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利用Reaxys快速获取海量文献和 专利中的关键化学信息

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Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的文献快速检索方法
 - Reaxys中物质理化性质的查询与结构反查
 - 利用Reaxys进行专利突破与全新分子的专利评估
 - Reaxys中结构面板详解，合成信息的检索与合成计划制作
- Q&A

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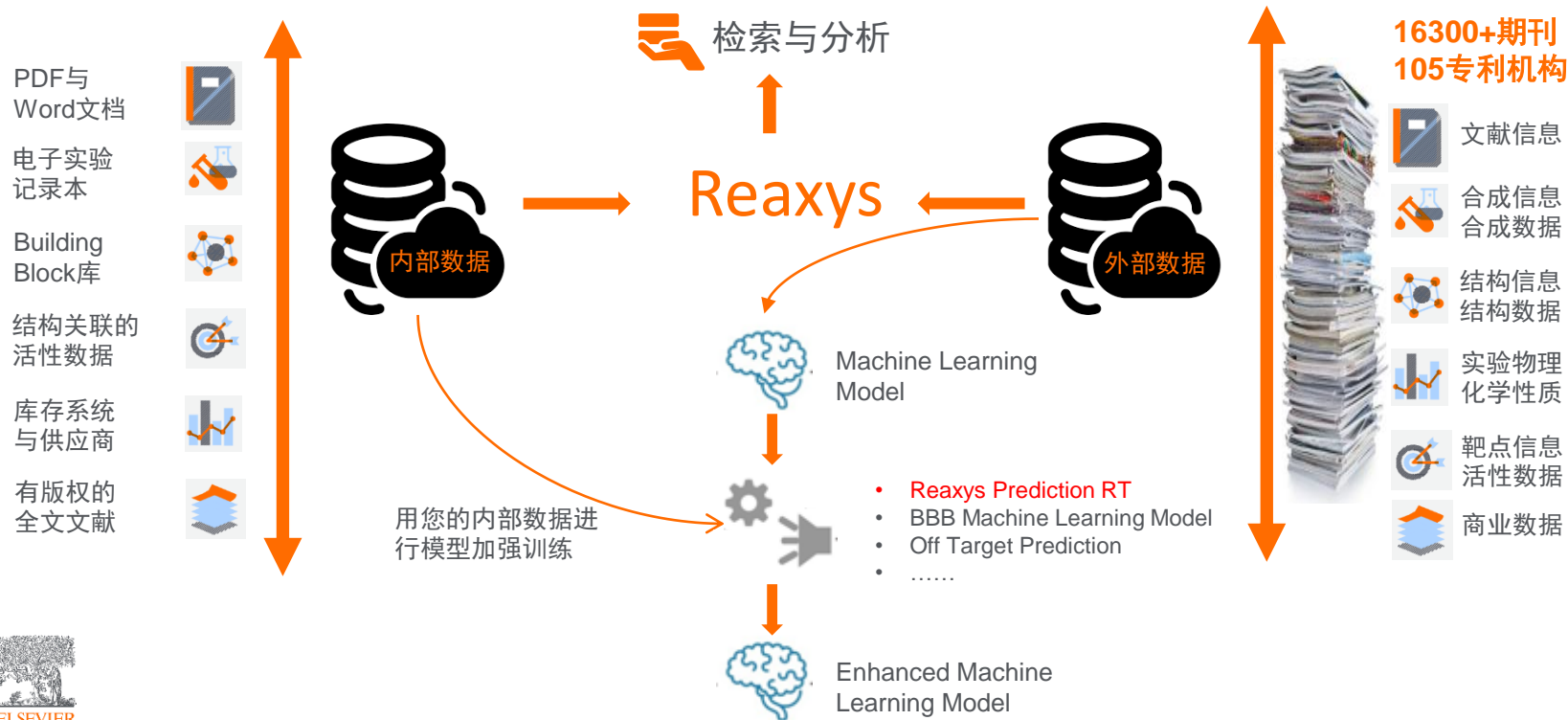
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Reaxys—从科学数据到数据科学的跨越

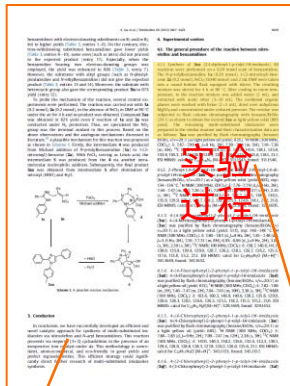
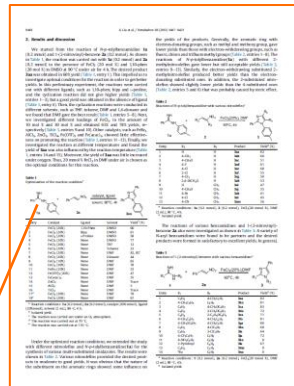
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Agenda

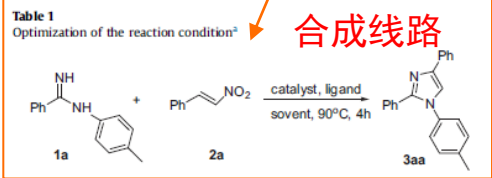
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- Q&A

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。

4.1.11. 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (3ak). 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (3ak) was purified by flash chromatography (hexanes/EtOAc, v/v=20:1) as an off white solid (yield: 41%), mp: 158–160 °C. ¹H NMR (300 MHz, CDCl₃): δ: 7.66–7.69 (d, *J*=9 Hz, 2H), 7.52–7.55 (m, 2H), 7.39–7.42 (m, 2H), 7.21–7.25 (m, 5H), 7.07–7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1. ESI HRMS: calcd for C₂₂H₁₉N₂Br [M+H]⁺: 403.0805, found: 403.0801.



- 新的催化剂
- 3+2环化加成
- 区域选择性
- 环保

3. Conclusion

In conclusion, we have successfully developed an efficient and novel catalytic approach for synthesis of multi-substituted imidazoles via nitroolefins and *N*-aryl benzamides. This reaction proceeds via stepwise [3+2] cycloaddition in the presence of an inexpensive iron catalyst under air. This methodology is convenient, atom-economical, and eco-friendly in good yields and prefect regioselectivities. This efficient strategy could significantly direct further research of multi-substituted imidazoles synthesis.

结论

实验过程

4.1. The general procedure of the reaction between nitroolefins and benzamides

4.1.1. Synthesis of 3aa (2,4-diphenyl-1-p-tolyl-1H-imidazole). All reactions were performed on a 0.20 mmol scale of benzamidine. The *N*-p-tolylbenzamide 1a (0.20 mmol), 1-(2-nitrovinyl)-benzene 2a (0.2 mmol), FeCl₃ (0.040 mmol) and 2 mL DMF were taken into a round bottom flask equipped with stirrer. The resulting mixture was stirred for 4 h at 90 °C. After cooling to room temperature, to the reaction mixture was added water (2 mL), and extracted with acetic ether (3×10 mL). The combined organic phases were washed with brine (2×5 mL), dried over anhydrous MgSO₄ and concentrated under reduced pressure. The residue was subjected to flash column chromatography with hexanes/EtOAc (20:1) as eluent to obtain the desired 3aa as light yellow solid (90% yield). The remaining multi-substituted imidazoles were

化合物性质数据

Reaxys对这篇全文的提炼—概览

Iron(III)-catalyzed synthesis of multi-substituted imidazoles via [3+2] cycloaddition reaction of nitroolefins and N-aryl benzamidines Cited 38 times

Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421]

Abstract [Index Terms](#) [Substances](#) (49) [Reactions](#) (23) [Full Text](#)

Abstract

A novel and efficient iron(III)-catalyzed synthesis of multi-substituted imidazoles via [3+2] cycloaddition of nitroolefins and N-aryl benzamidines under the air atmosphere had been developed. This methodology is convenient, atom-economical, general, and eco-friendly in good yields and perfect regioselectivities.

Index Terms

EMTREE drug term: 1,4 diphenyl 2 [4 (trifluoromethyl)phenyl] 1h imidazole • 2 (1,4 diphenyl 1h imidazol 2 yl)pyridine • 2 phenyl 1 (4 tolyl) 4 [4 (trifluoromethyl)phenyl] idazole • 2 phenyl 1,4 di(4 tolyl) 1h imidazole • 2,4 diphenyl 1 (4 tolyl) 1h imidazole • 4 (2 chlorophenyl) 2 phenyl 1 (4 tolyl) 1h imidazole • 4 (2,4 dimethoxyphenyl) 2 ph (4 tolyl) 1h imidazole • 4 (4 bromophenyl) 5 methyl 2 phenyl 1 (4 tolyl) 1h imidazole • 4 (4 chlorophenyl) 2 phenyl 1 (4 tolyl) 1h imidazole • 4 (4 chlorophenyl) 5 methyl 2 phenyl 1 (4 tolyl) 1h imidazole • 4 (4 fluorophenyl) 2 phenyl 1 (4 tolyl) 1h imidazole • 4 (4 methoxyphenyl) 2 phenyl 1 (4 tolyl) 1h imidazole • 4 [5 methyl 2 phenyl 1 (4 tolyl) 1h i 4 yl]benzonitrile • 5 methyl 2 phenyl 1,4 di(4 tolyl) 1h imidazole • alkene derivative • benzamide derivative • ferric ion • imidazole derivative • ligand • nitroolefin der • unclassified drug

EMTREE medical term: article • atmosphere • catalysis • catalyst • cycloaddition • drug structure • drug synthesis • green chemistry • priority journal • reaction optim • solvent effect • substitution reaction

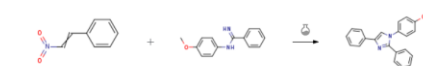
Author keyword: Benzamidines • Cycloaddition • Iron-catalyzed • Multi-substituted imidazoles • Nitroolefins

Reaxys index Terms: Fluorescence • Michael addition • cyclization reaction • cycloaddition • nucleophilic addition • organic reaction • oxidative cyclization • steric effe

23 Reactions out of 1 Documents, containing 49 Substances, 0 Targets

selected Sort by Reaxys Ranking

Limit To Exclude Export Hide Conditions

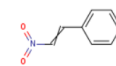


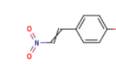
11 Hits 3 Conditions Find Similar Reaction ID: 35243549

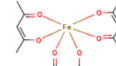
Conditions	Yield	Reference
With iron(III) chloride in N,N-dimethyl-formamide at 90°C, for 4h; Green chemistry; regioselective reaction; Experimental Procedure	85%	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract

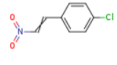
[+ Show all conditions](#) 1 hit out of 1

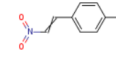
1 Cl_3Fe

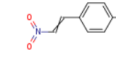
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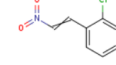
3 

4 

5 

6 

7 

8 

- Reaxys提炼全文中的：
- 题录，摘要，关键词
 - 物质结构，
 - 反应Scheme

Reaxys对全文中的化合物（产物）的相关数据提炼

4.1.11. 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (3ak). 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (3ak) was purified by flash chromatography (hexane/EtOAc, v/v=20:1) as an off white solid (yield: 41%), mp: 158–160 °C. ¹H NMR (300 MHz, CDCl₃): δ: 7.66–7.69 (d, J=9 Hz, 2H), 7.52–7.55 (m, 2H), 7.39–7.42 (m, 2H), 7.21–7.25 (m, 5H), 7.07–7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1. ESI HRMS: calcd for C₂₂H₁₉N₂Br [M+H]⁺: 403.0805, found: 403.0801.

4-(4-bromophenyl)-5-methyl-2-phenyl-1-(p-tolyl)-1H-imidazole
 C₂₂H₁₉N₂ 403.321 24040362 1462876-22-7

Hit Data - 6 Druglikeness Spectra - 3
 Identification Physical Data - 2

^ NMR Spectroscopy - 2 hits out of 2

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Original Text (NMR Spectroscopy)
Chemical shifts, Spectrum	¹ H	chloroform-d1	300	¹ H NMR (300 MHz, CDCl ₃): δ: 7.66-7.69 (d, J=9 Hz, 2H), 7.52-7.55 (m, 2H), 7.39-7.42 (m, 2H), 7.21-7.25 (m, 5H), 7.07-7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H)
Chemical shifts, Spectrum	¹³ C	chloroform-d1	100	¹³ C NMR (100 MHz, CDCl ₃): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1

Description (Mass Spectrometry)

high resolution mass spectrometry (HRMS), electrospray ionisation (ESI), spectrum

^ Hit Data - 6

- ✓ 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
- ✓ Mass Spectrometry - 1 hits out of 1

Label

3ak

Melting Point, °C

158 - 160

Colour & Other Properties

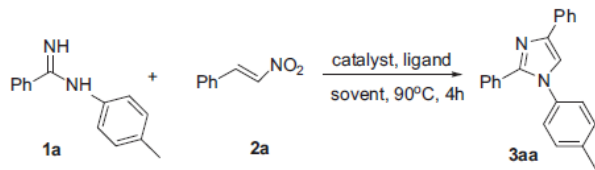
white

Peak

403.0801 m/z

Reaxys对全文中的化合物（催化剂）的相关数据提炼

Table 1
Optimization of the reaction condition^a



Entry	Catalyst	Ligand	Solvent	Yield ^b (%)
1	FeCl ₃ (20%)	1,10-Phen	DMSO	60
2	FeCl ₃ (20%)	Bipy	DMSO	61
3	FeCl ₃ (20%)	L-Proline	DMSO	58
4	FeCl ₃ (20%)	None	DMSO	77
5	FeCl ₃ (20%)	None	THF	12
6	FeCl ₃ (20%)	None	Toluene	23
7	FeCl ₃ (20%)	None	DMF	82, 82 ^c
8	FeCl ₃ (20%)	None	Dioxane	44
9	FeCl ₃ (10%)	None	DMF	65
10	FeCl ₃ (30%)	None	DMF	78
11	FeBr ₃ (20%)	None	DMF	53
12	Fe(OTf) ₃ (20%)	None	DMF	47
13	Fe(acac) ₃	None	DMF	55
14	ZnCl ₂	None	DMF	Trace
15	AlCl ₃	None	DMF	5
16	TiCl ₄	None	DMF	Trace
17 ^d	FeCl ₃ (20%)	None	DMF	79
18 ^e	FeCl ₃ (20%)	None	DMF	67

^a Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), catalyst (20% mmol), ligand (20%mmol), solvent (2 mL), 90 °C, 4 h.

^b Isolated yield.

^c The reaction was carried out under an O₂ atmosphere.

^d The reaction was carried out at 70 °C.

^e The reaction was carried out at 110 °C.

Cl₃Fe

iron(III) chloride

Cl₃Fe 162.206 11323458 Retrieve CAS RN

[Hit Data - 4](#) [Physical Data - 26](#)

[Identification](#) [Spectra - 58](#)

[Druglikeness](#) [Other Data - 128](#)

[Bioactivity \(All\)](#)

Hit Data - 4

Catalyst Investigation - 4 hits out of 303

Show/Hide columns

Investigated characteristic(s)	Specification of catalysis	Type of reaction (Catalyst Investigation)	Co-catalyst/co-substrate name	Reference
Catalytic activity	Regioselective catalysis	Cycloaddition		Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	[2,2]bipyridinyl	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	1,10-Phenanthroline	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	L-proline	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract

Reaxys对全文中的合成线路的相关数据提炼

Table 2
Reactions of *N*-*p*-tolylbenzimidine with various nitroolefins^a

Entry	R ₃	R ₄	Product	Yield ^b (%)
1	H	H	3a	82
2	4-CH ₃	H	3ab	60
3	4-CH ₃ O	H	3ac	51
4	4-F	H	3ad	61
5	4-Cl	H	3ae	68
6	2-Cl	H	3af	55
7	4-CF ₃	H	3ag	50
8	2,4-DiCH ₃ O	H	3ah	53
9	H	CH ₃	3ai	47
10	4-CH ₃ O	CH ₃	3aj	35
11	4-Br	CH ₃	3ak	41
12	4-Cl	CH ₃	3al	45
13	4-CN	CH ₃	3am	56

3. Conclusion

In conclusion, we have successfully developed an efficient and novel catalytic approach for synthesis of multi-substituted imidazoles via nitroolefins and *N*-aryl benzimidines. This reaction proceeds via stepwise [3+2] cycloaddition in the presence of an inexpensive iron catalyst under air. This methodology is convenient, atom-economical, and **eco-friendly** in good yields and perfect **regioselectivities**. This efficient strategy could significantly direct further research of multi-substituted imidazoles synthesis.

