



Reaxys 使用介绍

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今天的内容

- Reaxys基本介绍
- Reaxys的使用
 - Reaxys中化合物理化性质的检索
 - Reaxys中的结构面板与反应检索
 - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Reaxys—基于数据深度提炼的科研信息平台

16.000 期刊
(journals, books and patents)

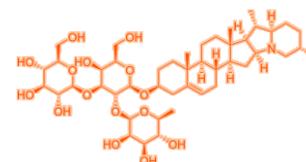
- **6000万文献**
 - (Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis, etc)
- **150万专利**
 - WPO, USPO, EPO [≈ mid 70's >]
 - PO: JP, KR, CN, TW [2015 >]
 - **2020年将扩展到100家专利机构**
- **38万书的章节**
 - Beilstein, Gmelin,



[自动抽提]



≈ 450 journals + PO
[人工抽提]



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](#) [v](#) Reactions [236](#) [v](#) 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 monodisubstituted substrates led to an increased mechanistic understanding.

Index terms

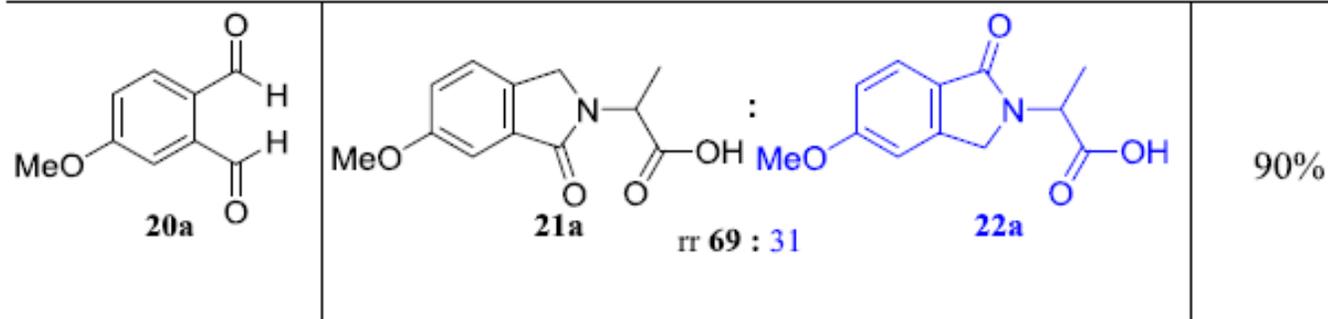
Author keyword: Condensation reaction, Mechanistic understanding, o-phthalaldehyde, Regioselectivity

EMTREE drug term: alanine, phthalaldehyde

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

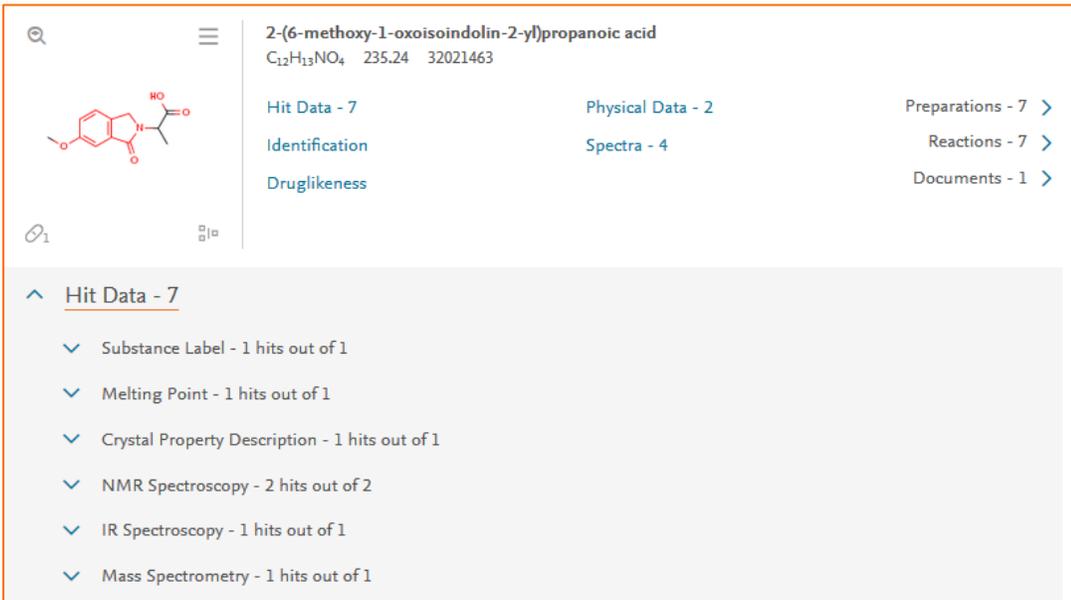
Reaxys Index Terms: Swern oxidation, condensation reaction, esterification, pure, reactivity, regioselectivity, separation method, tautomerization

4-substituted series



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-oxisoindolin-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

The reaction scheme shows the synthesis of two regioisomers, 21a and 22a, from alanine and 4-methoxyphthalaldehyde. Alanine (16) reacts with 4-methoxyphthalaldehyde (20a) to produce a mixture of 2-(6-methoxy-1-oxoisindolin-2-yl)propanoic acid (21a) and 2-(5-methoxy-1-oxoisindolin-2-yl)propanoic acid (22a).

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

1 Conditions Find Similar

Yield	Conditions	Reference
	In acetonitrile for 4h; Reflux; Inert atmosphere; Overall yield = 90 percent; Overall yield = 38 mg; regioselective reaction;	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239]

[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.

