



ELSEVIER

Elsevier Reaxys中化学信息的获取

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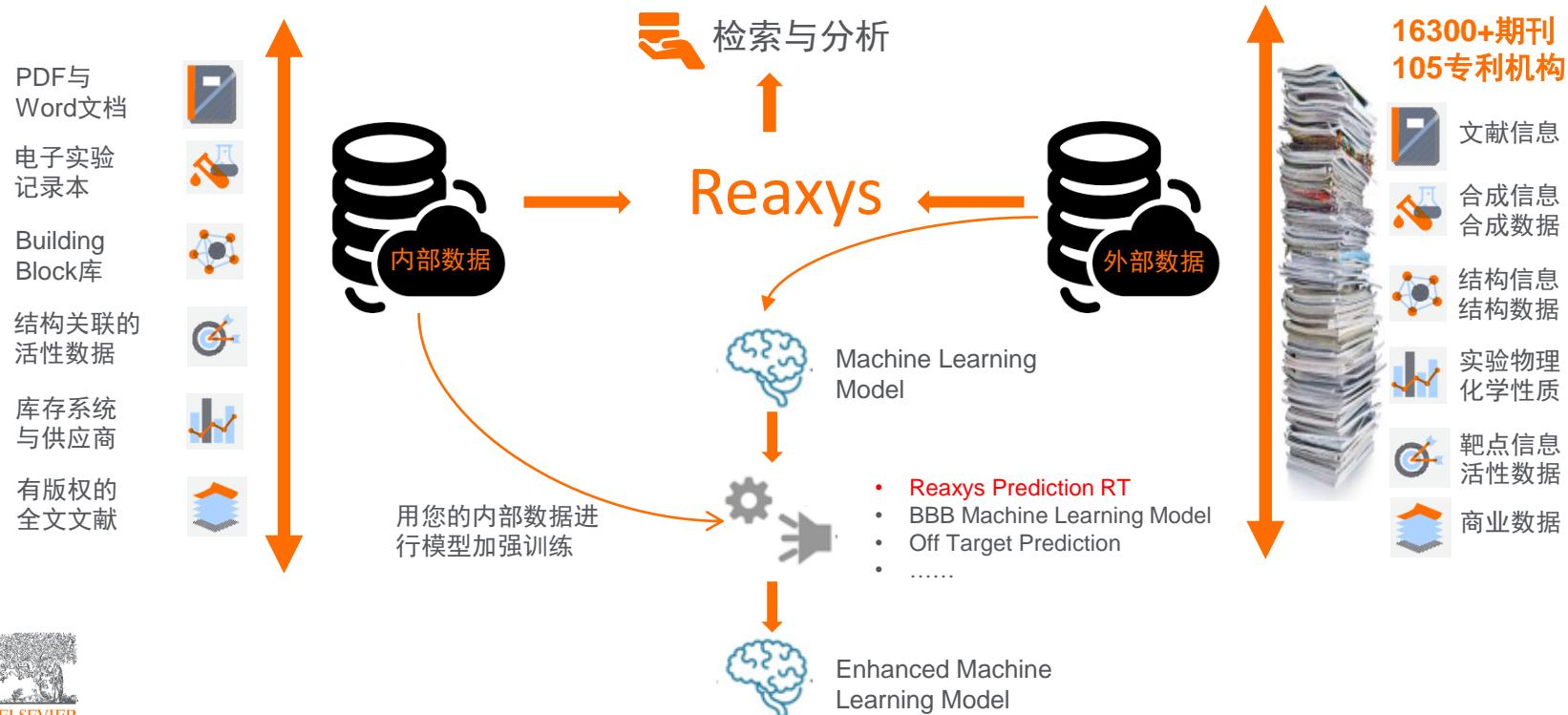
Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Reaxys—从科学数据到数据科学的跨越

Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘，且可以整合内部与外部化学相关学科科学数据的信息检索，分析，数据科学应用平台。



Reaxys对药学与化学文献中的科学数据的提炼

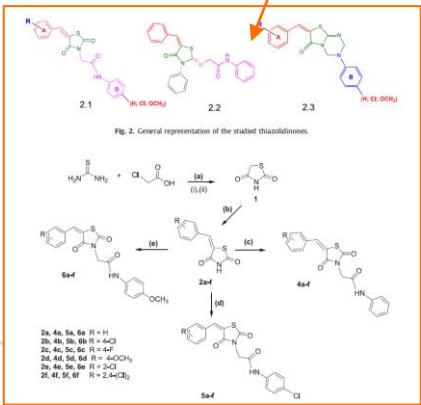
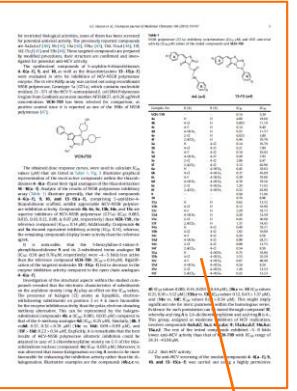
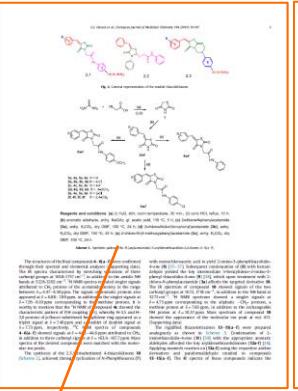


Table 1
NS5B polymerase (GT1a) inhibitory concentrations (IC_{50} μ M) and HCV anti-viral activity (EC_{50} μ M) values of the tested compounds and VCH-759.

Comds. No	R (A)	R (B)	IC_{50}	EC_{50}
VCH-759	—	—	0.14	5.29
4a	H	H	4.80	19.60
4b	4-Cl	H	0.085	11.10
4c	4-F	H	0.14	8.40
4d	4-CH ₃	H	0.25	11.57
4e	2-Cl	H	0.035	3.80
4f	2,4(Cl) ₂	H	0.44	10.78
5a	H	4-Cl	0.14	16.70
5b	4-Cl	4-Cl	0.21	7.80

4.1.6. 2-(5-(2-Chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-phenylacetamide (4e)

Yield: (3.36 g) 90%. **m.p.** 227–229 $^{\circ}$ C. **Rf:** 0.31. **IR ν cm⁻¹:** 3271 (NH), 1751, 1697, 1666 (C=O), 763 (C-Cl). **1 H NMR δ ppm:** 4.54 (s, 2H, CH_2), 7.07 (t, 1H, J =7.40 Hz, H-4 phenyl), 7.31 (t, 2H, J =7.94 Hz, H-3,5 phenyl), 7.54–7.58 (m, 4H, H-3,4,5,6 benzylidene), 7.64–7.69 (m, 2H, H-2,6 phenyl), 8.10 (s, 1H, C=CH), 10.41 (s, 1H, NH, exch. D_2 O). **13 C NMR δ ppm:** 44.5 (CH_2), 119.6, 124.2, 125.2, 128.6, 129.2, 129.3, 129.5, 130.8, 131.3, 132.6, 134.9, 138.7 (C–Ar, C–S, C=CH), 164.1, 165.3, 167.3 (C=O). **MS (m/z, %):** 372 (M^+ , 76), 374 (M^+ +2, 30), 93 (100). **Anal. Calcd.** for $C_{18}H_{13}ClN_2O_3S$ (372.83): C, 57.99%; H, 3.51%; N, 7.51. **Found:** C, 58.23; H, 3.48; N, 7.37.

实验 过程 具体化 合物描述

4.1.1. 2-(5-Unsubstitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-unsubstitutedphenyl acetamide 4a-f, 5a-f, 6a-f

A solution of the appropriate benzylidene thiazolidindione (2a-f) (10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol) in dry DMF (20 mL), was stirred at 100 $^{\circ}$ C for 30 min. The corresponding 2-chloro N-unsubstitutedphenyl acetamide (3a-c) (10 mmol) was added and stirring was continued at 100 $^{\circ}$ C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

一篇全文以及Support Information中有大量的数据，科研人员如果要获取，需要花费多的时间去阅读全文。

Reaxys对科学数据的提炼—题录, 摘要, 结构, 反应

☐ Anti-hepatitis-C virus activity and QSAR study of certain thiazolidinone and thiazolotriazine derivatives as potential NS5B polymerase inhibitors
1 Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. *European Journal of Medicinal Chemistry*, 2019, vol. 184, art. no. 111747]

Abstract

The present study reports on evaluation of anti-HCV activity and QSAR of certain arylidenethiazolidinone derivatives as potential inhibitors of HCV-NS5B polymerase. The pursued compounds involving, 5-arylen-3-arylacetamidothiazolidin-2,4-diones 4(a-f), 5-arylene-2-(N-arylacetamido)-iminothiazolidin-4-one (10) and their rigid counterparts 5-arylinethiazolidinotetrazines 13-15(a-f), were synthesized and their structures confirmed by spectral and elemental analyses. The results of NS5B polymerase inhibition assay revealed compound 4e, as the most active inhibitor ($IC_{50} = 0.035 \mu M$), which is four fold greater than that of the reference agent, VCH-759 ($IC_{50} = 0.14 \mu M$). Meanwhile, compounds 4b, 4c, 5a, and 5c, and 13b, 14, and 15c displayed equipotency to 2 fold higher activity than VCH-759 (IC_{50} values: 0.085, 0.14, 0.14, 0.10, 0.12, 0.09 and 0.07 μM , respectively). Assessment of the anti-HCV activity (GT1a) using human hepatoma cell line (HuH-7.5) illustrates superior activity of 4e ($EC_{50} = 3.80 \mu M$) relative to VCH-759 ($EC_{50} = 5.29 \mu M$). Cytotoxicity evaluation on, transformed normal cell lines (Human Liver Epithelial-2, THLE-2 and Prostatic Tubular Epithelial, RPTEC/TERT), demonstrate enhanced safety profile of 4e ($CC_{50} = 102.77, 161.37 \mu M$, respectively) compared to VCH-759 ($CC_{50} = 61.83, 81.28 \mu M$, respectively). Molecular docking of the synthesized derivatives to NS5B polymerase allosteric site (PDB: 2H1W) showed similar binding modes to that of the co-crystallized ligand. Moreover, QSAR models were established for the studied thiazolidinones and thiazolidinotetrazines to investigate the molecular characteristics contributing to the observed NS5B polymerase inhibition activity. The obtained results inspire further investigations of thiazolidinones and thiazolidinotetrazines aiming at affording more potent, safe and orally active non-nucleoside NS5B polymerase inhibitors as anti-HCV drug candidates.

Index Terms

Author keyword: 2D-QSAR, Anti-HCV, HCV-N55B polymerase, Molecular docking, Thiazolidinones, Thiazolotriazines.

EMTRE **medical term:** allosteric site, antiviral activity, Article, cell viability, controlled study, crystal structure, drug cytotoxicity, drug protein binding, drug synthesis, EC50, enzyme inhibition, hepatitis C, Hepatitis C virus, Hub, 7.5 cell line, human, human cell, IC50, in vitro study, molecular docking, nonhuman, selectivity index, two-dimensional quantitative structure activity relationship

Reaxys Index Terms: percent inhibition, 1,3-cycloaddition, Katritzky reaction, Mannich reaction, Molecular modeling, QSAR study, Scintillation inhibition, halogenation, hydrophobic surface, lipophilicity, luminescence, tautomerization, radial distribution function, surface area, tautomerization



Reaxys对科学数据的提炼—化合物标签，理化性质

1



2-(5-(2-chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-phenylacetamide
C₁₈H₁₃ClN₂O₅ 372.832 35110507

Hit Data - 7 Identification Druglikeness

Bioactivity (All) Physical Data - 2 Spectra - 4

Preparations - 1 > Reactions - 1 > Targets - 1 > Documents - 1 >

这个化合物在这篇文献中叫4e

Substance Label - 1 hits out of 1
Melting Point - 1 hits out of 1
Chromatographic Data - 1 hits out of 1
NMR Spectroscopy - 2 hits out of 2
IR Spectroscopy - 1 hits out of 1
Mass Spectrometry - 1 hits out of 1

Label Reference

4e Hassan, Ghanea S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747]
Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗

Melting Point, °C	Solvent (Melting Point)	Reference
227 - 229	ethanol	Hassan, Ghanea S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗

NMR Spectroscopy - 2 hits out of 2

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Temperature (NMR Spectroscopy), °C	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	¹ H	dimethylsulfoxide-d ₆	24.94	400.2	supporting information	Hassan, Ghanea S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗
Chemical shifts	¹³ C	dimethylsulfoxide-d ₆	24.84	100	supporting information	Hassan, Ghanea S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗

文献中出现的化合物性质，全部直接抽提，或者给出文献中出现的位置，方便科研人员直接获取，或节省查找阅读全文的时间。

Reaxys对科学数据的提炼—活性数据(所有活性数据在RMC模块中)

Compds. No	R (A)	R (B)	IC ₅₀	EC ₅₀
VCH-759	—	—	0.14	5.29
4a	H	H	4.80	19.60
4b	4-Cl	H	0.085	11.10
4c	4-F	H	0.14	8.40
4d	4-OCH ₃	H	0.25	11.57
4e	2-Cl	H	0.035	3.80
4f	2,4(Cl) ₂	H	0.44	10.78

In vitro: Efficacy - 2									
Quantitative Results									
pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Effect	Reference
7.46	IC ₅₀	0.035	μM	Hepatitis C virus subtype 1a	Inhibitor	N55B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus];Wild		anti-HCV	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗
5.42	EC ₅₀	3.8	μM		Inhibitor	N55B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus];Wild	Huh-7.5 cell line	anti-HCV	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗

Table 2

Cytotoxicity (CC₅₀, μM)^a and Selectivity index (SI)^b values of the tested compound and VCH-759.