1 Hits/Conditions [Find Similar](#) > Reaction ID: 36429699

Conditions	Yield	Reference
With iron(III) chloride in <i>N,N</i> -dimethyl-formamide at 90°C; for 4h; Green chemistry; regioselective reaction;	41%	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract >

[Experimental Procedure](#) >

11 The general procedure of the reaction between nitroolefins and benzimidines

General procedure: 4.1.1 Synthesis of **3aa** (2,4-diphenyl-1-*p*-tolyl-1*H*-imidazole) All reactions were performed on a 0.20mmol scale of benzimidine. The *N*-*p*-tolylbenzimidine **1a** (0.20mmol), 1-(2-nitrovinyl)-benzene **2a** (0.2mmol), FeCl₃ (0.040mmol) and 2mL DMF were taken into a round bottom flask equipped with stirrer. The resulting mixture was stirred for 4h at 90°C. After cooling to room temperature, to the reaction mixture was added water (2mL), and extracted with acetic ether (3x10mL). The combined organic phases were washed with brine (2x5mL), dried over anhydrous MgSO₄ and concentrated under reduced pressure. The residue was subjected to flash column chromatography with hexanes/EtOAc (20:1) as eluent to obtain the desired **3aa** as light yellow solid (90% yield). The remaining multi-substituted imidazoles were prepared in the similar manner and their characterization data are as follows: **3aa** was purified by flash chromatography (hexane/EtOAc, v/v=20:1) as light yellow oil (yield: 82%). 4.1.1.1
4-(4-Bromophenyl)-5-methyl-2-phenyl-1-*p*-tolyl-1*H*-imidazole (**3ak**)
4-(4-Bromophenyl)-5-methyl-2-phenyl-1-*p*-tolyl-1*H*-imidazole (**3ak**) was purified by flash chromatography (hexane/EtOAc, v/v=20:1) as an off white solid (yield: 41%), mp: 158-160 °C. ¹H NMR (300 MHz, CDCl₃): δ: 7.66-7.69 (d, J=9 Hz, 2H), 7.52-7.55 (m, 2H), 7.39-7.42 (m, 2H), 7.21-7.25 (m, 5H), 7.07-7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1. ESI HRMS: calcd for C₂₂H₁₉N₂Br [M+H]⁺: 403.0805, found: 403.0801.

实验过程与条件

Reaxys从文献中提炼出来的内容

文献记录:

>94.7 million

16300+期刊

105专利机构的专利

38万书的章节

化合物记录:

>170 million

期刊, 专利, 商品

2022年中前完成
105家专利机构中
专利物质的回溯

化学反应记录:

>57.8 million

单步多步反应, 同
时提炼文献与专利
中的实验过程

实验性质记录:

> 500 million

化合物实验数据,
并提炼实验数据检
测条件

生物活性记录:

> 41.9 million数据

> 35,000靶点

> 7.9 million化合物

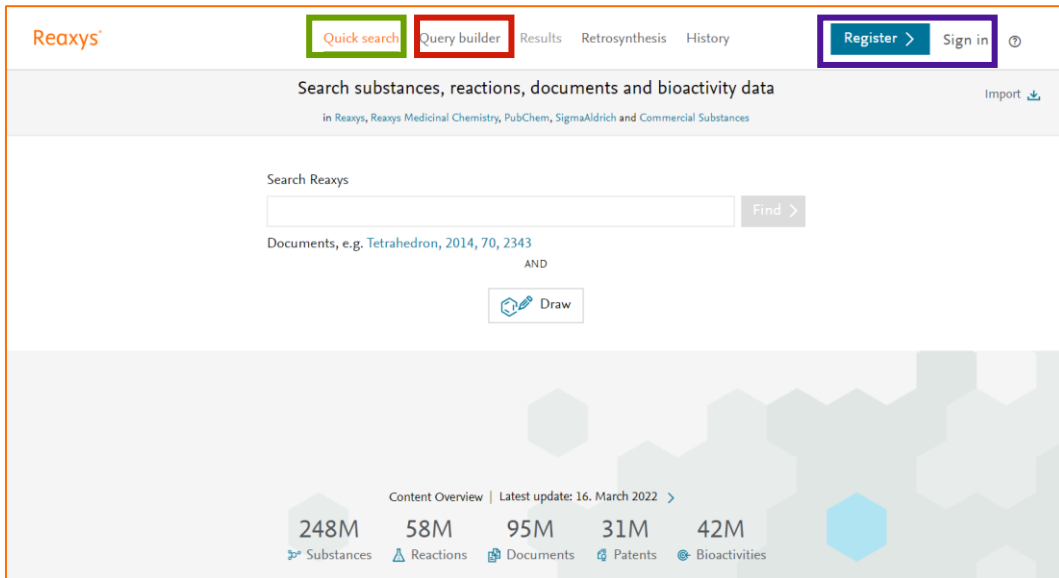
化合物在不同生物
体内活性数据

Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- **Reaxys中的化学科学数据获取**
 - Reaxys中的文献快速检索方法
 - Reaxys中物质理化性质的查询与结构反查
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Reaxys的登录界面

- IP范围内，浏览器输入www.Reaxys.com或asia.Reaxys.com,可以直接进行检索，推荐Chrome，Firefox浏览器。



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

Quick Search界面

The screenshot shows the Reaxys Quick Search interface. At the top, there is a navigation bar with the Reaxys logo, a 'Quick search' dropdown menu, and links for 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. On the right side of the navigation bar, the user's name 'Sam Yu' is displayed along with user and help icons.

Below the navigation bar is a search header area with the text 'Search substances, reactions, documents and bioactivity data' and an 'Import' button with a download icon. A sub-header indicates the search scope: 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances'.

The main search area features a 'Search Reaxys' input field with a 'Find >' button. An orange arrow points to this input field with the text: '可以输入关键词，物质名称，人名反应，以及各类组合' (Keywords, substance names, person names, reactions, and various combinations can be entered).

Below the search field, there is a 'Draw' button with a chemical structure icon. An orange arrow points to this button with the text: '可以输入具体结构，骨架结构，通式结构，以及包含上述结构的反应式进行检索' (Specific structures, skeletal structures, general structures, and reaction schemes containing these structures can be entered for search).

At the bottom of the interface, there is a 'Content Overview' section with the text 'Latest update: 16. March 2022 >'. Below this, five statistics are displayed: 248M Substances, 58M Reactions, 95M Documents, 31M Patents, and 42M Bioactivities.

Reaxys中的Query Builder是一种高级的组合检索模式

The screenshot displays the Reaxys Query Builder interface. At the top, there is a navigation bar with 'Quick search', 'Query builder' (selected), 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user 'Sam Yu' is logged in. Below the navigation bar, there is a search bar with 'Reactions' selected, and buttons for 'Targets', 'Substances', and 'Documents'. A toolbar contains 'Import', 'Save', 'Reset form', and 'Delete all'. Below the toolbar, there are icons for 'Current Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main area is a large grid with the text 'Drag & Drop to build a new query'. On the right side, there is a sidebar with 'Search fields' and a search icon. The sidebar includes 'Fields', 'Forms', 'History', 'Reaxys', 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'.

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

Query Builder的使用步骤，第一步是选择字段，第二步是输入条件，第三步是确定不同字段之间的逻辑关系

Agenda

- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - **Reaxys中的文献快速检索方法**
 - Reaxys中物质理化性质的查询与结构反查
 - 利用Reaxys进行专利突破与全新分子的专利评估
 - Reaxys中结构面板详解，合成信息的检索与合成计划制作
- Q&A

Case 1: 关键词检索—千金藤素 Covid-19

- Cepharanthine Covid-19

Quick search Query builder Results Retrosynthesis History Alerts

Search for Cepharanthine Covid-19

Search Reaxys

Cepharanthine Covid-19






Substance Properties, e.g. solubility of vitamin D3
AND

Content Overview | Latest update: 03. June 2022 >

257M	58M	97M	32M	42M
Substances	Reactions	Documents	Patents	Bioactivities

Reaxys中的检索结果

Results for Cepharanthine Covid-19 New Edit

 72 Documents	Filters Limit to > Exclude > Publication Year Document Type Authors/Inventors Current Patent Assignee Patent Office Journal Title Substance Classes Reaction Classes Index Terms (List) Index Terms (ReaxysTree) <input type="checkbox"/> Manually processed content only	93 Documents with 730 Substances, 0 Reactions, 10 Targets <input type="checkbox"/> 0 selected Limit To Exclude Export	<input type="checkbox"/> 1 SARS-CoV-2 M ^{PRO} inhibitors: identification of anti-SARS-CoV-2 M ^{PRO} compounds from FDA approved drugs Cited 11 times Bharadwaj, Shiv; Azhar, Esam Ibraheem; Kamal, Mohammad Amjad; Bajrai, Leena Hussein; Dubey, Amit; Jha, Kanupriya; Yadava, Umesh; Kang, Sang Gu; Dwivedi, Vivek Dhar [Journal of Biomolecular Structure and Dynamics, 2022, vol. 40, # 6, p. 2769 - 2784] Abstract Index Terms Full Text
 27 Substances		<input type="checkbox"/> 2 Trace Minerals, Vitamins and Nutraceuticals in Prevention and Treatment of COVID-19 Cited 4 times Srivastava, Ajay; Gupta, Ramesh C.; Doss, Robin B.; Lall, Rajiv [Journal of Dietary Supplements, 2022, vol. 19, # 3, p. 395 - 429] Abstract Index Terms Substances 12 Full Text	
 921 Documents		<input type="checkbox"/> 3 Computer-aided evaluation of anti-sars-cov-2 (3-chymotrypsin-like protease and transmembrane protease serine 2 inhibitors) activity of cepharanthine: An in silico approach Jain, Divya; Hossain, Rajib; Khan, Rasel Ahmed; Dey, Dipta; Toma, Tanzila Rahman; Islam, Mohammad Torequl; Janmeda, Pracheta; Hakeem, Khalid Rehman [Biointerface Research in Applied Chemistry, 2022, vol. 12, # 1, p. 768 - 780] Abstract Index Terms Substances 11 Full Text	
 241,484 Documents		Abstract hit: {...outbreak of COVID-19 pandemic caused by severe acute respiratory syndrome-Coronavirus-2 (SARS-CoV-2) has raised...}	
 1 Commercial Substances		Index Terms hit: {...Author keyword: COVID-19, drug repurposing...}	

Abstract hit: {...disease 2019 (COVID-19) was first officially diagnosed in the city of Wuhan, China...}

Index Terms hit: {...Author keyword: cepharanthine, coagulopathy...}

Abstract hit: {...molecular docking. Cepharanthine (CEP) exhibits antiviral activity in SARS-CoV at 9.5 µg/mL IC₅₀...}

Index Terms hit: {...3CL^{PRO}, Cepharanthine, COVID-19...}

Reaxys中对于文献检索结果的分析

The screenshot displays the Reaxys search results analysis interface, showing a sidebar with filter categories and four main panels for detailed filter views.

Filters Sidebar:

- 93
- Preview
- Limit to > Exclude >
- Publication Year
- Document Type
- Authors/Inventors
- Current Patent Assignee
- Patent Office
- Journal Title
- Substance Classes
- Reaction Classes
- Index Terms (List)
- Index Terms (ReaxysTree)
- Manually processed content only

Publication Year Panel:

Year	Count
<input type="checkbox"/> 2022	7
<input type="checkbox"/> 2021	36
<input type="checkbox"/> 2020	28

Filter by value ▾

Document Type Panel:

Document Type	Count
<input type="checkbox"/> review	33
<input type="checkbox"/> article	32
<input type="checkbox"/> patent	3
<input type="checkbox"/> note	1
<input type="checkbox"/> letter	1
<input type="checkbox"/> editorial	1

Current Patent Assignee Panel:

Assignee	Count
<input type="checkbox"/> rigel pharmaceuticals inc	1
<input type="checkbox"/> kowa company, ltd	1
<input type="checkbox"/> institut pasteur	1
<input type="checkbox"/> (no entry given)	68

Filter by value ▾

Journal Title Panel:

Journal Title	Count
<input type="checkbox"/> frontiers in pharmacology	7
<input type="checkbox"/> pharmacological reports	4
<input type="checkbox"/> pharmaceuticals	3
<input type="checkbox"/> molecules	2
<input type="checkbox"/> journal of medical virology	2
<input type="checkbox"/> current pharmaceutical d...	2
<input type="checkbox"/> current medicinal chemistry	2

Filter by value ▾ View more

Index Terms (List) Panel:

Clear selected ✕ ↓ ↑ Sort by Occurrence ▾ ✕

Index Term	Count
<input type="checkbox"/> agent	33
<input type="checkbox"/> antiviral	29
<input type="checkbox"/> occurrence	22
<input type="checkbox"/> nature	22
<input type="checkbox"/> in	22
<input type="checkbox"/> toxicity	16
<input type="checkbox"/> drug	16
<input type="checkbox"/> property	15
<input type="checkbox"/> pharmacokinetics	15
<input type="checkbox"/> structure	14
<input type="checkbox"/> pharmacological	14

1 2 3 ... 11 > Go to page > Limit to > Exclude >

Reaxys中的Index Terms (Reaxys Tree) 学科分类

71

Filters

Limit to > Exclude >

Preview

Publication Year ▾

Document Type ▾

Authors/Inventors ▾

Current Patent Assignee ▾

Patent Office ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

Index Terms (List) ▾

Index Terms (Reaxys Tree) 学科分类

Manually processed content only

ELSEVIER

Index Terms (ReaxysTree) ^

physico chemical proper... 41

chemical transformations 36

physico chemical analysi... 14

quantum chemical calcula... 7

[View more](#)

Index Terms (ReaxysTree) X

Index Terms (ReaxysTree)

- Index Terms (ReaxysTree) 72
- physico chemical properties 41
- chemical transformations 36
- physico chemical analysis methods 14
- quantum chemical calculation methods 7

Clear selected X

Limit to > Exclude >

利用树状图进行学科分类

Index Terms (ReaxysTree) ✕

- Index Terms (ReaxysTree) 72
 - physico chemical properties 41
 - chemical transformations 36
 - physico chemical analysis methods 14
 - quantum chemical calculation methods 7

点击箭头展开层级

Clear selected ✕ Lim

Index Terms (ReaxysTree) 4 ✕

- Index Terms (ReaxysTree) 72
 - physico chemical properties 41
 - chemical property 28
 - phase property 16
 - electrochemical property 9
 - acid / base behaviour 9
 - acidity 4
 - pKa 1
 - pH value 1
 - neutralization 4
 - protonation 1
 - substance spectroscopy 6
 - thermodynamic property 3

Selected search items:
acidity ✕

Clear selected ✕ 选择获取或者排除 Limit to > Exclude >

最后的检索结果

Computer-aided evaluation of anti-sars-cov-2 (3-chymotrypsin-like protease and transmembrane protease serine 2 inhibitors) activity of cepharanthine: An in silico approach

Jain, Divya; Hossain, Rajib; Khan, Rasel Ahmed; Dey, Dipta; Toma, Tanzila Rahman; Islam, Mohammad Torequl; Janmeda, Pracheta; Hakeem, Khalid Rehman [Biointerface Research in Applied Chemistry, 2022, vol. 12, # 1, p. 768 - 780]

Abstract [Index Terms](#) [Substances](#) 11 [Full Text](#)

全文链接，如果是OA或者学校已经订购可以直接打开

Abstract

3-chymotrypsin-like protease (3CL^{PRO}) is found in severe acute respiratory syndrome coronavirus (SARS CoV)-2, and transmembrane protease serine 2 (TMPRSS-2) in humans, both of them have a role in viral attachment and proliferation. 3CL^{PRO} and TMPRSS-2 are the most vital target for the discovery of an anti-corona virus. One efficient approach used to screen potential active compounds against specific target proteins, such as 3CL^{PRO} and TMPRSS-2, is molecular docking. Cepharanthine (CEP) exhibits antiviral activity in SARS-CoV at 9.5 μg/mL IC₅₀ level. This study aims to perform an in silico study on CEP against non-structural SARS-CoV-2 3CL^{PRO} and host transmembrane protease serine 2 protein. Molecular docking studies were carried out using compounds against 3CL^{PRO} and TMPRSS-2 proteins through Swiss model, Uniport, PROCHECK, Swiss PDB viewer, PyMol, and PyRx computerized software. CEP displayed strong binding interactions-8.5 and-7.4 Kcal/mol with the 3CL^{PRO}, and TMPRSS-2 proteins. In all cases, CEP showed better binding affinities than FDA-approved anti-corona virus drug (Camostat mesylate, CAM) is currently underused in COVID-19. CEP may be one of the potentials leads to fighting against SARS-CoV-2. Further in vivo studies should be required to support the findings of this study.