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- Reaxys小结与未来展望

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 [Substances](#) 49M [Reactions](#) 59M [Documents](#) 37M [Bioactivities](#)

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RELX Group™

Reaxys中的结果

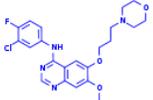
Quick search Query builder Results Synthesis planner History

Results for solubility of gefitinib New Edit

- 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 7,831 Documents, containing 130 Reactions, 1,103 Targets Reaxys - 1

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

1  **gefitinib**
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 3,436 Preparations - 83
Identification Physical Data - 98 Reactions - 130
Druglikeness Spectra - 75 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 [<i>Journal of Molecular Liquids</i> , 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 [<i>ACS Medicinal Chemistry Letters</i> , 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 [<i>Tetrahedron</i> , 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 [<i>Bioorganic and Medicinal Chemistry Letters</i> , 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

Sort by No of References ↓ Grid Heatmap

gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 3,436 Preparations - 83 >
Identification Physical Data - 98 Reactions - 130 >
Druglikeness Spectra - 75 Targets - 1,103 >
Documents - 7,831 >

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

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

直接获取化合物的理化性质或者谱图数据

Spectra - 77

- NMR Spectroscopy - 46
- IR Spectroscopy - 9
- Mass Spectrometry - 14
- UV/VIS 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

Solubility

Solubility Product

Reaxys ^

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](#)** [Documents](#)

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

<input type="checkbox"/>	ethane-1,2-diamine	23
<input type="checkbox"/>	ethane-1,2-diol	100
<input type="checkbox"/>	ethanesulfonic acid	1
<input checked="" type="checkbox"/>	ethanol	5,024
<input type="checkbox"/>	ethanol (99.4percent)	1
<input type="checkbox"/>	ethanol (99.8percent)	1
<input type="checkbox"/>	ethanol (99.9percent)	2
<input type="checkbox"/>	ethanol (99percent)	3
<input type="checkbox"/>	ethanolamine	3
<input type="checkbox"/>	ethyl acetate	1,062
<input type="checkbox"/>	ethyl benzoate	7
<input type="checkbox"/>	ethyl carbamate	6
<input type="checkbox"/>	ethyl nitrate	2

38 of 67 [Go to page >](#) Clear selected

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

Sort by No of References

Grid Heatmap

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

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……

Solubility (MCS) - 20 hits out of 429

Show/Hide columns

Solubility, g ⁻¹	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
	20	ethanol	Solubility: 0.012 mol/kg solvent	El-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	El-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	El-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	El-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	Kim; 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	Kim; Dunlap[<i>Journal of the American Chemical Society</i> , 1931, vol. 53, p. 393] Full Text Details >

Case 3: 如何用Reaxys快速筛选对“冠状病毒”有活性的化合物

- 获取文献中报道的对“RNA依赖的RNA聚合酶（RdRp）”有活性报道的化合物
- 希望这些化合物的IC50在um级别
- 视频操作：<https://www.bilibili.com/video/BV13A411b73P>（2分10秒开始）

The screenshot displays the Reaxys Query Builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted with an orange box), 'Results', 'Synthesis planner', and 'History'. On the right, there are 'Register >' and 'Sign in ?' buttons. Below the navigation bar, there are search field buttons for 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. A toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all', along with search field options: 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main query builder area shows a search for 'Target Name is rdrp'. Below this, a group of criteria is defined with 'AND' logic. The first criterion is 'Measurement Parameter is ic50|' (highlighted with an orange box). The second criterion is 'Measurement pX >= 6'. On the right side, the 'Search fields' panel shows 'PX' and 'Measurement pX'.

Tips:
利用Query Builder构建靶点，检测参数，以及参数大小的检索式

Reaxys中的结果

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

1.20 K Filters

Limit to > Exclude >

1,204 Substances out of 33 Documents, containing 2,896 Reactions, 6 Targets

0 Limit To Exclude Export Preparations

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

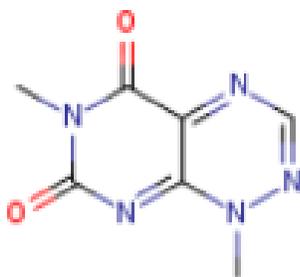
1 **toxoflavin**
C₇H₇N₅O₂ 193.165 21014 84-82-2
Identification Physical Data - 22 Preparations - 19 >
Druglikeness Spectra - 29 Reactions - 23 >
Bioactivity (Hit Data) Other Data - 3 Targets - 27 >
Bioactivity (All) Documents - 124 >

2 **3'-deoxycytidine**
C₉H₁₃N₃O₄ 227.22 616742 7057-33-2
Identification Bioactivity (All) Preparations - 54 >
Druglikeness Physical Data - 15 Reactions - 92 >
Bioactivity (Hit Data) Spectra - 31 Targets - 10 >
Documents - 44 >

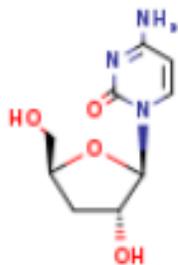
3 **3'-deoxyguanosine**
C₁₀H₁₃N₅O₄ 267.244 561508 3608-58-0
Identification Bioactivity (All) Preparations - 20 >
Druglikeness Physical Data - 12 Reactions - 55 >
Targets - 10 >