Code	THLE-2 cell line		RPTEC/TERT1 cell line	
	CC ₅₀	SI	CC ₅₀	SI
VCH-759	61.83	11.69	81.28	15.36
4e	102.77	27.04	161.37	42.47

^a CC₅₀ is the concentration of compounds that reduce the cell viability by 50%.

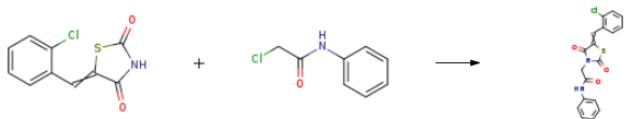
^b SI: is the ratio of CC₅₀ values on normal cells to EC₅₀ on hepatoma infected cell lines (Huh7.5).

Toxicity/Safety Pharmacology - 2

Quantitative Results

pX	Parameter	Value (quant)	Unit	Cell	Effect	Reference
3.99	CC ₅₀ (cytotoxic concentration)	102.77	μM	THLE-2 cell line	Cytotoxic	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗
3.79	CC ₅₀ (cytotoxic concentration)	161.37	μM	RPTEC/TERT1 cell line	Cytotoxic	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details ↗ Abstract ↗

Reaxys对科学数据的提炼—实验过程



1 Hits/Conditions ▾ Find Similar > Reaction ID: 52326456 ▾

Conditions

Stage #1: 5-(2-chlorobenzylidene)-2,4-thiazolidinedione With potassium carbonate In N,N-dimethyl-formamide at 100°C; for 0.5h;
Stage #2: N-chloroacetyl-aniline In N,N-dimethyl-formamide at 100°C; for 24h;

Experimental Procedure ▾

4.1.1. 2-(5-Un/substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-un/substitutedphenyl acetamide 4a-f, 5a-f, 6a-f

General procedure: A solution of the appropriate benzylidene thiazolidindione (2af)(10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol)in dry DMF (20 mL), was stirred at 100 °C for 30 min. The corresponding2-chloro N-un/sub phenyl acetamide (3a-c) (10 mmol)was added and stirring was continued at 100 °C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

4.1.1. 2-(5-Un/substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-un/substitutedphenyl acetamide 4a-f, 5a-f, 6a-f

A solution of the appropriate benzylidene thiazolidindione (**2a-f**) (10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol) in dry DMF (20 mL), was stirred at 100 °C for 30 min. The corresponding 2-chloro N-un/sub phenyl acetamide (**3a-c**) (10 mmol) was added and stirring was continued at 100 °C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

Reaxys将文献中报道的科学数据进行了抽提，归纳，标准化

The diagram illustrates the process of extracting and standardizing scientific data from literature into a database. It shows a flow from a journal article and a reaction scheme to a detailed data entry and a search results page.

Journal Article: A screenshot of a journal page from *European Journal of Medicinal Chemistry* is shown. It includes the title, authors, and a small image of the article content.

Reaction Scheme: A screenshot of a reaction scheme from *Chem* (Chemical Communications) is shown. It features a reaction diagram with reagents and products, and a caption: "Porous Ligand Creates New Reaction Route for General Single-Atom Palladium Catalyst for Selective Desulfonylation of Terminal Alkynes".

Bioactivity (All): A box containing a list of bioactivity categories with their counts: In vitro: Efficacy - 5709, In vivo: Animal Model - 817, Metabolism - 345, Pharmacokinetic - 816, and Toxicity/Safety Pharmacology - 2045.

Reaction Detail: A detailed reaction entry from Reaxys. It shows a reaction between 2-methoxy-4-(3-morpholino-propoxy)-3,4-dihydroquinazolin-4-one and 3-chloro-4-nitrophenylamine. The conditions are: Stage #1: 2-methoxy-4-(3-morpholino-propoxy)-3,4-dihydroquinazolin-4-one With thiourea, Na-dimethyl-formamide for 1h; Reflux; Stage #2: 3-chloro-4-nitrophenylamine In isopropyl alcohol for 1h; Reflux. The experimental procedure involves potassium carbonate in isopropyl alcohol at 80-85°C for 1h. The reference is: Shanghai Taicii International Pharmaceutical Co., Ltd., Li-Xin-Jian, Li-Jianhu, Ma-Yi-Ke, Chi-Wangshou, Sun-Li, Liu-Hai, (..) CN105151305, 2017, 8. Location in patent: Paragraph 0166, 0167, 0168, 0169. Full Text, Details, Abstract.

Gefitinib Entry: A detailed entry for gefitinib (C₂₂H₂₄N₄ClF₃O₃). It includes the chemical structure, physical data (446.909, 8949523, 184475-35-2), and links to identification, druglikeness, and bioactivity (All) data.

Search Results: A screenshot of the Reaxys search results page showing 10,992 documents, 74,211 substances, 79,080 reactions, and 2,355 targets. The results are filtered by 'Bcr-abl tyrosine kinase inhibitors as candidates for the treatment of covid-19: Molecular docking, pharmacophore modeling, admet studies'. Other results include 'Etiologic Role of Kinases in the Progression of Human Cancers and Its Targeting Strategies' and 'Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer'.

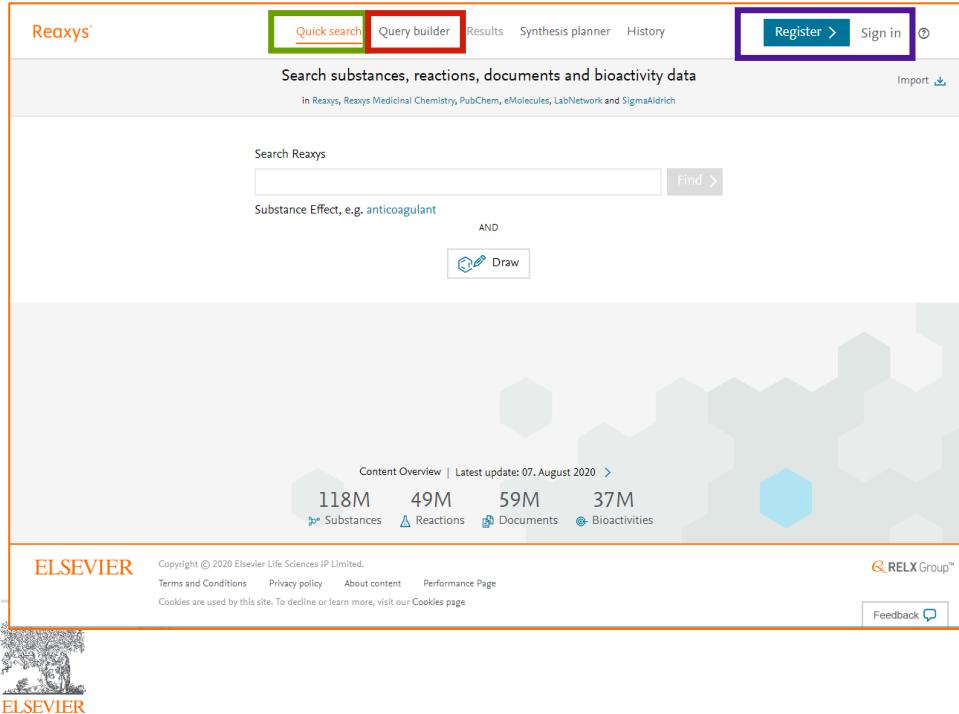
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- Q&A



Reaxys的登录界面

- IP范围内，浏览器输入www.Reaxys.com，可以直接进行检索，推荐Chrome，Firefox浏览器，
- 收藏夹收藏的链接建议只收藏www.Reaxys.com



Tips:

- 账号注册（可选），注册帐号后，可以使用提醒，结果集保存，结果导出功能（2020.8以后）
- Quick Search，快速检索，结构反应检索，或者输入自然语言，Reaxys智能分析语义进行检索。
- Query Builder，组合检索，利用Reaxys中的各种字段进行组合，实现不同检索需求。

视频介绍：

- Reaxys主界面：
<https://www.bilibili.com/video/BV1T5411L7Ec>
- Quick Search：
<https://www.bilibili.com/video/BV1az4y1C7ZL>
- Query Builder：
<https://www.bilibili.com/video/BV1UK4y1774Q>
- Reaxys账号注册与应用
<https://www.bilibili.com/video/BV1NA41147if>

Quick Search界面

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Sam Yu  

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Import 

Search Reaxys

可以输入关键词，物质名称，人名反应，以及各类组合

Substance Properties, e.g. solubility of vitamin D3

AND

 Draw

可以输入具体结构，骨架结构，通式结构，以及包含上述结构的反应式进行检索

Content Overview | Latest update: 16. March 2022

248M 58M 95M 31M 42M

 Substances  Reactions  Documents  Patents  Bioactivities



Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Case 1：关键词检索—锂硫电池

- Lithium–Sulfur Battery

Reaxys [Quick search](#) [Query builder](#) [Results](#) [Retrosynthesis](#) [History](#) [Alerts](#) Sam Yu  

Search for lithium–sulfur Battery [Import](#)

Search Reaxys [Find >](#)

Documents, e.g. publications about quasicrystals
AND

 Draw

Content Overview | Latest update: 16. March 2022 [>](#)

248M  Substances 58M  Reactions 95M  Documents 31M  Patents 42M  Bioactivities



Reaxys中的检索结果

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts Sam Yu

Results for lithium–sulfur Battery

New Edit

13,563 Documents Titles, Abstracts, Keywords : "lithium-sulfur", "Battery" Edit in Query Builder Create Alert

0 Substances Structure as drawn Edit in Query Builder Create Alert

17,799 Documents Titles, Abstracts, Keywords : "lithium-sulfur" Edit in Query Builder Create Alert

1,533,052 Documents Titles, Abstracts, Keywords : "Battery" Edit in Query Builder Create Alert

Reaxys

Quick search Query builder **Results** Retrosynthesis History Alerts Sam Yu

13,563 Documents with 1,792 Substances, 290 Reactions, 0 Targets

Filters Limit to > Exclude >

Publication Year Document Type Authors/Inventors Current Patent Assignee Patent Office Journal Title Substance Classes Reaction Classes Index Terms (List) Index Terms (ReaxysTree)

Manually processed content only

0 Limit To Exclude Export

1 A flame retardant separator modified by MOFs-derived hybrid for safe and efficient Li-S batteries
Wu, Na; Wang, Junling; Liao, Can; Han, Longfei; Song, Lei; Hu, Yuan; Mu, Xiaowei; Kan, Yongchun [Journal of Energy Chemistry, 2022, vol. 64, p. 372 - 384] Cited 4 times
Abstract Index Terms Substances Full Text

Abstract hit: {...for high-performance Lithium-Sulfur batteries (Li-S batteries). Robust carbon structure with large specific surface...}

2 Hybridized S cathode with N719 dye for a photo-assisted charging Li-S battery
Li, Jingfa; Ren, Changwei; Zhang, Linbiao; Jiang, Wenhao; Liu, Hongmin; Su, Jing; Li, Min [Journal of Energy Chemistry, 2022, vol. 65, p. 205 - 209]
Abstract Index Terms Full Text

Abstract hit: {...An integrated battery system, which integrates solar power and rechargeable battery in the...}

Index Terms hit: {...Hybridized cathode, Intergrated battery, Lithium-sulfur...}

3 Mitigating side reaction for high capacity retention in lithium-sulfur batteries
Cai, Yong; Jin, Qi; Zhao, Kaixin; Ma, Xinzhi; Zhang, Xitan [Chinese Chemical Letters, 2022, vol. 33, # 1, p. 457 - 461]
Abstract Index Terms Full Text

Reaxys中对于文献检索结果的分析

13.56 K

Preview

Filters

Publication Year

Document Type

Authors/Inventors

Current Patent Assignee

Patent Office

Journal Title

Substance Classes

Reaction Classes

Index Terms (List)

Index Terms (ReaxysTree)

Manually processed content only

Limit to > Exclude >

Filter by value < View more

View more

Publication Year

2022 337

2021 2,311

2020 2,237

2019 2,068

2018 1,638

2017 1,293

2016 1,026

Filter by value < View more

Document Type

patent 8,873

article 4,106

review 371

conference paper 152

note 16

conference review 15

short survey 12

View more

Current Patent Assignee

lg chem co,ltd 1,107

chinese academy of scie... 489

samsung sdi co,ltd 340

robert bosch stiftung 267

bosch (w/o bsh) 267

global graphene group 260

central south university 220

Filter by value < View more

Journal Title

journal of power sources 281

acs applied materials an... 269

electrochimica acta 251

journal of materials che... 179

energy storage materials 138

chemical engineering jo... 135

advanced energy materials 113

Filter by value < View more

Index Terms (List)

reaction 3,254

spectroscopy 2,838

surface 2,555

ray 2,544

x 2,542

diffusion 2,484

electrode 2,404

behavior 2,280

area 2,279

kinetics 2,250

... 2,246

Clear selected < > Sort by Occurrence < >

1 2 3 ... 47 Go to page

Limit to > Exclude >

Reaxys中的Index Terms (Reaxys Tree) 学科分类

The screenshot illustrates the Reaxys search interface, specifically focusing on the 'Index Terms (ReaxysTree)' filter. The interface is divided into several sections:

- Top Left:** Displays a total of 13.56 K results and a 'Preview' button.
- Filters Section:** A vertical list of filters including 'Publication Year', 'Document Type', 'Authors/Inventors', 'Current Patent Assignee', 'Patent Office', 'Journal Title', 'Substance Classes', 'Reaction Classes', 'Index Terms (List)', and 'Index Terms (ReaxysTree)'. The 'Index Terms (ReaxysTree)' filter is highlighted with a red box.
- Index Terms (ReaxysTree) List:** A modal window showing a list of index terms with counts: physico chemical prop... 4,036, chemical transformati... 3,628, physico chemical analy... 3,496, and quantum chemical cal... 1,000. A 'View more' button is present at the bottom.
- Index Terms (ReaxysTree) Tree:** A hierarchical tree view of the index terms. The root node 'Index Terms (ReaxysTree)' has four children: 'physico chemical properties', 'chemical transformations', 'physico chemical analysis methods', and 'quantum chemical calculation methods'. Each node is accompanied by a colored circular icon representing its count: 13,563 (dark grey), 4,036 (medium grey), 3,628 (light grey), 3,496 (very light grey), and 1,000 (white).
- Bottom Buttons:** 'Clear selected' (with an X icon), 'Limit to >', and 'Exclude >'.