Index Terms

Author keyword: 3CL^{PRO} • Cepharanthine • COVID-19 • Molecular docking • PkCSM, Swiss-ADME • TMPRSS2

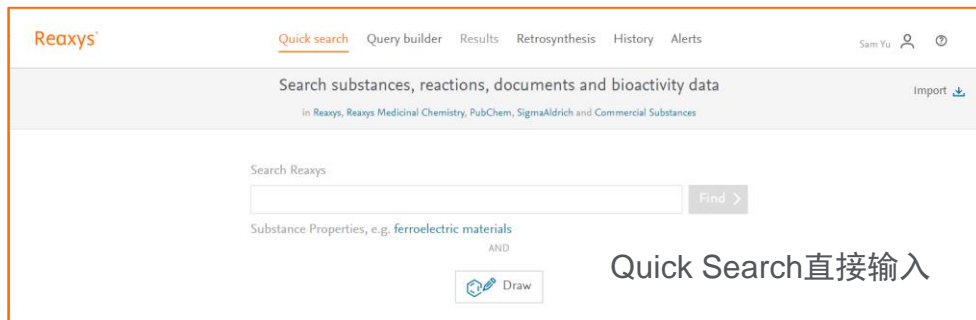
Reaxys Index Terms: Hydrogen bond • IC50 • LD50 • Permeability • Pi-pi interaction • antiviral agent • bioavailability • hydrophobic surface • hydrophobicity • lipophilicity • occurrence in nature • pharmacokinetics • reactivity • toxicity

Agenda

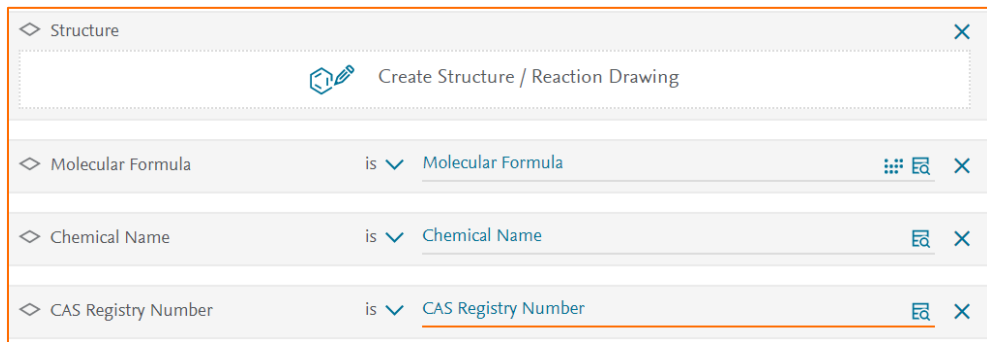
- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的文献快速检索方法
 - **Reaxys中物质理化性质的查询与结构反查**
 - 利用Reaxys进行专利突破与全新分子的专利评估
 - Reaxys中结构面板详解，合成信息的检索与合成计划制作
- Q&A

Reaxys中的结构获取物质的常用方法小结

- Reaxys中获取物质的方法
 - 物质名称
 - 物质分子式
 - 物质结构式
 - CAS No



Quick Search直接输入



Query Builder选择不同字段

Case 2: Reaxys中化合物理化性质的快速获取

The screenshot shows the Reaxys search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' are in the center. On the right, the user name 'Sam Yu' and profile icons are visible. Below the navigation bar, a search bar contains the text 'solubility of gefitinib' with a 'Find >' button. Above the search bar, the text 'Search for solubility of gefitinib' and an 'Import' button are present. Below the search bar, the text 'Search Reaxys' is followed by a dropdown menu showing 'solubility of gefitinib'. Below the dropdown, the text 'Substance Properties, e.g. solubility of vitamin D3' and 'AND' are displayed. A 'Draw' button is also visible. At the bottom, a 'Content Overview' section shows the latest update date as '16. March 2022' and five categories with their respective counts: 248M Substances, 58M Reactions, 95M Documents, 31M Patents, and 42M Bioactivities.

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Sam Yu

Search for solubility of gefitinib Import

Search Reaxys

solubility of gefitinib Find >

Substance Properties, e.g. solubility of vitamin D3

AND

Draw

Content Overview | Latest update: 16. March 2022 >

248M 58M 95M 31M 42M

Substances Reactions Documents Patents Bioactivities

Tips:

快速获取某个化合物溶解性数据。

Reaxys中的结果

Reaxys Quick search Query builder Results Retrosynthesis History Alerts

Results for solubility of gefitinib

- 1 Substances Structure: as drawn AND Property: solubility
- 417 Documents Titles, Abstracts, keywords: 'solubility', 'gefitinib'
- 569,958 Documents Titles, Abstracts, keywords: 'solubility'
- 33,750 Documents Titles, Abstracts, keywords: 'gefitinib'
- 6 Commercial Substances Structure: as drawn AND Property: solubility

gefitinib
C22H24N4ClFO3 446.909 8949523 184475-35-2

Hit Data - 6
 Identification
 Druglikeness
 Bioactivity (All)

Physical Data - 123
 Spectra - 89
 Other Data - 4,498

Preparations - 85
 Reactions - 164
 Targets - 1,170
 Documents - 12,124

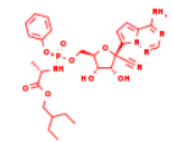
Hit Data - 6
 Solubility (MCS) - 6 hits out of 6

抽提的数据包括具体的数值，
或者相关的文字性描述

Solubility (MCS) - 6 hits out of 6

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent/Solubility (MCS)	Location	Comment (Solubility (MCS))	Reference
	in pure solvent	37	aq. phosphate buffer		Solubility: 0.05 g/100g solvent	Sun, Yamin <i>Journal of the Indian Chemical Society</i> , 2022, vol. 99, # 1, art. no. 100260 Full Text Details Abstract
					soluble in water, pH dependent water solubility	Alamy, Raid G.; Fletcher, John; Khoder, Mouhamad; Mustafa, Wesam W. <i>JAAPS PharmSciTech</i> , 2022, vol. 23, # 1, art. no. 48 Full Text Details Abstract
					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; Shaheer, Fayaz <i>Journal of Molecular Liquids</i> , 2020, vol. 299, art. no. 112211 Full Text Cited 44 times Details Abstract
					soluble in water and 1-octanol	Wu, Kuen-Da; Chen, Grace Shihyuy; 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 6 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 Cited 2 times Details Abstract
0.0021	in pure solvent	20	water			Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Wei; Dong, Xiaochun <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, vol. 23, # 19, p. 5385-5388 Full Text Cited 28 times Details Abstract

Reaxys中理化性质



1

[Shopping Cart](#) [Close](#) [Zoom](#) [More](#) [Add to Favorites](#)

(2S)-2-ethylbutyl 2-(((S)-(((2R,3S,4R,5R)-5-(4-aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-5-cyano-3,4-dihydroxytetrahydrofuran-2-yl)methoxy)(phenoxy)phosphoryl)amino)propanoate

C₂₇H₃₅N₆O₈P 602.584 29506468 1809249-37-3

[Identification](#) [Bioactivity \(All\)](#) [Spectra - 21](#) [Preparations - 79 >](#)
[Druglikeness](#) [Physical Data - 20](#) [Other Data - 89](#) [Reactions - 85 >](#)
[Targets - 14 >](#)
[Documents - 108 >](#)

Physical Data - 20

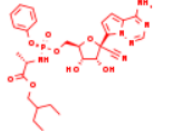
- [Melting Point - 3](#)
- [Chromatographic Data - 6](#)
- [Crystal Phase - 3](#)
- [Crystal Property Description - 3](#)
- [Optical Rotatory Power - 2](#)
- [Space Group - 3](#)

Optical Rotatory Power - 2

[Show/Hide columns v](#)

Type (Optical Rotatory Power)	Concentration (Optical Rotatory Power)	Length of Path, cm	Solvent (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength (Optical Rotatory Power), nm	Temperature (Optical Rotatory Power), °C	Location	Reference
[alpha]	0.2 g/100ml	5	dichloromethane	-24	589	25	supporting information	Chen, Jianzhong; Huo, Xiaohong; Li, Panpan; Wang, Mo; Wu, Zhengxing; Yuan, Qianjia; Zhang, Lu; Zhang, Wanbin; Zhang, Zhenfeng; Zou, Yashi [<i>Angewandte Chemie - International Edition</i> , 2020, vol. 59, # 47, p. 20814 - 20819][<i>Angew. Chem.</i> , 2020, vol. 132, # 47, p. 21000 - 21005,6] Full Text Cited 18 times Details > Abstract >
[alpha]	1 g/100ml		methanol	-21	589	21		Siegel, Dustin; Hui, Hon C.; Doerffler, Edward; Clarke, Michael O.; Chun, Kwon; Zhang, Lijun; Neville, Sean; (...); Warren, Travis K.; Mackman, Richard L. [<i>Journal of Medicinal Chemistry</i> , 2017, vol. 60, # 5, p. 1648 - 1661] Full Text Cited 302 times Details > Abstract >

Reaxys中的谱图



(2S)-2-ethylbutyl 2-(((S)-(((2R,3S,4R,5R)-5-(4-aminopyrrolo[2,1-f[1,2,4]triazin-7-yl)-5-cyano-3,4-dihydroxytetrahydrofuran-2-yl)methoxy)(phenoxy)phosphoryl)amino)propanoate
C₂₇H₃₅N₆O₈P 602.584 29506468 1809249-37-3

Identification Bioactivity (All) Spectra - 21 Preparations - 79 >
Druglikeness Physical Data - 20 Other Data - 89 Reactions - 85 >
Targets - 14 >
Documents - 108 >

Spectra - 21

- ✓ NMR Spectroscopy - 15
- ✓ IR Spectroscopy - 1
- ✓ Mass Spectrometry - 5

NMR Spectroscopy - 15 Show/Hide columns ▾

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	¹ H	d(4)-methanol	600	supporting information	Gannedi, Veeranjanyulu; Villuri, Bharath Kumar; Reddy, Sivakumar N.; Ku, Chiao-Chu; Wong, Chi-Huey; Hung, Shang-Cheng]Journal of Organic Chemistry, 2021, vol. 86, # 7, p. 4977 - 4985 Full Text ↗ Cited 4 times ↗ Details > Abstract >
Chemical shifts	¹³ C	chloroform-d1	151	supporting information	Gannedi, Veeranjanyulu; Villuri, Bharath Kumar; Reddy, Sivakumar N.; Ku, Chiao-Chu; Wong, Chi-Huey; Hung, Shang-Cheng]Journal of Organic Chemistry, 2021, vol. 86, # 7, p. 4977 - 4985 Full Text ↗ Cited 4 times ↗ Details > Abstract >
Chemical shifts, Spectrum	¹³ C	chloroform-d1	151	supporting information	Gannedi, Veeranjanyulu; Villuri, Bharath Kumar; Reddy, Sivakumar N.; Ku, Chiao-Chu; Wong, Chi-Huey; Hung, Shang-Cheng]Journal of Organic Chemistry, 2021, vol. 86, # 7, p. 4977 - 4985 Full Text ↗ Cited 4 times ↗ Details > Abstract >

Case 3: 特定条件下理化性质的获取

- 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

The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs: "Quick search", "Query builder" (active), "Results", "Synthesis planner", and "History". On the right, there are "Register" and "Sign in" buttons. Below the navigation, there is a "Search in:" section with buttons for "Reactions", "Targets", "Substances", and "Documents". A toolbar contains icons for "Import", "Save", "Reset form", and "Delete all". The main search area shows a query structure: "Molecular Formula" is linked to "Molecular Formula" with the operator "is". Below this, a blue "AND" button is followed by a "Solubility" section. The "Solubility" section includes a "Find any" checkbox and a "Hide fields" link. It lists several sub-fields: "Solubility, g·l-1", "Saturation", "Temperature (Solubility (MCS)), °C", "Solvent (Solubility (MCS))", and "Ratio of Solvents". On the right side, a "Search fields" panel is open, showing a search for "solubility" and a list of results: "Solubility" and "Solubility Product". An orange arrow points from the "Solubility" result in the "Search fields" panel to the "Solubility" section in the main query builder. Another orange arrow points from the "Molecular Formula" result in the "Search fields" panel to the "Molecular Formula" section in the main query builder.

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 Q 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](#) > [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

<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

Navigation: < 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

Solubility, g ⁻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 4: “特定研究领域” 的催化剂选择

- 检索可用于立体选择性催化的含Fe的催化剂

The screenshot shows the Reaxys search 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 with a help icon. Below the navigation, there are search filters: Reactions >, Targets >, Substances >, and Documents >. A search bar contains the text 'catalyst'. Below the search bar, there are icons for Import, Save, Reset form, and Delete all. In the center, there are icons for Structure, Molecular Formula (highlighted with an orange arrow), CAS RN, and TI, AB & KW. The main search area shows a query builder with two conditions: 'Molecular Formula is Molecular Formula' and 'Catalyst Investigation is Investigated characteristic(s)'. The 'Catalyst Investigation' condition is expanded to show several sub-fields: 'Investigated characteristic(s)', 'Specification of catalysis', 'Classification of catalysis', 'Type of reaction', and 'Co-catalyst/co-substrate name'. On the right side, there is a 'Search fields' dropdown menu with 'catalyst' selected. Below it, there are expandable sections for 'Catalyst Investigation' and 'Reagent/Catalyst'. An orange arrow points from the 'Molecular Formula' icon in the search bar area to the 'Investigated characteristic(s)' field in the query builder. A tip box on the right contains the text: 'Tips : 手动添加MF 与 Catalyst Investigation的字段.'

Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in ?