Reaxys直接给出符合条件的化合物，大量节省了科研人员阅读文献，并查找数据的时间，可以通过各自的Hit Data查看具体数据

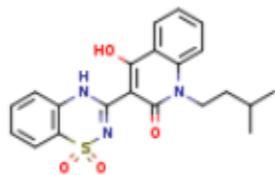
Reaxys中的结果



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



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



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
7.1	IC50	=	0.08	μM	Hepatitis C virus (strain DELTA 21)	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Dhanak, Dashyant; Duffy, Kevin J.; Johnston, Victor K.; Lin-Goerke, Juili; Darcy, Michael; Shaw, Antony N.; Gu, Baohua; (...) Keenan, Richard M.; Sarisky, Robert T. [Journal of Biological Chemistry , 2002, vol. 277, # 41 p. 38322 - 38327] Full Text ↗ Cited 172 times ↗ Details > Abstract

利用HeatMap看结构与靶点关系

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

1,204 Substances out of 33 Documents, containing 2,896 Reactions, 6 Targets

Limit To Exclude Export Preparations No of References Grid Heatmap

toxoflavin
C₇H₇N₅O₂ 193.165 21014 84-82-2

Identification Physical Data - 22 Preparations - 19 >
Druglikeness Spectra - 29 Reactions - 23 >
Bioactivity (Hit Data) Other Data - 3 Targets - 27 >
Bioactivity (All) Documents - 124 >

3'-deoxycytidine
C₉H₁₃N₃O₄ 227.22 616742 7057-33-2

Identification Bioactivity (All) Preparations - 54 >
Druglikeness Physical Data - 15 Reactions - 92 >
Bioactivity (Hit Data) Spectra - 31 Targets - 10 >
Documents - 44 >

3'-deoxyguanosine
C₁₀H₁₃N₅O₄ 267.244 561508 3608-58-0

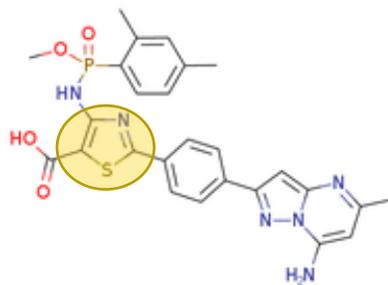
Identification Bioactivity (All) Preparations - 20 >
Druglikeness Physical Data - 12 Reactions - 55 >

利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

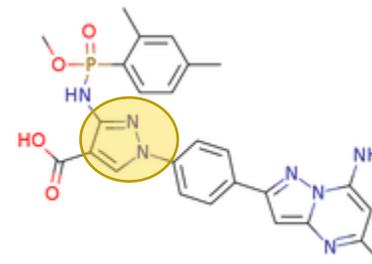


一些非常有意思的结构

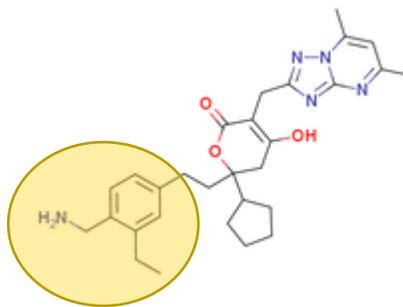
		RNA-dependent RNA polymerase	
Substances		Targets	
5-thiazolec... ylamine]	●		9.5
(E)-N-(4-(... fonamide	●		9.5
IDX17119	●		9.4
20673525	●		9.3
5-thiazolec... l-amine]	●		9.1
20673509	●		9.1
20673487	●		9.1
29885944	●		9
27259279	●		9
6-cyclope... an-2-one	●		9
(6R)-6-cy... an-2-one	●		9
6-cyclope... an-2-one	●		9
6-cyclope... an-2-one	●		9
6-cyclope... an-2-one	●		9
N-(4-((3-(t... fonamide	●		8.9
5-[2-(4-flu... boxamide	●		8.7
(1aR,12b... boxamide	●		8.7
20673500	●		8.7
N-[4-(2-(2... cetamide	●		8.7
6-cyclope... an-2-one	●		8.7
6-cyclope... an-2-one	●		8.7
N-(2-[4-(2... cetamide	●		8.7
6-cyclope... an-2-one	●		8.7