利用树状图进行学科分类

Index Terms (ReaxysTree)

13,563
4,036
3,628

Index Terms (ReaxysTree) 2266

13,563
4,036
3,102
2,721
2,593
2,266
426
54
7
233
166
50
5

Clear selected

Selected search items:
behavior as electrode

Clear selected

选择获取或者排除

Limit to >

Exclude >

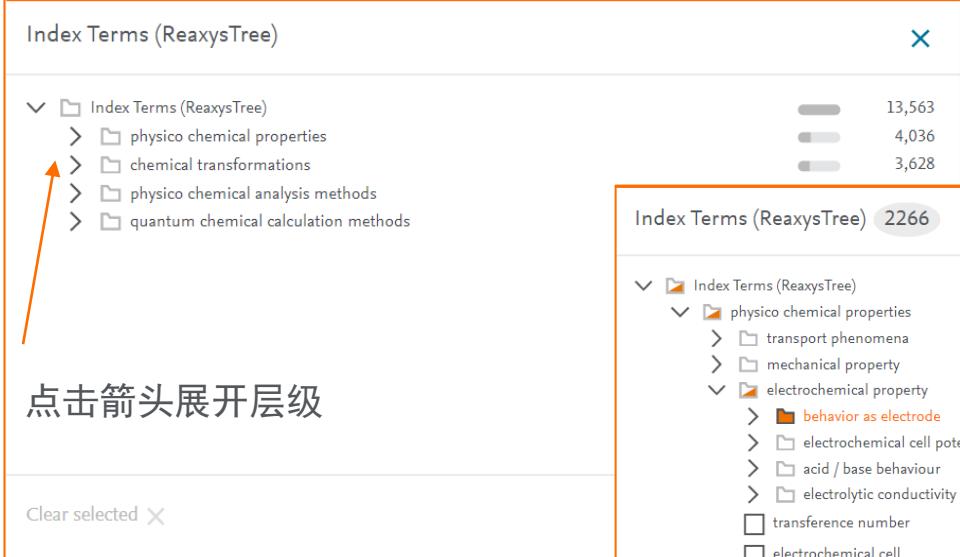


Diagram illustrating the use of a tree状图 (tree diagram) for subject classification. The interface shows a hierarchical tree of index terms on the left and a detailed view of a selected branch on the right. The tree structure is as follows:

- Index Terms (ReaxysTree)
 - Index Terms (ReaxysTree)
 - physico chemical properties
 - transport phenomena
 - mechanical property
 - electrochemical property
 - behavior as electrode
 - electrochemical cell potential
 - acid / base behaviour
 - electrolytic conductivity
 - transference number
 - electrochemical cell
 - electrocatalytic property
 - decomposition potential

The 'Selected search items' section contains 'behavior as electrode'. Action buttons at the bottom include 'Clear selected', '选择获取或者排除' (Select Get or Exclude), 'Limit to >', and 'Exclude >'. The Elsevier logo is visible in the bottom left corner.

最后的检索结果

Reaxys

Quick search Query builder **Results** Retrosynthesis History Alerts

Sam Yu  

2,266 Documents with 1,199 Substances, 65 Reactions, 0 Targets

Filters

2.27 K

13.56 K

Preview

Limit to > Exclude >

Publication Year Document Type Authors/Inventors Current Patent Assignee Patent Office Journal Title Substance Classes Reaction Classes Index Terms (List) Index Terms (ReaxysTree)  Manually processed content only

0 selected Limit To Exclude Export

Sort by Publication Year  Heatmap 

Hybridized S cathode with N719 dye for a photo-assisted charging Li-S battery

Li, Jingfa; Ren, Changwei; Zhang, Linbiao; Jiang, Wenhao; Liu, Hongmin; Su, Jing; Li, Min [Journal of Energy Chemistry, 2022, vol. 65, p. 205 - 209]

Abstract  Index Terms  Full Text 

Abstract hit: {...An integrated battery system, which integrates solar power and rechargeable battery in the...}

Index Terms hit: {...Hybridized cathode, Intergrated battery, Lithium-sulfur...}

Intagliated Cu substrate containing multifunctional lithiophilic trenches for Li metal anodes

Park, Sunwoo; Ahn, Kihyeon; Lim, Hyung-Kyu; Jin, Hyoung-Joon; Han, Seungyong; Yun, Young Soo [Chemical Engineering Journal, 2022, vol. 428]

Abstract  Index Terms  Substances  4  Full Text 

Index Terms hit: {...Lithium metal anode, Lithium metal battery, Lithium metals...}

A new flame-retardant polymer electrolyte with enhanced Li-ion conductivity for safe lithium-sulfur batteries

Li, Hongping; Kuai, Yixi; Yang, Jun; Hirano, Shin-ichi; Nuli, Yanna; Wang, Jiulin [Journal of Energy Chemistry, 2022, vol. 65, p. 616 - 622]

Abstract  Index Terms  Substances  4  Full Text 

Abstract hit: {...fireproof quasi-solid-state battery system...}

Index Terms hit: {...Lithium-ion conductivity, Lithium-sulfur battery, Polymer electrolyte...}

Nano storage-boxes constructed by the vertical growth of MoS₂ on graphene for high-performance Li-S batteries

Cited 1 times  Feedback 

全文链接，如果是OA或者学校已经订购
可以直接打开

Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Case 2：快速获取化合物的理化性质

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Sam Yu  

Search for solubility of gefitinib Import 

Search Reaxys

solubility of gefitinib  

Substance Molecular Formula, e.g. Pt(PPh₃)₃

AND

 Draw

Tips:
快速获取某个化合物
溶解性数据。

Content Overview | Latest update: 07. February 2022 

179M 57M 86M 41M

 Substances  Reactions  Documents  Bioactivities

 ELSEVIER

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Remote access Terms and Conditions Privacy policy About content

 RELX Group™

Reaxys中的结果

Quick search Query builder Results Synthesis planner History

Results for solubility of gefitinib

New Edit

1 Substances Structure: as drawn AND Property: solubility Preview Results View Results

178 Documents Titles, Abstracts, Keywords: "solubility", "gefitinib" Preview Results View Results

341,792 Documents Titles, Abstracts, Keywords: "solubility" Preview Results View Results

23,178 Documents Titles, Abstracts, Keywords: "gefitinib" Preview Results View Results

1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References Grid Heatmap

gefitinib C22H24N4ClFO3 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All)

Identification Physical Data - 115

Druglikeness Spectra - 80

Other Data - 4,132

Preparations - 83

Reactions - 148

Targets - 1,149

Documents - 9,928

1 Hit Data - 4

Solubility (MCS) - 4 hits out of 4

抽提的数据包括具体的数值，或者相关的文字性描述

Solubility (MCS) - 4 hits out of 4						Show/Hide columns 
Solubility, g l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					freely soluble in DMSO,THP and PEG-400, sparingly soluble in 2-butanol and slightly soluble in 1-butanol, IPA, ethanol, methanol, EG and PG	Alanazi, Abdullah; Alshehri, Sultan; Altamimi, Mohammad; Shakeel, Faiyaz [Journal of Molecular Liquids, 2020, vol. 299, art. no. 112211] Full Text  Details  Abstract 
					soluble in water and 1-octanol	Wu, Kuen-Da; Chen, Grace Shiahuy; Liu, Jia-Rong; Hsieh, Chen-En; Chem, Ji-Wang [ACS Medicinal Chemistry Letters, 2019, vol. 10, # 1, p. 22 - 26] Full Text  Cited 1 times  Details  Abstract 
0.009832	in pure solvent	25	water	supporting information		Wang, Xin-Xin; Tian, Fei-Yang; Liu, Ming; Chen, Kai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu [Tetrahedron, 2019, vol. 75, # 37, art. no. 130488] Full Text  Details  Abstract 
0.0021	in pure solvent	20	water			Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Weili; Dong, Xiaochun [Bioorganic and Medicinal Chemistry Letters, 2013, vol. 23, # 19, p. 5385 - 5388] Full Text  Cited 22 times  Details  Abstract 



Reaxys中化合物更多的理化性质

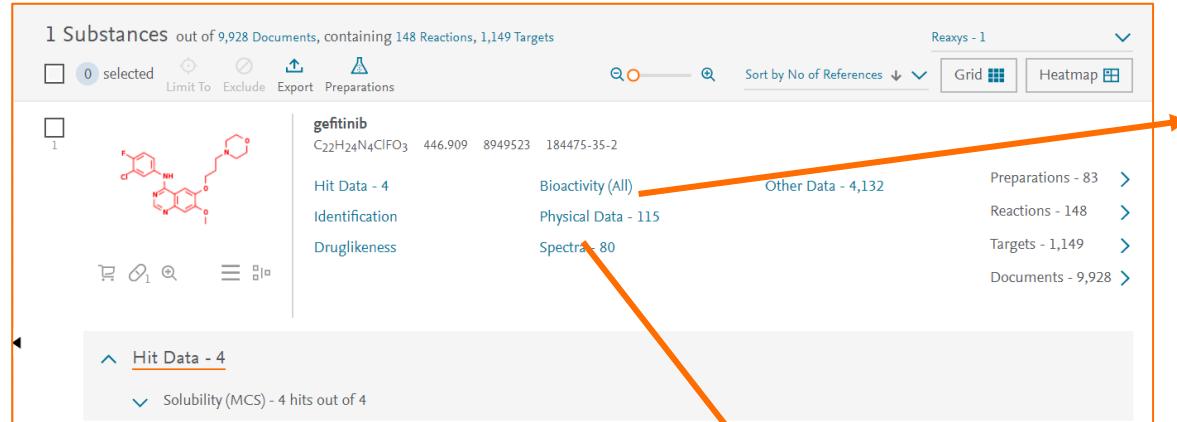
1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

gefinitib
C₂₂H₂₄N₄ClF₃ 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 4,132
Identification Physical Data - 115 Preparations - 83
Druglikeness Spectra - 80 Reactions - 148
Spectra - 80 Targets - 1,149
Documents - 9,928

Hit Data - 4
Solubility (MCS) - 4 hits out of 4



直接获取化合物的理化性质或者谱图数据

Physical Data - 115

- ▼ Melting Point - 27
- ▼ Density - 1
- ▼ Association (MCS) - 12
- ▼ Chromatographic Data - 5
- ▼ Conformation - 1
- ▼ Crystal Phase - 9
- ▼ Crystal Property Description - 25
- ▼ Crystal System - 2
- ▼ Dissociation Exponent - 3
- ▼ Further Information - 1

Spectra - 80

- ▼ NMR Spectroscopy - 46
- ▼ IR Spectroscopy - 9
- ▼ Mass Spectrometry - 17
- ▼ UV/VIS Spectroscopy - 6
- ▼ Raman Spectroscopy - 1
- ▼ Fluorescence Spectroscopy - 1



