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Elsevier Reaxys中化学信息的获取

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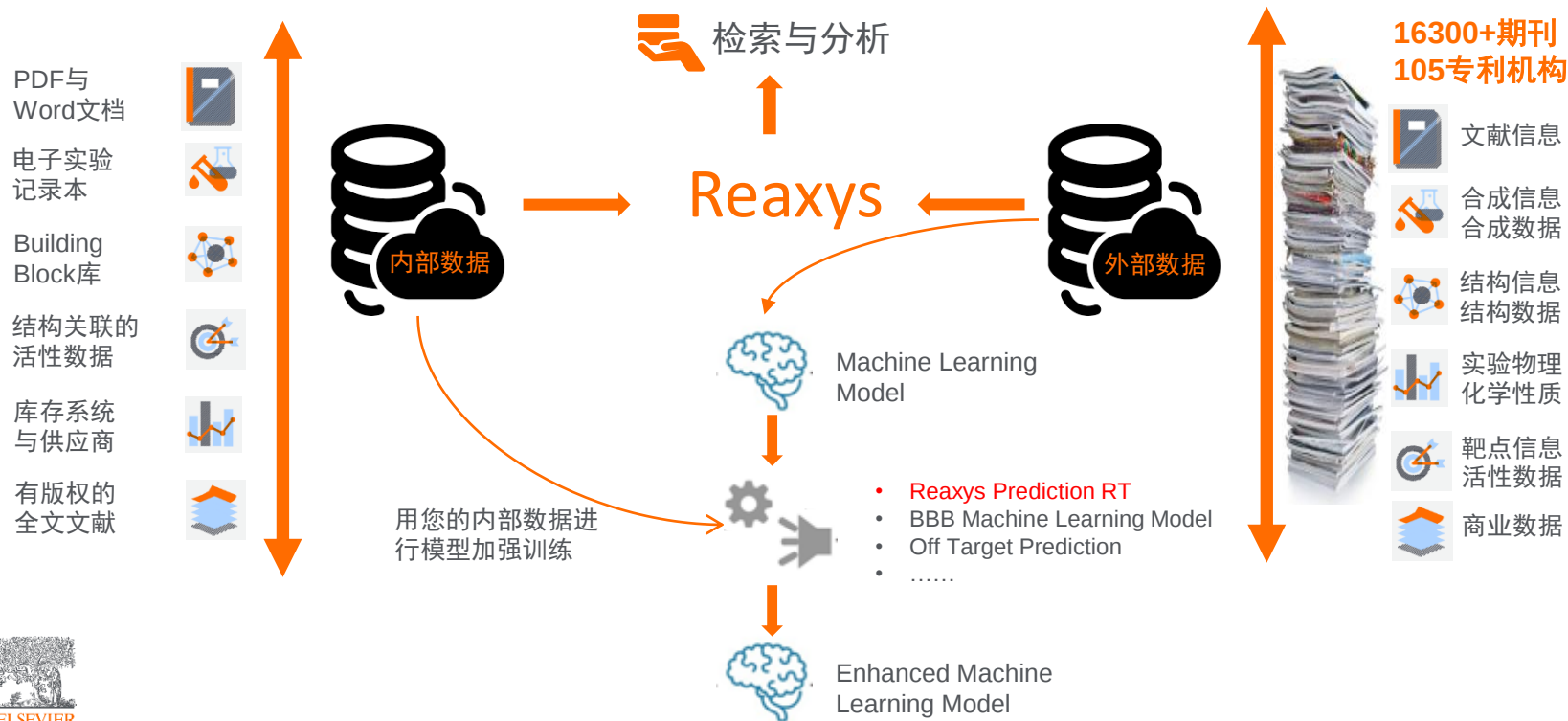


Agenda

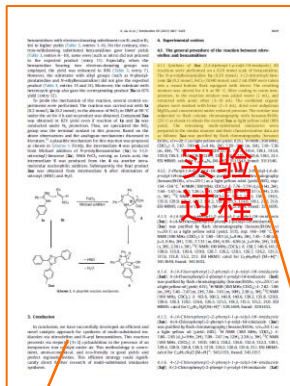
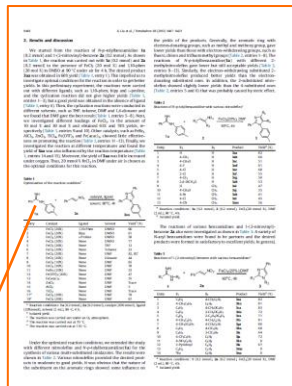
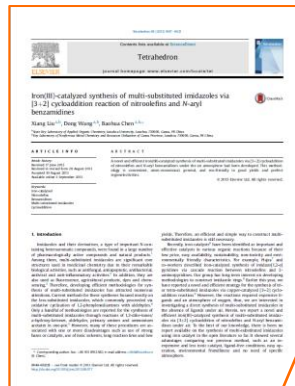
- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的科技文献检索与分析
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 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A

