



ELSEVIER

Elsevier Reaxys使用介绍

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Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物性数据的查询与反向检索
 - Reaxys中的结构面板与复杂反应定义
 - Reaxys中的实用小案例
- Q&A

什么是Reaxys

Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘的**化学及相关学科**的科研信息平台

6,000万文献

(Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis, etc)

150万专利

WPO, USPO, EPO [≈ mid 70's >]

PO: JP, KR, CN, TW [2015 >]

2020年将扩展到100家专利机构

38万书的章节

Beilstein, Gmelin,

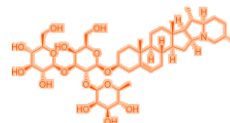
16,000 期刊
(journals, books and patents)



[自动抽提]



≈ 450 journals + PO
[人工抽提]

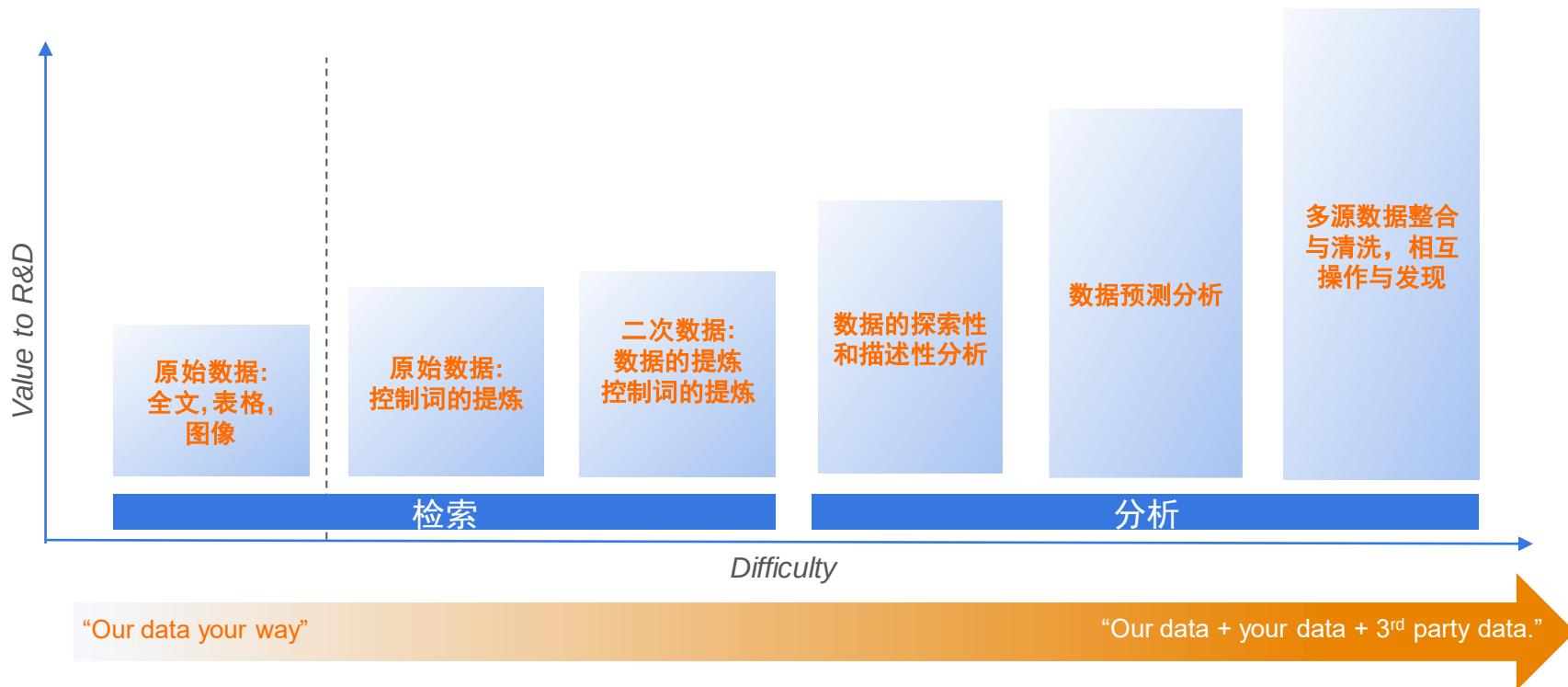


Reaxys的战略是为化学研究的全生命周期，提供完整的化学生态系统



不断利用AI/ML技术， 引领数据库到解决方案的行业升级

Reaxys等Elsevier Life Science
全线产品都在朝解决方案方向发展



越来越多的AI/ML技术融入到数据库中

靶点预测

Target prediction					
Target	Common name	Uniprot ID	Target Class	Probability*	Known actives (30/29)
Adenosine receptor A2a	ADORA2A	P09274	Membrane receptor		564 / 465
Adenosine receptor A2b	ADORA2B	P09275	Membrane receptor		179 / 230
Adenosine receptor A1	ADORA1	P05042	Membrane receptor		488 / 581
Adenosine receptor A3	A3A	P33795	Membrane receptor		690 / 636
Neurexophilin Y receptor type 5	NPY5R	Q18761	Membrane receptor		209 / 149
Carbamazepine receptor 1	CNR1	P21554	Membrane receptor		1418 / 305
5-Hydroxytryptamine receptor 2A	HTR2A	P08223	Membrane receptor		108 / 42
5-Hydroxytryptamine receptor 2C	HTR2C	P08335	Membrane receptor		54 / 34
Carbamazepine receptor 2	CNR2	P34972	Membrane receptor		1603 / 133
Corticocapsin-releasing factor receptor 1	CRFR1	P34988	Membrane receptor		218 / 125
Sodium-dependent serotonin transporter	SERT	P18445	Transporter		12 / 33
Phosphatidylinositol 3-OH kinase catalytic subunit delta isoform	PIK3CD	Q03039	Enzyme		100 / 136
Cathepsin L1	CTSL	P07711	Cysteine Protease		159 / 65
Epidermal growth factor receptor	EGFR	P05533	Tyr Kinase		674 / 53
Cyclin-dependent kinase 2	CDK2	P04941	Ser_Thr Kinase		160 / 118

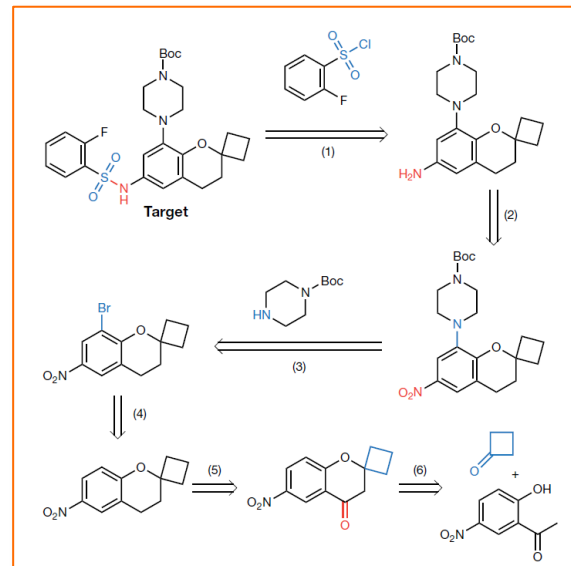
利用动物临床前数据预测药物临床安全性



MMP分析



合成预测

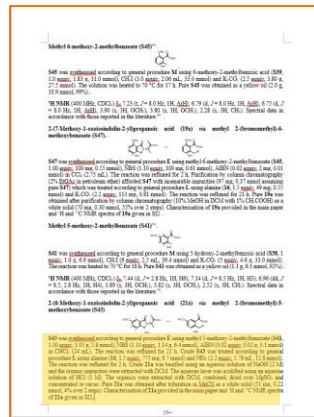
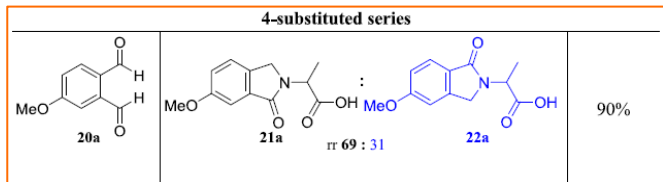
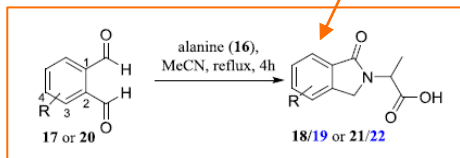
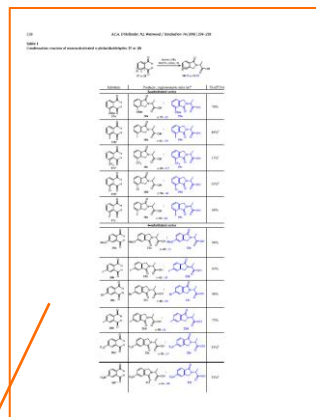


Elsevier Life Science Solution中已经开始融入不同领域的AI技术

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
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 - Reaxys中物性数据的查询与反向检索
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- Q&A

一篇常见的化学相关文献的构成



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。

21a; Mp: 194–196 °C; IR ν_{max} cm⁻¹ (thin film) 3370 (O–H stretch), 1730 (C=O stretch), 1636 (C=O stretch), 1493 (C=C stretch), 1456 (C–H bend), 1447 (C–H bend), 1196 (C–O stretch), 1022, 770; ¹H NMR (500 MHz, CD₃OD) δ 7.48 (d, *J* = 8.5 Hz, 1H, H4), 7.29 (d, *J* = 2.5 Hz, 1H, H7), 7.19 (dd, *J* = 8.5, 2.5 Hz, 1H, H5), 5.00 (q, *J* = 7.5 Hz, 1H, CH), 4.54 (d, *J* = 17.0 Hz, 1H, H3), 4.48 (d, *J* = 17.0 Hz, 1H, H3), 3.86 (s, 3H, OCH₃), 1.61 (d, *J* = 7.5 Hz, 3H, CH₃); ¹³C NMR (125 MHz, CD₃OD) δ 174.8 (COOH), 171.0 (C1), 161.6 (C6), 135.8 (C3a), 134.3 (C7a), 125.2 (C4), 121.0 (C5), 107.4 (C7), 56.1 (OCH₃), 51.2 (CH), 48.4 (C3), 15.9 (CH₃); HRMS (ES⁺) *m/z* calculated for C₁₂H₁₄NO₄ [M+H]⁺: 236.0917; found: 236.0921. See S11 part IX for experimental procedure and S12 for ¹H and ¹³C NMR spectra.