Reaxys中与化合物分析有关文献的获取

1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

Reaxys - 1 Grid Heatmap

Sort by No of References

gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 4,132

Identification Physical Data - 115

Druglikeness Spectra - 80

Preparations - 83 >

Reactions - 148 >

Targets - 1,149 >

Documents - 9,928 >

Hit Data - 4

Solubility (MCS) - 4 hits out of 4

Reaxys®

9,928 Documents with 61,309 Substances, 72,101 Reactions, 2,279 Targets

0 selected Limit To Exclude Export

1 Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer
Karuppasamy, Ramanathan; Veerappapillai, Shanthi; Maiti, Sayoni; Shin, Woong-Hee; Khara, Daisuke [Seminars in Cancer Biology, 2021, vol. 68, p. 84 - 91]
Abstract < Index Terms < Substances (48) < Full Text >
Hit Substances (1) <

2 Repurposing of plant alkaloids for cancer therapy: Pharmacology and toxicology
Effert, Thomas; Oesch, Franz [Seminars in Cancer Biology, 2021, vol. 68, p. 143 - 163]
Abstract < Index Terms < Substances (43) < Full Text >
Hit Substances (1) <

3 Repurposing old drugs as new inhibitors of the ubiquitin-proteasome pathway for cancer treatment
Yang, Huanjie; Chen, Xin; Li, Kai; Cheaito, Hassan; Yang, Qianqian; Wu, Guojun; Liu, Jinbao; Dou, Q. Ping [Seminars in Cancer Biology, 2021, vol. 68, p. 105 - 122]
Abstract < Index Terms < Substances (64) < Full Text >
Hit Substances (1) <

4 Kinases as potential targets for treatment of pulmonary hypertension and right ventricular dysfunction
Weiss, Astrid; Boehm, Mario; Egemenazarov, Bakytbek; Grimmling, Friedrich; Savai Pullamsetti, Soni; Kwapiszewska, Grazyna; Schermuly, Ralph T. [British Journal of Pharmacology, 2021, vol. 178, #1, p. 31 - 53]
Abstract < Index Terms < Substances (28) < Full Text >
Hit Substances (1) <

Results

Quick search Query builder Synthesis planner History Alerts

9,928 Documents with 61,309 Substances, 72,101 Reactions, 2,279 Targets

0 selected Limit To Exclude Export

1 Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer
Karuppasamy, Ramanathan; Veerappapillai, Shanthi; Maiti, Sayoni; Shin, Woong-Hee; Khara, Daisuke [Seminars in Cancer Biology, 2021, vol. 68, p. 84 - 91]
Abstract < Index Terms < Substances (48) < Full Text >
Hit Substances (1) <

2 Repurposing of plant alkaloids for cancer therapy: Pharmacology and toxicology
Effert, Thomas; Oesch, Franz [Seminars in Cancer Biology, 2021, vol. 68, p. 143 - 163]
Abstract < Index Terms < Substances (43) < Full Text >
Hit Substances (1) <

3 Repurposing old drugs as new inhibitors of the ubiquitin-proteasome pathway for cancer treatment
Yang, Huanjie; Chen, Xin; Li, Kai; Cheaito, Hassan; Yang, Qianqian; Wu, Guojun; Liu, Jinbao; Dou, Q. Ping [Seminars in Cancer Biology, 2021, vol. 68, p. 105 - 122]
Abstract < Index Terms < Substances (64) < Full Text >
Hit Substances (1) <

4 Kinases as potential targets for treatment of pulmonary hypertension and right ventricular dysfunction
Weiss, Astrid; Boehm, Mario; Egemenazarov, Bakytbek; Grimmling, Friedrich; Savai Pullamsetti, Soni; Kwapiszewska, Grazyna; Schermuly, Ralph T. [British Journal of Pharmacology, 2021, vol. 178, #1, p. 31 - 53]
Abstract < Index Terms < Substances (28) < Full Text >
Hit Substances (1) <

Cited 1 times

ELSEVIER

Reaxys中的文献分析工具

9.93 K
1
Preview

Filters

Limit to > Exclude >

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

Document Type ▾

Authors ▾

Patent Assignee ▾

Patent Office ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

Manually processed content only

Index Terms (ReaxysTree)

- physico chemical properties 4,729
- chemical transformations 4,540
- physico chemical analysis... 1,658
- quantum chemical calculati... 196

[View more](#)

Index Terms (ReaxysTree)

- Index Terms (ReaxysTree)
 - physico chemical properties 9,928
 - chemical transformations 4,729
 - physico chemical analysis methods 4,540
 - separation method 1,658
 - spectroscopical analysis 781
 - fluorescence spectroscopy 760
 - luminescence spectroscopy 267
 - mass spectrometry 245
 - NMR spectroscopy 116
 - IR spectroscopy 55
 - Raman spectroscopy 35
 - photoelectron emission spectroscopy 28
 - ESR 12

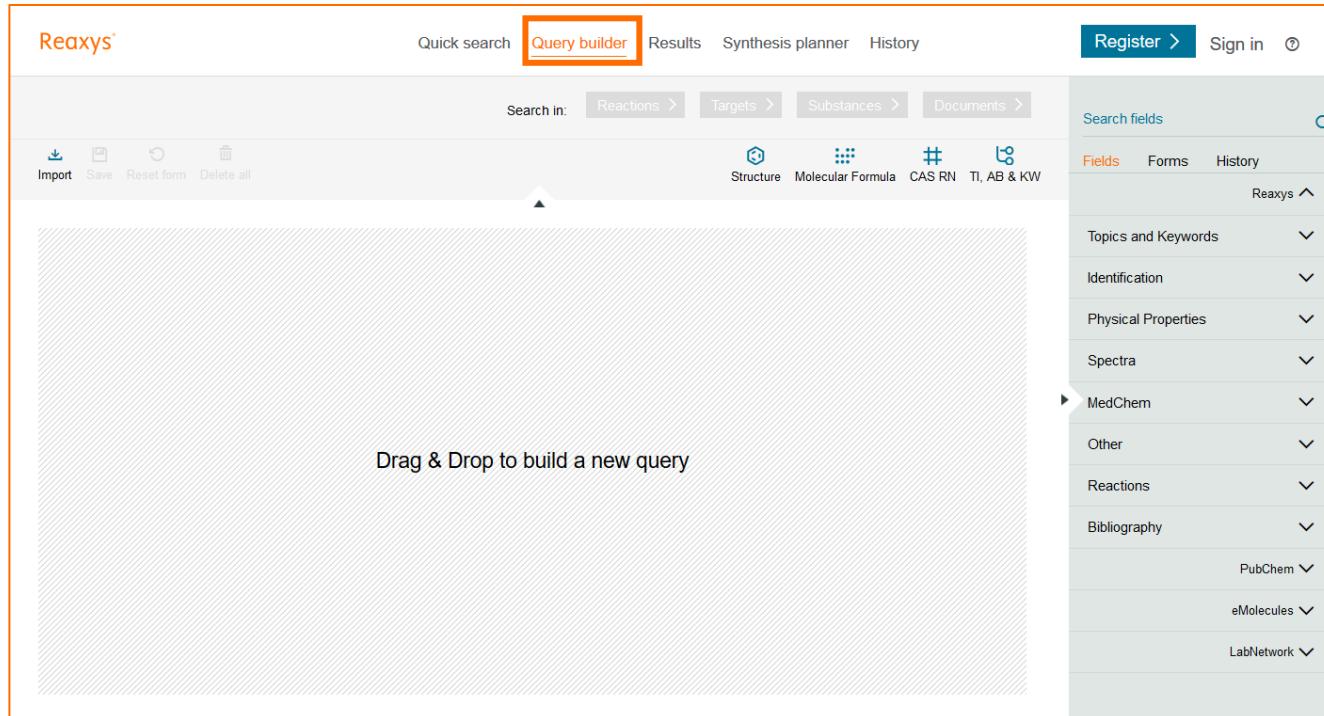
[Clear selected](#) X

Limit to > Exclude >

Reaxys中与分析有关的文献分类

Case 3：理化性质的高级应用

- 获取KCl在乙醇中的溶解度



Reaxys中的Query Builder可以按照一定的规则构建检索式，Reaxys一共提供180+字段和字段组，科研人员可以自由的对这些字段和字段组进行组合，同时Reaxys也根据一些常见的需求，内置了多种检索策略模板，如“天然产物”，“hERG”等

检索策略的构建

Reaxys

Quick search [Query builder](#) Results Synthesis planner History [Register](#) [Sign in](#) [?](#)

Search in: [Reactions](#) [Targets](#) [Substances](#) [Documents](#)

[Import](#) [Save](#) [Reset form](#) [Delete all](#)

Structure Molecular Formula CAS RN TI, AB & KW

AND

Find any [Hide fields](#)

Solubility, g·l⁻¹

Saturation

Temperature (Solubility (MCS)), °C

Solvent (Solubility (MCS))

Ratio of Solvents

Search fields [X](#)

Solubility

Solubility Product

Tips:
手动添加MF与
Solubility的字段

条件的输入

Reaxys

Quick search [Query builder](#) Results Synthesis planner History

Search in: Reactions > Targets > **Substances >** [Solvents](#)

Import Save Reset form Delete all

Molecular Formula is KCl

AND

Solubility

Find any Hide fields

- = Solubility, g 1-1
- is Saturation
- = Temperature (Solubility (MCS)), °C
- is ethanol
- is Ratio of Solvents

Step1: 输入分子式KCl

Step2: 在溶剂一块选择乙醇

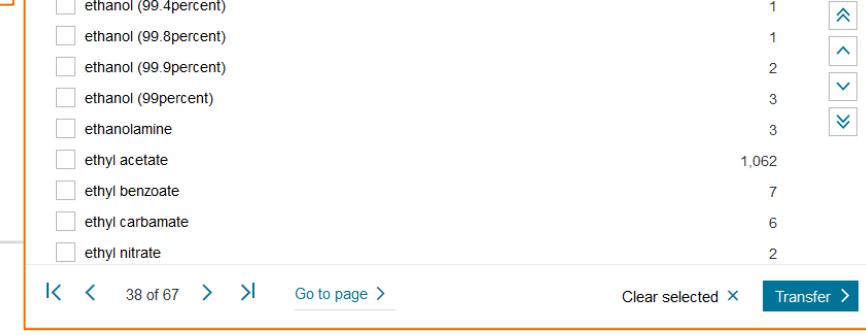
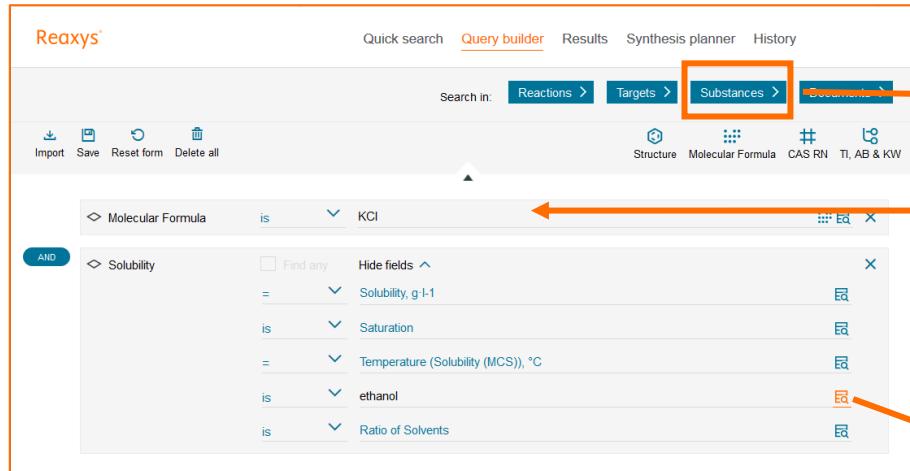
Step3: 进行物质检索

Solvent (Solubility (MCS)) 1

eth

Substance	Count
ethane-1,2-diamine	23
ethane-1,2-diol	100
ethanesulfonic acid	1
ethanol	5,024
ethanol (99.4percent)	1
ethanol (99.8percent)	1
ethanol (99.9percent)	2
ethanol (99percent)	3
ethanolamine	3
ethyl acetate	1,062
ethyl benzoate	7
ethyl carbamate	6
ethyl nitrate	2

< < 38 of 67 > > Go to page > Clear selected Transfer >



ELSEVIER

最后的结果

1 Substances out of 7,363 Documents, containing 4,322 Reactions, 68 Targets

Reaxys - 1

0 selected Limit To Export Preparations Sort by No of References Grid Heatmap

1 CIK potassium chloride CIK 74.5513 3534978

Hit Data - 20 Bioactivity (All) Other Data - 791 Preparations - 415 >

Identification Physical Data - 2,976 Reactions - 4,322 >

Druglikeness Spectra - 184 Targets - 68 >

Documents - 7,363 >

Hit Data - 20

Solubility (MCS) - 20 hits out of 429

^ Solubility (MCS) - 20 hits out of 429

Show/Hide columns

Solubility, g l ⁻¹	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
20	ethanol	Solubility: 0.012 mol/kg solvent	Ei-Dossoki[<i>Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical</i> , 2005, vol. 44, # 8, p. 1594 - 1596]	Full Text Cited 6 times Details Abstract
25	ethanol	Solubility: 0.025 mol/kg solvent	Ei-Dossoki[<i>Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical</i> , 2005, vol. 44, # 8, p. 1594 - 1596]	Full Text Cited 6 times Details Abstract
30	ethanol	Solubility: 0.037 mol/kg solvent	Ei-Dossoki[<i>Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical</i> , 2005, vol. 44, # 8, p. 1594 - 1596]	Full Text Cited 6 times Details Abstract
35	ethanol	Solubility: 0.043 mol/kg solvent	Ei-Dossoki[<i>Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical</i> , 2005, vol. 44, # 8, p. 1594 - 1596]	Full Text Cited 6 times Details Abstract
0.320571	ethanol		Abakshin, V. A.; Eliseeva, O. V.; Krasnoperova, A. P.; Lebedeva, L. T.; Krestov, G. A.[<i>Doklady Physical Chemistry</i> , 1991, vol. 317, p. 303 - 306][<i>Dokl. Phys. Chem. (Transl. of Dokl. Akad. Nauk.)</i> , 1991, vol. 317, p. 1140 - 1143]	Full Text Details
20	ethanol	Solubility: 1.270E0 mol/1000mol solvent	Kirm; Dunlap[<i>Journal of the American Chemical Society</i> , 1931, vol. 53, p. 393]	Full Text Details
45	ethanol	Solubility: 1.277E0 mol/1000mol solvent	Kirm; Dunlap[<i>Journal of the American Chemical Society</i> , 1931, vol. 53, p. 393]	Full Text Details

