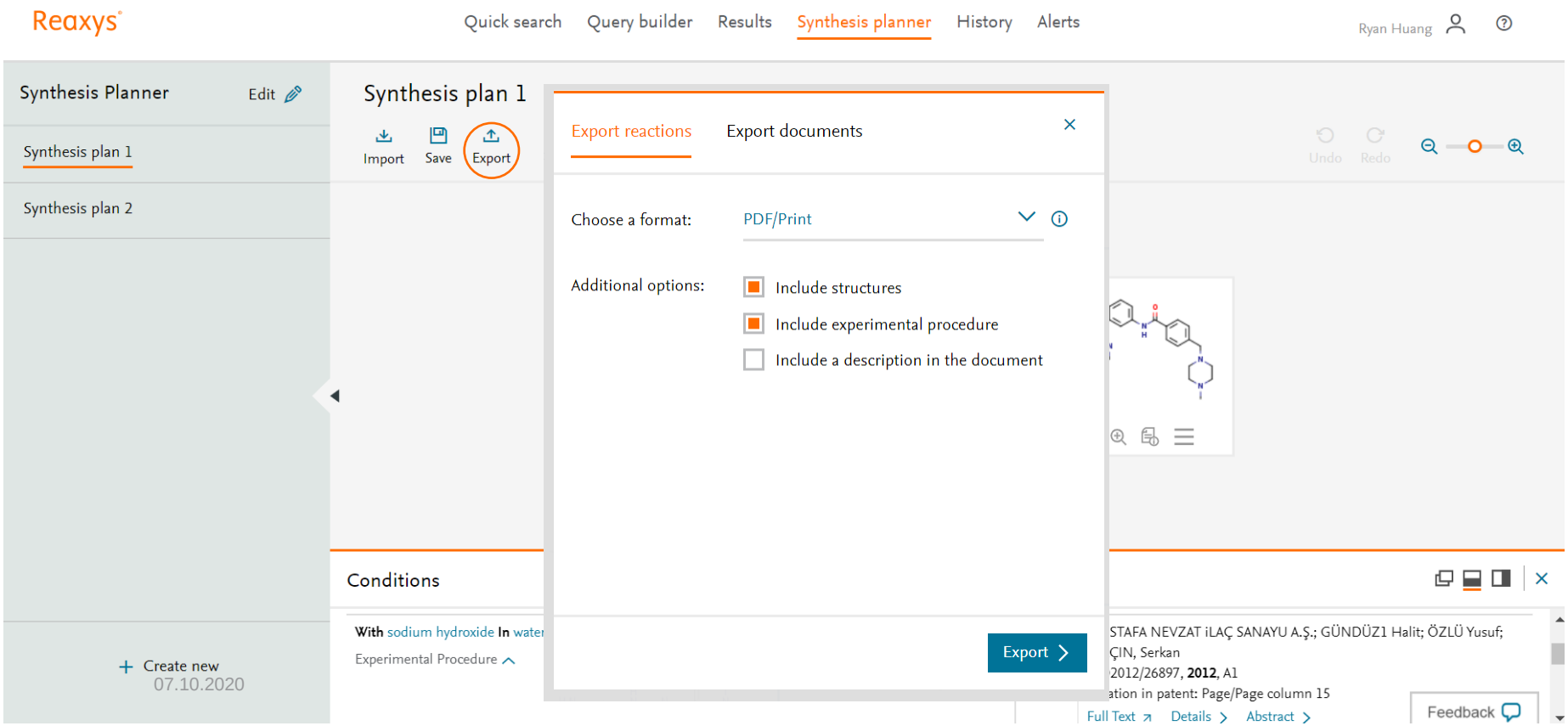
逆合成路徑規劃


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
15
170
Preview
Filters
Limit to
Exclude
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
1 selected
Limit To
Exclude
Export
Syn-Plan
Hide Conditions
Sort by Reaxys Ranking
Experimental Procedure
加入合成計畫
SKRABANJA Vida
WO2011/157450, 2011, A1
Location in patent: Page/Page column 19
Full Text
Details
Abstract
1 out of 1
7
1 Conditions
Find Similar
Reaction ID: 32644292
Conditions
Yield
Reference
With sodium hydroxide In water at 0 - 55°C; pH=9 - 9.5;
Experimental Procedure
99.26%
MUSTAFA NEVZAT iLAÇ SANAYU A.Ş.; GÜNDÜZ1 Halit; ÖZLÜ Yusuf; YALÇIN, Serkan
WO2012/26897, 2012, A1
Location in patent: Page/Page column 15
Full Text
Details
Abstract
1 out of 1
Feedback