22a; Mp: 191–193 °C; IR ν_{max} cm⁻¹ (thin film) 3229 (O–H stretch), 1717 (C=O stretch), 1628 (C=O stretch), 1611 (C=C stretch), 1558 (C=C stretch), 1506 (C=C stretch), 1447 (C–H bend), 1435 (C–H bend), 1298 (C–N stretch), 1206 (C–O stretch), 1086, 1026, 845, 775; ¹H NMR (500 MHz, CD₃OD) δ 7.68 (d, *J* = 8.5 Hz, 1H, H7), 7.13 (d, *J* = 2.0 Hz, 1H, H4), 7.04 (dd, *J* = 8.5, 2.2 Hz, 1H, H6), 4.98 (q, *J* = 7.5 Hz, 1H, CH), 4.57 (d, *J* = 17.0 Hz, 1H, H3), 4.50 (d, *J* = 17.0 Hz, 1H, H3), 3.88 (s, 3H, OCH₃), 1.60 (d, *J* = 7.5 Hz, 3H, CH₃); ¹³C NMR (125 MHz, CD₃OD) δ 174.8 (COOH), 171.0 (C1), 164.9 (C5), 146.2 (C3a), 125.6 (C7), 125.4 (C7a), 116.3 (C6), 108.8 (C4), 56.2 (OCH₃), 50.9 (CH), 48.4 (C3), 15.9 (CH₃); HRMS (ES⁺) *m/z* calculated for C₁₂H₁₄NO₄ [M+H]⁺: 236.0917; found: 236.0921. See S11 part IX for experimental procedure and S12 for ¹H and ¹³C NMR spectra.

2-(6-Methoxy-1-oxoisindolin-2-yl)propanoic acid (21a) via methyl 2-(bromomethyl)-5-methoxybenzoate (S43)

S43 was synthesised according to general procedure E using methyl 5-methoxy-2-methylbenzoate (S41, 1.00 equiv, 1.05 g, 5.8 mmol), NBS (1.10 equiv, 1.14 g, 6.4 mmol), AIBN (0.02 equiv, 0.02 g, 0.1 mmol) in CHCl₃ (24 mL). The reaction was refluxed for 21 h. Crude **S43** was treated according to general procedure L using alanine (**16**, 1.5 equiv, 775 mg, 8.7 mmol) and NEt₃ (2.2 equiv, 1.78 mL, 12.8 mmol). The reaction was refluxed for 2 h. Crude **21a** was basified using an aqueous solution of NaOH (2 M) and the organic impurities were extracted with DCM. The aqueous layer was acidified using an aqueous solution of HCl (1 M). The organics were extracted with DCM, combined, dried over MgSO₄ and concentrated *in vacuo*. Pure **21a** was obtained after trituration in MeCN as a white solid (51 mg, 0.22 mmol, 4% over 2 steps). Characterisation of **21a** provided in the main paper and ¹H and ¹³C NMR spectra of **21a** given in S12.



Reaxys对这篇全文的提炼

- ☐ Assessment of the regioselectivity in the condensation reaction of unsymmetrical o-phthalaldehydes with alanine

1

D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239]

[Abstract](#) [Index Terms](#) [Substances](#) 103 [Reactions](#) 236 [Full Text](#) [↗](#)

Abstract

One approach for the synthesis of isoindolinones, a privileged bioactive heterocyclic core structure, involves a condensation reaction of o-phthalaldehydes with a suitable nitrogen-containing nucleophile. This fascinating reaction is revisited here in the context of the use of o-phthalaldehydes that contain additional substituents in the aromatic ring, leading to a detailed analysis of the regioselectivity of the reaction. Eleven monosubstituted o-phthalaldehydes were synthesised and reacted with alanine. The regioselectivity observed across the eleven substrates led to the identification of a disubstituted substrate that reacted with very high control. A gram-scale reaction followed by esterification gave the major regioisomer in high yield. In addition, the regioselectivity observed on reaction of two novel monosubstituted substrates led to an increased mechanistic understanding.

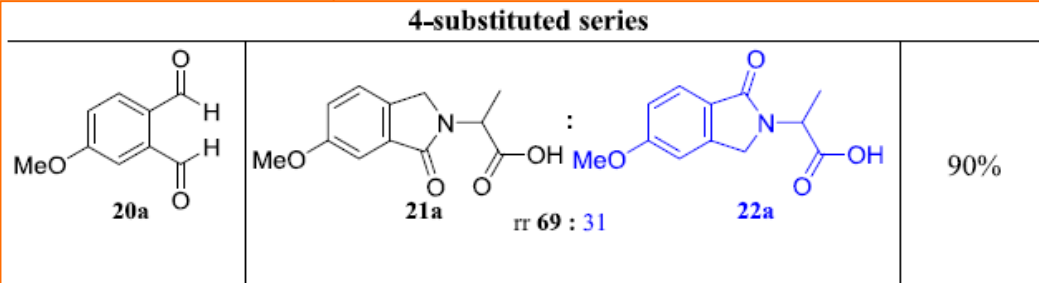
Index terms

Author keyword: Condensation reaction, Mechanistic understanding, o-phthalaldehyde, Regioselectivity

EMTREE drug term: alanine, phthalaldehyde

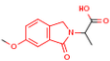
EMTREE medical term: Article, esterification, polymerization, priority journal, regioselectivity, synthesis

Reaxys Index Terms: Swern oxidation, condensation reaction, esterification, pure, reactivity, regioselectivity, separation method, tautomerization



Reaxys对于文献中的结构与反应都做了提炼

Reaxys对文献中的化合物的结构化数据提炼



2-(6-methoxy-1-oxoisindolin-2-yl)propanoic acid
C₁₂H₁₃NO₄ 235.24 32021463

Hit Data - 7 Physical Data - 2 Preparations - 7 >
Identification Spectra - 4 Reactions - 7 >
Druglikeness Documents - 1 >

Hit Data - 7

- Substance Label - 1 hits out of 1
- Melting Point - 1 hits out of 1
- Crystal Property Description - 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

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。

Label	Reference
21a	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Melting Point, °C	Reference
194 - 196	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Colour & Other Properties	Location	Reference
white	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	¹ H	d(4)-methanol	500	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract
Chemical shifts, Spectrum	¹³ C	d(4)-methanol	125.8	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Reaxys对原文反应的提炼 (21a)

Reaction ID: 47133770

2

1 Conditions Find Similar

Yield Conditions Reference

In acetonitrile for 4h; Reflux; Inert atmosphere; Overall yield = 90 percent; Overall yield = 38 mg; regioselective reaction;

Experimental Procedure

General procedure: Alanine (16, 1.2 equiv.) was added to a solution of unsymmetrical o-phthalaldehyde (1.0 equiv.) in anhydrous MeCN (3.8 mL per mmol of o-phthalaldehyde). The reaction mixture was heated at reflux for 4 h under a nitrogen atmosphere. The solution was then cooled to rt before being concentrated in vacuo to afford the crude mixture of regioisomers.