Search in: Reactions > Targets > Substances > Documents >

Search fields
Q catalyst X

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Reaxys ^

◇ Molecular Formula is Molecular Formula

AND

◇ Catalyst Investigation Find any Hide fields ^

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

◇ Catalyst Investigation

◇ Reagent/Catalyst

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

条件的输入

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

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula contains Fe

AND

◇ Catalyst Investigation

- 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

Search

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

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

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

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

Hit Data - 2
Catalyst Investigation - 2 hits out of 25

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

Case 5: 可见光下特定溶剂中呈现特定颜色的化合物

- 获取在可见光下，水溶液中呈现出紫罗兰色的化合物

检索前提:

一个化合物在可见光下显示什么颜色，需要知道他能吸收什么样的波长

波长 (nm)	吸收颜色	可见颜色
400 ~ 450	紫	黄绿
450 ~ 480	蓝	黄
480 ~ 490	绿蓝	橙
490 ~ 500	蓝绿	红
500 ~ 560	绿	红紫
560 ~ 580	黄绿	紫
580 ~ 610	黄	蓝
610 ~ 650	橙	绿蓝
650 ~ 760	红	蓝绿

Reaxys中的检索策略

- Query Builder下用UV/VIS字段进行检索

The screenshot shows the Reaxys Query Builder interface. The search fields dropdown menu is open, displaying the search term 'uv'. An orange arrow points from the text '查找紫外可见光字段' to the search input field.

查找紫外可见光字段

The screenshot shows the Reaxys Query Builder interface with the 'UV/VIS Spectroscopy' field expanded. The 'Hide fields' button is highlighted with an orange box. The expanded field shows the following options:

Field	Operator	Field Name	Field Type
is	is	Description (UV/VIS Spectroscopy)	Text
is	is	Solvent (UV/VIS Spectroscopy)	Text
=	=	Absorption Maxima (UV/VIS), nm	Text
=	=	Ext./Abs. Coefficient, l·mol ⁻¹ cm ⁻¹	Text

添加吸收光波长和溶剂

Reaxys[®] Quick search Query builder Results Retrosynthesis History Alerts

Search in: Reactions > Targets > Substances > Documents >

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

◇ UV/VIS Spectroscopy Find any Hide fields ^

is ✓ Description (UV/VIS Spectroscopy

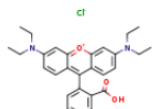
is ✓ water;h2o ← 输入条件

= ✓ 560-580

= ✓ Ext./Abs. Coefficient, l·mol⁻¹cm⁻¹

最后的结果

1



rhodamine B
C₁₃H₆O(N(C₂H₅)₂)₂C₆H₄COOH(4+)*... 479.019 4091619 81-88-9

Hit Data - 6 Bioactivity (All) Other Data - 92

Identification Physical Data - 699

Druglikeness Spectra - 706

Preparations - 14 >

Reactions - 1,244 >

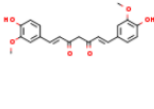
Targets - 7 >

Documents - 34,671 >

Hit Data - 6

UV/VIS Spectroscopy - 6 hits out of 453

2



curcumin
(HOC₆H₃(OCH₃)CHCHCO)₂CH₂ 368.386 2306965 458-37-7

Hit Data - 1 Bioactivity (All) Other Data - 2,560

Identification Physical Data - 273

Druglikeness Spectra - 507

Preparations - 28 >

Reactions - 1,278 >

Targets - 628 >

Documents - 29,483 >

Hit Data - 1

UV/VIS Spectroscopy - 1 hits out of 223

UV/VIS Spectroscopy - 6 hits out of 453

Description (UV/VIS Spectroscopy)	Solvent (UV/VIS Spectroscopy)	Location	Absorption Maxima (UV/VIS), nm	Ext./Abs. Coefficient, l·mol ⁻¹ ·cm ⁻¹	Reference
Spectrum	water		560		Bai, Yan; Chen, Lin-Lin; Dang, Dong-Bin; Li, Dan; Li, Ya-Min; Liu, Xin-Yu; Tan, Xiao-Li Journal of Solid State Chemistry, 2022, vol. 305, art. no. 122694 Full Text > Details > Abstract >
Spectrum	water	supporting information	560		Feng, Yongqiang; Sakaki, Masoud; Kim, Jae-hyun; Huang, Jianfeng; Kajiyoshi, Koji New Journal of Chemistry, 2018, vol. 42, # 24, p. 20212 - 20218 Full Text > Cited 6 times > Details > Abstract >

UV/VIS Spectroscopy - 1 hits out of 223

Description (UV/VIS Spectroscopy)	Solvent (UV/VIS Spectroscopy)	Absorption Maxima (UV/VIS), nm	Reference
Spectrum	dimethyl sulfoxide, water, sodium hydroxide	571	Kim, Sung-Hoon; Gwon, Seon-Yeong; Burkinshaw, Son, Young-A Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2010, vol. 76, # 3-4, p. 384 - 387 Full Text > Cited 18 times > Details > Abstract >

如果还有更多的需求

- 获取在可见光下，水溶液中呈现出紫罗兰色的化合物，且该化合物必须包含以下片段

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' are in the center. The user 'Sam Yu' is logged in on the right. Below the navigation bar, there are search filters for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar includes 'Import', 'Save', 'Reset form', and 'Delete all' on the left, and 'Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW' on the right. The main workspace is divided into two sections. The top section, titled 'Structure', contains a chemical structure of phenol (a benzene ring with an -OH group) and the text 'On all atoms'. The bottom section, titled 'UV/VIS Spectroscopy', is connected to the main query by an 'AND' button. It contains a list of search criteria: 'Description (UV/VIS Spectroscopy)', 'water:h2o', '560-580', and 'Ext./Abs. Coefficient, l·mol⁻¹cm⁻¹'. A right-hand sidebar lists various search fields such as 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', 'Bibliography', 'PubChem', and 'Commercial Substances'.

最后的结果

127 Substances out of 43,776 Documents, containing 17,443 Reactions, 716 Targets

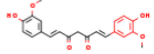
0 selected Limit To Exclude Export Preparations

Reaxys - 127

Sort by No of References

Grid Heatmap

1



curcumin
(HO₂C₆H₃(OCH₃)CHCHCO)₂CH₂ 368.386 2306965 458-37-7

Hit Data - 1 Bioactivity (All) Other Data - 2,560

Identification Physical Data - 273

Druglikeness Spectra - 507

Preparations - 28 >

Reactions - 1,278 >


Targets - 628 >

Documents - 29,483 >

Hit Data - 1

UV/VIS Spectroscopy - 1 hits out of 223

2



2-amino-phenol
HO(C₆H₄)NH₂ 109.128 606075 95-55-6

Hit Data - 1 Bioactivity (All) Other Data - 34

Identification Physical Data - 371

Druglikeness Spectra - 199

Preparations - 231 >

Reactions - 15,180 >

Targets - 30 >

Documents - 8,759 >

Hit Data - 1

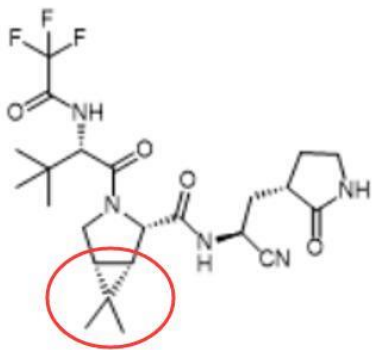
UV/VIS Spectroscopy - 1 hits out of 68

Agenda

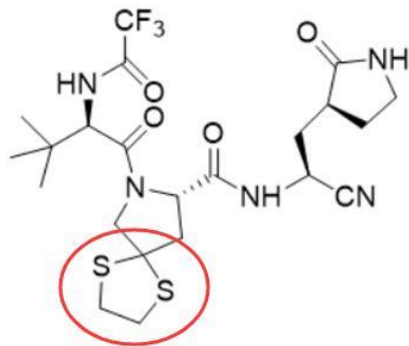
- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的文献快速检索方法
 - Reaxys中物质理化性质的查询与结构反查
 - 利用Reaxys进行专利突破与全新分子的专利评估
 - Reaxys中结构面板详解，合成信息的检索与合成计划制作
- Q&A

Case 6: 利用Reaxys中的专利数据进行专利突破

- 2023年1月底，国家药监局发布公告，批准先声药业的新冠口服药物“先诺欣”在国内上市。从作用机制看，先声药业的“先诺欣”和辉瑞的Paxlovid是相同的，且也是和Ritonavir组合包装的抗病毒药物。“先诺欣”的活性成分先诺特韦和辉瑞的Nirmatrelvir非常相像。




辉瑞：Nirmatrelvir



先声：先诺特韦

寻找专利突破点需要先调研原研专利

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
(19) World Intellectual Property Organization
International Bureau
(43) International Publication Date
16 December 2021 (16.12.2021)  (10) International Publication Number
WO 2021/250648 A1

(5) International Patent Classification:
C07D 207/267 (2006.01) C07D 401/02 (2006.01)
C07D 403/02 (2006.01) C07D 497/04 (2006.01)
C07D 403/14 (2006.01) A61K 31/4015 (2006.01)
A61P 31/14 (2006.01) A61K 31/025 (2006.01)

(21) International Application Number:
PCT/IB2021/057281

(22) International Filing Date:
06 August 2021 (06.08.2021)

(25) Filing Language:
English

(26) Publication Language:
English

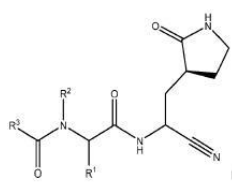
(30) Priority Data:
63/073,982 03 September 2020 (03.09.2020) US
63/141,435 29 January 2021 (29.01.2021) US
63/170,158 02 April 2021 (02.04.2021) US
63/194,241 28 May 2021 (28.05.2021) US

(71) Applicant: **PFIZER INC.**, [US/US], 235 East 42nd Street, New York, New York 10017 (US).

(72) Inventor: **OWEN, Dafydd Rhys**, c/o Pfizer Inc., 610 Main Street, Cambridge, Massachusetts 02139 (US); **PETERSERSON, Martin Youngjin**, 3 Gilson Road, Littleton, Massachusetts 01469 (US); **REISE, Matthew Richard**, c/o Pfizer Inc., 445 Eastern Point Road, Building 98, Cromton, Connecticut 06340 (US); **SAMMONS, Matthew Forrest**, c/o Pfizer Inc., 610 Main Street, Cambridge, Massachusetts 02139 (US); **TUTTLE, Jamison Bryce**, c/o Pfizer Inc., 610 Main Street, Cambridge, Massachusetts 02139 (US); **VERHOEST, Patrick Robert**, c/o Pfizer Inc., 610 Main Street, Cambridge, Massachusetts 02139 (US); **WEL, Linaqing**, c/o Pfizer Inc., 445 Eastern Point Road, Building 98, Cromton, Connecticut 06340 (US); **YANG, Qiang**, c/o Pfizer Inc., 610 Main Street, Cambridge, Massachusetts 02139 (US).

(84) Title: NITRILE-CONTAINING ANTIVIRAL COMPOUNDS

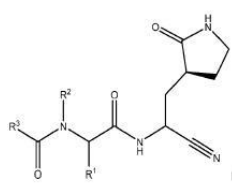
E1 is a compound of E45 or E59, hereinbelow, of Formula I



or a pharmaceutically acceptable salt thereof, wherein R¹ is selected from the group consisting of C₁-C₆ alkyl which is optionally substituted with a cyano or with one to five fluoro; C₂-C₆ alkynyl; and (C₁-C₆ cycloalkyl)-C₁-C₃ alkyl which is optionally substituted with one to two substituents selected from trifluoromethyl and C₁-C₃ alkyl or with one to five fluoro; R² is hydrogen or R² and R¹ taken together with the nitrogen and carbon atoms to which they are attached are a pyrrolidine or piperidine ring which is optionally substituted with one to four R^{2a}; R^{2b} at each occurrence is independently selected from the group consisting of fluoro, C₁-C₃ alkyl optionally substituted with one to three fluoro and C₁-C₃ alkoxy optionally substituted with one to three fluoro; or two R^{2b} groups when

(7) Abstract: The invention relates to compounds of Formula (I*) wherein R¹, R², R^{2a}, R^{2b}, p, q and q' are as defined herein, pharmaceutical compositions comprising the compounds, methods of treating coronavirus infection such as COVID-19 in a patient by administering therapeutically effective amounts of the compounds, and methods of inhibiting or preventing replication of coronaviruses such as SARS-CoV-2 with the compounds.

E1 is a compound of E45 or E59, hereinbelow, of Formula I



or a pharmaceutically acceptable salt thereof, wherein R¹ is selected from the group consisting of C₁-C₆ alkyl which is optionally substituted with a cyano or with one to five fluoro; C₂-C₆ alkynyl; and (C₁-C₆ cycloalkyl)-C₁-C₃ alkyl which is optionally substituted with one to two substituents selected from trifluoromethyl and C₁-C₃ alkyl or with one to five fluoro; R² is hydrogen or R² and R¹ taken together with the nitrogen and carbon atoms to which they are attached are a pyrrolidine or piperidine ring which is optionally substituted with one to four R^{2a}; R^{2b} at each occurrence is independently selected from the group consisting of fluoro, C₁-C₃ alkyl optionally substituted with one to three fluoro and C₁-C₃ alkoxy optionally substituted with one to three fluoro; or two R^{2b} groups when

专利当中对于骨架结构的描述极其复杂，理解起来费时费力。

attached to adjacent carbons and taken together with the carbons to which they are attached are a fused C₃-C₆ cycloalkyl which is optionally substituted with one to four R^{2b}; or two R^{2b} groups when attached to the same carbon and taken together with the carbon to which they are attached are a spiro C₃-C₆ cycloalkyl which is optionally substituted with one to four R^{2b}; R^{2b} at each occurrence is independently selected from fluoro, C₁-C₃ alkyl optionally substituted with one to three fluoro, and C₁-C₃ alkoxy optionally substituted with one to three fluoro; R² is selected from the group consisting of C₁-C₆ alkyl, C₁-C₆ alkoxy, (C₁-C₆ alkoxy)-C₁-C₆ alkyl, C₂-C₆ alkynyl, C₂-C₆ alkenyloxy, C₃-C₁₂ cycloalkyl optionally fused with a 5- to 6-membered heteroaryl or phenyl, (C₃-C₁₂ cycloalkyl)-C₁-C₆ alkyl, C₃-C₁₂ cycloalkoxy, (C₃-C₁₂ cycloalkoxy)-C₁-C₆ alkyl, 4- to 12-membered heterocycloalkyl which is optionally fused with a 5- to 6-membered heteroaryl or phenyl and wherein said heterocycloalkyl comprises one to four heteroatoms independently selected from N, O and S(O)_n, (4- to 12-membered heterocycloalkyl)-C₁-C₆ alkyl wherein said heterocycloalkyl moiety comprises one to four heteroatoms independently selected from N, O and S(O)_n, C₆-C₁₀ aryl optionally fused with a C₆-C₆ cycloalkyl or a 4- to 7-membered heterocycloalkyl, (C₆-C₁₀ aryl)-C₁-C₆ alkyl, 5- to 10-membered heteroaryl comprising one to five heteroatoms independently selected from N, O and S, which is optionally fused with a C₆-C₆ cycloalkyl; (5- to 10-membered heteroaryl)-C₁-C₆ alkyl wherein the heteroaryl moiety comprises one to five heteroatoms independently selected from N, O and S, (C₆-C₁₀ aryl)-(5- to 10-membered heteroaryl)- wherein the heteroaryl moiety comprises one to five heteroatoms independently selected from N, O and S, (5- to 10-membered heteroaryl)-C₁-C₆ alkyl wherein the heteroaryl moiety comprises one to five heteroatoms independently selected from N, O and S, (5- to 6-membered heteroaryl)-(5- to 6-membered heteroaryl)- wherein each heteroaryl moiety comprises one to four heteroatoms independently selected from N, O and S, (4- to 7-membered heterocycloalkyl)-(5- to 6-membered heteroaryl)- wherein the heterocycloalkyl moiety comprises one to three heteroatoms independently selected from N, O and S(O)_n and the heteroaryl moiety comprises one to four heteroatoms independently selected from N, O and S, (5- to 6-membered heteroaryl)-(4- to 7-membered heterocycloalkyl)- wherein the heterocycloalkyl moiety comprises one to three heteroatoms independently selected from N, O and S, where each R² group is optionally substituted with one to five R⁴; R⁴ at each occurrence is independently selected from the group consisting of oxo, halo, hydroxy, cyano, phenyl, benzyl, amino,