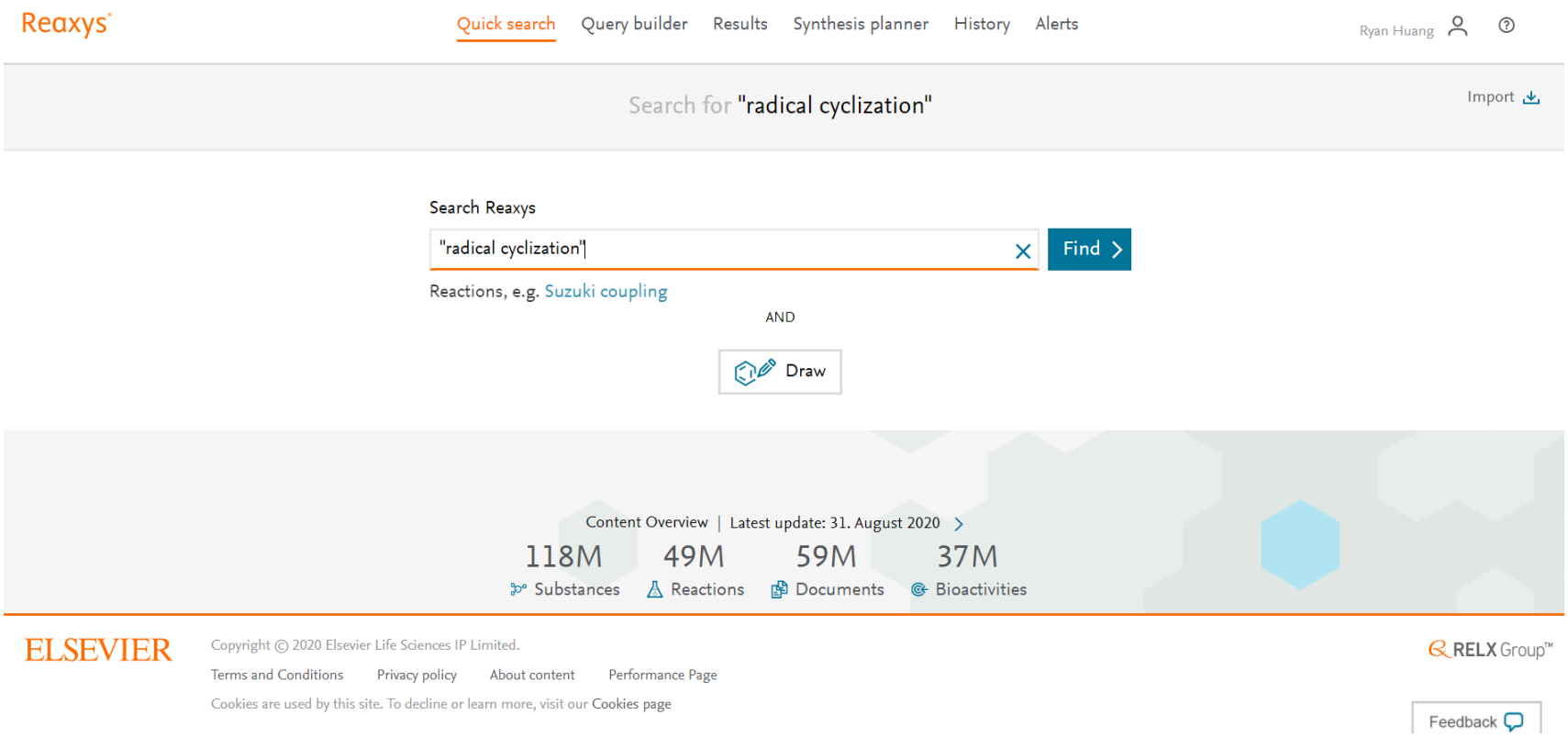
逆合成路徑規劃


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Synthesis Planner
Edit
Synthesis plan 1
Synthesis plan 2
Create new
07.10.2020
Synthesis plan 1
Import
Save
Export
Undo
Redo
Synthesize
Manually
Autoplan
Substance Availability
Accelrys' ACD
CambridgeSoft ACX
Labnetwork
Sigma Aldrich
eMolecules
2 HCl
1
99.26%
Conditions
With sodium hydroxide In water at 0 - 55°C; pH=9 - 9.5;
Experimental Procedure
99.26%
MUSTAFA NEVZAT iLAÇ SANAYU A.Ş.; GÜNDÜZ1 Halit; ÖZLÜ Yusuf; YALÇIN, Serkan
WO2012/26897, 2012, A1
Location in patent: Page/Page column 15
Full Text
Details
Abstract
Feedback

逆合成路徑規劃


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Synthesis Planner
Edit
Synthesis plan 1
Synthesis plan 2
Create new
07.10.2020
Synthesis plan 1
Import
Save
Export
Undo
Redo
Export reactions
Export documents
Choose a format:
PDF/Print
Additional options:
Include structures
Include experimental procedure
Include a description in the document
Export
Conditions
With sodium hydroxide In water
Experimental Procedure
STAFA NEVZAT iLAÇ SANAYU A.Ş.; GÜNDÜZ1 Halit; ÖZLÜ Yusuf;
ÇIN, Serkan
2012/26897, 2012, A1
ation in patent: Page/Page column 15
Full Text
Details
Abstract
Feedback