4.3.9. 2-(6-Methoxy-1-oxoisindolin-2-yl)propanoic acid (**21a**) with 2-(5-methoxy-1-oxoisindolin-2-yl)propanoic acid (**22a**)

A mixture of **21a** and **22a** was synthesised according to general procedure **B** using 4-methoxyphthalaldehyde (**20a**, 1.0 equiv., 30 mg, 0.18 mmol) and alanine (**16**, 1.2 equiv., 19 mg, 0.22 mmol). A

Reaxys从文献中提炼出来的内容

文献 Database

>63 million records

源自16000本刊以及
7大专利机构的专利
(2020年将扩大到
100家)

化合物 Database

>150 million

源自文献专利中的
报道, 供应商品库
(2020将继续扩大
供应商名录)

化学反应Database

>53 million

单步多步反应, 同
时提炼文献与专利
中的实验过程

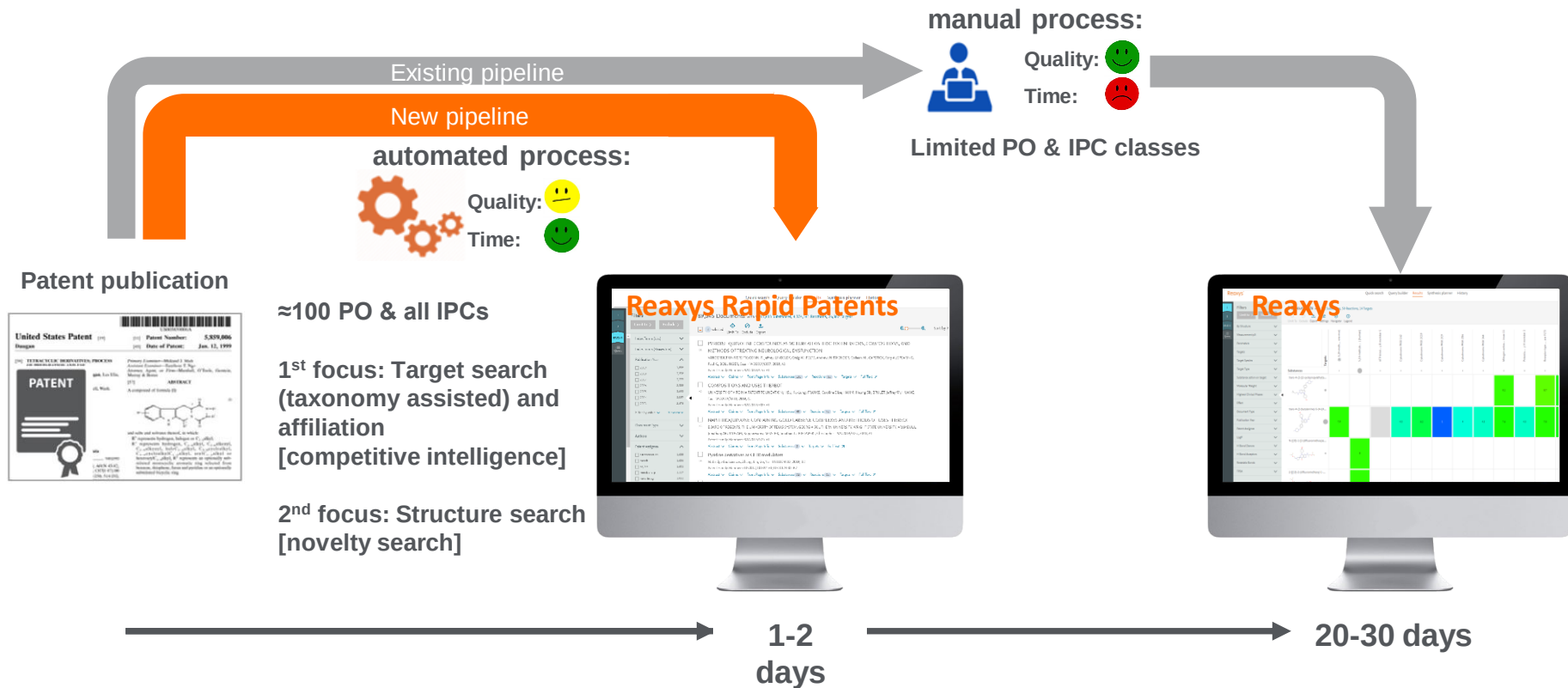
性质 Database

> 500 million

化合物实验数据,
并提炼实验数据检
测条件

Reaxys 2020年专利计划

2020年专利奖扩大到100家专利机构的专利

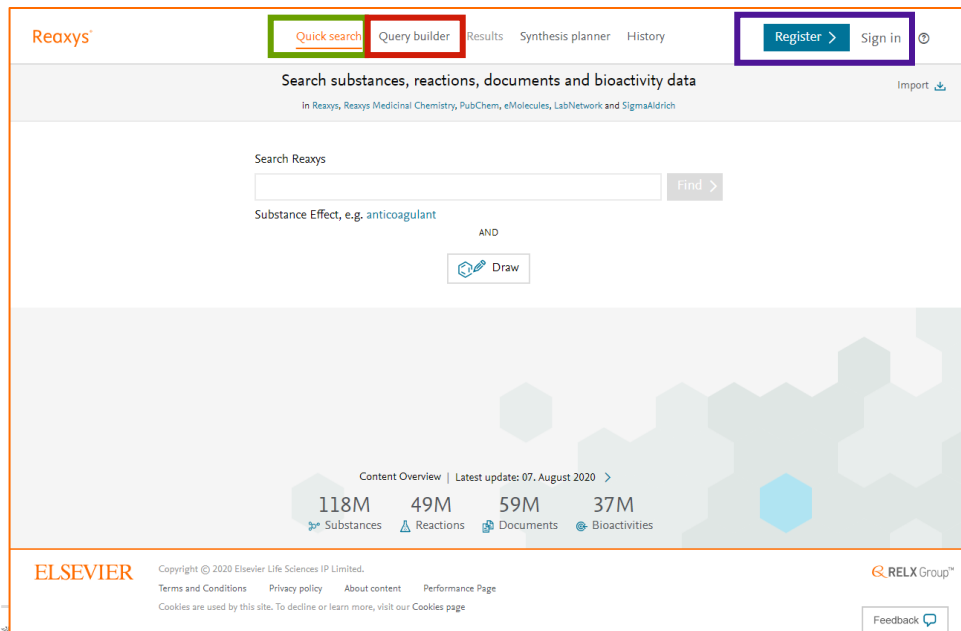


Agenda

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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:

1. 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）
2. 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。
3. 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:

1. Reaxys主界面: <https://b23.tv/av92441795>
2. Quick Search: <https://b23.tv/av92445805>
3. Query Builder: <https://b23.tv/av92565153>

Case 1: 快速获取化合物的理化性质

Reaxys[®]

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

Register > Sign in ⓘ

Search for solubility of gefitinib [Import](#)

Search Reaxys

solubility of gefitinib [×](#) [Find >](#)

Substance Properties, e.g. [ferroelectric materials](#)

AND

[Draw](#)

Tips:
快速获取某个化合物
溶解性数据。

Content Overview | Latest update: 30. March 2020 >

118M

49M

59M

37M

Substances

Reactions

Documents

Bioactivities

ELSEVIER

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RELX Group™

Reaxys中的结果

Quick search Query builder Results Synthesis planner History

Results for **solubility of gefitinib** New Edit

Icon	Count	Type	Filters	Preview Results	View Results
Substances	1	Structure AND Property	solubility	Preview Results	View Results
Documents	178	Titles, Abstracts, Keywords	"solubility", "gefitinib"	Preview Results	View Results
Documents	341,792	Titles, Abstracts, Keywords	"solubility"	Preview Results	View Results
Documents	23,178	Titles, Abstracts, Keywords	"gefitinib"	Preview Results	View Results

1 Substances out of 7,831 Documents, containing 130 Reactions, 1,103 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
 Identification
 Druglikeness

Bioactivity (All)
 Physical Data - 98
 Spectra - 75

Other Data - 3,436
 Preparations - 83
 Reactions - 130
 Targets - 1,103
 Documents - 7,831

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; Chern, 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, Zhao; Wang, Feng; Zhao, Wei; 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 7,831 Documents, containing 130 Reactions, 1,103 Targets

0 selected Limit To Exclude Export Preparations

Reaxys - 1

Sort by No of References ↓

Grid Heatmap

gefitinib
C22H24N4ClFO3 446.909 8949523 184475-35-2

Hit Data - 4
Identification
Druglikeness

Bioactivity (All)
Physical Data - 96
Spectra - 75

Other Data - 8,436
Preparations - 83
Reactions - 130
Targets - 1,103
Documents - 7,831

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 - 104

- ✓ Melting Point - 25
- ✓ Association (MCS) - 12
- ✓ Chromatographic Data - 5
- ✓ **Conformation - 1**
- ✓ Crystal Phase - 7
- ✓ Crystal Property Description - 24
- ✓ Crystal System - 1
- ✓ Dissociation Exponent - 3
- ✓ Further Information - 1
- ✓ Interatomic Distances and Angles - 2

Spectra - 77

- ✓ NMR Spectroscopy - 46
- ✓ IR Spectroscopy - 9
- ✓ Mass Spectrometry - 14
- ✓ UVVIS Spectroscopy - 6
- ✓ Raman Spectroscopy - 1

Case 2: 理化性质的高级应用

- 获取KCl在乙醇中的溶解度

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

Drag & Drop to build a new query

Search fields

Fields Forms History

Reaxys ^

Topics and Keywords v

Identification v

Physical Properties v

Spectra v

MedChem v

Other v

Reactions v

Bibliography v

PubChem v

eMolecules v

LabNetwork v

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

◇ Molecular Formula is Molecular Formula

AND ◇ Solubility

Find any Hide fields ^

= Solubility, g·l⁻¹

is Saturation

= Temperature (Solubility (MCS)), °C

is Solvent (Solubility (MCS))

is Ratio of Solvents

Search fields
solubility

Reaxys ^

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

Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula is ▾ KCl

AND

◇ Solubility

☐ Find any Hide fields ^

= ▾ Solubility, g l-1

is ▾ Saturation

= ▾ Temperature (Solubility (MCS)), °C

is ▾ ethanol

is ▾ Ratio of Solvents

Step3: 进行物质检索

Step1: 输入分子式KCl

Step2: 在溶剂一块选择乙醇

Solvent (Solubility (MCS)) 1

eth

☐	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 >

最后的结果

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

0 selected Limit To Exclude Export Preparations

potassium chloride
CIK 74.5513 3534978

Hit Data - 20 Bioactivity (All) Other Data - 791 Preparations - 415
Identification 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	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	25	ethanol	Solubility: 0.025 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	30	ethanol	Solubility: 0.037 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	35	ethanol	Solubility: 0.043 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 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. [Doklady Physical Chemistry, 1991, vol. 317, p. 303 - 306][Dokl. Phys. Chem. (Transl. of Dokl. Akad. Nauk.), 1991, vol. 317, p. 1140 - 1143] Full Text Details
	20	ethanol	Solubility: 1.270E0 mol/1000mol solvent	Kirm; Dunlap [Journal of the American Chemical Society, 1931, vol. 53, p. 393] Full Text Details
	45	ethanol	Solubility: 1.277E0 mol/1000mol solvent	Kirm; Dunlap [Journal of the American Chemical Society, 1931, vol. 53, p. 393] Full Text Details

Reaxys直接给出具体的数据和数据的文献出处，其实也可以设定更多的条件，如温度.....