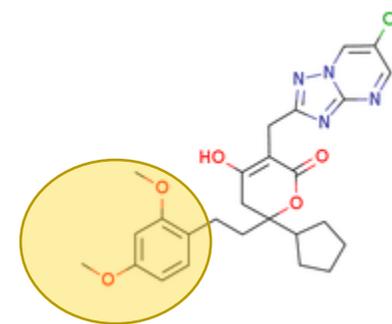
PX=9.5



PX=9.4



PX=8.0

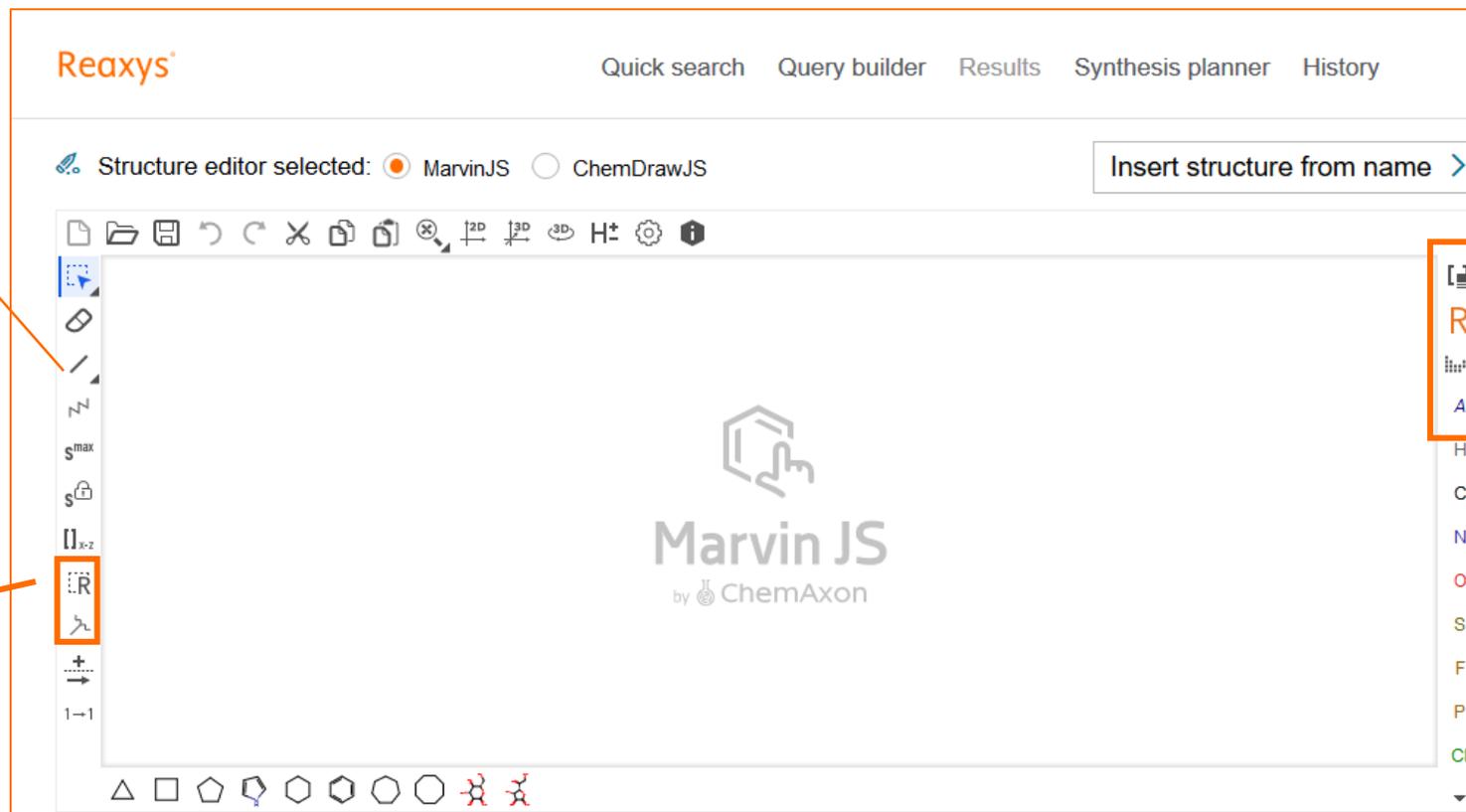


PX=7.7

今天的内容

- Reaxys基本介绍
- Reaxys的使用
 - Reaxys中化合物理化性质的检索
 - Reaxys中的结构面板与反应检索
 - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Reaxys中的结构面板



R基团定义工具

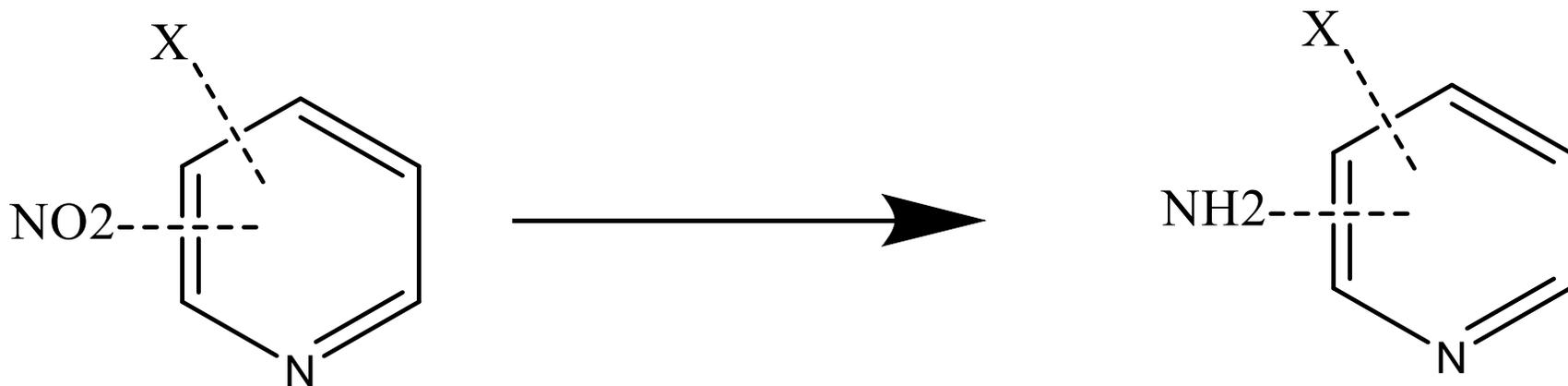
缩写官能团，通用官能团，原子列表/列表非原子属性列表

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

Case 4: 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

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

最后的结果

Reaxys® Quick search Query builder **Results** Synthesis planner

624
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

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

0 selected
Limit To Exclude Export Syn-Plan Show Conditions

1

6 Conditions Find Similar > Reaction ID: 149845

2

7 Conditions Find Similar > Reaction ID: 22895930

3

1

6 Conditions Find Similar > Reaction ID: 149845

Conditions	Yield	Reference
With hydrogen In methanol at 20°C; for 2h; Experimental Procedure	96%	LIFESCI PHARMACEUTICALS, INC.; MCDONALD, Andrew; QIAN, Shawn WO2017/1936, 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. WO2007/47793, 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;		Talik; Plazek [Roczniki Chemii, 1956, vol. 30, p. 1139,1145.][Chem.Abstr., <1957> 12089] Full Text > Details >