Case 4: “特定研究领域”的催化剂选择

- 检索可用于立体选择性催化的含Fe的催化剂

The screenshot shows the Reaxys Query builder interface. The search bar at the top contains the text "catalyst". Below the search bar, there are buttons for "Reactions >", "Targets >", "Substances >", and "Documents >". On the left, there are buttons for "Import", "Save", "Reset form", and "Delete all". On the right, there are buttons for "Structure", "Molecular Formula", "CAS RN", and "TI, AB & KW". The "Molecular Formula" button is highlighted with a red arrow. Below these buttons, there are two search fields: "Molecular Formula" and "Catalyst Investigation". The "Molecular Formula" field has a dropdown menu with "is" and "is not" options, and a sub-field "Molecular Formula" with a search bar. The "Catalyst Investigation" field has a dropdown menu with "Find any" and "Hide fields" options, and a sub-field "Investigated characteristic(s)" with a search bar. A red arrow points from the "Search fields" search bar to the "Investigated characteristic(s)" search bar. A red box on the right contains the text "Tips : 手动添加MF 与 Catalyst Investigation的字段.".

Reaxys

Quick search [Query builder](#) Results Synthesis planner History

Register > Sign in ?

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Molecular Formula

AND

Catalyst Investigation

Investigated characteristic(s)

Specification of catalysis

Classification of catalysis

Type of reaction

Co-catalyst/co-substrate name

Search fields

catalyst

Tips : 手动添加MF 与 Catalyst Investigation的字段.

条件的输入

Search in: Reactions > Targets > **Substances >** Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

AND

◆ Molecular Formula contains Fe

◆ Catalyst Investigation

- Find any Hide fields
- is Investigated characteristic(s)
- is stereoselective catalysis
- is Classification of catalysis
- is Type of reaction
- is Co-catalyst/co-substrate name

Specification of catalysis 1

	Search
<input type="checkbox"/> chemoselective catalysis	2,481
<input type="checkbox"/> immobilised catalyst	452
<input type="checkbox"/> phase-transfer catalysis	419
<input type="checkbox"/> regioselective catalysis	2,516
<input checked="" type="checkbox"/> stereoselective catalysis	9,365

Step1: 输入分子式Fe，并将逻辑关系改成“Contains”，即只要分子式中包含Fe，就检索出来

Step2: Specification of Catalysis部分选择立体选择性催化

Step3: 进行物质检索

最后的结果

Reaxys

Quick search Query builder **Results** Synthesis planner History Register > Sign in ?

311 Substances out of 33,712 Documents, containing 28,346 Reactions, 70 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References ▾ Grid Heatmap

311

Query

Filters

Limit to > Exclude >

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases Available Data Document Type Publication Year Patent Assignee LogP

1

 ferrocene
((C₅H₅)₂Fe) 186.036 11756767 102-54-5

Hit Data - 2 Bioactivity (All) Other Data - 241 Preparations - 896 >
Identification Physical Data - 3,483 Reactions - 3,636 >
Druglikeness Spectra - 514 Targets - 1 >
Documents - 13,609 >

Hit Data - 2

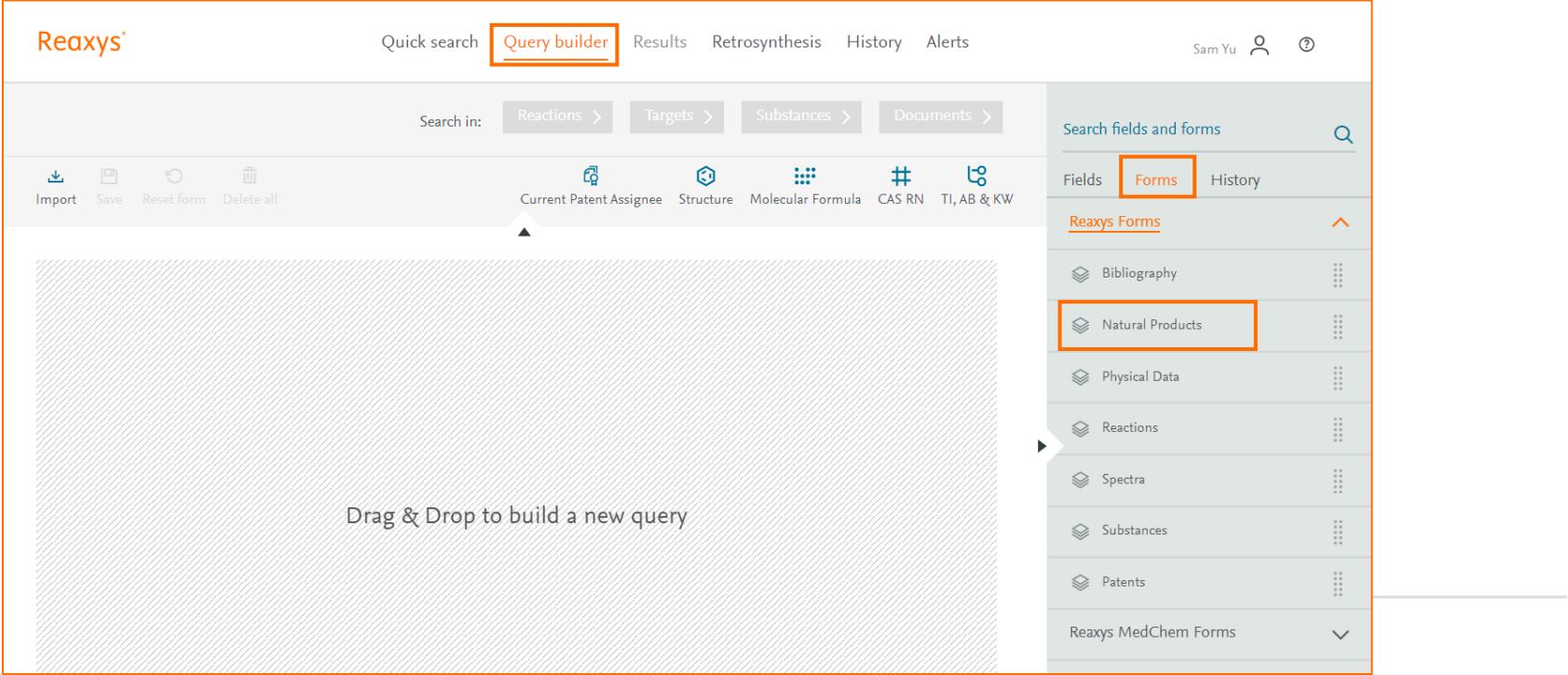
Catalyst Investigation - 2 hits out of 25

Reaxys给出的结果与证据

Investigated characteristic(s)	Specification of catalysis	Type of reaction (Catalyst Investigation)	Location	Co-catalyst/co-substrate name	Reference
Catalytic activity, Diastereomeric excess	Stereoselective catalysis	Olefination		bathophenanthroline	Gao, Pin; Wu, Hao; Yang, Jun-Cheng; Guo, Li-Na [Organic Letters, 2019, vol. 21, # 17, p. 7104 - 7108] Full Text > Details > Abstract >
Catalytic activity, Diastereomeric excess	Stereoselective catalysis	Annulation	supporting information		Hou, Zhong-Wei; Yan, Hong; Song, Jin-Shuai; Xu, Hai-Chao [Chinese Journal of Chemistry, 2018, vol. 36, # 10, p. 909 - 915] Full Text > Cited 26 times > Details > Abstract >

Case 5：活性天然产物的获取

- 检索包含特定结构的天然产物，并做活性分析



The screenshot shows the Reaxys search interface. The top navigation bar includes 'Quick search', 'Query builder' (which is highlighted with a red box), 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user 'Sam Yu' is logged in. The main search area has a 'Search in:' dropdown set to 'Reactions' and a large central area with a 'Drag & Drop to build a new query' placeholder. Below this are search icons for 'Current Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. On the left, there are buttons for 'Import', 'Save', 'Reset form', and 'Delete all'. The right sidebar is titled 'Search fields and forms' and shows a list of fields under the 'Forms' tab. The 'Natural Products' option is highlighted with a red box. Other listed fields include Bibliography, Physical Data, Reactions, Spectra, Substances, and Patents. A 'Reaxys MedChem Forms' section is also present at the bottom of the sidebar.

添加天然产物模块

- 添加结构和勾选天然产物

Reaxys

Quick search [Query builder](#) Results Retrosynthesis History Alerts

Sam Yu  

Search in: [Reactions >](#) [Targets >](#) [Substances >](#) [Documents >](#)

 Import  Save  Reset form  Delete all

 Current Patent Assignee  Structure  Molecular Formula  CAS RN  TI, AB & KW

 Natural Products

 Structure

CC(=O)Oc1ccccc1

On all atoms

 AND  Isolated from Natural... Find any Show fields  (Isolated from Natural Source) 

Search fields 

Fields Forms History

Reaxys

Topics and Keywords

Identification

Physical Properties

Spectra

MedChem

Other

Reactions

Bibliography

最后的结果

Reaxys®

Quick search Query builder **Results** Retrosynthesis History Alerts

Sam Yu ?

1,605 Substances out of 333,243 Documents, containing 214,279 Reactions, 2,039 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References Grid Bioactivity Visualization

benzoic acid
C6H5CO2H 122.123 636131 65-85-0

Hit Data - 85 Bioactivity (All) Other Data - 1,072 Preparations - 7,354 >
Identification Physical Data - 2,992 Reactions - 33,818 >
Druglikeness Spectra - 466 Targets - 120 >
Documents - 49,271 >

Hit Data - 85
Isolated from Natural Source - 85 hits out of 85

salicylic acid
C6H4(O)C(=O)O Isolated from Natural Source - 85 hits out of 85

Hit Data - 124 Isolated from Natural Source Location Reference
Identification culture of Streptomyces netropsis WLXQ55-4; isolated from the rhizosphere soil of Clematis mandshurica Rupr. collected from Zhanwanhe Village, Yingermen Town, Qingyuan County, Fushun City, Liaoning Province, China (28°55'59" N, 115°3'19" E) Chen, Hong; Chen, Zhicong; Liu, Tao; Si, Tong; Zhang, Lingxiao; Zhang, Songya; Zhu, Jing [Molecules, 2021, vol. 26, # 8, art. no. 2147]
Druglikeness stems and leaves of Piper suippia; collected in Monlong, Mae Rim district, Chiang Mai province, (18°55'08.0" N 98°50'09.1" E) northern Thailand, September 2016 Kanokmedhakul, Kwanjai; Kanokmedhakul, Somdej; Lakornwong, Waranya; Masranoi, Jariya; Suwanphakdee, Chalermpol; Tontapha, Sarawut; Yahuafai, Jantana [Natural Product Research, 2021]
Show/Hide columns

每一个化合物都给出是天然产物的证据

活性的分析

1.60 K

Search

Filters

Limit to > Exclude >

By Structure

Measurement pX

Targets

Parameters

Substances

Measurement pX 3

>11 - 12 5

>10 - 11 3

>9 - 10 11

>8 - 9 14

>7 - 8 44

>6 - 7 108

>5 - 6 226

View more

14 Substances out of 38 Documents, containing 2,502 Reactions, 13 Targets

0 selected Limit To Exclude Export Preparations Sort by No of References

salicylic acid

C₆H₄(OH)(CO₂H) 138.123 774890 69-72-7

Hit Data - 50 Identification Druglikeness Bioactivity (Hit Data) Spectra - 268

Identification Bioactivity (All) Other Data - 2,110

Druglikeness Physical Data - 1,841

124

1 Hit Data - 50

Isolated from Natural Source - 50 hits out of 50

In vitro: Efficacy - 1

Quantitative Results

Show/Hide columns

pX	Parameter	Value (qual)	Value (quant)	Unit	Target	Reference
9.6	IC50	=	254	pM	Prostaglandin G/H synthase 1:Wild	Current Patent Assignee: EURO CELTIQUE S.A. - US2002/99049, 2002, A1 Full Text > Details > Abstract >