由關鍵字搜尋反應式


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Search for "radical cyclization"
Import
Search Reaxys
"radical cyclization"
Find
Reactions, e.g. Suzuki coupling
AND
Draw
Content Overview | Latest update: 31. August 2020
118M
Substances
49M
Reactions
59M
Documents
37M
Bioactivities
ELSEVIER
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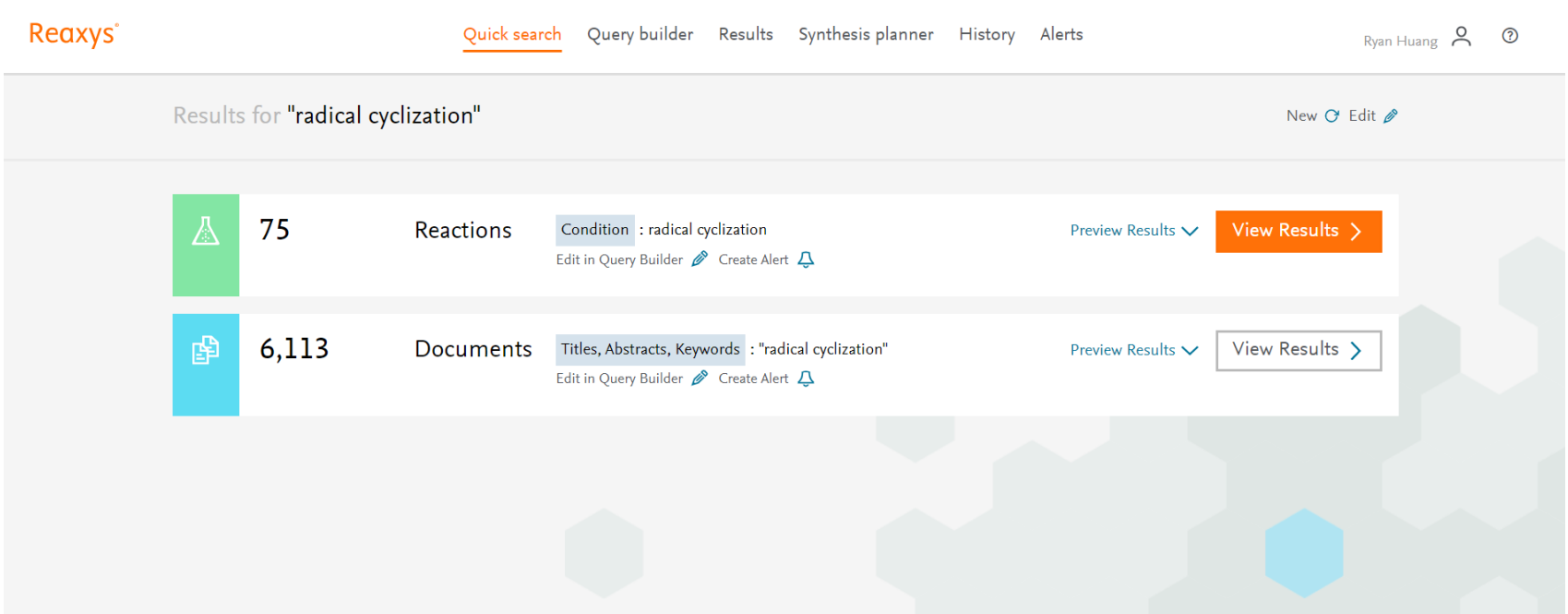
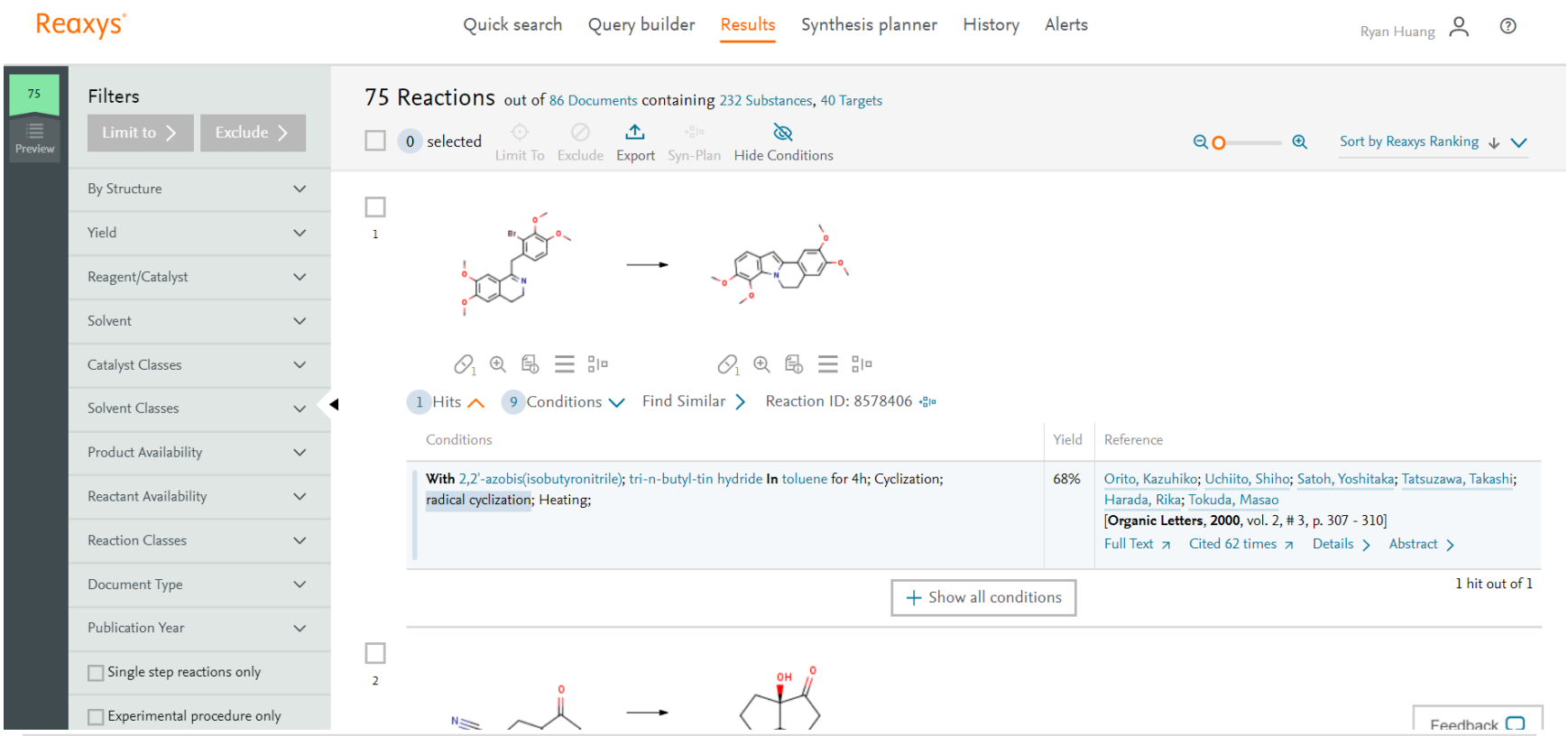
Terms and Conditions
Privacy policy
About content
Performance Page
Cookies are used by this site. To decline or learn more, visit our Cookies page
RELX Group™
Feedback