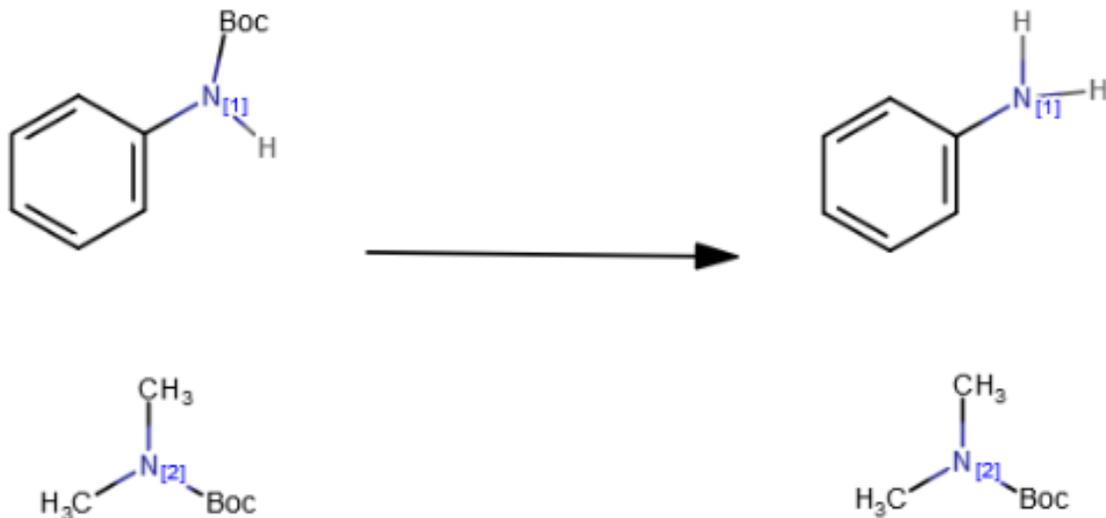
Experimental Procedure

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. t.

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 5: 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

The screenshot displays the Reaxys software interface. At the top, there are navigation links: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". On the right, there are buttons for "Register >" and "Sign in". Below the navigation, the "Structure editor selected" section shows "MarvinJS" selected over "ChemDrawJS". A search bar contains the text "Insert structure from name >".

The main workspace shows a chemical reaction scheme. The reactants are N-benzyloxycarbonylamine (Boc-NH-Ph) and N,N-dimethyl-N-benzyloxycarbonylamine (Boc-N(CH₃)₂-Ph). An arrow points to the products: benzylamine (NH₂-Ph) and N,N-dimethylbenzylamine (N(CH₃)₂-Ph). The nitrogen atoms in the structures are labeled with atom mapping numbers [1] and [2].

On the right side, there is a search configuration panel titled "Search this structure as:". It includes several radio buttons and checkboxes:

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

An orange box highlights the "+ More options" button, with an arrow pointing to a detailed view of its settings:

- Ignore Atom Mappings
- Keep fragments
 - Separate
 - Together

At the bottom of the interface, there are buttons for "Clear", "Cancel", and "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

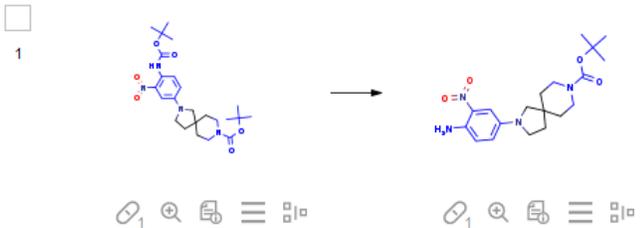
Limit to > Exclude >

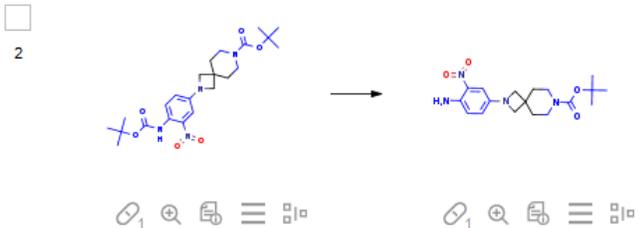
By Structure > Yield > Reagent/Catalyst > Solvent > Catalyst Classes > Solvent Classes > Product Availability > Reactant Availability > Reaction Classes > Document Type > Publication Year >

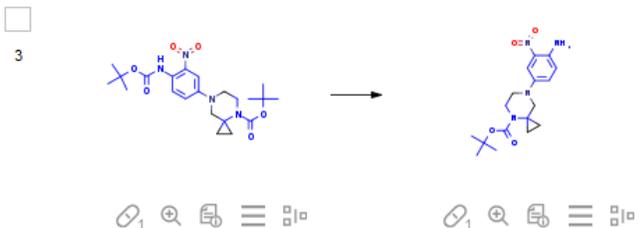
Single step reactions only
 Experimental procedure only