通过Reaxys对专利的提炼快速了解突破点

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Search for WO 2021/250648 Import

Search Reaxys

WO 2021/250648 Find

Documents, e.g. Tetrahedron, 2014, 70, 2343

AND

Draw

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Results for WO 2021/250648 New Edit

51 Documents Patent: WO 2021/250648 Preview Results View Results

0 Documents Titles, Abstracts, Keywords: "WO 2021/250648"

Reaxys中通过简单的链接，获取原研专利中的所有物质

Quick search Query builder Results Retrosynthesis History Alerts

51 Documents with 1,048 Substances, 424 Reactions, 1 Targets

0 Limit To Exclude Export

1 Nitrile-containing antiviral compounds
Current Patent Assignee: PFIZER INC - US11541034, 2023, B2
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2021266232 C1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Index Terms Claims Bibliographic Info Substances (514) Full Text

2 NITRILE-CONTAINING COMPOUNDS USEFUL AS ANTIVIRAL AGENTS FOR THE TREATMENT OF A CORONAVIRUS INFECTION
Current Patent Assignee: PFIZER INC - HRP20221379, 2023, T1
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Claims Bibliographic Info Full Text

3 Nitrile-containing compounds useful as antiviral agents for the treatment of a coronavirus infection
Current Patent Assignee: PFIZER INC - ES2932173, 2023, T3
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Bibliographic Info Full Text

4 NITRILE-CONTAINING COMPOUNDS USEFUL AS ANTIVIRAL AGENTS FOR THE TREATMENT OF A CORONAVIRUS INFECTION
Current Patent Assignee: PFIZER INC - PL3953330, 2023, T3
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Bibliographic Info Full Text

5 Nitrile-containing compounds useful as antiviral agents for the treatment of a coronavirus infection
Current Patent Assignee: PFIZER INC - MD3953330, 2023, T2
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Bibliographic Info Full Text

6 NITRILE-CONTAINING COMPOUNDS USEFUL AS ANTIVIRAL AGENTS FOR THE TREATMENT OF A CORONAVIRUS INFECTION
Current Patent Assignee: PFIZER INC - SI3953330, 2023, T1
Patent Family Members: AR123111 A1; AU2021266232 B1; AU2022202158 A1; AU2022202158 B2; ...
Abstract Claims Bibliographic Info Full Text

专利中的物质，并利用MW筛选出没有分子量报道的物质

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

1,048 Substances out of 51 Documents, containing 424 Reactions, 1 Targets

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

Filters

- By Structure
- Measurement pX
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Available Data
- Document Type
- Publication Year
- Current Patent Assignee
- LogP
- H Bond Donors
- H Bond Acceptors

1-ethyl-(3-(3-dimethylamino)propyl)-carbodiimide hydrochloride
ClH^+C_8H_{17}N_3 191.704 5764110 25952-53-8

Identification Bioactivity (All) Spectra - 18
Druglikeness Physical Data - 17 Other Data - 60

Preparations - 8
Reactions - 480
Targets - 6
Documents - 89,567

benzyl bromide
(C_6H_5)CH_2Br 171.037 385801 100-39-0

Identification Bioactivity (All) Spectra - 1
Druglikeness Physical Data - 216 Other Data - 1

di-tert-butyl dicarbonate
((C_4H_9)OC(O))_2O 218.25 1911173 24424-99-5

Identification Physical Data - 31 Other Data - 1
Druglikeness Spectra - 19

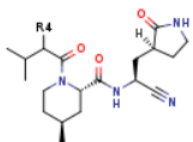
Molecular Weight 1 Clear selected Sort by Occurrence

- >300 - 300
- >132 - 144
- >576 - 588
- >84 - 96
- >96 - 108
- >72 - 84
- >60 - 72
- >648 - 660
- >636 - 648
- >600 - 612
- (no entry given)

< 1 2 Limit to Exclude

最后的结果

1



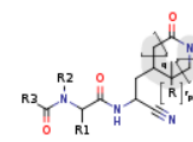
Reaxys ID: 39439325
39439325

Hit Data - 7
Identification
Other Data - 5

Hit Data - 7

- Substance Label - 1 hits out of 1
- Patent-Specific Data - 1 hits out of 1
- Use - 5 hits out of 5

2



Reaxys ID: 39439326
39439326

Hit Data - 7
Identification
Other Data - 5

Hit Data - 7

- Substance Label - 1 hits out of 1
- Patent-Specific Data - 1 hits out of 1
- Use - 5 hits out of 5

这是保护范围最大的Markush结构

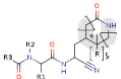
Identification

Reaxys ID: 39439326

- Substance Label - 1
- Patent-Specific Data - 1
- Markush Details**

从Markush Detail中寻找突破点

Markush Details




Label	Value	Size	Attributes	Substituted by	Frequency
q	0-2				
p	0-2				
r	q'				
R	hydroxy				
	oxo				
R1	allyl	1-6C		\$a\$	0-5
	alkenyl	2-6C			
	{(acycloalkyl(3-6)-alkyl(1-3			\$b\$	0-5
R2	hydrogen				
R3	allyl	1-8C		\$c\$	0-5
	alkoxy	1-8C		\$d\$	0-5
	{alkoxy(1-6)-alkyl(1-6			\$e\$	0-5
	alkenyl	2-6C		\$f\$	0-5
	alkynyl	2-6C		\$g\$	0-5
	acycloalkyl	3-12C	o fused with <\$a\$>	\$h\$	0-5
	{(acycloalkyl(3-12)-alkyl(1-6			\$i\$	0-5
	acycloalkoxy	3-12C		\$j\$	0-5
	{(acycloalkoxy(3-12)-alkyl(1-6			\$k\$	0-5
	heterocycloalkyl	4-12	o fused with <\$a\$>; 1-4 N, O, S(O)<\$m\$>	\$l\$	0-5
	{heterocycloalkyl(4-12)-alkyl(1-6			\$m\$	0-5
	aryl	6-10C	o fused with <\$a\$>	\$n\$	0-5
	{aryl(6-10)-alkyl(1-6			\$o\$	0-5
	heteroaryl	5-10	1-5 N, O, S; o fused <\$a\$>	\$p\$	0-5
	{heteroaryl(5-10)-alkyl(1-6			\$q\$	0-5
	{aryl(6-10)-{heteroaryl(5-10)			\$r\$	0-5
	{heteroaryl(5-10)-alkyl(1-6			\$s\$	0-5

也可以将Reaxys中的Markush Detail下载下来用表格的形式进行研究：

Reaxys®

Reaxys © 2014/2015 View a Markush

Type of Substances: markush structure
Name: or a molecule or hybrid thereof, or a pharmacologically acceptable salt of said compound, solvate or hydrate thereof

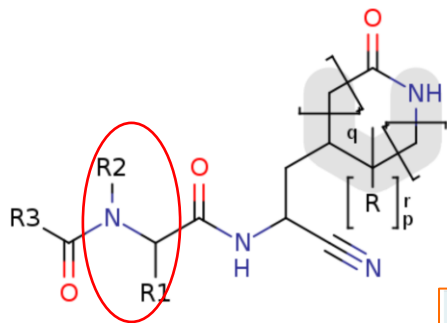


Label	Value	Size	Attributes	Substituted by	Frequency
q	0-2				
p	0-2				
r	q'				
R	hydroxy				
	oxo				
R1	allyl	1-6C		<\$a\$>	0-5
	alkenyl	2-6C			
	{(cycloalkyl(3-6)-alkyl(1-3			<\$b\$>	0-5
R2	hydrogen				
R3	allyl	1-8C		<\$c\$>	0-5
	alkoxy	1-8C		<\$d\$>	0-5
	{alkoxy(1-6)-alkyl(1-6			<\$e\$>	0-5
	alkenyl	2-6C		<\$f\$>	0-5
	alkynyl	2-6C		<\$g\$>	0-5
	cycloalkyl	3-12C	o fused with <\$a\$>	<\$h\$>	0-5
	{(cycloalkyl(3-12)-alkyl(1-6			<\$i\$>	0-5
	acycloalkoxy	3-12C		<\$j\$>	0-5
	{(acycloalkoxy(3-12)-alkyl(1-6			<\$k\$>	0-5
	heterocycloalkyl	4-12	o fused with <\$a\$>; 1-4 N, O, S(O)<\$m\$>	<\$l\$>	0-5
	{heterocycloalkyl(4-12)-alkyl(1-6			<\$m\$>	0-5
	aryl	6-10C	o fused with <\$a\$>	<\$n\$>	0-5
	{aryl(6-10)-alkyl(1-6			<\$o\$>	0-5
	heteroaryl	5-10	1-5 N, O, S; o fused <\$a\$>	<\$p\$>	0-5
	{heteroaryl(5-10)-alkyl(1-6			<\$q\$>	0-5
	{aryl(6-10)-{heteroaryl(5-10)			<\$r\$>	0-5
	{heteroaryl(5-10)-alkyl(1-6			<\$s\$>	0-5

Reaxys®

Label	Value	Size	Attributes	Substituted by	Frequency
q	0-2				
p	0-2				
r	q'				
R	hydroxy				
	oxo				
R1	allyl	1-6C		<\$a\$>	0-5
	alkenyl	2-6C			
	{(acycloalkyl(3-6)-alkyl(1-3			<\$b\$>	0-5
R2	hydrogen				
R3	allyl	1-8C		<\$c\$>	0-5
	alkoxy	1-8C		<\$d\$>	0-5
	{alkoxy(1-6)-alkyl(1-6			<\$e\$>	0-5
	alkenyl	2-6C		<\$f\$>	0-5
	alkynyl	2-6C		<\$g\$>	0-5
	cycloalkyl	3-12C	o fused with <\$a\$>	<\$h\$>	0-5
	{(cycloalkyl(3-12)-alkyl(1-6			<\$i\$>	0-5
	acycloalkoxy	3-12C		<\$j\$>	0-5
	{(acycloalkoxy(3-12)-alkyl(1-6			<\$k\$>	0-5
	heterocycloalkyl	4-12	o fused with <\$a\$>; 1-4 N, O, S(O)<\$m\$>	<\$l\$>	0-5
	{heterocycloalkyl(4-12)-alkyl(1-6			<\$m\$>	0-5
	aryl	6-10C	o fused with <\$a\$>	<\$n\$>	0-5
	{aryl(6-10)-alkyl(1-6			<\$o\$>	0-5
	heteroaryl	5-10	1-5 N, O, S; o fused <\$a\$>	<\$p\$>	0-5
	{heteroaryl(5-10)-alkyl(1-6			<\$q\$>	0-5
	{aryl(6-10)-{heteroaryl(5-10)			<\$r\$>	0-5
	{heteroaryl(5-10)-alkyl(1-6			<\$s\$>	0-5

寻找简单的描述来进行突破

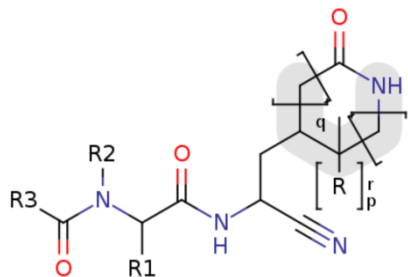


专利保护点:

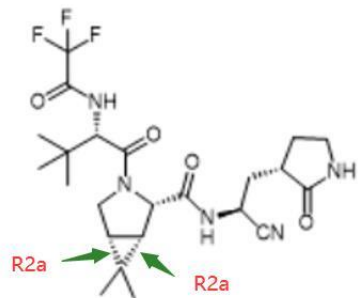
1. R1+R2=吡咯烷, 或哌啶, 且可以被R2a取代, 那突破点是否可以定在不一样的环?
2. R2a+R2a=3-6个C的环烷基, 或者3-6个C的螺环烷基, 那突破点是否可以是不一样的螺环? 先声用螺杂环进行了突破。

R1+R2	pyrrolidine			R2a	0-4
	piperidine			R2a	0-4
R2a	fluoro				
	hydroxy				
	alkyl	1-6C		fluoro	0-3
	alkoxy	1-6C		fluoro	0-3
R2a+R2a	cycloalkyl	3-6C		R2b	0-4
	spiro cycloalkyl	3-6C		R2b	0-4

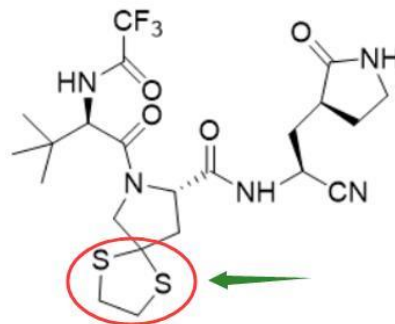
先声药业的突破点



5 attached to adjacent carbons and taken together with the carbons to which they are attached are a fused C₃-C₆ cycloalkyl which is optionally substituted with one to four R^{2b}; or two R^{2a} groups when attached to the same carbon and taken together with the carbon to which they are attached are a spiro C₃-C₆ cycloalkyl which is optionally substituted with one to four R^{2b}; R^{2b} at each occurrence is independently selected from fluoro, C₁-C₃ alkyl optionally substituted with one to three fluoro, and C₁-C₃ alkoxy optionally substituted with one to three fluoro; R³ is selected from the group consisting of C₁-C₈ alkyl, C₁-C₈ alkoxy, (C₁-C₈ alkoxy)-C₁-C₆ alkyl, C₂-C₈ alkenyl, C₂-C₆ alkynoxy, C₃-C₁₂ cycloalkyl optionally fused with a 5- to 6-membered heteroaryl or phenyl, (C₃-C₁₂



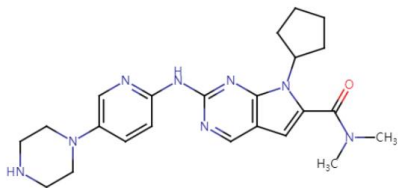
辉瑞:
1: R¹+R²=吡咯烷
2: R^{2a}+R^{2a}=环烷烃



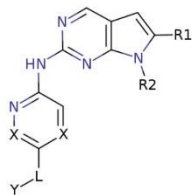
先声:
1: R¹+R²=吡咯烷
2: R^{2a}+R^{2a}=5元螺杂环

类似的策略可以继续用到CDK4/6的专利突破上

诺华CDK4/6药物Ribociclib

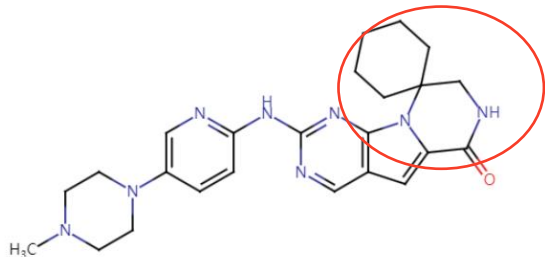


诺华保护的Markush



发现诺华保护的R1和R2都是单独的取代基团

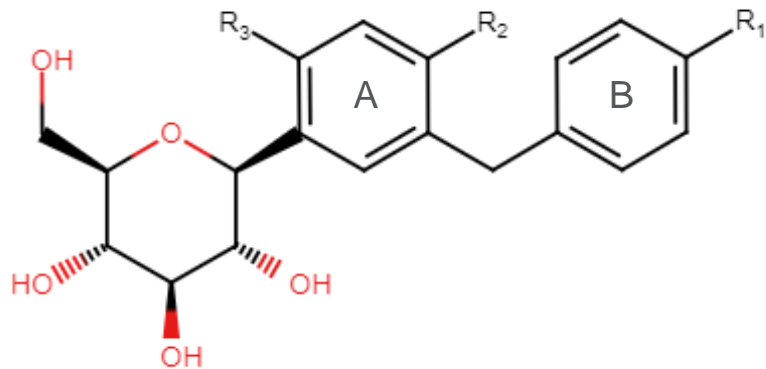
R^1 is C_{1-8} alkyl, CN, $C(O)OR^4$ or $CONR^5R^6$, a 5-14 membered heteroaryl group, or a 3-14 membered cycloheteroalkyl group;
 R^2 is C_{1-8} alkyl, C_{3-14} cycloalkyl, or a 5-14 membered heteroaryl group, and wherein R^2 may be substituted with one or more C_{1-8} alkyl, or OH;