由關鍵字搜尋反應式


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
Results for "radical cyclization"
New
Edit
75
Reactions
Condition : radical cyclization
Edit in Query Builder
Create Alert
Preview Results
View Results
6,113
Documents
Titles, Abstracts, Keywords : "radical cyclization"
Edit in Query Builder
Create Alert
Preview Results
View Results

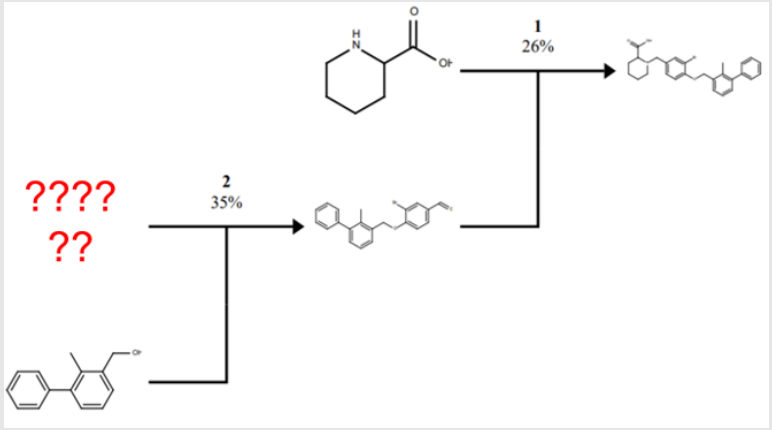
由關鍵字搜尋反應式


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Ryan Huang
75
Preview
Filters
Limit to
Exclude
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
75 Reactions out of 86 Documents containing 232 Substances, 40 Targets
0 selected
Limit To
Exclude
Export
Syn-Plan
Hide Conditions
Sort by Reaxys Ranking
1
1 Hits
9 Conditions
Find Similar
Reaction ID: 8578406
Conditions
Yield
Reference
With 2,2'-azobis(isobutyronitrile); tri-n-butyl-tin hydride In toluene for 4h; Cyclization; radical cyclization; Heating;
68%
Orito, Kazuhiko; Uchiito, Shiho; Satoh, Yoshitaka; Tatsuzawa, Takashi; Harada, Rika; Tokuda, Masao
[Organic Letters, 2000, vol. 2, # 3, p. 307 - 310]
Full Text
Cited 62 times
Details
Abstract
Show all conditions
1 hit out of 1
2
Feedback

問題5

循著線索追到附近的實驗室大樓，遠遠看到酒吧撞見的科學家在大廳咆嘯，臉色發青似乎酒醒了一半。

上前遞還他遺落的餐巾紙後，他感激的邀請你到他的實驗室，並央求你協助填入該物質合成計畫中消失的環節?



Reaxys具有長遠的歷史，提供創新所需的資訊

1817: First edition of
Gmelin Handbook

1881: First edition of
Beilstein Handbook

1989: Beilstein and Gmelin database go online

1992: CrossFire launched

2009:
Reaxys
launched

2013/2014:
Complete overhaul of Reaxys and content expansion including RMC

2016: New Reaxys launched

全新介面推出

2017: New Reaxys Medicinal Chemistry (RMC) module

藥物化學模組

2020:
AI-assisted Predicted Retrosynthesis Tool

AI輔助逆合成“預測”工具

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Reaxys predictive retrosynthesis solution combines unparalleled Reaxys content with AI & ML technologies

One of the most cited works in the fields of predictive retrosynthesis has been enabled by a partnership between Elsevier, Dr. Marwin Segler and Prof. Dr. Mark Waller

Reaxys predictive retrosynthesis tool in news


nature

604 | NATURE | VOL 555 | 29 MARCH 2018

Planning chemical syntheses with deep neural networks and symbolic AI


Game Changer: Scientist Mark Waller Next level with AI-Driven Synthesis

Mark Waller
Professor
Department of Physics,
International Center of Quantum and Molecular Structures, Shanghai, China

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

NEWS · 28 MARCH 2018

Need to make a molecule? Ask this AI for instructions

Artificial-intelligence tool that has digested nearly every reaction ever performed could transform chemistry.