Case 3: “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. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, and History. On the right, there are buttons for Register > and Sign in ?.

Below the navigation tabs, there is a search bar with the text "Search in:" and four buttons: Reactions >, Targets >, Substances >, and Documents >. Below these buttons are icons for Import, Save, Reset form, and Delete all.

In the center, there are icons for Structure, Molecular Formula (selected), CAS RN, and TI, AB & KW.

The main query builder area shows two conditions:

- Molecular Formula** is **Molecular Formula**
- Catalyst Investigation** is **Investigated characteristic(s)**

The "Catalyst Investigation" condition is expanded, showing a list of fields:

- Investigated characteristic(s)
- Specification of catalysis
- Classification of catalysis
- Type of reaction
- Co-catalyst/co-substrate name

On the right side, there is a "Search fields" panel with a search bar containing "catalyst". Below the search bar, there are two expandable sections: "Catalyst Investigation" and "Reagent/Catalyst".

An orange arrow points from the "Molecular Formula" icon in the center to the "Catalyst Investigation" section in the "Search fields" panel.

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

◇ Molecular Formula contains ▼ Fe

AND

◇ 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

Step3: 进行物质检索

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

Specification of catalysis 1

☐ chemoselective catalysis	2,481
☐ immobilised catalyst	452
☐ phase-transfer catalysis	419
☐ regioselective catalysis	2,516
☒ stereoselective catalysis	9,365

最后的结果

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

311 Filters

Limit to > Exclude >

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

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

Hit Data - 2

Catalyst Investigation - 2 hits out of 25

Show/Hide columns

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 4: 获取在可见光下，水溶液中呈现蓝色的化合物

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

UV/VIS Spectroscopy Find any Hide fields ^

- is Description (UV/VIS Spectroscopy)
- is Solvent (UV/VIS Spectroscopy)
- = Absorption Maxima (UV/VIS), nm
- = Ext./Abs. Coefficient, l-mol-1cm-1

Search fields Q UV

Reaxys ^

UV/VIS Spectroscopy

如果想呈现蓝色，那么需要吸收580-600nm的光

Solvent (UV/VIS Spectroscopy) Search

☐ (2)h8-toluene	66
☐ (cd3)2co=acetone-d6	2
☐ (ph 3.5)	1
☐ (ph 5.5)	1
☐ (ph 6.8)	1
☐ (ph 7)	1
☐ (ph 7.0)	1
☐ (ph 8.9)	4
☐ 1,1,1-trichloro-ethane	73
☐ 1,1,1-trichloroethane	9
☐ 1,1,1-trideuteromethanol	8
☐ 1,1,2,2-tetrachloro-ethane	206
☐ 1,1,2,2-tetrachloroethane	204
☐ 1,1,2,2-tetrachloroethylene	68

1 of 107 Go to page >

Clear selected x Transfer >

选择溶剂的时候，建议将分子式，物质名称都输入下，比如水，需要同时查询Water和H2O。

最后的检索策略与结果

物质检索。

Reaxys

Quick search Query builder Results Synthesis planner History

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

UV/VIS Spectroscopy

Find any Hide fields

is Description (UV/VIS Spectroscopy)

is h2o:water

= 580-600

= Ext./Abs. Coefficient, I

Reaxys

Quick search Query builder Results Synthesis planner History

Register Sign in

0 selected Limit To Exclude Export Preparations

Sort by No of References Grid Heatmap

3

methylen blue
C12H9NS(N(CH3)2)2[1+].[Cl-]=C12H9... 319.858 3599847 152071-32-4

Hit Data - 2
Identification
Druglikeness

Bioactivity (All)
Physical Data - 983
Spectra - 374

Other Data - 633
Preparations - 29
Reactions - 288
Targets - 79
Documents - 25,082

Hit Data - 2
UV/VIS Spectroscopy - 2 hits out of 252

Description (UV/VIS Spectroscopy)	Solvent (UV/VIS Spectroscopy)	Absorption Maxima (UV/VIS), nm	Reference
Spectrum	water	680, 665	Ponade/Kone, Sibagatulle(Russian Chemical Bulletin, 2011, vol. 60, # 4, p. 676-678) Full Text Details Abstract
Absorption maxima	H2O	680, 665	Myosh, Norio; Tomita, Gai(Zeitschrift für Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, 1980, vol. 35, # 4, p. 741-745) Full Text Details Abstract

4

rhodamine B
C13H9O(N(C2H5)2)2(C6H4COOH)[1+].[H+] 479.019 4091619 81-88-9

Hit Data - 1
Identification
Druglikeness

Bioactivity (All)
Physical Data - 593
Spectra - 678

Other Data - 91
Preparations - 13
Reactions - 1,089
Targets - 6
Documents - 25,082

Hit Data - 1
UV/VIS Spectroscopy - 1 hits out of 430

Description (UV/VIS Spectroscopy)	Solvent (UV/VIS Spectroscopy)	Absorption Maxima (UV/VIS), nm	Reference
Spectrum	water	554, 582	Prubash, Kasiogan; Senthil Kumar, Puvaneswaran; Pandian, Selvar; Karthiappan, Swaminathan [Research on Chemical Intermediates, 2019, vol. 45, # 3, p. 1147-1157] Full Text Details Abstract

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物性数据的查询与反向检索
 - Reaxys中的结构面板与复杂反应定义
 - Reaxys中的实用小案例
- Q&A

Reaxys中的结构面板



R基团定义工具

Reaxys

Quick search Query builder Results Synthesis planner History

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS

Insert structure from name >

The interface shows a central workspace with the Marvin JS logo. On the left is a vertical toolbar with various drawing tools. On the right is a vertical panel with a list of functional groups and atoms. At the bottom is a row of chemical structures.

缩写官能团，通用官能团，原子列表/列表非原子属性列表

一些常见的功能使用视频

常用功能	视频链接
最基本功能	https://www.bilibili.com/video/av92474230
不定位键	https://www.bilibili.com/video/av92568326
通用/缩写官能团	https://www.bilibili.com/video/av92474816
原子列表与列表非	https://www.bilibili.com/video/av92571129
R基团定义	https://www.bilibili.com/video/av92569854
原子锁定与环锁定	https://www.bilibili.com/video/av92833557
G Group与通用原子	https://www.bilibili.com/video/BV1Tp4y1y7SS
原子属性列表	https://www.bilibili.com/video/BV1B54y197G6
盐，自由基，同位素	https://www.bilibili.com/video/BV1pg4y1z7AB

一些简单案例视频

常用功能	视频链接
合成计划的制作	https://www.bilibili.com/video/av92577710
机理性文献查询	https://www.bilibili.com/video/av92580572
反应定义基本操作	https://www.bilibili.com/video/av92574819
反应条件的定义	https://www.bilibili.com/video/av92581106

Case 5: 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://b23.tv/BV1KZ4y147PQ>

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

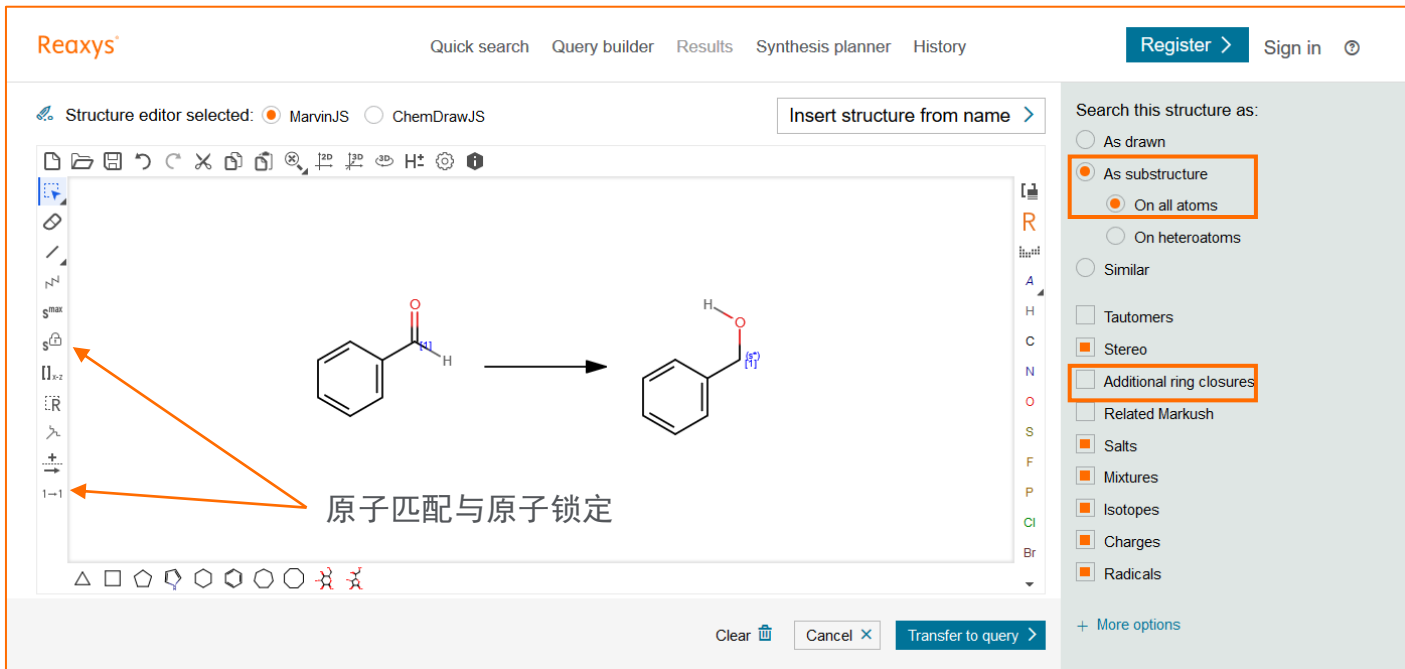
Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS Insert structure from name >