Reaxys—从科学数据到数据科学的跨越

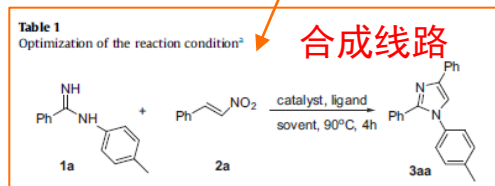
Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘，且可以整合内部与外部化学相关学科科学数据的信息检索，分析，数据科学应用平台。



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。



- 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 perfect 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

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.

Reaxys对这篇全文的提炼—概览

1 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] imidazole • 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 phenyl 1 (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 imidazol 2 yl]benzonitrile • 5 methyl 2 phenyl 1,4 di(4 tolyl) 1h imidazole • alkene derivative • benzamide derivative • ferric ion • imidazole derivative • ligand • nitroolefin derivative • unclassified drug

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

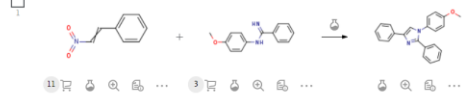
Author keywords: Benzamidines • Cycloaddition • Iron-catalyzed • Multi-substituted imidazoles • Nitroolefins

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

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

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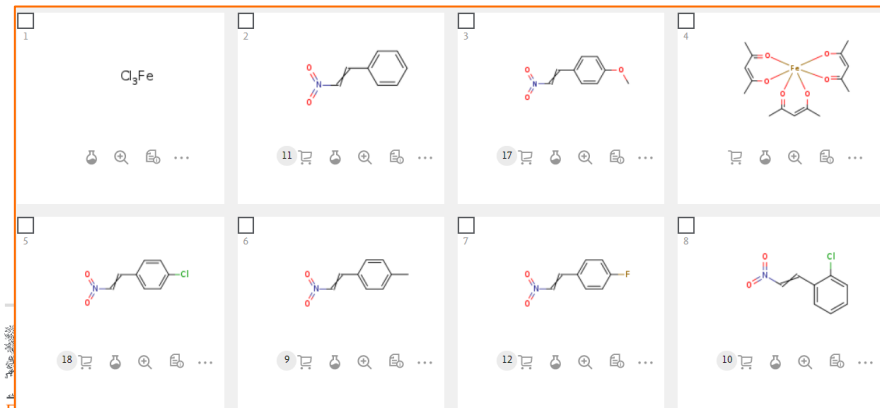
1



11 Hits [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



Grid of chemical structures showing various substituted nitroolefins and benzamidines used in the reaction. The structures are numbered 1 through 10, showing different substituents on the phenyl rings, including trifluoromethyl, chlorophenyl, and dimethoxyphenyl groups.

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.

46

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

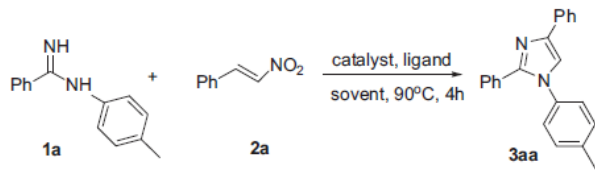
white

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.

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

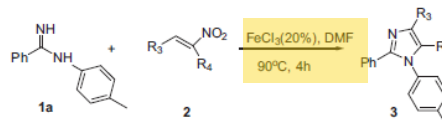
Catalyst Investigation - 4 hits out of 303

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

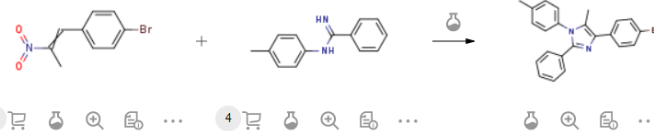


Entry	R ₃	R ₄	Product	Yield ^b (%)
1	H	H	3a	82
2	4-CH ₃	H	3ab	60
3	4-CH ₃ O	H	3ac	51
4	4-F	H	3ad	61
5	4-Cl	H	3ae	68
6	2-Cl	H	3af	55
7	4-CF ₃	H	3ag	50
8	2,4-DiCH ₃ O	H	3ah	53
9	H	CH ₃	3ai	47
10	4-CH ₃ O	CH ₃	3aj	35
11	4-Br	CH ₃	3ak	41
12	4-Cl	CH ₃	3al	45
13	4-CN	CH ₃	3am	56

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 benzamidines. 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.