Advantages of Reaxys RT over other RTs

- Not reliant on extracting and encoding rules by hand (manually)
- Integrate own custom building block libraries or proprietary reaction data
- System solves retrosynthesis for almost twice as many molecules
- Thirty times faster than the traditional computer-aided methods

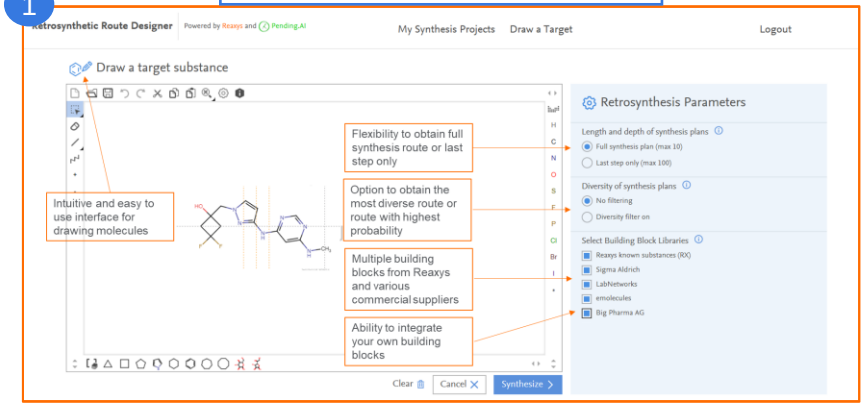
Value of predictive retrosynthesis

- New idea generation: find routes to make novel compounds
- Time saving: reduce time and effort in developing synthesis routes
- R&D cost reduction: improve synthesis success
- Knowledge augmentation: a digital assistant to help chemists navigate route designs

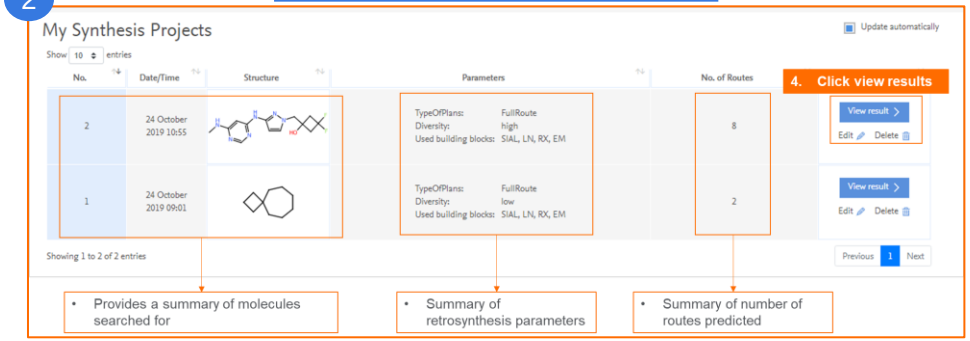
MOCK UP OF THE TECHNOLOGY PREVIEW VERSION

Reaxys predictive retrosynthesis augments your expertise & helps drive innovation