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

原子匹配与原子锁定



Reaxys中的结果

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Register > Sign in ⓘ

10.11 K 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

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

☐ 0 Limit To Exclude Export Syn-Plan Show Conditions

Reaxys Ranking ↓

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

Conditions	Yield	Reference
With formic acid, [(η ⁵ -C ₅ H ₅)Ru(k ¹ -P-PPH ₂ Py)(PPh ₃)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(η ⁵ -cyclopentadienyl)hafnium dihydride In isopropyl alcohol at 80°C; for 8h;	91%	Nakano, Tatsuya; Umano, Shigetoshi; Kino, Yoshio; Ishii, Yasutaka; Ogawa, Masaya [Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757] Full Text > Details > Abstract >
With sodium tetrahydroborate 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 WO2018/217266, 2018, A1 Location in patent: Page/Page column 52, 53 Full Text > Details > Abstract >

1

O=Cc1ccc(C=O)cc1 $\rightarrow$ OCCc1ccc(C=O)cc1

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

[查看物质详情](#)

4-(hydroxymethyl)benzaldehyde

HOCc1ccc(C=O)cc1
136.15
878348
52010-97-6



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

[View Details](#) 

合成计划按钮

更多与物质相关操作

Options ✕

- Find Similar
- View related Markush
- View details

- Copy structure to query
- Copy reaction to query
- Use as filter
- Open in database

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

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

☐ >95 - 100 924

☐ >90 - 95 835

☐ >85 - 90 614

☐ >80 - 85 456

☐ >75 - 80 375

☐ >70 - 75 287

☐ >65 - 70 223

Filter by value > View more

Reagent/Catalyst

☐ sodium tetrahydroborate 7,079

☐ methanol 1,387

☐ potassium carbonate 1,236

☐ water 690

☐ lithium aluminium tetrahydride 639

☐ hydrogen 620

☐ hydrogenchloride 599

Filter by value > View more

Solvent

☐ methanol 4,014

☐ tetrahydrofuran 3,375

☐ ethanol 2,025

☐ water 1,395

☐ dichloromethane 1,268

☐ n,n-dimethyl-formamide 1,105

☐ toluene 515

Filter by value > View more

Document Type

☐ article 7,543

☐ patent 3,181

☐ review 68

☐ conference paper 44

☐ letter 11

☐ short survey 4

☐ note 4

View more

Publication Year

☐ 2020 393

☐ 2019 788

☐ 2018 834

☐ 2017 780

☐ 2016 921

☐ 2015 829

☐ 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

> Solvent Classes	10,112
> 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

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 X

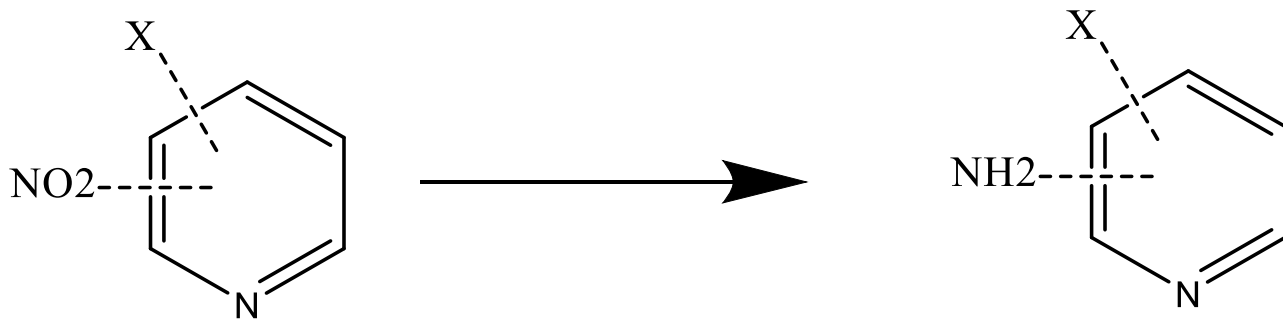
- ▼ Catalyst Classes 10,112
 - ▼ active center 8,926
 - > B 7,587
 - > Al 956
 - > Pd 803
 - ▼ Cu 288
 - ☐ copper(I) iodide 160
 - ☐ copper 40
 - ☐ copper(II) oxide 35
 - ☐ copper(I) chloride 13
 - ☐ copper diacetate 11
 - ☐ copper oxide-chromium oxide 10

Clear selected X

Limit to > Exclude >

Case 6: 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/BV1ua4y147q2>

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 >

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 Filters

Limit to > Exclude >

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

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

0 selected Limit To Exclude Export Syn-Plan Show Conditions

1

2

3

6 Conditions Find Similar > Reaction ID: 149845

7 Conditions Find Similar > Reaction ID: 22895930

1

Conditions

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

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

With iron, acetic acid Erwärmen des Reaktionsgemisches mit HgCl₂ und Zink;

Yield	Reference
96%	LIFESCI PHARMACEUTICALS, INC., MCDONALD, Andrew, QIAN, Shawn WO2017/1936, 2017, A2 Location in patent: Paragraph 00159 Full Text > Details > Abstract >
95%	UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC. WO2007/47793, 2007, A2 Location in patent: Page/Page column 87 Full Text > Details > Abstract >
	Talik, Plazek [Roczniki Chemii, 1956, vol. 30, p. 1139,1145;][Chem.Abstr., <1957> 12089] Full Text > Details >

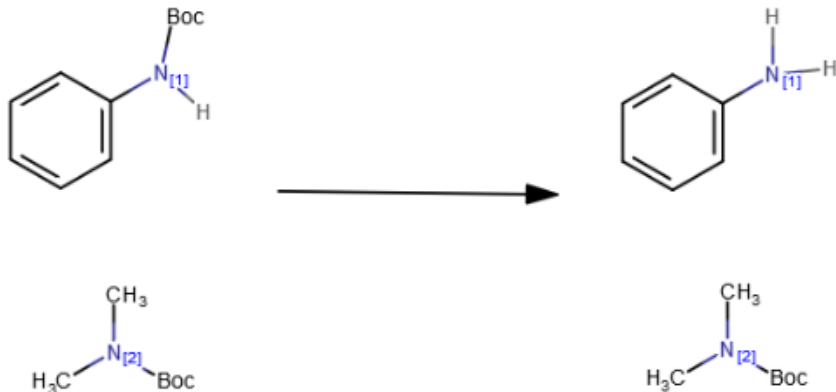
Experimental Procedure

4-Amino-2-chloro-3-nitropyridine (6.0 g, 34.57 mmol) in 150 mL of ethanol was hydrogenated over Raney nickel catalyst (6.0 g wet) for 4h at room temperature under 1.0 atm of H₂ atmosphere. After addition of 4.0 g of celite to the solution, the mixture was stirred vigorously and filtered over celite pad. The filtrate was concentrated and purified with silica gel column chromatography (CH₂Cl₂:MeOH = 20:1 v/v) to give 2-Chloro-3,4-diaminopyridine (4.72 g, 32.84 mmol) in 95% yield. ¹H-NMR (DMSO, 500 MHz) δ 7.31 (d, J = 5.0, 1H), 6.45 (d, J = 5.0, 1H), 5.79 (s, 2H), 4.68 (s, 2H); ¹³C-NMR (DMSO, 125 MHz) δ 143.41, 138.03, 135.61, 126.66, 108.73, 1.