G1治疗与先声药业在R1+R2上做了突破，做了成环的突破

Markush Details					
Label	Value	Size	Attributes	Substituted by	Frequency
R2	alkyl	1-8C		<\$a>	0-?
	cycloalkyl	3-14C		<\$a>	0-?
	heteroaryl	5-14		<\$a>	0-?
R1	alkyl	1-8C			
	CN				
	$C(O)O<R4>$				
	$CON<R5><R6>$				
	heteroaryl	5-14			
	cycloheteroalkyl	3-14			

CASE 7: Reaxys中的全新化合物专利评估



- 保持AB环和glucose的主要活性部分，考虑R₁,R₂,R₃的变构
- R₁为小位阻烷基，烷氧基，环烷基
- R₂为H, F, Cl, CF₃, Me, Et
- R₃为H, 或者短的烷基，烷氧基，醚，H, 且允许和自身成环

Reaxys中通式结构的专利评估

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

获取结构的同时，也获取专利中的通式结构

Clear Cancel x Transfer to query >

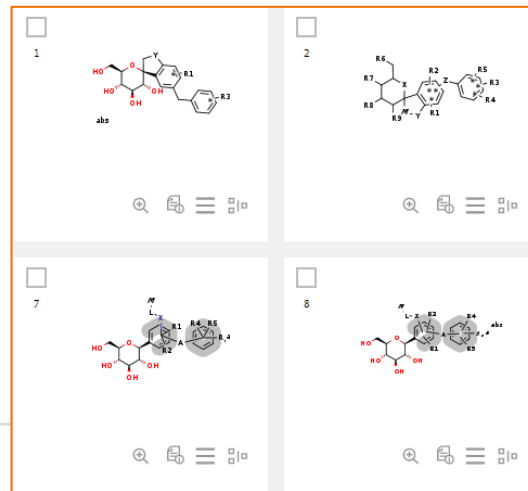
Reaxys中的结果

133 Substances out of 17 Documents, containing 302 Reactions, 2 Targets

0 selected Limit To Exclude Export Preparations

<input type="checkbox"/> 1 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 2 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 3 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 4 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>
<input type="checkbox"/> 7 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 8 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 9 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 10 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>
<input type="checkbox"/> 13 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 14 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 15 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	<input type="checkbox"/> 16 <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>

Reaxys除了给出具体的结构，还能给出涉及这些结构的Markush通式



利用分子量筛选获取所有的Markush结构

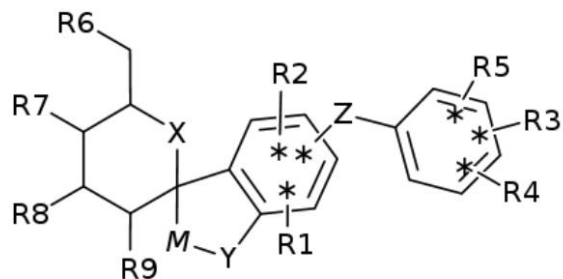
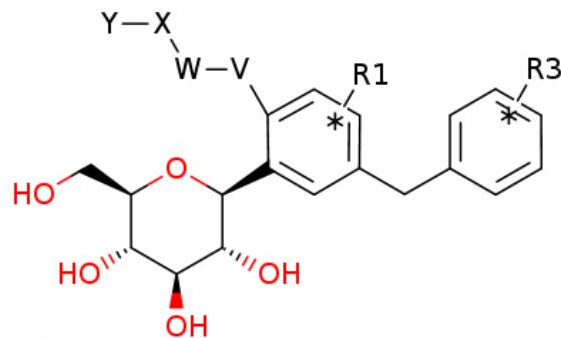
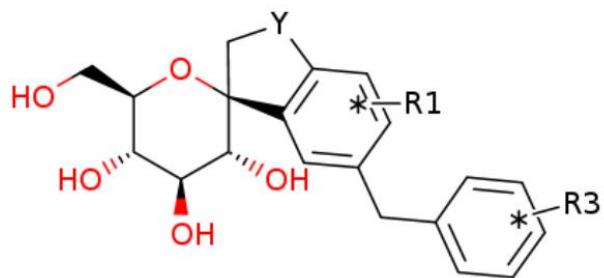
The screenshot displays a search interface with a 'Filters' sidebar on the left and a 'Molecular Weight' filter panel on the right. The 'Filters' sidebar includes categories like 'By Structure', 'Measurement pX', 'Highest Clinical Phases', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', 'Number of Fragments', 'Availability', 'Availability in other databases', 'Available Data', and 'Document Type'. The 'Molecular Weight' panel shows a list of ranges with checkboxes and counts. An expanded view of the 'Molecular Weight' filter shows a list of ranges from '>864 - 876' to '>540 - 552', plus a '(no entry given)' option. The interface includes 'Limit to' and 'Exclude' buttons at the bottom of the filter panels.

Molecular Weight Range	Count
>408 - 420	4
>420 - 432	5
>432 - 444	9
>444 - 456	22
>456 - 468	23
>468 - 480	11
>480 - 492	6

Molecular Weight Range	Count
>864 - 876	1
>768 - 780	1
>744 - 756	1
>720 - 732	1
>708 - 720	1
>636 - 648	1
>612 - 624	1
>588 - 600	1
>576 - 588	1
>540 - 552	1
(no entry given)	13

由于Markush结构是没有分子量的，所以可以通过分子量筛选获取所有的通式结构

一些比较有意思的Markush结构



Tips:

- 这些Markush结构，和我们设计的结构非常的相似，如何突破专利，需要详细阅读专利Claim部分
- Reaxys可以帮助大家大大缩短阅读全文的时间

Reaxys对于专利中Markush的提炼

Reaxys ID: 13022958
13022958

Identification
Other Data - 24

Documents - 1 >



Identification

Reaxys ID: 13022958

Substance Label

Patent-Specific Data - 1

Location in Patent	Reference
Claim 10	Chen, Yuanwei; Feng, Yan; Xu, Baihua; Lv, Binhua; Dong, Jiajia; Seed, Brian; Hadd, Michael J. - US2007/275907, 2007, Abstract > Full Text > Details > Abstract >

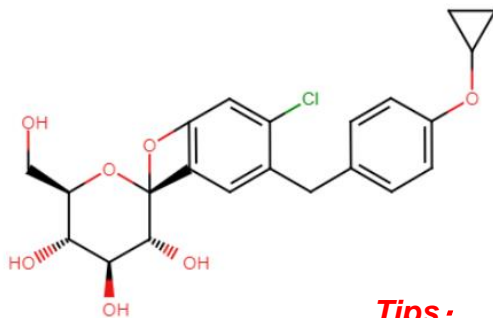
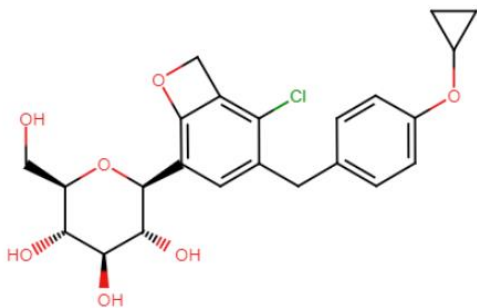
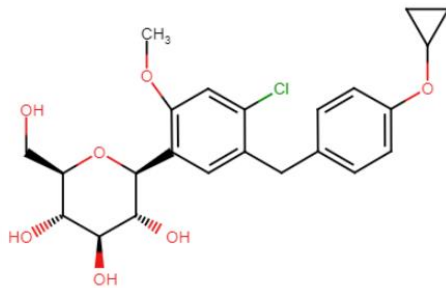
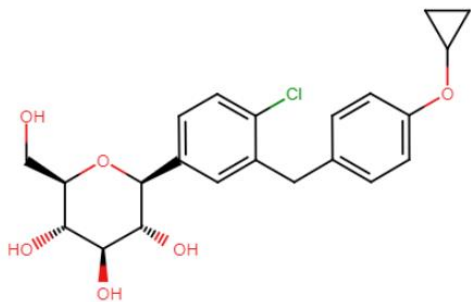
Markush Details



Label	Value	Size	Attributes	Substituted by
Y	(C#H2)n			
	(C#H2)mC#H=C#H			
	C#H=C#H(C#H2)m			
	C#H2C#H=C#HC#H2			
	(C#H2)mC(O)			
	C(O)(C#H2)m			
	C(O)N#H(C#H2)m			
	(C#H2)mN#HC(O)			
	C(O)O(C#H2)m			
	(C#H2)mSO2			
R1	SO2(C#H2)m			
	(O)C(C#H2)mC(O)			
	hydrogen			
	halo			
	allyl	1-6C		\$dSe;\$f\$g
	alkenyl	2-6C		\$dSe;\$f\$g
	alkynyl	2-6C		\$dSe;\$f\$g
	cycloalkyl	3-10C	1-2 methylene groups o replaced by <\$h>	\$dSe;\$f\$g
	Scycloalkyl1310-\$alkyl13			
	(\$alkenyl24)\$alkyloxy13			

提炼了出现的位置和Markush的结构细节。

评估完专利后，设计一些全新化合物（假设下列结构无专利问题）



Tips:

案例制作当天，Reaxys中没有相同结构。


Agenda


- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的文献快速检索方法
 - Reaxys中物质理化性质的查询与结构反查
 - 利用Reaxys进行专利突破与全新分子的专利评估
 - Reaxys中结构面板详解，合成信息的检索与合成计划制作
- Q&A


Reaxys中的结构面板


Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >



铅笔	单键	双键	三键
芳香键	单键上	单键下	单键上或下
双键顺或反	顺反或未定义	单键或双键	单键或芳香键
双键或芳香键	不确定键	配位键	不定位键


 缩写官能团, 用于定义一些常见的缩写官能团



 **Generic Group**, 用于定义一些通用官能团



 元素周期表, 用于定义不同的元素, 并包含 Atom List Not List 功能



 S^{\max} 开放取代功能, 适用于AsDrawn检索



  原子锁定功能, 适用于AsSubstructure功能



 $||_{x,z}$ 重复基团定义工具

  Smart R功能, 用于 R 基团自定义功能


  R Group Attachment, 用于 R 基团自定义时末端原子定义


  Make/break, 用于规定化学反应时断裂的键


  Protect, 用于保护化学键不变


  反应箭头, 反应方向


 1-1 原子匹配工具, 用于定义化学反应前后匹配原子


 **R**


 A


 H


 C


 N


 O


 S


 F

 P

 Cl

 Br

 I

Clear  Cancel × Transfer to query >

结构面版功能合集

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

Case 8: Reaxys中最简单的反应定义与筛选

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

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 side, there are buttons for "Register >" and "Sign in".

The main workspace shows a chemical reaction: benzaldehyde (a benzene ring with a formyl group, O=Cc1ccccc1) reacting to form benzyl alcohol (a benzene ring with a hydroxymethyl group, OCCc1ccccc1). The reaction is indicated by a right-pointing arrow.

Below the reaction, the text "原子匹配与原子锁定" (Atom matching and atom locking) is written. Two orange arrows point from this text to the left-hand side of the reaction, specifically to the carbonyl carbon and the oxygen atom of the benzaldehyde reactant.

On the right side of the interface, there is a search filter panel titled "Search this structure as:". It contains several options with 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

At the bottom of the interface, there are buttons for "Clear", "Cancel", and "Transfer to query".

Reaxys中的结果

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

11,06 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

11,063 Reactions out of 7,929 Documents, containing 14,783 Substances, 2,966 Targets

0 Limit To Exclude Export **Show Conditions** Reaxys Ranking

Show/Hide Conditions, 选择显示/隐藏条件

1 79 72

63 Conditions Find Similar > Reaction ID: 2407606

2 114 85

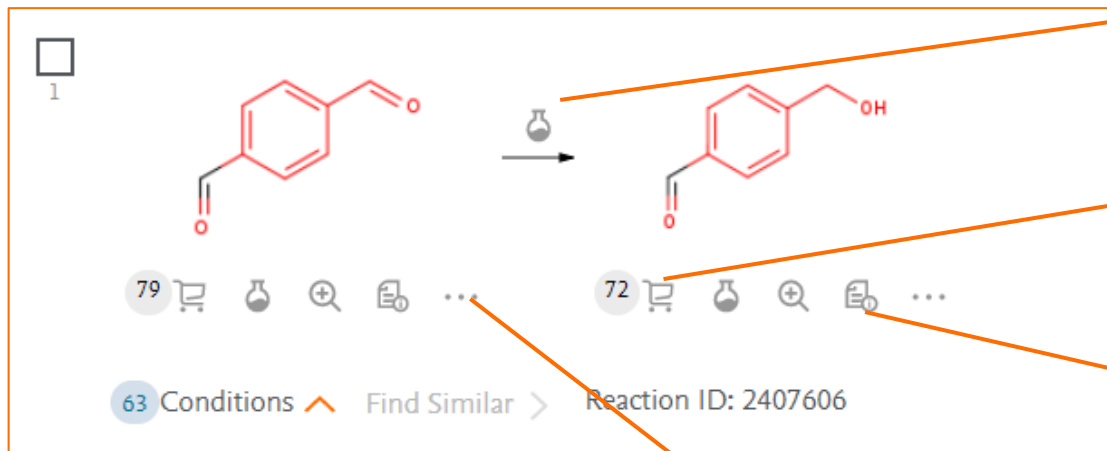
38 Conditions Find Similar > Reaction ID: 305004

3

Conditions	Yield	Reference
With sodium tetrahydroborate in tetrahydrofuran, ethanol at 0°C, for 7h;	97%	Bahn, Yong-Sun; Cheong, Eunji; Choi, Ji Won; Hwang, Hyoung; Kim, Byungseon; Kim, Myeon; Jeong, Kim, Jun Woo; [...] Seo, Seon Hee; Yeon, Seul Ki [Journal of Medicinal Chemistry, 2021] Full Text > Details > Abstract >
With formic acid; [Pt-Cl5H3]Ru2(K1-P-PPH2P)(PPH3)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 22 times > Details > Abstract >
With bis[15-cyclopentadienyl]hafnium dihydride in isopropyl alcohol at 80°C, for 8h;	91%	Nakano, Tatsuya; Umami, Shigetoshi; Kino, Yoshio; Ishii, Yasutaka; Ogawa, Masaru [Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757] Full Text > Cited 48 times > Details > Abstract >

Feedback

Reaxys的一条反应的界面



进行合成计划

查看商业来源

4-(hydroxymethyl)benzaldehyde ×

HCOC6H4CH2OH 136.15 878348 52010-97-6

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

[View Details >](#)