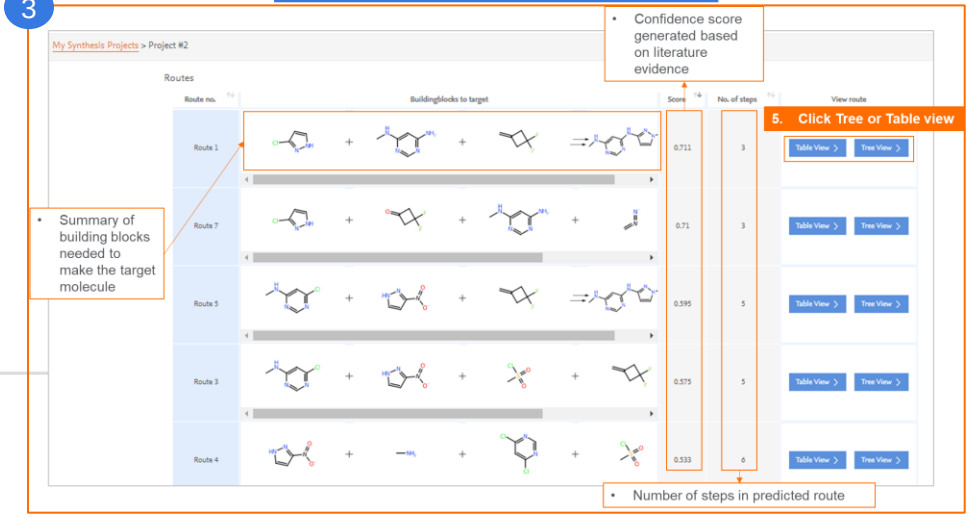
1 Start your search



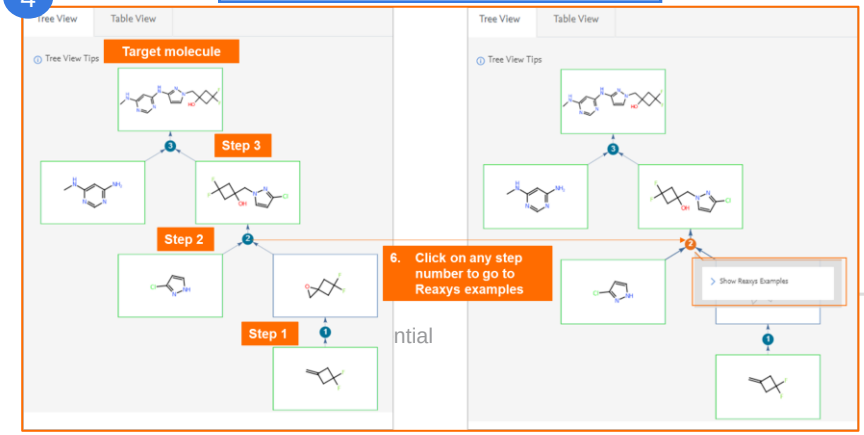
2 Project summary



3 Routes summary



4 Detailed route view



Reaxys predictive retrosynthesis – our USP

1. **AI and ML training dataset:** Predicted algorithm trained on largest (>15m) chemistry reaction dataset, with ~400,000 rules auto-extracted
   a) Reaxys data is powering the world's leading AI and ML development in predictive chemistry including MIT, SRI, Univ. of Cambridge and AstraZeneca
   b) Training dataset also included 100 million negative chemical reactions (virtual) to enable scientifically robust predictions

2. **Technology:** The only retrosynthesis solution based on auto-extracted rules and deep learning algorithm (3 neural networks coupled with Monte-Carlo tree search) i.e. similar technology that powered AlphaGo
   a) This technology also enables the ability to easily update the model so that predictions keep pace with innovation in chemistry published

3. **Scientifically robust:** Predictions have been tested using three approaches:
   a) The false positive rate of the filter (that is, incorrect reactions passing the filter) is 1.5% indicating very good performance
   b) Time split validation (basically we are trying to predict the future and by doing this we can get a good feeling about how well our model is performing) indicated that the model performed quite well when we analysed many drug molecules and the nice feature is that not only is the accuracy quite good but also that these deep neural networks are very fast
   c) 'Chemical Turing Test' – double blinded test with organic chemists (45 PhDs and Post-docs) indicated high quality and robustness of predicted routes

4. **Augmentable and customizable:** Ability to customize by adding your own building block library and augmentable by adding your own chemistry reactions data

NEWS · 28 MARCH 2018

Need to make a molecule? Ask this AI for instructions

Artificial-intelligence tool that has digested nearly every reaction ever performed could transform chemistry.

An artificial-intelligence tool could help scientists plan multi-step chemical reactions. Credit: Roger Mayne Archive/Mary Evans Picture Library

https://www.nature.com/articles/d41586-018-03977-w

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MENU

nature

Article | Published: 29 March 2018

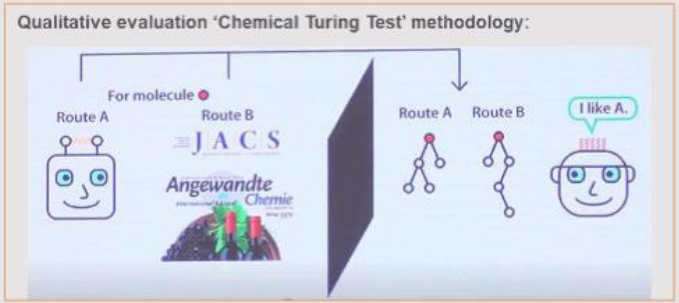
Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler, Mike Preuss & Mark P. Waller

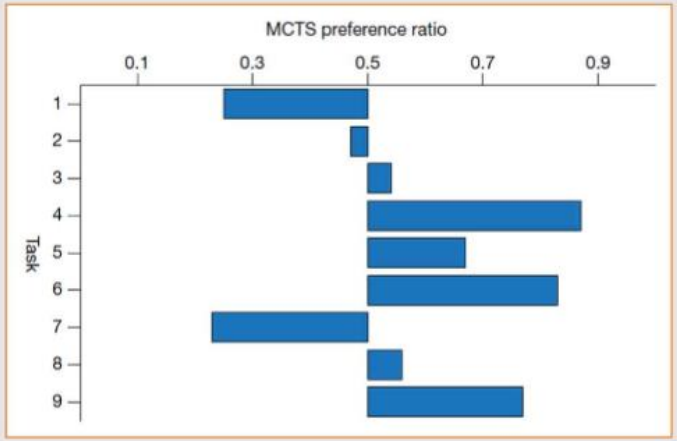
Nature **555**, 604–610(2018) | Cite this article

Abstract

To plan the syntheses of small organic molecules, chemists use retrosynthesis, a problem-solving technique in which target molecules are recursively transformed into increasingly simpler precursors. Computer-aided retrosynthesis would be a valuable tool but at present it is slow and provides results of unsatisfactory quality. Here we use Monte Carlo tree search and symbolic artificial intelligence (AI) to discover retrosynthetic routes. We combined Monte Carlo tree search with an



Qualitative evaluation result: No significant difference in expert choice



Expert choose Reaxys predictive retrosynthesis route (57%) versus literature route (43%) *p=0.26*