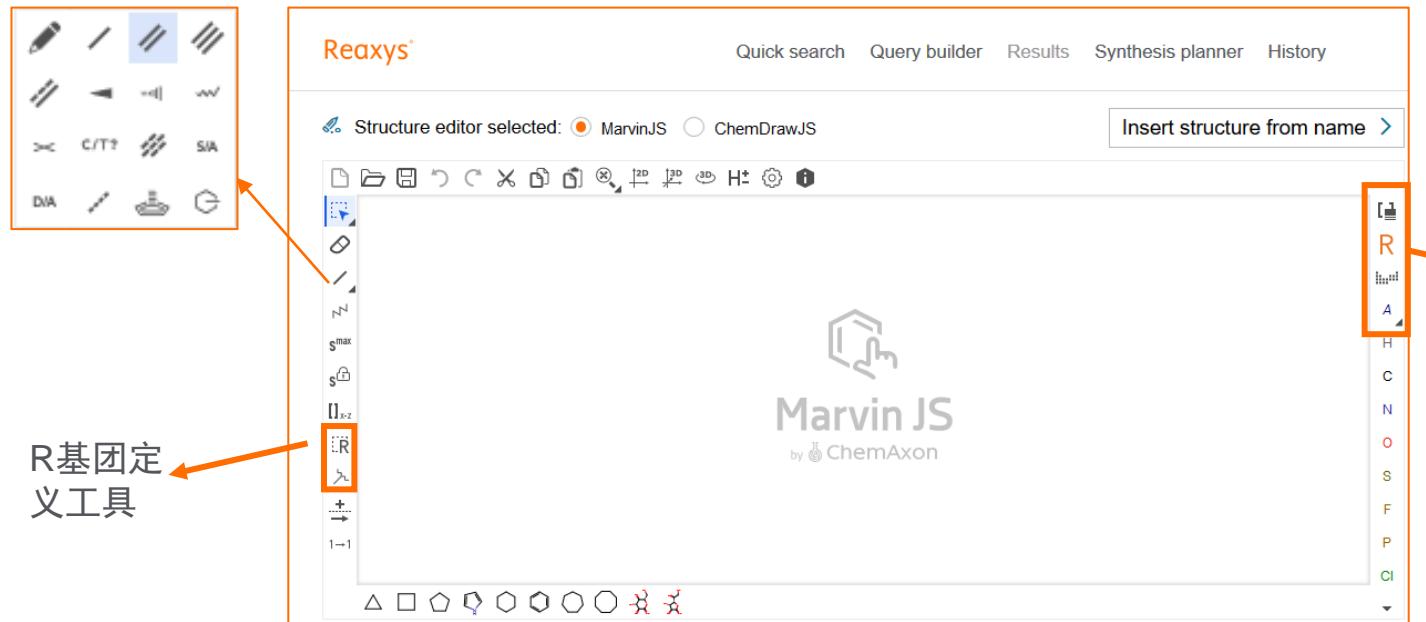
ELSEVIER

Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Reaxys中的结构面板



一些常见的功能使用视频

2022新版结构面板	视频链接		
1-最基本功能	https://www.bilibili.com/video/BV1Jm4y1F7hG		
2-不定位键	https://www.bilibili.com/video/BV1xP4y127G9		
3-缩写写官能团	https://www.bilibili.com/video/BV16K411o72c		
4-通用官能团与G	https://www.bilibili.com/video/BV16P4y1y7QA		
5-原子列表与列表非	https://www.bilibili.com/video/BV1w84y117yD		
6,7-R基团的使用与讨论	<p>R基团与Linker: https://www.bilibili.com/video/BV1Ze4y1p7hx</p> <p>讨论1: 基本使用方法和逻辑</p>	<p>关于R基团的讨论 https://www.bilibili.com/video/BV1w14y1n7dD</p> <p>讨论2: 取代基的控制</p>	<p>讨论3: As Draw的控制</p>
8,9,10-检索模式的讨论	https://www.bilibili.com/video/BV1rG4y1V7Hw	https://www.bilibili.com/video/BV1aG4y1G7cb	https://www.bilibili.com/video/BV1k14y1n76d
11-反应的基本定义	https://www.bilibili.com/video/BV17W4y1p7p1		
12-配位化合物同位素盐	https://www.bilibili.com/video/BV15v4y1R7xb		
13,14-原子属性列表		<p>属性列表讨论 (上)</p> https://www.bilibili.com/video/BV1UM411B7rQ	<p>属性列表讨论 (下)</p> https://www.bilibili.com/video/BV1KW4y1T7Pv
15-键的控制	https://www.bilibili.com/video/BV1LD4y1h79d		
16-More Option	https://www.bilibili.com/video/BV1U84y147ao		



Case 6: Reaxys中最简单的反应定义与筛选

- 检索以下核心结构反应并进行反应筛选操作
- 视频操作过程
 - <https://www.bilibili.com/video/BV1BT4y1F7vT>

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in ?

Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >

原子匹配与原子锁定

Search this structure as:

As drawn

As substructure

On all atoms

On heteroatoms

Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

Clear Cancel Transfer to query > + More options

ELSEVIER

Reaxys中的结果

Reaxys®

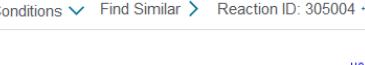
Quick search Query builder **Results** Synthesis planner History Register > Sign in ?

10,112 Reactions out of 7,263 Documents containing 13,573 Substances, 2,788 Targets

0 Limit To Exclude Export Syn-Plan Show Conditions

1  55 Conditions Find Similar Reaction ID: 2407606

2  38 Conditions Find Similar Reaction ID: 305004

3 

Show/Hide Conditions, 选择显示/隐藏条件

1  55 Conditions Find Similar Reaction ID: 2407606

With formic acid; $[(n\text{Pr}_2\text{C}_5\text{H}_5)\text{Ru}(\text{C}_1\text{P}-\text{PPh}_2\text{Py})(\text{PPh}_3)\text{Cl}]$; sodium hydroxide **In** water; acetonitrile at 80°C; for 8h;

92% Kumar, Prashant; Singh, Ashish Kumar; Sharma, Sanjeev; Pandey, Daya Shankar
[Journal of Organometallic Chemistry, 2009, vol. 694, # 22, p. 3643 - 3652]
Full Text > Cited 21 times > Details > Abstract >

With bis($n\text{C}_5\text{H}_5$ -cyclopentadienyl)hafnium dihydride **In** isopropyl alcohol at 80°C; for 8h;

91% Nakano, Tatsuya; Umeno, Shigetoshi; Kino, Yoshi; Ishii, Yasutaka; Ogawa, Masaya
[Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757]
Full Text > Details > Abstract >

With sodium tetrahydorbate **In** ethanol at 0°C; for 1h;
Experimental Procedure

91% AKITA INNOVATIONS LLC; BARDON, Kevin M.; MINNS, Richard A.; SELFRIDGE, Scott D.; TAKIFF, Larry; ADAMS, Timothy
W02018/217266, 2018, A1
Location in patent: Page/Page column 52; 53
Full Text > Details > Abstract >

10.11 K Preview

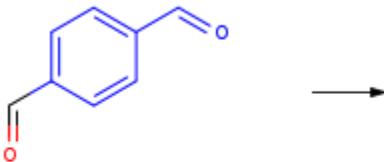
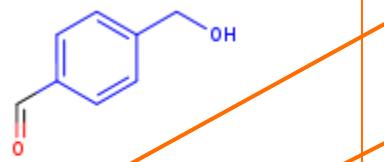
Filters Limit to > Exclude >

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

ELSEVIER

Reaxys的一条反应的界面

1   

55 [Conditions](#) [Find Similar](#) > Reaction ID: 2407606 

查看商业来源 

查看物质详情 

更多与物质相关操作 

4-(hydroxymethyl)benzaldehyde
HCOC₆H₄CH₂OH 136.15 878348 52010-97-6

Identification Physical Data - 28 Preparations - 35
Druglikeness Spectra - 84 Reactions - 745
Bioactivity (All) Targets - 1
Documents - 251

[View Details >](#)

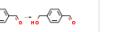
查看条件 

寻找相似反应 

合成计划按钮 

Find Similar Reactions... 

Click on one of the hyperlinks below for getting similar reactions according to the selected scope:
the reactions were determined by regarding similar transition states based on your reaction query

Query Reaction	Tight 	Near 	Medium 	Wide 	Widest 
	1,612	6,822	6,827	6,878	40,060

 ELSEVIER

Options 

- > Find Similar
- > View related Markush
- > View details
- > Copy structure to query
- > Copy reaction to query
- > Use as filter
- > Open in database

Reaxys的筛选操作

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

Yield	
<input type="checkbox"/> >95 - 100	924
<input type="checkbox"/> >90 - 95	835
<input type="checkbox"/> >85 - 90	614
<input type="checkbox"/> >80 - 85	456
<input type="checkbox"/> >75 - 80	375
<input type="checkbox"/> >70 - 75	287
<input type="checkbox"/> >65 - 70	223

[Filter by value](#) [View more](#)

Reagent/Catalyst	
<input type="checkbox"/> sodium tetrahydroborate	7,079
<input type="checkbox"/> methanol	1,387
<input type="checkbox"/> potassium carbonate	1,236
<input type="checkbox"/> water	690
<input type="checkbox"/> lithium aluminium tetrahydride	639
<input type="checkbox"/> hydrogen	620
<input type="checkbox"/> hydrochloric acid	599

[Filter by value](#) [View more](#)

Solvent	
<input type="checkbox"/> methanol	4,014
<input type="checkbox"/> tetrahydrofuran	3,375
<input type="checkbox"/> ethanol	2,025
<input type="checkbox"/> water	1,395
<input type="checkbox"/> dichloromethane	1,268
<input type="checkbox"/> n,n-dimethyl-formamide	1,105
<input type="checkbox"/> toluene	515

[Filter by value](#) [View more](#)

Document Type	
<input type="checkbox"/> article	7,543
<input type="checkbox"/> patent	3,181
<input type="checkbox"/> review	68
<input type="checkbox"/> conference paper	44
<input type="checkbox"/> letter	11
<input type="checkbox"/> short survey	4
<input type="checkbox"/> note	4

[View more](#)

Publication Year	
<input type="checkbox"/> 2020	393
<input type="checkbox"/> 2019	788
<input type="checkbox"/> 2018	834
<input type="checkbox"/> 2017	780
<input type="checkbox"/> 2016	921
<input type="checkbox"/> 2015	829
<input type="checkbox"/> 2014	755

[Filter by value](#) [View more](#)

Tips:

常见的一些反应筛选工具，
如:收率, 催化剂/试剂, 溶剂,
文献类型, 出版年限等



Reaxys中的一些特殊筛选工具—溶剂分类

Solvent Classes ^

- Low boiling (<100°C) 8,385
- Green 6,424
- Protic 6,352
- Aprotic apolar 4,172
- Yellow 4,056
- Aprotic dipolar 3,179
- Red 3,119
- High boiling (>150°C) 1,354
- Middle boiling(100°C - 150°C) 912
- Inorganic 88

[View more](#)

Solvent Classes X

▼ Solvent Classes

- > Low boiling (<100°C) 10,112
- > Green 8,385
- > Protic 6,424
- > Aprotic apolar 6,352
- > Yellow 4,172
- > Aprotic dipolar 4,056
- > Red 3,179
- > High boiling (>150°C) 3,119
- > Middle boiling(100°C - 150°C) 1,354
- > Inorganic 912

[Clear selected](#) X

[Limit to >](#) [Exclude >](#)



Reaxys中的一些特殊筛选工具—催化剂分类

Catalyst Classes

- active center 8,926
- heterogeneous 297
- organism / enzymes 52

[View more](#)

Catalyst Classes

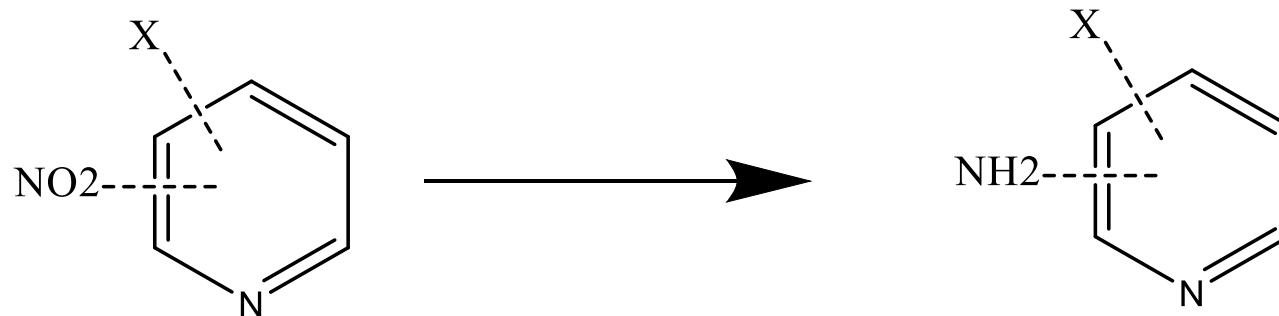
- Catalyst Classes
 - active center
 - > B 10,112
 - > Al 8,926
 - > Pd 7,587
 - Cu 956
 - copper(I) iodide 803
 - copper 288
 - copper(II) oxide 160
 - copper(I) chloride 40
 - copper diacetate 35
 - copper oxide-chromium oxide 13
 - copper(II) acetate 11
 - copper(II) iodide 10