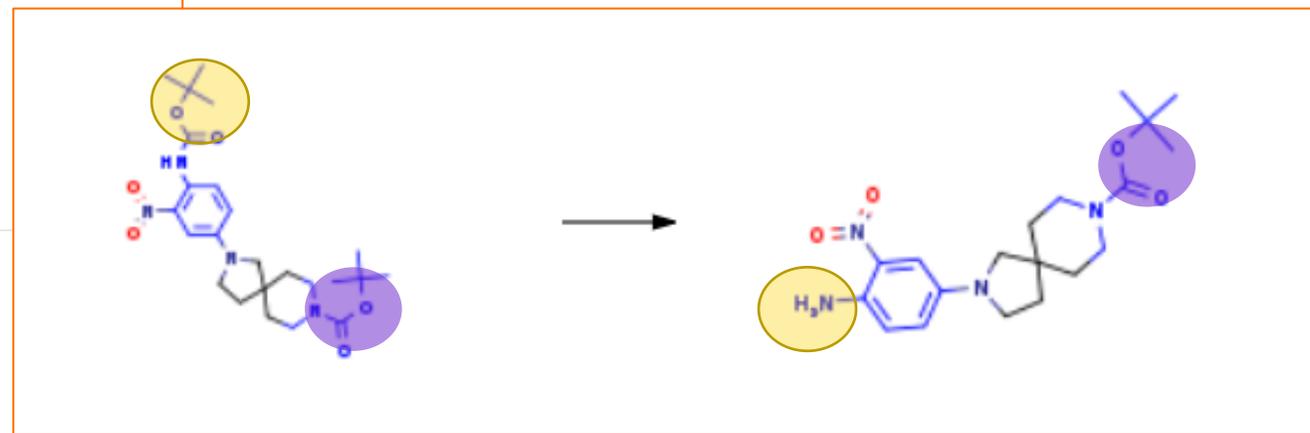
12 Reactions out of 8 Documents containing 22 Substances, 5 Targets

0 Limit To Exclude Export Syn-Plan Show Conditions

1 
1 Conditions Find Similar > Reaction ID: 51038227

2 
1 Conditions Find Similar > Reaction ID: 51038186

3 

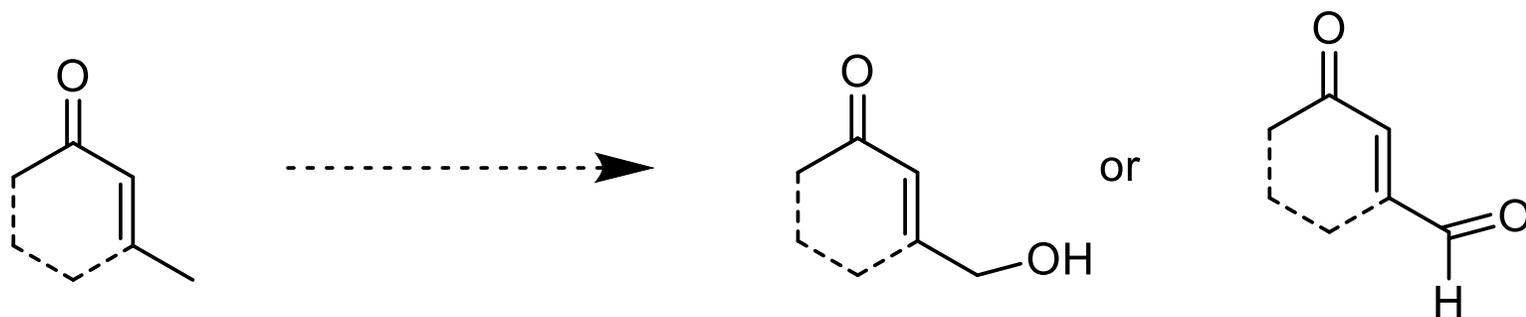


今天的内容

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 - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Case Study 6:

- 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CH₂OH, CHO是有底物的CH₃变化过来

Reaxys中的结构绘制

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

- 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

By Structure Limit to > Exclude >

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

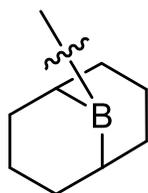
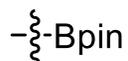
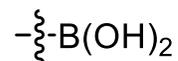
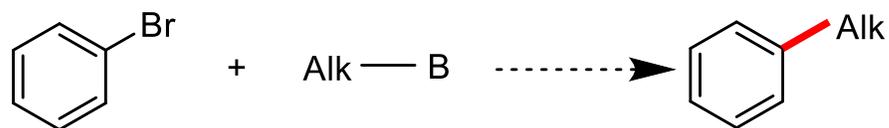
1 
1 Conditions Find Similar Reaction ID: 39179987

2 
1 Conditions Find Similar Reaction ID: 53952384

3 

Case Study 7:

- 获取以下反应性对比的文献（收率）



(9-BBN)

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 >

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中的结果

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

444 Filters
Limit to > Exclude >

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

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

0 Limit To Exclude Export Syn-Plan Show Conditions

1 Conditions Find Similar > Reaction ID: 23313056

2 Conditions Find Similar > Reaction ID: 28287724

3

直接获取这些反应的文献

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

317 Filters
Limit to > Exclude >

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

317 Documents with 823 Substances, 444 Reactions, 115 Targets

0 Limit To Exclude Export Publication Year Heatmap

1 Potassium trimethylsilanolate enables rapid, homogeneous suzuki-miyaura cross-coupling of boronic esters
Delaney, Connor P.; Kassel, Vincent M.; Denmark, Scott E. [ACS Catalysis, 2020, vol. 10, # 1, p. 73 - 80]
Abstract Index Terms Substances 107 Reactions 62 Full Text
Hit Reactions 1