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 7: 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/av92577868>

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 >

Reaxys可以直接设定这些片段在一个结构中

- ☐ Ignore Atom Mappings
- ☒ Keep fragments
 - ☐ Separate
 - ☒ Together

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

By Structure ▾

Yield ▾

Reagent/Catalyst ▾

Solvent ▾

Catalyst Classes ▾

Solvent Classes ▾

Product Availability ▾

Reactant Availability ▾

Reaction Classes ▾

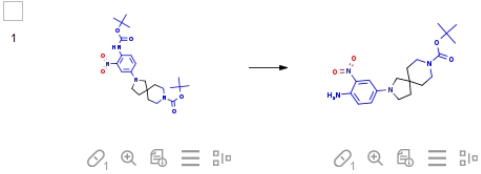
Document Type ▾

Publication Year ▾

☐ Single step reactions only

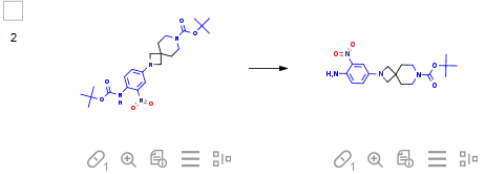
☐ Experimental procedure only

1



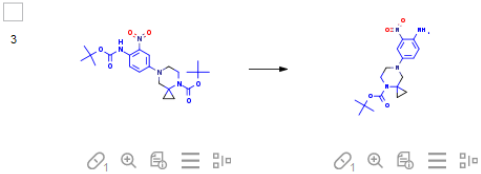
1 Conditions Find Similar > Reaction ID: 51038227

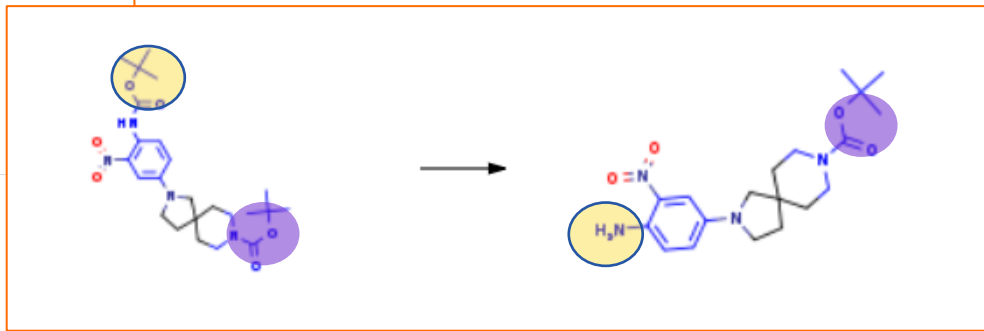
2



1 Conditions Find Similar > Reaction ID: 51038186

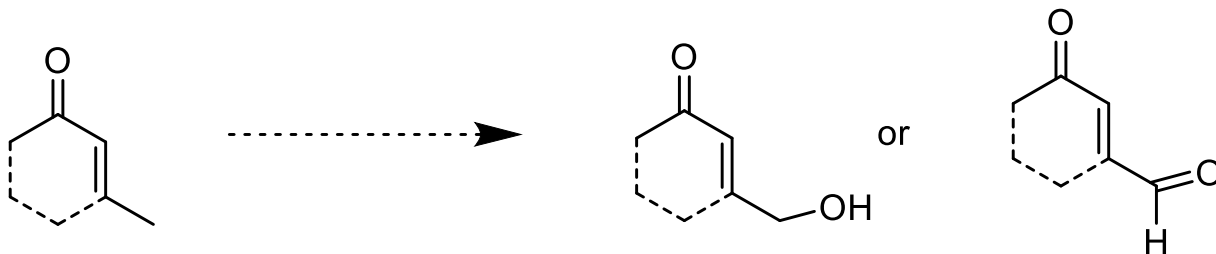
3





Case 8: 涉及环系变化的反应定义

- 获取以下反应



Requirement:

- 虚线部分是大于5个C原子的环
- 结构中不能发生互变异构
- 产物的 CH_2OH , CHO 是有底物的 CH_3 变化过来
- 视频操作（结构类似）：

<https://b23.tv/S08u6p>

Reaxys中的定义

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 >

定义方法:

- R基团定义工具，定义侧链
- S*定义侧链CH₂OH，以及底物CH₃无取代
- 重复基团定义工具，定义环的大小
- 无互变异构

最后的结果

Reaxys®

Quick search Query builder Results Synthesis planner History

63 Reactions out of 41 Documents containing 92 Substances, 72 Targets

☐ 0 selected Limit To Exclude Export Syn-Plan Show Conditions

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



1 Conditions Find Similar > Reaction ID: 39179987

2



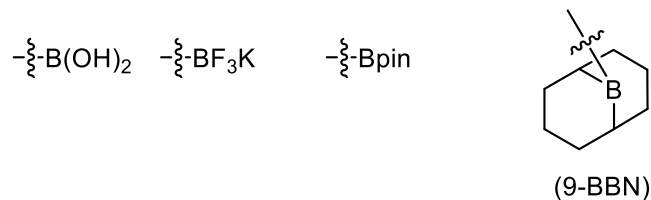
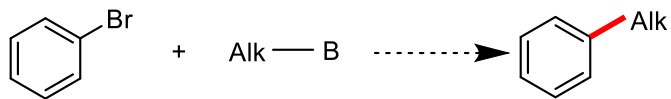
1 Conditions Find Similar > Reaction ID: 53952384

3



Case Study 9:

- 获取以下反应性对比的文献（收率）



Requirement:

- 希望获得在一篇文献中讨论过同一个B试剂和不同底物反应的对比
- ALK也可以是醚

Reaxys中的解决方案

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

Structure editor selected: ☒ MarvinJS ☐ ChemDrawJS Insert structure from name >

Structure editor interface showing a chemical reaction scheme:

Reaction scheme: A benzene ring with a bromine atom (Br) and a substituent R₁ (labeled [1]) reacts with a borane reagent (R₁-BH₂) to form a product: a benzene ring with a substituent R₁ (labeled [1]).

Below the reaction scheme, the substituent R₁ is defined as:

R₁ = ALK AOX

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 X Transfer to query >

Reaxys中的结果

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Alerts Sam Yu

444 Reactions out of 317 Documents containing 823 Substances, 115 Targets

Limit To Exclude Limit To Exclude Export Syn-Plan Show Conditions

1

2

3

Conditions Find Similar Reaction ID: 23313056

Conditions Find Similar Reaction ID: 28287724

Conditions Find Similar Reaction ID: 28287724

直接获取这些反应的文献

Reaxys Quick search Query builder **Results** Synthesis planner History Alerts Sam Yu

317 Documents with 823 Substances, 444 Reactions, 115 Targets

Limit To Exclude Limit To Exclude Export Publication Year Heatmap

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

1 Potassium trimethylsilylanolate enables rapid, homogeneous suzuki-miyaura cross-coupling of boronic esters [Cited 1 times](#)

2 SPERO THERAPEUTICS, INC.; BROWN, Pamela; DAWSON, Michael; SIMONOVIC, Mona; BOAKES, Steven; DUPERCHY, Esther; RIVERS, Dean; LESTER, Ray; COLEMAN, Scott - WO2020/2325, 2020, A1

3 Ligand assessment for the suzuki-miyaura cross coupling reaction of aryl and heteroaryl bromides with n-butylboronic acid. The advantages of buchwald's s-phos

4 PHENYL-N-QUINOLINE DERIVATIVES FOR TREATING A RNA VIRUS INFECTION

Reaxys中的结果

Enabling the Cross-Coupling of Tertiary Organoboron Nucleophiles through Radical-Mediated Alkyl Transfer

Primer, David N.; Molander, Gary A. [Journal of the American Chemical Society, 2017, vol. 139, # 29, p. 9847 - 9850]

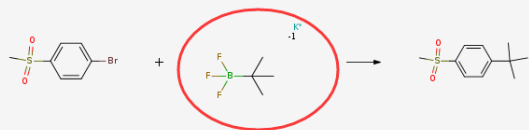
Abstract ▾ Index Terms ▾ Substances 88 ▾ Reactions 58 ▾ Full Text ↗

Hit Reactions 8 ^

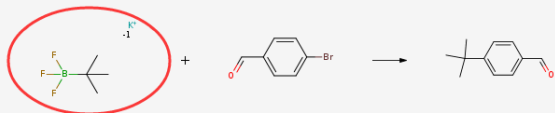
Hit Reactions



1 Conditions ▾ Find Similar > Reaction ID: 45928116



1 Conditions ▾ Find Similar > Reaction ID: 45928165



1 Conditions ▾ Find Similar > Reaction ID: 45928175

专门找Hit Reaction >1的文献，先进行预览，看是否存在相同硼试剂，不同底物的。

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物性数据的查询与反向检索
 - Reaxys中的结构面板与复杂反应定义
 - Reaxys中的实用小案例
- Q&A

Case 10: 化合物的文献定位

这是一篇常见的化学文献，包含：

1. 16页PDF全文
2. 2个Supporting Information的Word文档，一个是44页，一个37页

已知文献中报道了这个化合物，如何在上述的97页文档中找到有关这个化合物的描述？

Tetrahedron 74 (2018) 234–239

Contents lists available at ScienceDirect

Tetrahedron

Journal homepage: www.elsevier.com/locate/tet

Assessment of the regioselectivity in the condensation reaction of unsymmetrical *o*-phthalaldehydes with alanine

Agathe C.A. D'Hollander, Nicholas J. Westwood*

School of Chemistry and Biomolecular Sciences Research Complex, University of St Andrews and ErciCHEM, North Haugh, St Andrews, Fife, KY16 9ST, UK

ARTICLE INFO

Article history:
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Keywords:
o-phthalaldehyde
Condensation reaction
Regioselectivity
Mechanistic understanding

ABSTRACT

One approach for the synthesis of isoindolones, a privileged bioactive heterocyclic core structure, involves a condensation reaction of *o*-phthalaldehydes with a suitable nitrogen-containing nucleophile. This fascinating reaction is revisited here in the context of the use of *o*-phthalaldehydes that contain additional substituents in the aromatic ring leading to a detailed analysis of the regioselectivity of the reaction. Eleven monosubstituted *o*-phthalaldehydes were synthesised and reacted with alanine. The regioselectivity observed across the eleven substrates led to the design of a disubstituted substrate that reacted with very high control. A gram-scale reaction followed by esterification gave one major regioisomer in high yield. In addition, the regioselectivity observed on reaction of two novel mono-deuterated substrates led to an increased mechanistic understanding.