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NEW

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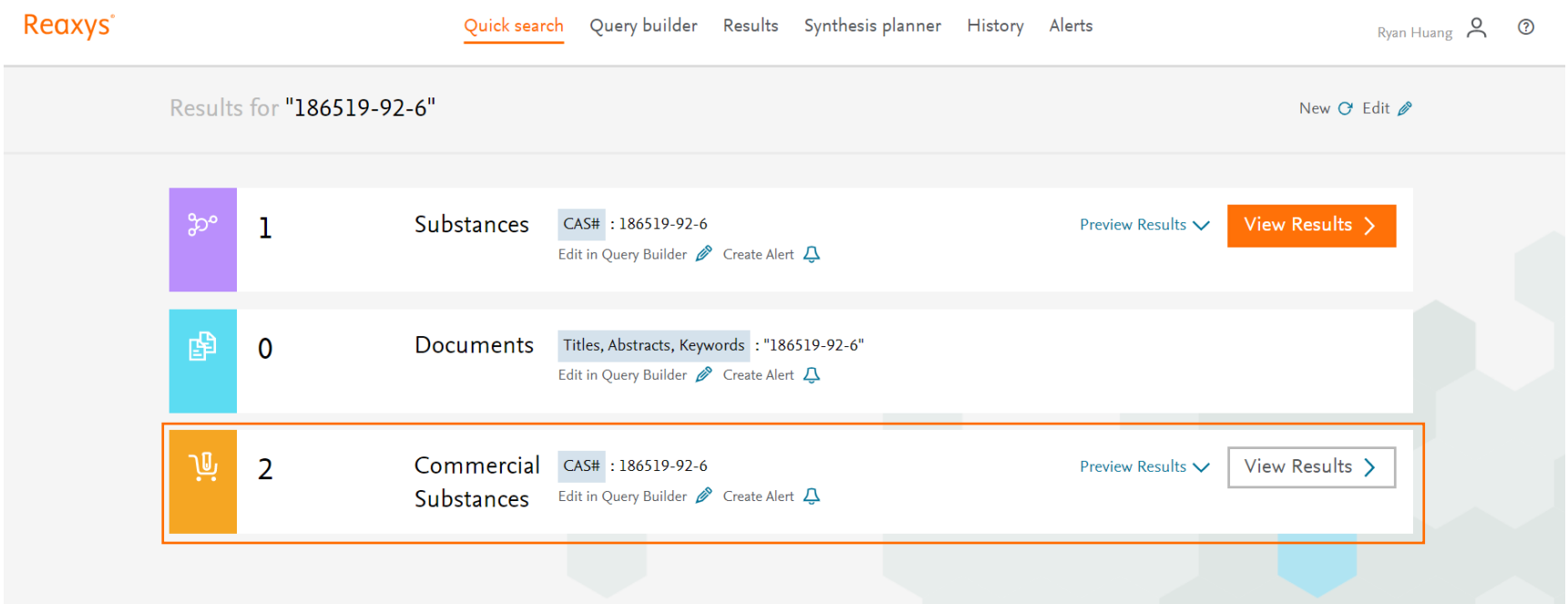
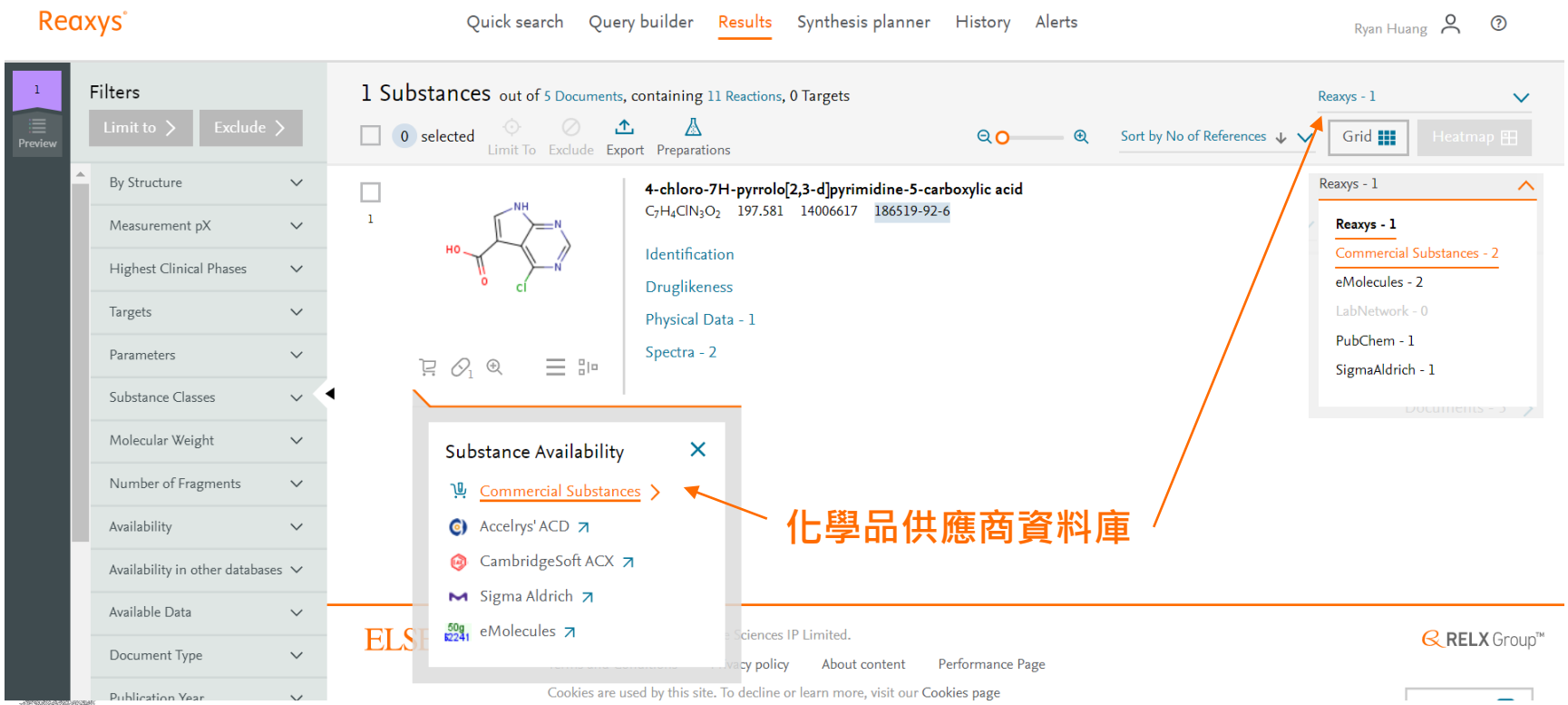
新增分類”Commercial Substances”於預視頁面