21



11
4

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; Experimental Procedure	41%	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract

11 The general procedure of the reaction between nitroolefins and benzamidines

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 benzamidine. 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**) 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

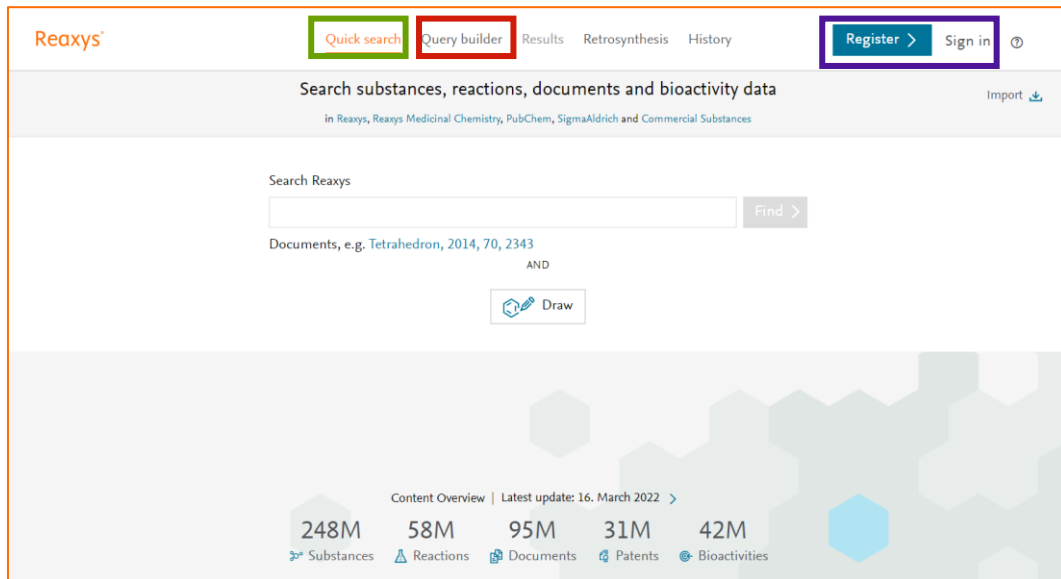
化合物在不同生物
体内活性数据

Agenda

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 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A

Reaxys的登录界面

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



Tips:

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

视频介绍:

1. Reaxys主界面：
<https://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

Reaxys®

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Sam Yu  

Search substances, reactions, documents and bioactivity data [Import](#) 

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

Search Reaxys

Find >

Substance Properties, e.g. solubility of vitamin D3

AND

 Draw

可以输入关键词，物质名称，人名反应，以及各类组合

可以输入具体结构，骨架结构，通式结构，以及包含上述结构的反应式进行检索

Content Overview | Latest update: 16. March 2022 >

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

Agenda

- Reaxys介绍与内容
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 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A

Case 1: 关键词检索—锂硫电池

- Lithium–Sulfur Battery

The screenshot displays 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 'Sam Yu' is logged in. Below the navigation bar, a search bar contains the text 'lithium-sulfur Battery'. To the right of the search bar is a 'Find >' button. Above the search bar, the text 'Search for lithium-sulfur Battery' is displayed, along with an 'Import' button. Below the search bar, there is a 'Search Reaxys' label and a 'Documents, e.g. publications about quasicrystals' suggestion. Below this, the word 'AND' is displayed. A 'Draw' button with a chemical structure icon is also visible. At the bottom, a 'Content Overview' section shows the latest update date as '16. March 2022' and provides counts for various content types: 248M Substances, 58M Reactions, 95M Documents, 31M Patents, and 42M Bioactivities.