2 COMPOUNDS
SPERO THERAPEUTICS, INC.; BROWN, Pamela; DAWSON, Michael; SIMONOVIC, Mona; BOAKES, Steven; DUPERCHY, Esther; RIVERS, Dean; LESTER, Roy; COLEMAN, Scott - WO2020/2325, 2020, A1
Patent Family Members: WO2020/2325 A1
Abstract Claims Front Page Info Substances 88 Reactions 50 Full Text
Hit Reactions 1

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
Jagusch, Thomas; Lehnemann, Bernd; Meudt, Andreas; Nerdinger, Sven; Neuner, Sandro; Scherer, Stefan; Schottenberger, Herwig; Snieckus, Victor [Heterocycles, 2020, vol. 101, # 2, p. 631 - 644]
Abstract Index Terms Substances 11 Reactions 4 Full Text
Hit Reactions 2

4 PHENYL-N-QUINOLINE DERIVATIVES FOR TREATING A RNA VIRUS INFECTION
ABIVAX; CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE; UNIVERSITE DE MONTPELLIER; INSTITUT CURIE; SCHERRER, Didier; TAZI, Jamal; MAHUTEAU-BETZER, Florence; NAJMAN, Romain; SANTO, Julien; APOLIT, Cécile - WO2020/11810, 2020, A1
Patent Family Members: EP3594206 A1; WO2020/11810 A1
Abstract Claims Front Page Info Substances 111 Reactions 50 Full Text
Hit Reactions 1

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

Reaction 1: 4-bromobenzonitrile + $\text{K}^+ \text{[t-Bu-BF}_3\text{]}^-$ → 4-(tert-butyl)benzotrile

Reaction 2: 4-bromobenzene sulfonamide + $\text{K}^+ \text{[t-Bu-BF}_3\text{]}^-$ → 4-(tert-butyl)benzene sulfonamide

Reaction 3: $\text{K}^+ \text{[t-Bu-BF}_3\text{]}^-$ + 4-bromobenzaldehyde → 4-(tert-butyl)benzaldehyde

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。

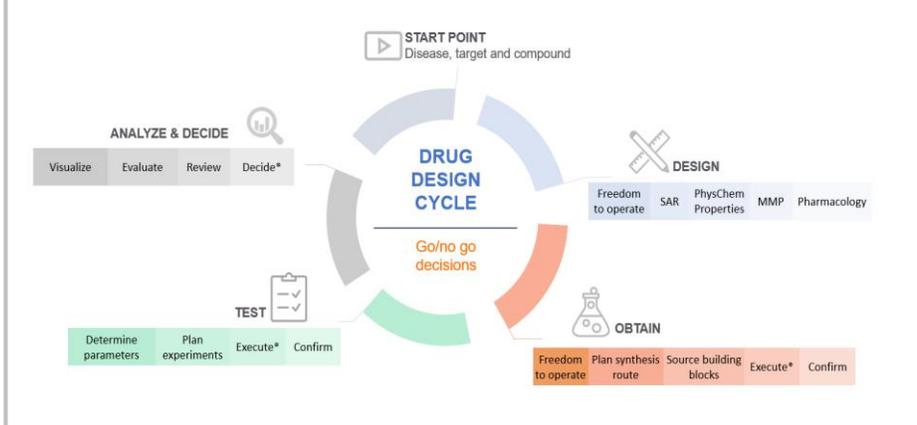
今天的内容

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- Reaxys的使用
 - Reaxys中化合物理化性质的检索
 - Reaxys中的结构面板与反应检索
 - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Reaxys已经开始嵌入药物研发流程中信息的获取, 分析, 预测

“Workflow Solution”

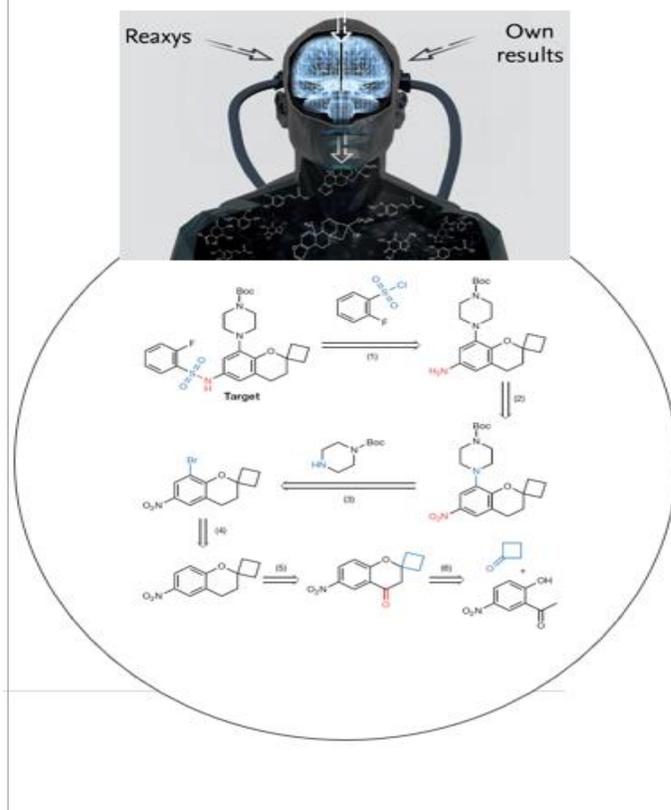
面向早期药物发现和开发的,以客户为中心的工作流解决方案



现在的Reaxys可以提供从传统数据库, AI模型预测, 专业数据服务等多种服务类型, 以满足药物研发全流程中的信息需求。

“Predictive Retrosynthesis”