[Clear selected](#)

[Limit to >](#) [Exclude >](#)

Case 7：结构中有特殊需求的反应定义

- 检索以下反应
 - 吡啶环上存在一个硝基，一个卤素，且这两个官能团处于**邻位**
 - 反应过后硝基还原成氨基
 - 定义难点：如果确保NO₂和卤素处于邻位



视频操作过程：

<https://www.bilibili.com/video/BV1si4y177as>

Reaxys中的结构定义

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

+ More options

Clear Cancel Transfer to query >

最后的结果

Reaxys[®]

Quick search Query builder **Results** Synthesis planner

624 Reactions out of 434 Documents containing 791 Substances, 37 Targets

0 selected Limit To Exclude Export Syn-Plan Show Conditions

1 
Conditions Find Similar Reaction ID: 149845

2 
Conditions Find Similar Reaction ID: 22895930

3 
Conditions Find Similar Reaction ID: 149845

1 
Conditions Find Similar Reaction ID: 149845

With hydrogen in methanol at 20°C; for 2h;
Experimental Procedure

96% LIFESCI PHARMACEUTICALS, INC.; McDONALD, Andrew; QIAN, Shawn
WO20171936, 2017, A2
Location in patent: Paragraph 00159
Full Text > Details > Abstract

With hydrogen, nickel in ethanol at 20°C; under 760.051 Torr; for 4h;
Experimental Procedure

95% UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC
WO200747793, 2007, A2
Location in patent: Page/Page column 87
Full Text > Details > Abstract

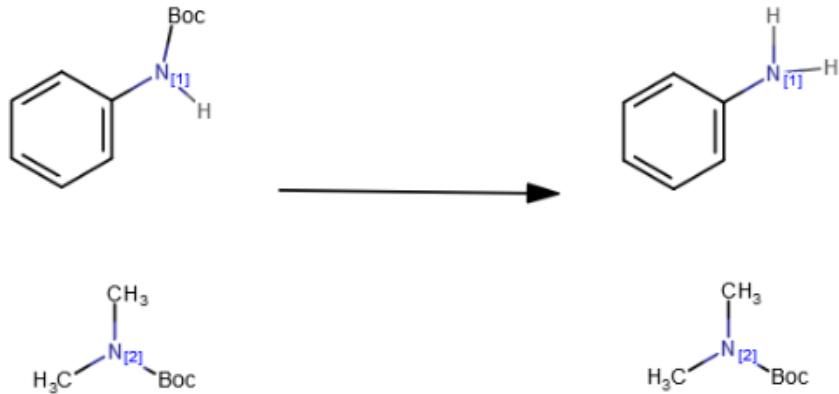
With iron, acetic acid Erwärmen des Reaktionsgemisches mit $HgCl_2$ und Zink;
Experimental Procedure

Talk; Plazek
[Roczniki Chemii, 1956, vol. 30, p. 1139-1145.]Chem. Abstr., <1957> (1269)
Full Text > Details > Abstract

Reaxys将相同scheme的反应全部整合成1条反应，在同样的反应下列举不同的反应条件。

Case 8：选择性氧化还原脱保护反应的定义

- 结构中两个带Boc的片段，两个片段以任意的形式相接在一个分子中
- 反应过后把其中一个片段的Boc脱掉，但是另外一个Boc不变



视频操作过程：

<https://www.bilibili.com/video/BV1Vv411r7Bc>

Reaxys中的结构定义

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in ?

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

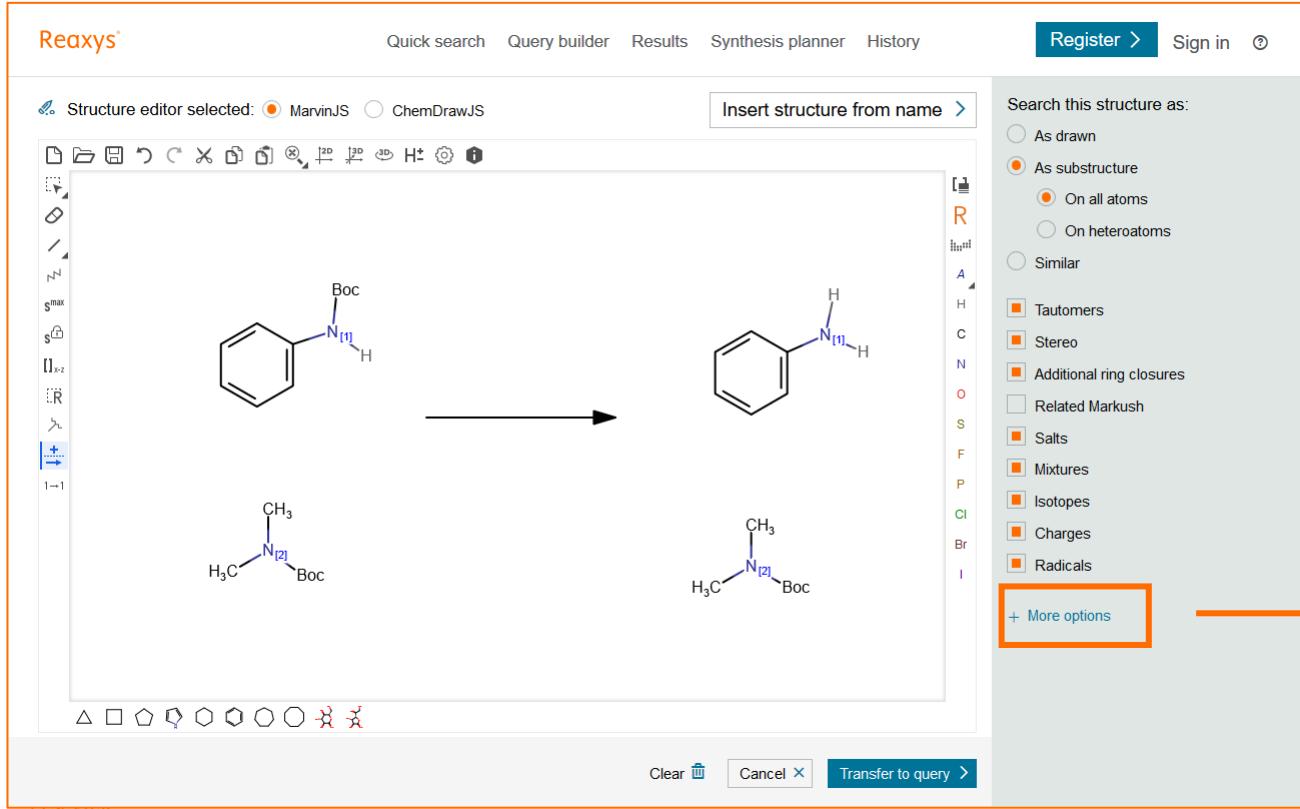
- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Ignore Atom Mappings

Keep fragments

Separate Together



Chemical structures in the editor:

- Benzyl Boc group: Cc1ccccc1N(Boc)2
- Methyl Boc group: CCN(Boc)2
- Joined structure: Cc1ccccc1N(Boc)2CCN(Boc)2

Toolbars and buttons:

- Structure editor toolbar: File, Open, Save, Print, Zoom, etc.
- Bottom buttons: Clear, Cancel, Transfer to query >

Reaxys可以直接设定这些片段在一个结构中

Reaxys中结果

Reaxys

Quick search Query builder **Results** Synthesis planner History

12

Filters

Limit to > Exclude >

12 Reactions out of 8 Documents containing 22 Substances, 5 Targets

0 Limit To Exclude Export Syn-Plan Show Conditions

1

2

3

1 Conditions Find Similar Reaction ID: 51038227

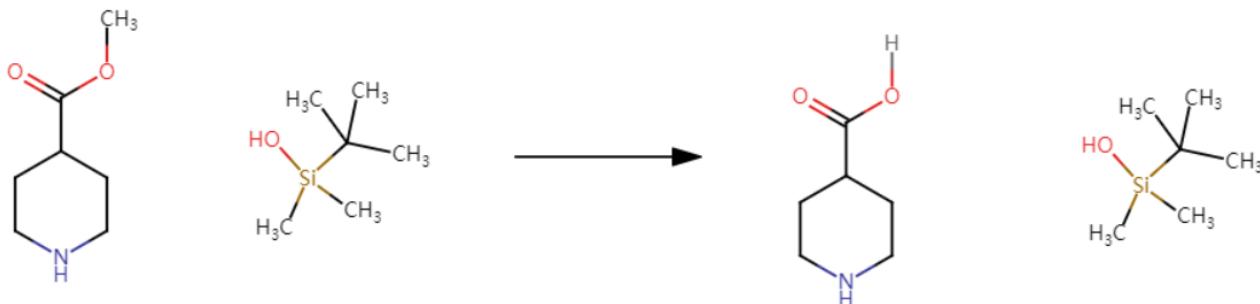
1 Conditions Find Similar Reaction ID: 51038186

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

Case 9：检索结果不理性时的拓展策略

- 在硅基存在的情况下，水解脂基
- 检索结果不太好，如何扩展结果



视频操作: <https://www.bilibili.com/video/BV14A41147gL>

利用Reaxys的碎片反应检索策略

Reaxys

Quick search Query builder Results Synthesis planner History Alerts

Sam Yu

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear Cancel Transfer to query >

Feedback

最后的结果

Reaxys®

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

Sam Yu

Filters

2 Reactions out of **2 Documents**, containing **4 Substances**, **0 Targets**

0 selected

Sort by Reaxys Ranking

1

2

Find Similar Reactions...

Click on one of the hyperlinks below for getting similar reactions according to the selected scope:
the reactions were determined by regarding similar transition states based on your reaction query

Query Reaction	Tight	Near	Medium	Wide	Widest
	1	616	2,529	178,600	182,332

ELSEVIER Copyright © 2020 Elsevier Life Sciences
Terms and Conditions Privacy policy
Cookies are used by this site. To decline

发现检索到的结果中并没有Si

Reaxys[®]

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

Sam Yu  

616

2

Preview

Filters

Limit to > Exclude >

616 Reactions out of 383 Documents, containing 1,112 Substances, 99 Targets

0 selected     

   Sort by Reaxys Ranking 

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



 Find Similar > Reaction ID: 34846790 

2



 Find Similar > Reaction ID: 36184173 

3



这些反应的反应中心与之前的反应相同，但是需要考虑原有反应条件，如含Si。

Feedback 

限定Si

616

2

Preview

Filters

Limit to > Exclude >

By Structure

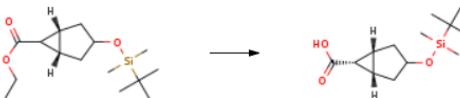
 X

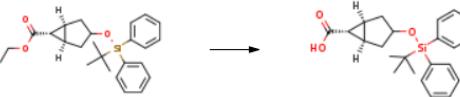
On all atoms



15 Reactions out of 14 Documents, containing 26 Substances, 0 Targets

0 selected Limit To Exclude Export Syn-Plan Show Conditions

1 

2 

3 

Conditions Find Similar Reaction ID: 46668291 [View](#)

Conditions Find Similar Reaction ID: 49144740 [View](#)

Case 10：Reaxys中合成计划的制作

- 针对具体的化合物进行合成计划制作
 - 需要自行注册账号才可以使用这个功能
 - 可以直接从物质界面，或者反应界面直接进入，也可以通过Retrosynthesis功能进入

The screenshot shows the Reaxys interface with the following components:

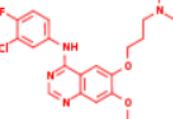
- Left Panel (Compound Information):** Displays the chemical structure of Gefitinib (C₂₂H₂₄N₄ClFO₃, 446.909, 8949523, 184475-35-2). It includes tabs for Identification, Bioactivity (All), Spectra - 89, Druglikeness, Physical Data - 123, and Other Data - 4,498. A red box highlights the "Retrosynthesis" button in the bottom right corner.
- Right Panel (Synthesis Plan):** Shows a retrosynthetic reaction scheme. Gefitinib is shown reacting with 4-fluorobiphenyl-4-amine to produce a product. A red box highlights the "Retrosynthesis" button in the bottom right corner of this panel as well.
- Bottom Navigation Bar:** Includes links for Quick search, Query builder, Results, Retrosynthesis (highlighted with a red box), History, and Alerts.

视频操作过程：

<https://www.bilibili.com/video/BV1oL411u7yP>

从具体物质出发的合成计划制作

1



96    ...

Synthesize

> Find preparations

> Create retrosynthesis plans

Parameters

Predicted  

20 full routes (up to)
3 identical reaction steps per project (up to)
3 identical building blocks per project (up to)
10 min processing time
STD SIAL LN EM U2 U5 T1 RSM3 RSM4 RSM5 building blocks

Published  

5 full routes (up to)
5 branches per step (up to)
5 steps per route (up to)
Don't Stop at commercial building blocks
50% yield per step (assumed, if not published)

目前没有开通AI模块

编辑条件

Always show screen before creating plan 

条件的编辑及结果

Length & depth of synthesis plans i

Full routes: 5 给几条, 给全部还是只给最后一步?