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1. Introduction

The isoindolones make up an important class of bioactive molecules that includes the known drugs Pazinotone (1),^{1a} Indoprofen (2)^{3b} and Chlorhalidone (3)^{1c} (Fig. 1a).

Common methods of obtaining isoindolones that are unsymmetrical in the aromatic ring, for example compound 4 (Fig. 1b), include selective reduction of 5,7-reductive amination-cyclisation of 6¹ or 7¹ with a primary amine (RNH₂) and, of interest here, the condensation reaction of *o*-phthalaldehyde (8) with a primary amine (RNH₂).^{1,2,4–6}

To date, the majority of studies performed on this condensation reaction have focused on evaluating the scope of the amine nucleophile that can be tolerated in the reaction,^{1–3,5a,b,8} and/or proposing potential reaction mechanisms.^{5a,b,9} In contrast, examples of the use of this condensation reaction with monosubstituted *o*-phthalaldehydes are rare (S11 part 1). One report describes a regioselectivity of 1:1 for the products 11–12 resulting from the condensation of 9 with 10 (Scheme 1a).⁷ However, the observed regioselectivity was measured only after filtration or purification by column chromatography. Isolated yields for the formation of a single isomer, 14 in most cases, resulting from the condensation of 13 with various amines have also been reported (Scheme 1b).⁸

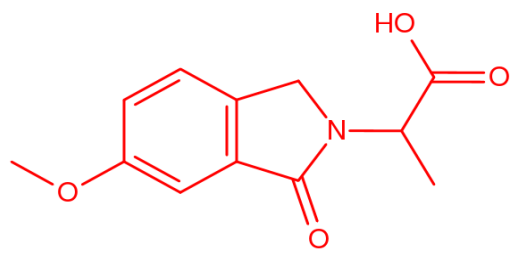
Other studies have provided only isolated yield(s) after purification (for one or for each isomer), incomplete regioisomeric ratio (rr) data within a series or have claimed to form a single regioisomer (no yield provided) without discussing the other possible isomer (S11 part 1).^{7–9}

The work reported here revisits this issue by presenting a detailed study of the regiochemical outcome of the condensation of alanine (16) with 3-monosubstituted *o*-phthalaldehydes 17 (to give 18 and 19, Scheme 1c) and with 4-monosubstituted *o*-phthalaldehydes 20 (to give 21 and 22, Scheme 1d). Based on the initial results, the design of a highly regioselective substrate was achieved consistent with an improved understanding of the reaction. Further mechanistic insights were provided by the use of novel mono-deuterated substrates.

2. Results and discussions

2.1. Synthesis of monosubstituted *o*-phthalaldehydes

Five 3-substituted *o*-phthalaldehydes 17a–e were synthesised using 2–5 step routes involving either a Swern oxidation of the corresponding diol 23 or an acetal deprotection of the corresponding monoacetal 24 or diacetal 25 (Scheme 2 and S11 part B.1 for more details). It should be noted that the synthesis of pure samples of 17a–e was particularly challenging (in line with literature reports¹⁰) with significant decomposition occurring during purification attempts and on storage. In several cases freshly



Reaxys中的检索

- Query Builder联合化合物结构与文献DOI号

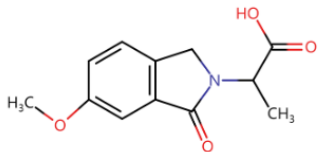
Reaxys® Quick search Query builder Results Synthesis planner History Register > Sign in ?

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

◇ DOI is 10.1016/j.tet.2017.11.035

AND ◇ Structure


As drawn

Search fields

Fields Forms History

Reaxys ^

Topics and Keywords v

Identification v

Physical Properties v

Spectra v

MedChem v

Other v

Reactions v

Bibliography v

PubChem v

eMolecules v

Feedback

Reaxys中的结果

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Register > Sign in ⓘ

1 **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 >

1 Substances out of 1 Documents, containing 7 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations

Reaxys - 1

Grid Heatmap

2-(6-methoxy-1-oxoisindolin-2-yl)propanoic acid
C₁₂H₁₃NO₄ 235.24 32021463

Hit Data - 7 Druglikeness Spectra - 4 Preparations - 7 >
Identification Physical Data - 2 Reactions - 7 >
Documents - 1 >

Hit Data - 7

- Substance Label - 1 hits out of 1
- Melting Point - 1 hits out of 1
- Crystal Property Description - 1 hits out of 1
- NMR Spectroscopy - 2 hits out of 2
- IR Spectroscopy - 1 hits out of 1

Substance Label - 1 hits out of 1

Label	Reference
21a	D'Hollander, Agathe C.A.; Westwood, Nicholas J. [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239] Full Text > Cited 3 times > Details > Abstract >

+ Load More

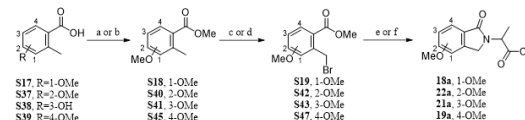
全文检索21a定位化合物

2.2. Regioselectivity of the condensation reaction of mono-substituted *o*-phthalaldehydes

The mono-substituted *o*-phthalaldehydes **17a-e** and **20a-f** were refluxed for 4 h with alanine (**16**, 1.2 equivalents) in anhydrous acetonitrile before the reaction was concentrated *in vacuo*. The crude reaction mixtures (except when specified, [Table 1](#)) were then analysed using a quantitative ^1H NMR experiment. A baseline correction was applied using MestReNova-9 software and integrations were calculated relative to one proton on deconvoluted peaks (see [Fig. 2](#) for an example of the analysis applied to the formation of **18a/19a** and [S11 part III.1](#) for the rest of the NMR analysis; also see the experimental section below for a detailed explanation of the analytical protocol used).

In two of the condensation reactions the structure of the major regioisomer was identified by comparison with the ^1H NMR spectrum of a pure sample of one of the regioisomers (for **18a/19a**, **21a/22a**, for the synthesis of authentic isomers see [S11 part III.2](#)). In the rest of the cases, advanced NMR techniques (HSQC, HMBC, COSY) applied to the crude reaction mixture were used to assign the structure of the major regioisomer. Considering the analysis of the regioisomeric mixture of **18b/19b** as an example ([Fig. 3](#)), the proximity of a carbonyl was observed to shift the signal corresponding to the aromatic H7 proton in **18b** and the methyl H1' protons in **19b** downfield ([Fig. 3a](#) and [b](#)). Identification of H7 in **18b** was further validated by its correlation with C1 in the HMBC analysis of the regioisomeric mixture ([Fig. 3a](#)). In contrast, H4 in **19b** showed a correlation with C3 in this HMBC analysis ([Fig. 3c](#)). Using the correlations observed in the COSY spectrum ([Fig. 3d](#)), the signals corresponding to H5 and H6 for **18b** and **19b** were finally assigned. The value of the integrals in the 1D quantitative ^1H NMR

III.2. Synthesis of pure isoindolinones **18a**, **19a**, **21a** and **22a**.



Scheme S 10: Synthesis of **18a**, **19a**, **21a** and **22a**. Reagents and conditions: (a) MeOH, H_2SO_4 , reflux, 7–24 h, quant. for **S18**, 84% for **S40**; (b) MeI, K_2CO_3 , DMF, 70 °C 17–18 h, 92% for **S41**, 99% for **S45**; (c) NBS, AIBN, CHCl_3 , reflux, 2.5–21.0 h, 97% for **S19**, crude **S42** and **S43** were directly used in the next step; (d) NBS, AIBN, CCl_4 , reflux, 2 h, crude **S47** was directly used in the next step; (e) alanine (**16**), MeOH, K_2CO_3 , reflux 19–21 h, 61% for **18a**, 55% (2 steps) for **19a**; (f) alanine (**16**), MeOH, NEt_3 , reflux 2–23 h, 4% (2 steps) for **21a**, 4% (2 steps) for **22a**.

Esterification of **S17**, **S37**, **S38** and **S39** was achieved in excellent yield using iodomethane or methanol with sulfuric acid (Scheme S 10).⁸ Radical monobromination⁹ of **S18**, **S40**, **S41** formed **S19**, **S42**, **S43** which were directly reacted⁹ with alanine (**16**) to obtain **18a**, **22a** and **21a** respectively. To investigate the poor yield over two steps (2% for **18a**, 4% for **21a** and 4% for **22a**), radical monobromination of **S18** was repeated and the succinimide side product from *N*-bromosuccinimide was removed by a basic wash using NaOH (1 M) leading to pure **S19** in 97% yield. Reaction of **S19** with **16** and NEt_3 afforded **18a** in only 8% yield. However, concentration of the aqueous phase showed **S44** as the major product (identified by NMR spectroscopy ([Figure S 5](#)) and supported by mass spectrometric analysis (HRMS (ES^+) m/z calculated for $\text{C}_{16}\text{H}_{26}\text{NO}_3$ [M] $^+$: 280.1907; found: 280.1910) along with the remaining NEt_3 and alanine (**16**). Formation of **S44** was prevented by reacting **S19** with K_2CO_3 instead of NEt_3 to provide **18a** in good yield. This optimisation could be applied for the synthesis of **21a** and **22a** but was not performed since sufficient material was available.