基于深度神经网络算法的全新化合物合成路线设计

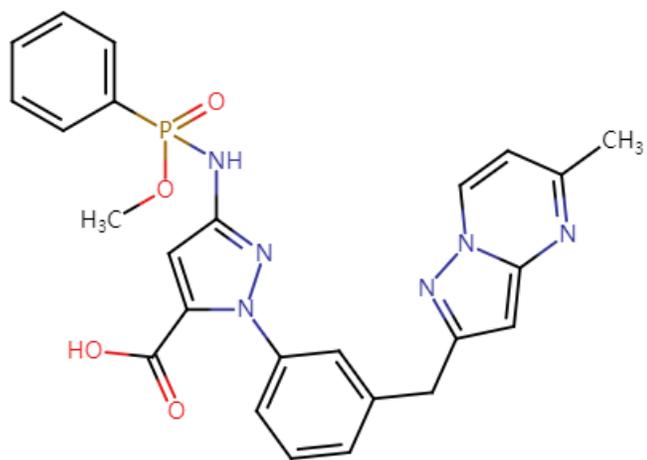


“MMP Analysis and Target Prediction”

将MMP与深度学习相结合, 预测药物可能毒性与毒性



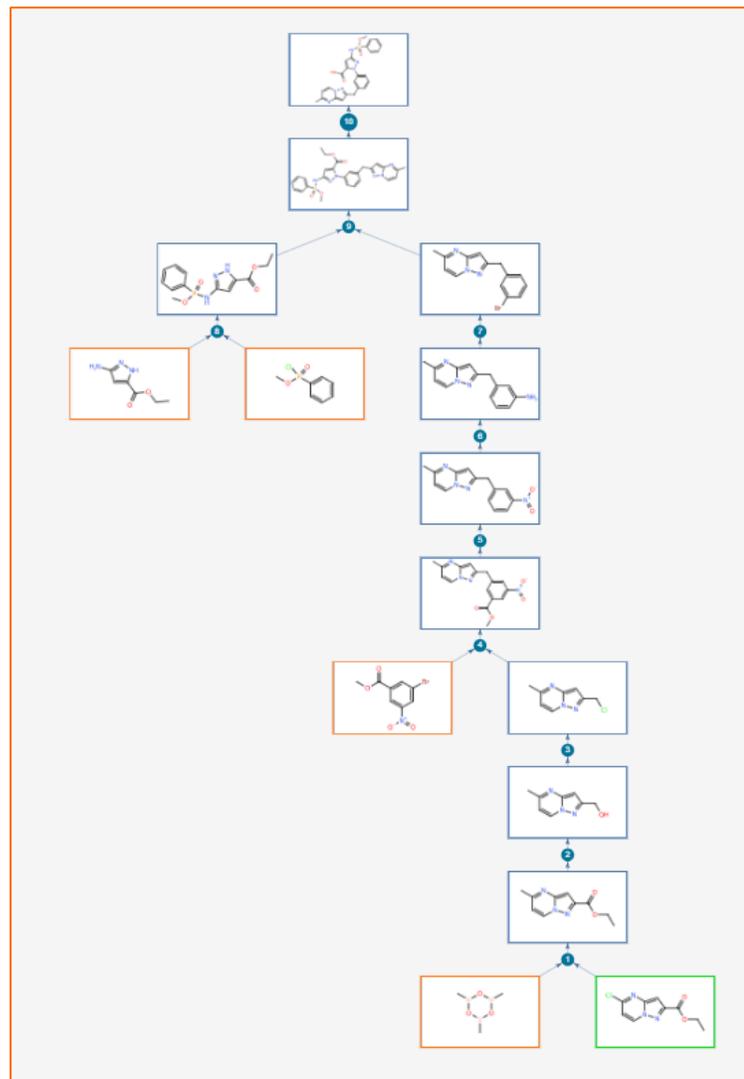
Reaxys逆合成模块



该结构是Case 3中根据现有活性化合物设计出来的全新结构，无文献报道，无合成线路报道。

Route no.	Buildingblocks to target	Route confidence score	No. of steps	View route
1		0.78	10	Table View > Tree View >
2		0.758	10	Table View > Tree View >
3		0.75	12	Table View > Tree View >

Reaxys逆合成模块结果呈现—所有起始原料都可以购买的到



Step no.	Reaction	Step confidence score	
1		0.93	Show Reaxys Examples >
2		1	Show Reaxys Examples >
3		1	Show Reaxys Examples >
4		0.96	Show Reaxys Examples >
5		1	Show Reaxys Examples >
6		1	Show Reaxys Examples >
7		0.99	Show Reaxys Examples >

2020年Reaxys变化之一—扩大专利覆盖范围与数据提炼范围

- 7 个专利机构(US, EP, WO, JP, CH, KR; TW)
- 选择性收入专利族(覆盖90%化学相关专利)
- 自动与手动的数据提炼(基于全文)
- 药物化学数据仅源自US, EP and WO
- 录入时间:
 - 自动: 5-10 days
 - 手动:
 - 30 days Reaxys
 - 45 days RMC

- 100 专利机构(from TotalPatents)
- 所有专利族
- 选择更多的专利范围, 用于手动数据提炼, (10% of additional patents expected)
- 录入时间:
 - 自动: 1-2 days
 - 手动:
 - 20 days Reaxys
 - 30 days RMC

~2019Q4

H2 2020

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
- Reaxys培训中心网址：

<https://www.elsevier.com/zh-cn/rd-solutions/pharma-and-life-sciences-solutions/life-sciences-online-training-center>

Thank you

Sam Yu(俞靚)

Elsevier Life Science Customer Consultant

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Phone: 18930408012