查看条件

寻找相似反应

查看物质详情

更多与物质相关操作

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

Options ×

- [Find Similar](#)
- [View related Markush](#)
- [View details](#)
- [Copy structure to query](#)
- [Copy reaction to query](#)
- [Use as filter](#)
- [Open in database](#)

Reaxys的筛选操作

Filters

Limit to > Exclude >

- By Structure ▾
- Yield ▾
- Reagent/Catalyst ▾
- Solvent ▾
- Catalyst Classes ▾
- Solvent Classes ▾
- Product Availability ▾
- Reactant Availability ▾
- Reaction Classes ▾
- Document Type ▾
- Publication Year ▾
- Single step reactions only
- Experimental procedure only

Yield ^

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

Filter by value ▾ [View more](#)

Document Type ^

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

[View more](#)

Reagent/Catalyst ^

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

Filter by value ▾ [View more](#)

Publication Year ^

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

Filter by value ▾ [View more](#)

Solvent ^

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

Filter by value ▾ [View more](#)

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 ^

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

[View more](#)

Solvent Classes ×

✓ <input type="checkbox"/> Solvent Classes	<input type="checkbox"/>	10,112
> <input type="checkbox"/> Low boiling (<100°C)	<input type="checkbox"/>	8,385
> <input type="checkbox"/> Green	<input type="checkbox"/>	6,424
> <input type="checkbox"/> Protic	<input type="checkbox"/>	6,352
> <input type="checkbox"/> Aprotic apolar	<input type="checkbox"/>	4,172
> <input type="checkbox"/> Yellow	<input type="checkbox"/>	4,056
> <input type="checkbox"/> Aprotic dipolar	<input type="checkbox"/>	3,179
> <input type="checkbox"/> Red	<input type="checkbox"/>	3,119
> <input type="checkbox"/> High boiling (>150°C)	<input type="checkbox"/>	1,354
> <input type="checkbox"/> Middle boiling(100°C - 150°C)	<input type="checkbox"/>	912
> <input type="checkbox"/> Inorganic	<input type="checkbox"/>	88

Clear selected × Limit to > Exclude >

Reaxys中的一些特殊筛选工具—催化剂分类

Catalyst Classes ^

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

[View more](#)

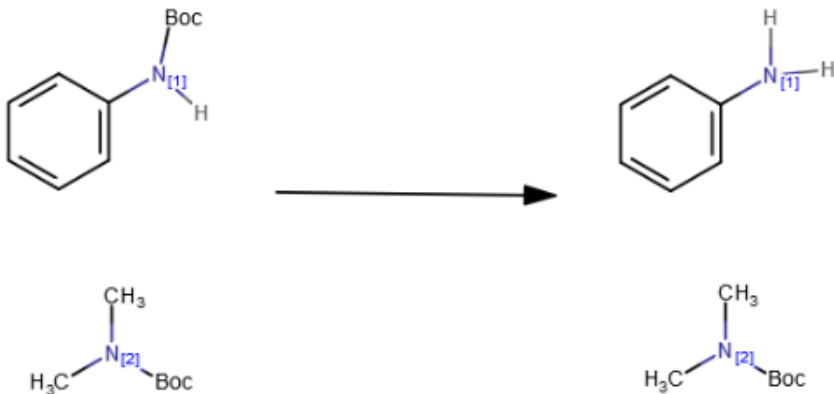
Catalyst Classes ×

- ▼ Catalyst Classes 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 × Limit to > Exclude >

Case 9: 选择性氧化还原脱保护反应的定义

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



视频操作过程:

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

Reaxys中的结构定义

Reaxys

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

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

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

- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Ignore Atom Mappings

Keep fragments

- Separate
- Together

Clear Cancel Transfer to query >

Reaxys可以直接设定这些片段在一个结构中

Reaxys中结果

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

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

Limit to > Exclude >

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

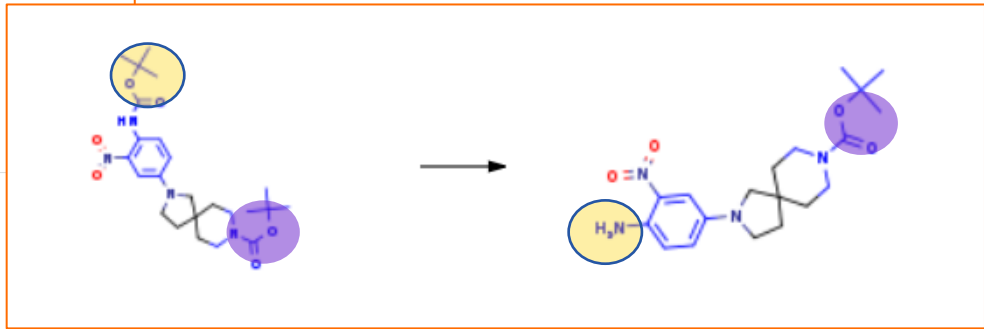
Single step reactions only
 Experimental procedure only

1 0 Limit To Exclude Export Syn-Plan Show Conditions

1 Conditions Find Similar > Reaction ID: 51038227

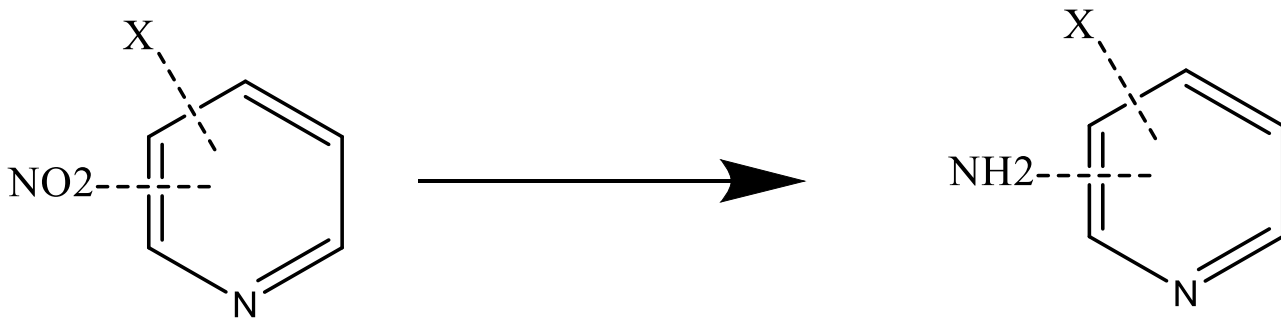
2 2 1 Conditions Find Similar > Reaction ID: 51038186

3 3



Case 10: 结构中有特殊需求的反应定义

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



视频操作过程:

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

Reaxys中的结构定义

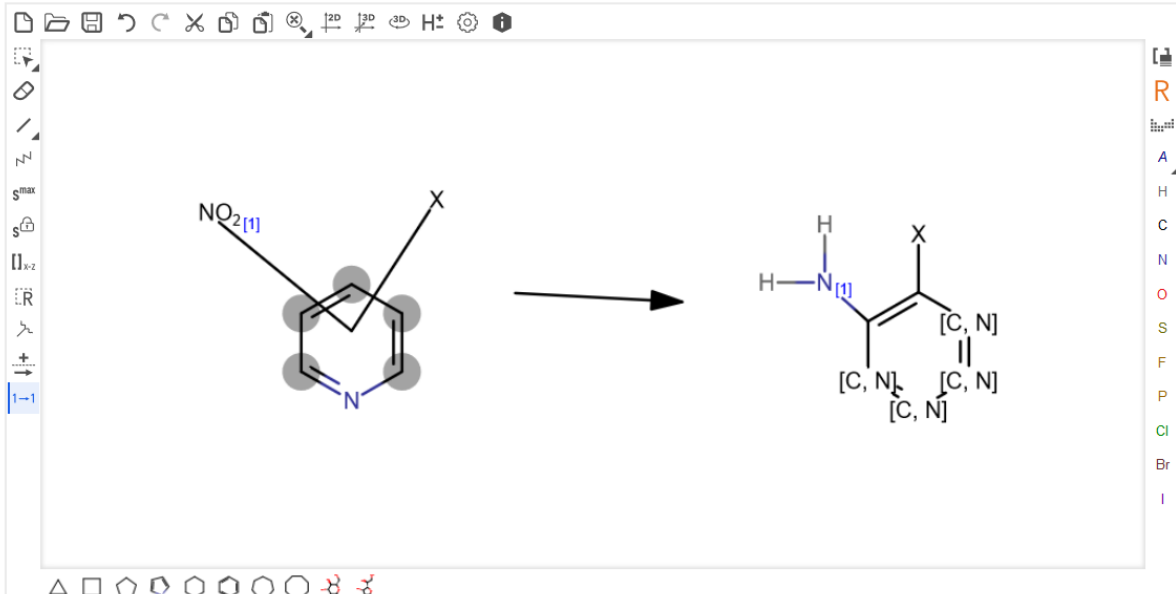
Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in ⓘ

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >




Search this structure as:

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

- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear  Cancel × Transfer to query >

最后的结果

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

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

Limit to > Exclude >

0 selected 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

2

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. 1130,1145.][Chem.Abstr., <1957> 12089] Full Text > Details >

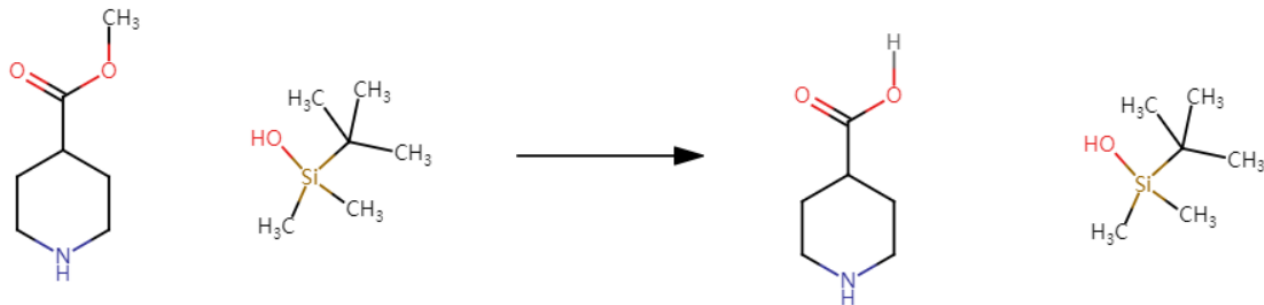
Experimental Procedure

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 11: 检索结果不理性时的拓展策略

- 在硅基存在的情况下，水解脂基
- 利用Reaxys中的碎片反应检索，只能获取2条反应，如何扩展结果

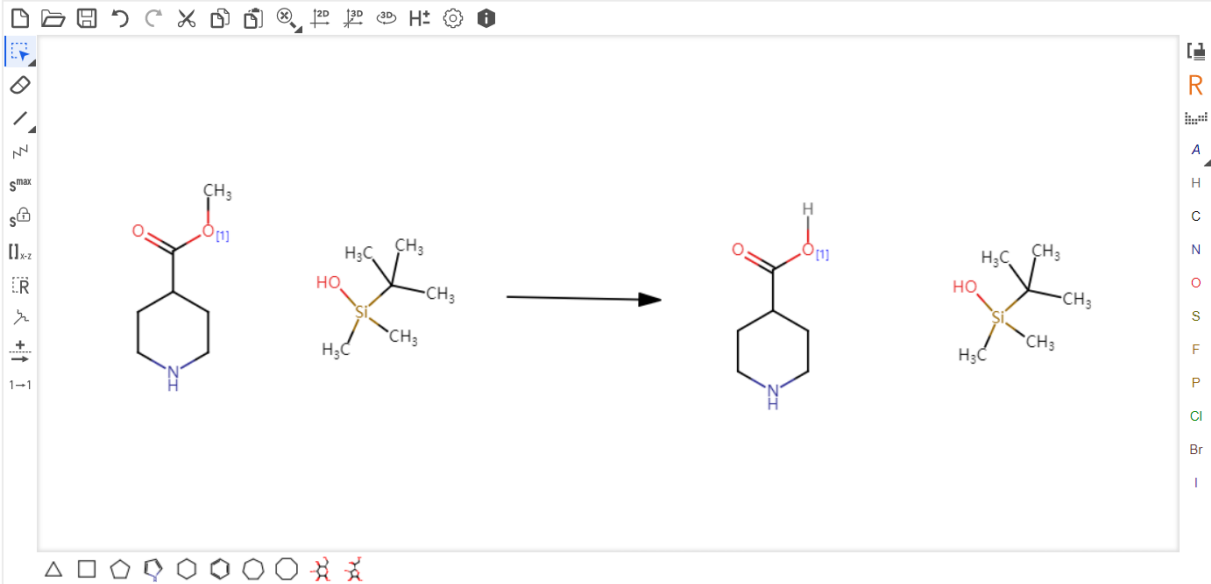


视频操作: <https://www.bilibili.com/video/BV14A41147gL>

利用Reaxys的碎片反应检索策略

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

Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >






Search this structure as:

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

Tautomers
 Stereo
 Additional ring closures
 Related Markush
 Salts
 Mixtures
 Isotopes
 Charges
 Radicals

+ More options

Clear  Cancel  Transfer to query >

Feedback 

最后的结果

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

2 Filters Limit to > Exclude > 0 selected Limit To Exclude Export Syn-Plan Show Conditions Sort by Reaxys Ranking

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

1 Conditions Find Similar > Reaction ID: 54802545

2 Conditions Find Similar > Reaction ID: 37

Find Similar Reactions...