用于文献中化合物信息的快速定位。

Case 11: 关键词检索时词语之间距离的设定

- 希望在主题，摘要，关键词中进行检索Optoelectronics Materials
- Optoelectronics与Materials两单词之间距离小于3，且Optoelectronics在Materials之前

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

◇ Titles, Abstracts & K...

is

Optoelectronic*

✕

◇ Titles, Abstracts & K...

is

Material*

✕

OR

AND

NOT

NEAR

NEXT

PROXIMITY

Tips:

1. 逻辑关系的选择, And, Or, Not

2. Near没有前后次序, Next有前后次序

Search fields

Fields Forms History

Reaxys

Topics and Keywords

◇ Substance Properties & Comments

◇ Reaction Data & Conditions

◇ Titles, Abstracts & Keywords

◇ All Keywords

Identification



Reaxys中的结果

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

3,27 K Filters Limit to > Exclude >

3,269 Documents with 6,860 Substances, 5,864 Reactions, 0 Targets

0 selected Limit To Exclude Export

Sort by Cited By ↓ Heatmap

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

1 A DNA-based method for rationally assembling nanoparticles into macroscopic materials Cited 5220 times
Mirkin, Chad A.; Letsinger, Robert L.; Mucic, Robert C.; Storhoff, James J. [Nature, 1996, vol. 382, # 6592, p. 607 - 609]
Abstract Index Terms Full Text
Abstract hit: {...useful optical, optoelectronic and material properties that derive from their small (nanoscopic) size....}

2 Nanocrystals of Cesium Lead Halide Perovskites (CsPbX₃, X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut Cited 2501 times
Protesescu, Loredana; Yakunin, Sergii; Bodnarchuk, Maryna I.; Krieg, Franziska; Caputo, Riccarda; Hendon, Christopher H.; Yang, Ruo Xi; Walsh, Aron; Kovalenko, Maksym V. [Nano Letters, 2015, vol. 15, # 6, p. 3692 - 3696]
Abstract Index Terms Substances 11 Reactions 5 Full Text
Abstract hit: {...are newcomer optoelectronic materials that have attracted enormous attention as solution-deposited absorbing layers...}

3 Organic materials for electronic and optoelectronic devices Cited 1546 times
Shirota, Yasuhiko [Journal of Materials Chemistry, 2000, vol. 10, # 1, p. 1 - 25]
Abstract Index Terms Full Text
Abstract hit: {...electronic and optoelectronic devices. The materials studied include amorphous molecular materials, titanyl phthalocyanine,...}

4 Thin-film transistor fabricated in single-crystalline transparent oxide semiconductor Cited 1536 times
Nomura, Kenji; Ohta, Hiromichi; Ueda, Kazushige; Kamiya, Toshio; Hirano, Masahiro; Hosono, Hideo [Science, 2003, vol. 300, # 5623, p. 1269 - 1272]
Abstract Index Terms Full Text
Index Terms hit: {...Irradiation, Optoelectronic devices, Semiconductor materials...}

5 Aggregation-induced emission: The whole is more brilliant than the parts Cited 1483 times
Mei, Ju; Hong, Yuning; Lam, Jacky W. Y.; Qin, Anjun; Tang, Youhong; Tang, Ben Zhong [Advanced Materials, 2014, vol. 26, # 31, p. ...]

Sort search results X

Relevance
Publication Year
Document Type
Cited By ↑↓

有订购Scopus，可以直接获取引文

Case 12: 专利Claim中的关键词检索

- Query Builder中Patent: Claim字段
- 如检索自愈材料
 - Self-heal*
 - Material*

The screenshot displays the Reaxys Query Builder interface. At the top, navigation links include 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History'. On the right, there are buttons for 'Register >' and 'Sign in'.

The main search area features a 'Search in:' dropdown with options: 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. Below this, a toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all'. To the right of the toolbar are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'.

The query builder shows two conditions in a list:

- Condition 1: Patents: Claims is self-heal* (with a dropdown arrow next to 'is' and a search icon).
- Condition 2: Patents: Claims is materia* (with a dropdown arrow next to 'is' and a search icon).

An 'AND' button is located to the left of the second condition.

On the right side, a 'Search fields' sidebar is visible, containing a search icon and a list of fields: 'Fields', 'Forms', and 'History'. Below these are expandable sections: 'Reaxys ^', 'Topics and Keywords ^', 'Identification ^', 'Physical Properties ^', 'Spectra ^', and 'MedChem ^'.

The Elsevier logo is visible in the bottom left corner.

Reaxys中的结果

Reaxys®

Quick searchQuery builderResultsSynthesis plannerHistory

Register >Sign in ⓘ

398

Filters

Limit to >Exclude >

Index Terms (List) >

Index Terms (ReaxysTree) >

Publication Year >

Document Type >

Authors >

Patent Assignee >

Journal Title >

Substance Classes >

Reaction Classes >

398 Documents with 1,855 Substances, 1,096 Reactions, 261 Targets

☐ 0 selectedLimit ToExcludeExport

Sort by Publication Year ↓

Heatmap

☐ SELF-HEALING COMPOSITE AND DEVICE INCLUDING SELF-HEALING FILM

1 Samsung Electronics Co., Ltd.; THE BOARD OF TRUSTEES OF THE LELAND STANFORD JUNIOR UNIVERSITY; Yun, Youngjun; Son, Donghee; Kang, Jiheong; Bao, Zhenan; Vardoulis, Orestis - US2020/2501, 2020, A1
Patent Family Members: US2020/2501 A1
[Abstract](#) > [Claims](#) > [Front Page Info](#) > [Full Text](#) >

Claims hit: {...1. A self-healing composite comprising a matrix including an elastomer, and conductive nanostructures embedded in...}

☐ DEVICE AND METHOD FOR SEALING A MEMBRANE

2 UNIVERSITAET ZÜRICH; DEVAUD, Yannick; MILLERET, Vincent; ZIMMERMANN, Roland; EHRBAR, Martin; OCHSENBEIN, Nicole - US2020/8788, 2020, A1
Patent Family Members: CA3052225 A1; WO2018/141951 A1; CN110446467 A; EP3576637 A1; US2020/8788 A1; ...
[Abstract](#) > [Claims](#) > [Front Page Info](#) > [Full Text](#) >

Claims hit: {...is a self-expandable patch (120).5. The membrane closure device (100) according to claim...}

☐ ORGANOID ARRAYS

3 Ecole Polytechnique Fédérale de Lausanne; HOEHNEL, Sylke; BRANDENBERG, Nathalie; LUTOLF, Matthias - US2020/10797, 2020, A1
Patent Family Members: EP3296018 A1; WO2018/50862 A1; EP3515600 A1; US2020/10797 A1
[Abstract](#) > [Claims](#) > [Front Page Info](#) > [Full Text](#) >

Claims hit: {...cell compatible material that supports organoid development and maintenance, more preferably wherein the cell...}

☐ HEALTH MONITORING GARMENT AND SYSTEM

4 Cornerstone Research Group, Inc.; Young, Trang T.; Cridge, Mark C.; Miller, Scott A.; Nieman, Joshua E.; Cupp, Gary N.; Cable, Kristin M. - US2020/22431, 2020, A1
Patent Family Members: US2020/22431 A1; WO2020/23479 A1
[Abstract](#) > [Claims](#) > [Front Page Info](#) > [Full Text](#) >

ELSEVIER

Case 13: 结果集的逻辑处理

- Query Builder中History选择多个结果集，进行逻辑处理

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, and History. On the right, there are buttons for Register and Sign in. Below the navigation, there is a search bar with tabs for Reactions, Targets, Substances, and Documents. Below the search bar, there are icons for Import, Save, Reset form, and Delete all. To the right of these icons are icons for Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main area displays a list of document sets. The first set has 398 Documents and the query: documents: (PBIB.CLAIMS is "self-heal") AND (PBIB.CLAIMS is "materia"). The second set has 263 Documents and the query: documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material"). An orange arrow points to the 'AND' button between the two document sets. On the right side, there is a sidebar with tabs for Search fields, Fields, Forms, and History (selected). Below the History tab, there is a list of recent document sets, including the two shown in the main area.

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

398 Documents documents: (PBIB.CLAIMS is "self-heal") AND (PBIB.CLAIMS is "materia")

AND

263 Documents documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material")

Search fields

Fields Forms **History**

Recent

398 Documents documents: (PBIB.CLAIMS is "self-heal") AND (PBIB.CLAIMS is "materia")

398 Documents documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material")

263 Documents documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material")

574 Documents documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material")

241 Documents documents: (PBIB.CLAIMS is "self-healing") AND (PBIB.CLAIMS is "material")

只能对相同类型的结果集进行And, Or, Not操作

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物性数据的查询与反向检索
 - Reaxys中的结构面板与复杂反应定义
 - Reaxys中的实用小案例
- Q&A

Reaxys小结

- 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Query Builder检索帮助科研人员通过简便的方式，获得精准，跨学科精确答案
- 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
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Thank you