- Quick Search輸入CAS#，或畫結構搜尋您要購買的物質



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



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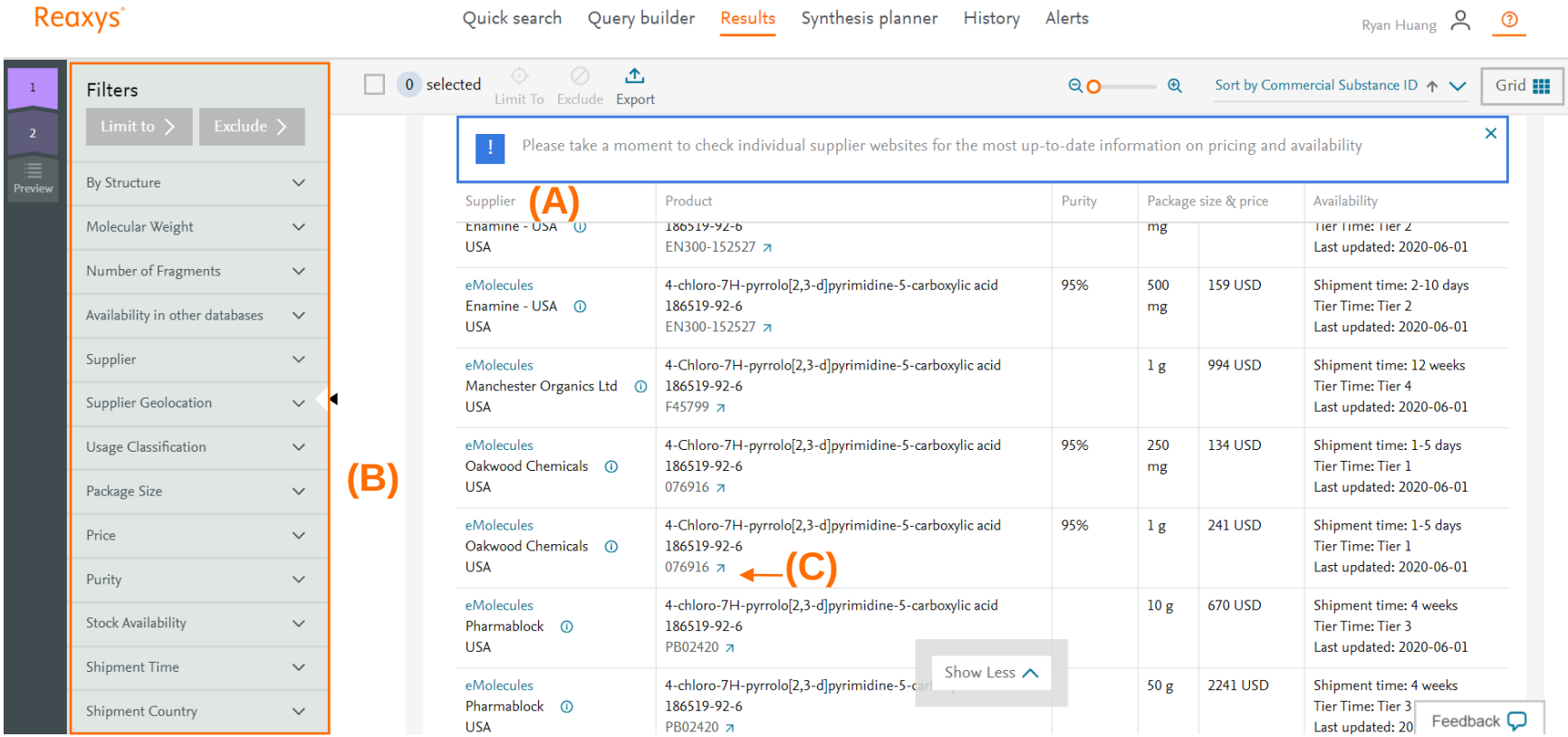

你可以在 Reaxys找甚麼?

- 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**」

>118 Million
有機、無機及有機金屬物質
>500 Million
公開實驗數據(物性、光譜、生物活性等)

>49 Million
化學反應(反應條件、溶劑、催化劑及產率等)

>54 M 文獻記錄
>16,000 期刊，專利
涉及有機化學，材料化學，生物醫藥，地球科學，工程等多種領域

>20,000 藥物作用標的
>33 M 生物活性資料點
結構活性關係資料
動物活體細胞研究
細胞外療效
藥物動力學
毒性資料
安全性資料

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Thank you

歡迎來信諮詢

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