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

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

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

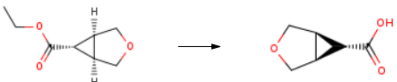
发现检索到的结果中并没有Si


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


616 Filters
2 Limit to > Exclude >
Preview

By Structure <v>
Yield <v>
Reagent/Catalyst <v>
Solvent <v>
Catalyst Classes <v>
Solvent Classes <v>
Product Availability <v>
Reactant Availability <v>
Reaction Classes <v>
Document Type <v>
Publication Year <v>
 Single step reactions only
 Experimental procedure only

616 Reactions out of 383 Documents, containing 1,112 Substances, 99 Targets
0 selected Limit To Exclude Export Syn-Plan Show Conditions
Sort by Reaxys Ranking <v>

1 
5 Conditions <v> Find Similar > Reaction ID: 34846790

2 
4 Conditions <v> Find Similar > Reaction ID: 36184173

3 

这些反应的反应中心与之前的反应相同，但是需要考虑原有反应条件，如含Si。

Feedback

限定Si

616

Filters

2

Limit to > Exclude >

Preview

By Structure

SiH_4


On all atoms

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

0 selected

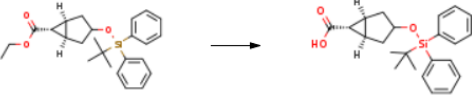
Limit To Exclude Export Syn-Plan Show Conditions

1




1 Conditions Find Similar Reaction ID: 46668291

2



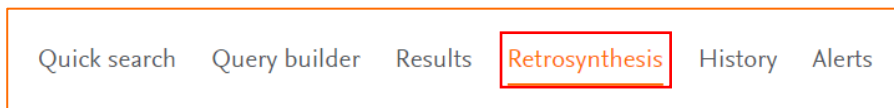
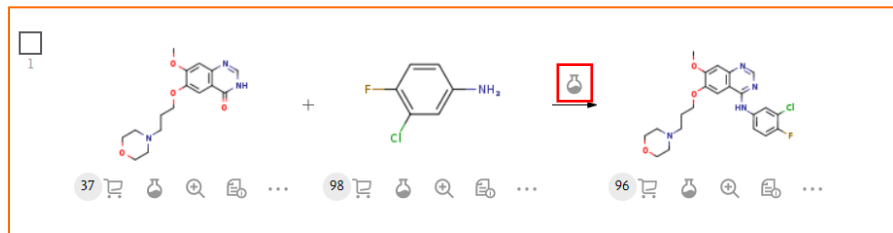
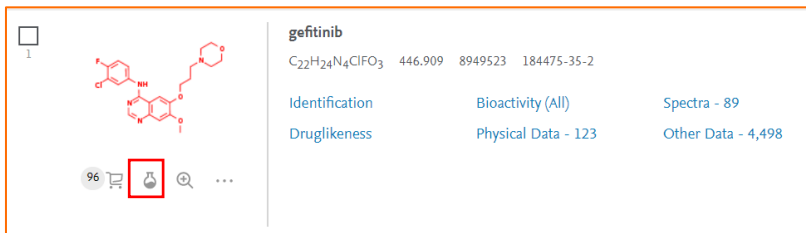
2 Conditions Find Similar Reaction ID: 49144740

3



Case 12: Reaxys中合成计划的制作

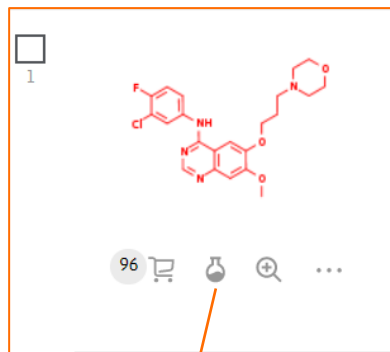
- 针对具体的化合物进行合成计划制作
 - 需要自行注册账号才可以用这个功能
 - 可以直接从物质界面，或者反应界面直接进入，也可以通过Retrosynthesis功能进入



视频操作过程:

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

从具体物质出发的合成计划制作



Synthesize

> Find preparations

> Create retrosynthesis plans

Parameters

Predicted ⓘ

20 full routes (up to)

3 identical reaction steps per project (up to)

3 identical building blocks per project (up to)

10 min processing time

STD SIAL LN EM U2 U5 T1 RSM3 RSM4 RSM5 building blocks

Edit

AI逆合成预测

Published ⓘ

5 full routes (up to)

5 branches per step (up to)

5 steps per route (up to)

Don't Stop at commercial building blocks

50% yield per step (assumed, if not published)

Edit

编辑条件

Always show screen before creating plan

Create Plans >

条件的编辑及结果

Length & depth of synthesis plans ⓘ

Full routes: 5 Last step only

Branches per step: 5

Max. number of steps: 5

Stop searching if building block is commercially available Yes No

Assumed yield for reactions without a given yield

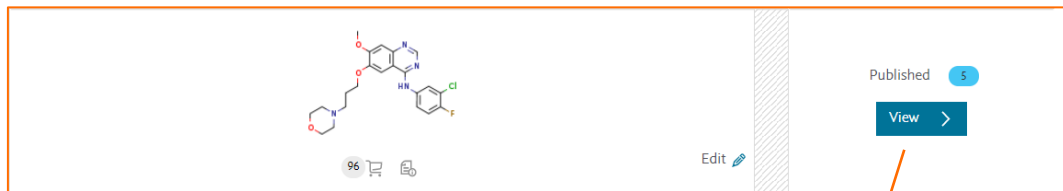
0% ————— 100%

给几条，给全部还是只给最后一步？

设定最大分支，最大步数

底物是否可购买

每一步收率



Published Route #1

Published Route #2

Published Route #3

Tree view >

Table view >

Tree view >

Table view >

Tree view >

Table view >

Feedback

结果的呈现

Export Legend

Hide conditions Tree view Table view

Published route #1

Step 1 Step 2 Step 3 Step 4

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

Step 1 Step 2 Step 3 Step 4

96.7 % Step 5

75 % Step 4

99.9 % Step 3

92.14 % Step 6

93.3 % Step 2

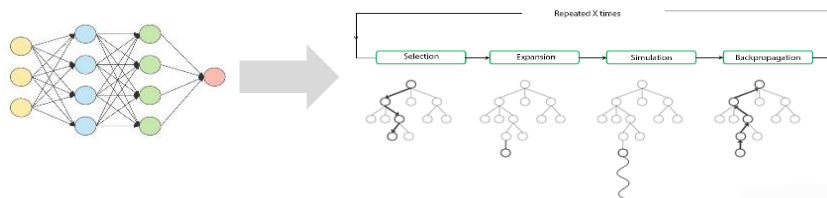
90.7 % Step 1

- Show Conditions/Reaxys Examples
- Add reaction step (one step only)
- Delete prior step(s)
- Copy reaction

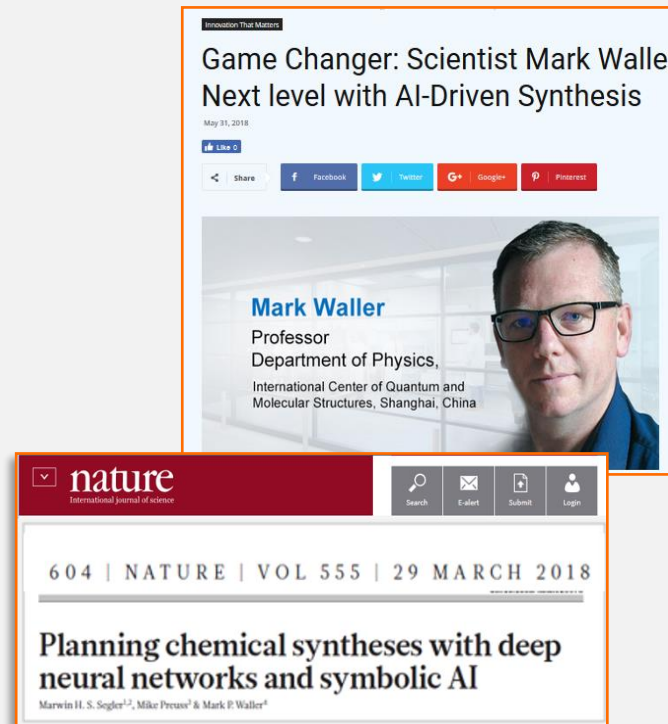
Feedback

关于Reaxys 小分子逆合成预测工具简单介绍

- Waller et al. wrote one of **the most cited works in the field of predictive retrosynthesis**, designing a predictive model based on neural networks and Monte-Carlo Tree search, that:
 - ✓ Learns transformation rules from data
 - ✓ Learns to prioritize rules
 - ✓ Learns to predict reactions
 - ✓ Uses modern efficient search methods



3 neural networks and Monte-Carlo-Tree-Search

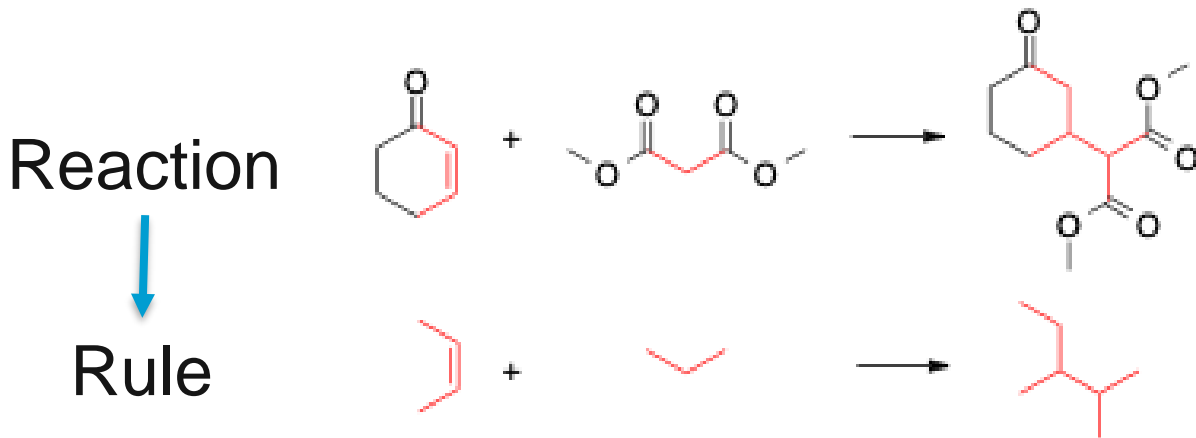


Reaxys-AI实现了自动化提取规则

Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler^{1,2}, Mike Preuss³ & Mark P. Waller⁴

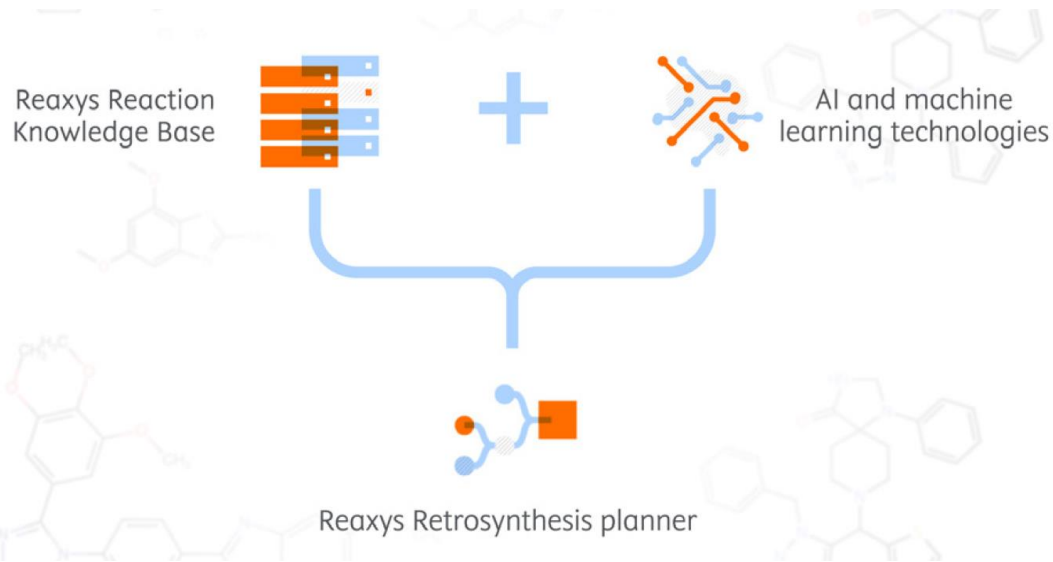
- 核心反应规则从Reaxys数据中获得
作者从来自Reaxys数据库的12.4M的**单步反应**中，提取反应转换规则。



301,671条及17,134条规则分别被应用于**拓展策略**与**快速落子策略神经网络**中

Reaxys 能提供最高质量的化学数据用于模型训练

- 预测逆合成模型的成功取决于算法和实验数据的质量



Reaxys data is key component of reaction knowledge base that is helping AstraZeneca to embed predictive algorithms in their drug development projects

Reaxys data is helping Jensen group transform the design of industrial processes for chemical and drug manufacturing

MIT Jensen Research Group
MIT Department of Chemical Engineering

From 12.5 million published single-step reactions tabulated in the Reaxys database, they prepared a library of 163,723 rules. Transformations with stereochemistry were included.

Elsevier collaboration with leading academics and the use of Reaxys data powers the most significant developments in predictive retrosynthesis algorithms

Walter Lab - Predictive Retrosynthesis

Reaxys empowers cutting edge research at MIT



Best Chemistry Predictive Analytics Specialists 2020

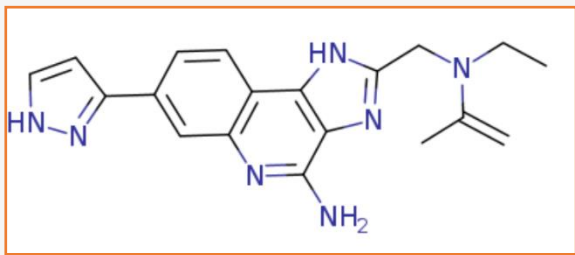
可以结合客户数据训练模型为客户定制RT工具

Reaxys RT –界面简洁使用方便

The screenshot displays the Reaxys RT Retrosynthesis interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis (selected), and History. The user is identified as Peter van Straaten. The main area shows a table of predicted routes for a target molecule. The table has columns for 'No. of steps', 'Route overview', and 'Confidence'. Five red circles with numbers 1 through 5 highlight specific features: 1. A red box around the 'Predicted Route #1' label in the first row. 2. A red box around a reaction step in the first row. 3. A red box around the '5 steps' label in the fifth row. 4. A red box around the 'Route overview' icon in the second row. 5. A red box around the confidence score '0.867' in the second row. The bottom of the interface shows 'Results per page' set to 60 and a page navigation arrow.

No. of steps	Route overview	Confidence
7 steps		
4 steps		0.867
5 steps		0.8
4 steps		0.6
5 steps		0.576
5 steps		0.3

- 1 同时查看，经典路线，文献路线，AI预测路线，便于对比
- 2 从商业化化合物的角度构建，修正预测路线
- 3 设计路线的反应步数
- 4 对和路线的概况预览
- 5 对合成路线的评分排序



卤素与烯烃的加成

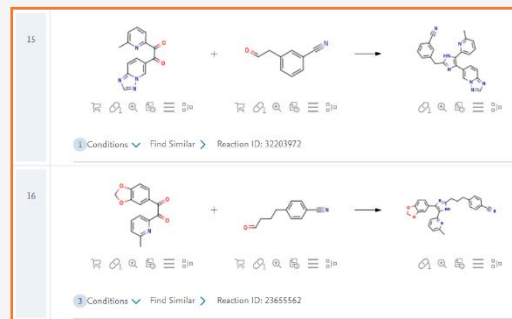
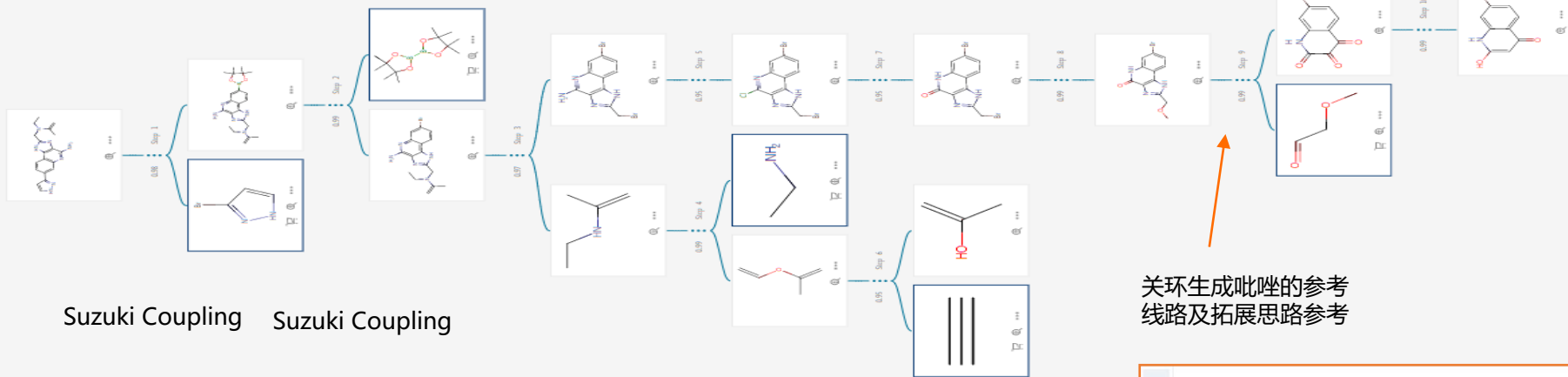
Cl转化成NH2

共轭环上OH的氯化

甲氧基变成Br

关环生成吡唑

氧化



总结

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





ELSEVIER

Q&A





Thank you