Last step only

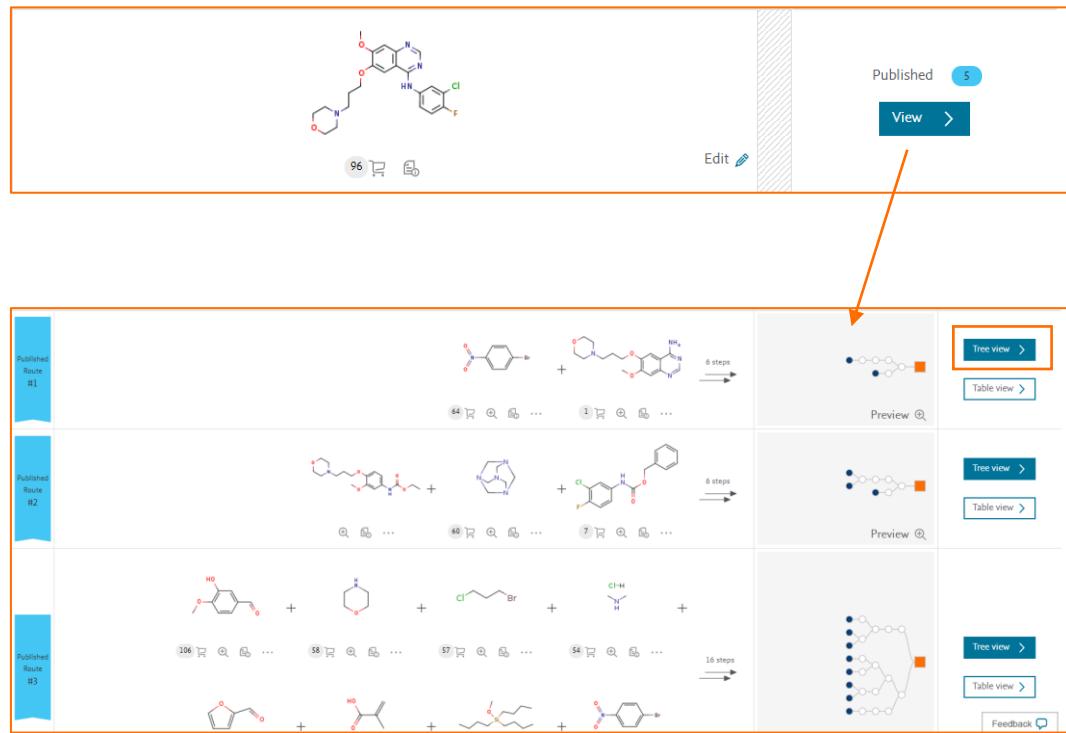
Branches per step: 5 设定最大分支, 最大步数

Max. number of steps: 5 底物是否可购买

Stop searching if building block is commercially available Yes No

Assumed yield for reactions without a given yield 每一步收率

0% 100%



结果的呈现

Export  Legend 

Hide conditions  Tree view  Table view 

Rotate  Fit view  Copy route 

Published route #1

Step 1	Step 2	Step 3	Step 4	Yield	Reference
With sodium hydroxide In water at 30 - 70°C; for 1.5h; pH=11 - 13; Experimental Procedure 	90.7%	Current Patent Assignee: JEIL PHARMA HOLDINGS INC - KR2015/1936, 2015, A Location in patent: Paragraph 0096; 0097; 0106; 0107 Full Text  Details  Abstract 			

Chemical reaction steps:

- Step 1: O=Cc1ccc(Br)cc1 (90.7% yield)
- Step 2: O=Cc1ccc(F)cc1 (95.3% yield)
- Step 3: O=Cc1ccc(F)cc1 (99.9% yield)
- Step 4: O=Cc1ccc(F)cc1 (75% yield)
- Step 5: O=Cc1ccc(F)cc1 (96.7% yield)
- Step 6: O=Cc1ccc(F)cc1 (92.14% yield)

Reaction conditions: With sodium hydroxide In water at 30 - 70°C; for 1.5h; pH=11 - 13; Experimental Procedure 

Yield: 90.7%

Reference: Current Patent Assignee: JEIL PHARMA HOLDINGS INC - KR2015/1936, 2015, A Location in patent: Paragraph 0096; 0097; 0106; 0107 Full Text  Details  Abstract 

Show Conditions/Reaxys Examples 

Add reaction step (one step only) 

Delete prior step(s) 

Copy reaction 

Feedback 

ELSEVIER

Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Case 11：化合物的文献定位

Chem

CelPress

Article

Porous Ligand Creates New Reaction Route: Bifunctional Single-Atom Palladium Catalyst for Selective Distannylation of Terminal Alkynes

Wen-Yong Huang, Guo-Qing Wang, Wen-Hao Li, ..., Hai-Tao Tang, Ying-Ming Pan, Yun-Jie Ding
https://pubs.acs.org/doi/10.1021/acs.joc.0c00426
Panjin University (Y.-M.P.)
yjup@163.com (Y.-J.D.)

HIGHLIGHTS
Design single-atom-site catalyst based on organic synthesis mechanism
Utilizing pores, ligands, and SAS for synergistic controlling reaction pathways
• 21 examples
• Up to 89% yield
• Cheap Sn source
• Recyclable catalyst
• 1.7 wt% Pd loading SASC
• High reactivity: TON up to 779
• High Selectivity: 2 only, *r/r* up to 100:1

A highly selective distannylation of terminal alkynes was achieved

We proposed a unique research concept of "mechanism-oriented catalyst design": The structural elements of single-atom catalyst are designed according to the requirements of organic synthesis mechanism. This concept is totally different from the previous "electrocatalysis" single-atom-site research concept. This work suggests that single-atom-site catalysts not only afford an efficient platform for transforming homogeneous reactions into heterogeneous reactions, but also possess many interesting potentials in developing new synthetic reactions and solving homogeneous reaction problems.

3 DESIGN
MECHANISM
ORIENTED
Catalyst

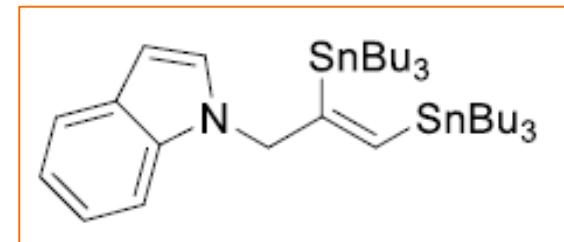
Huang et al., Chem 4, 2000–2015
September 10, 2020 © 2020 Duiker Inc.
https://doi.org/10.1021/acs.joc.0c00426

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这是一篇常见的化学文献，包含：

1. 15页PDF全文
2. 52页Support Information文档

已知文献中报道了这个化合物，如何在上述的67页文档中找到有关这个化合物的描述？



视频操作过程：

<https://www.bilibili.com/video/BV1gA411x7KE>

Reaxys中的检索

- Query Builder联合化合物结构与文献DOI号

Reaxys

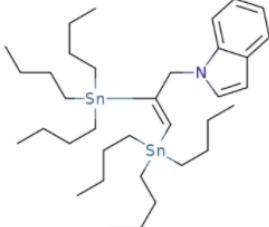
Quick search **Query builder** Results Synthesis planner History Alerts

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Structure



As drawn

AND

DOI is 10.1016/j.chempr.2020.06.020

Reaxys中的结果

1 Substances out of 1 Documents, containing 1 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References Grid Heatmap

1 (Z)-1-(2,3-bis(tributylstannyl)allyl)-1H-indole
C₃₅H₆₃NSn₂ 735.312 36450188

Hit Data - 6 Identification Druglikeness Spectra - 3 Preparations - 1 >
Physical Data - 2 Reactions - 1 >
Documents - 1 >

1 Hit Data - 6 Substance Label - 1 hits out of 1

Substance Label - 1 hits out of 1

Chromatographic Data - 1 hits out of 1

Crystal Property Description - 1 hits out of 1

NMR Spectroscopy - 2 hits out of 2

Mass Spectrometry - 1 hits out of 1

3j Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, - 2313]

Full Text > Details > Abstract >

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全文检索3J定位化合物

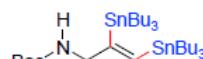
N-containing terminal alkynes



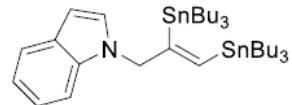
3j 89% (100:1)



3k 58% (25:1)



3n 81% (100:1)



(Z)-1-(2,3-bis(tributylstannyl)allyl)-1*H*-indole 3j: colorless oil. Petroleum ether as eluent for column chromatography (3j, $R_f = 0.75$; 2j, $R_f = 0.4$, 42% of alkyne was isolated and recovered); ^1H NMR (400 MHz, CDCl_3) $\delta = 7.52$ (1H, d, $J = 7.8$ Hz), 7.15 (1H, d, $J = 8.2$ Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, $J = 3.1$ Hz), 6.46 (1H, s, $J = 168.4$ Hz, 65.5 Hz), 6.40 (1H, d, $J = 3.1$ Hz), 4.78 (2H, d, $J = 1.3$ Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ^{13}C NMR (400 MHz, CDCl_3) $\delta = 160.6$, 144.4, 160.1, 29.2, 29.1, 27.4, 27.3, 13. $\text{C}_{35}\text{H}_{63}\text{KNSn}_2[\text{M}+\text{K}]^+$ 774.2630,

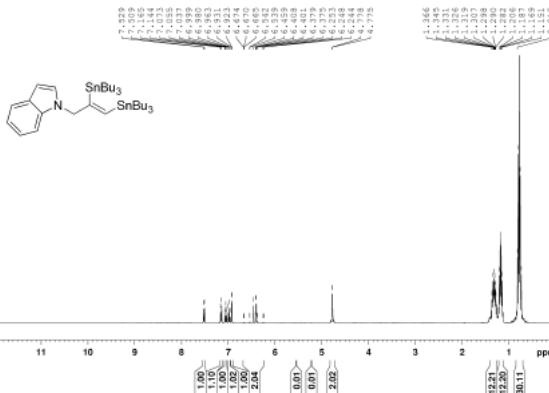


Figure S45. ^{13}C NMR of 3j.

Case 12: 机理性文献的检索

- Query Builder中结构与Subject Study联合检索
- 视频操作: <https://www.bilibili.com/video/BV1pK4y1E7Qx>

The screenshot shows the Reaxys Query Builder interface. The search query is:

Structure: R1C=CH2 + Sn-H -> Sn-C=C-R1

Subject Studied: mechanism

The search results pane on the right is highlighted with an orange box and shows a reaction mechanism diagram. The diagram illustrates the addition of a vinyl tin hydride intermediate to a Sn-H bond, resulting in a product where the Sn atom is bonded to two hydrogens and the vinyl group.

最后的结果

Reaxys

Quick search Query builder Results Synthesis planner History Alerts Sam Yu ?

1 Filters Limit to > Exclude >

1 Reactions out of 1 Documents, containing 3 Substances, 0 Targets

0 Limit To Exclude Export Syn-Plan Hide Conditions

Reaxys Ranking ▾

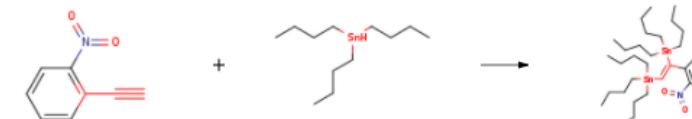
1 By Structure Yield Reagent/Catalyst Solvent Catalyst Classes Solvent Classes Product Availability Reactant Availability Reaction Classes Document Type Publication Year

1 Hits/Conditions Find Similar Reaction ID: 54835337

With porous vinyl functionalized tri(2-methoxyphenyl)phosphine derived polymer supported palladium **In** tetrahydrofuran at 25°C; Mechanism; Schlenk technique; Sealed tube; stereoselective reaction; Experimental Procedure

Conditions	Yield	Reference
With porous vinyl functionalized tri(2-methoxyphenyl)phosphine derived polymer supported palladium In tetrahydrofuran at 25°C; Mechanism; Schlenk technique; Sealed tube; stereoselective reaction; Experimental Procedure	82%	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie [Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text > Details > Abstract >

1 hit out of 1



Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的关键词检索
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A



Reaxys小结

- Reaxys拥有便捷的使用方式，IP范围内授权，不限制同时登录人数，可以自由注册ID。
- Reaxys从大量文献中摘取和物质性质相关的所有数据，帮助科研人员获得标准化，规范化，格式化的物性数据列表及参考文献
- Reaxys中的结构面板，能实现科研人员绝大部分的结构绘制要求，帮助科研人员用最直接的方式获得相应的物质和反应
- Elsevier Life Science线上服务：
 - 添加微信小助手ELS-LSS邀请进用户群：获取最新的咨询以及Q&A
 - 关注B站Up主（非官方）：ELS生命科学，获取所有Elsevier Life Science数据库的使用视频
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Thank you