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

Search for lithium-sulfur Battery Import

Search Reaxys

lithium-sulfur Battery Find >

Documents, e.g. publications about quasicrystals

AND

Draw

Content Overview | Latest update: 16. March 2022 >

248M 58M 95M 31M 42M

Substances Reactions Documents Patents Bioactivities

Reaxys中的检索结果

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

Results for lithium-sulfur Battery New Edit

Icon	Count	Type	Titles, Abstracts, Keywords	Actions
	13,563	Documents	"lithium-sulfur", "Battery"	Preview Results View Results
	0	Substances	Structure : as drawn	Edit in Query Builder Create Alert
	17,799	Documents	"lithium-sulfur"	Edit in Query Builder Create Alert
	1,533,052	Documents	"Battery"	Edit in Query Builder Create Alert

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

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

Limit To Exclude Export Publication Year Heatmap

13.56 K Preview

Filters

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

1 A flame retardant separator modified by MOFs-derived hybrid for safe and efficient Li-S batteries Cited 4 times
Wu, Na; Wang, Junling; Liao, Can; Han, Longfei; Song, Lei; Hu, Yuan; Mu, Xiaowei; Kan, Yongchun [Journal of Energy Chemistry, 2022, vol. 64, p. 372 - 384]
Abstract Index Terms Substances 3 Full Text

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

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

Reaxys中对于文献检索结果的分析

13.56 K

Preview

Filters

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

☐ 2022	337
☐ 2021	2,311
☐ 2020	2,237
☐ 2019	2,068
☐ 2018	1,638
☐ 2017	1,293
☐ 2016	1,026

Filter by value View more

Journal Title

☐ journal of power sources	281
☐ acs applied materials an...	269
☐ electrochimica acta	251
☐ journal of materials che...	179
☐ energy storage materials	138
☐ chemical engineering jo...	135
☐ advanced energy materials	113

Filter by value View more

Document Type

☐ patent	8,873
☐ article	4,106
☐ review	371
☐ conference paper	152
☐ note	16
☐ conference review	15
☐ short survey	12

View more

Current Patent Assignee

☐ lg chem co,ltd	1,107
☐ chinese academy of scie...	489
☐ samsung sdi co,ltd	340
☐ robert bosch stiftung	267
☐ bosch (w/o bsh)	267
☐ global graphene group	260
☐ central south university	220

Filter by value View more

Index Terms (List)

Clear selected X

Sort by Occurrence

☐ reaction	3,254
☐ spectroscopy	2,838
☐ surface	2,555
☐ ray	2,544
☐ x	2,542
☐ diffusion	2,484
☐ electrode	2,404
☐ behavior	2,280
☐ area	2,279
☐ kinetics	2,250
☐ se	2,246

1 2 3 ... 47 > Go to page

Limit to > Exclude >

Reaxys中的Index Terms (Reaxys Tree) 学科分类

The image shows the Reaxys interface with the 'Index Terms (Reaxys Tree)' filter selected in the left sidebar. The sidebar also shows a '13.56 K' count and a 'Preview' button. The main panel displays the 'Index Terms (ReaxysTree)' filter with a 'View more' link. An arrow points from the 'View more' link to a detailed view of the 'Index Terms (ReaxysTree)' filter, which shows a hierarchical tree structure with counts for each term.

Filters

Limit to > Exclude >

Publication Year ▾

Document Type ▾

Authors/Inventors ▾

Current Patent Assignee ▾

Patent Office ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

☐ Manually processed content only

Index Terms (ReaxysTree) ^

☐ physico chemical prop... 4,036

☐ chemical transformati... 3,628

☐ physico chemical analy... 3,496

☐ quantum chemical cal... 1,000

[View more](#)

Index Terms (ReaxysTree) X

- Index Terms (ReaxysTree) 13,563
 - physico chemical properties 4,036
 - chemical transformations 3,628
 - physico chemical analysis methods 3,496
 - quantum chemical calculation methods 1,000

Clear selected X

Limit to > Exclude >

利用树状图进行学科分类

Index Terms (ReaxysTree) ✕

✓ Index Terms (ReaxysTree) 13,563

> physico chemical properties 4,036

> chemical transformations 3,628

> physico chemical analysis methods

> quantum chemical calculation methods

点击箭头展开层级

Clear selected ✕

Index Terms (ReaxysTree) 2266 ✕

✓ Index Terms (ReaxysTree) 13,563

✓ physico chemical properties 4,036

> transport phenomena 3,102

> mechanical property 2,721

✓ electrochemical property 2,593

> behavior as electrode 2,266

> electrochemical cell potential 426

> acid / base behaviour 54

> electrolytic conductivity 7

☐ transference number 233

☐ electrochemical cell 166

☐ electrocatalytic property 50

☐ decomposition potential 5

Selected search items:

behavior as electrode ✕

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



ELSEVIER

最后的检索结果

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

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

0 selected Limit To Exclude Export

Sort by Publication Year ↓ Heatmap

Filters

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

physico chemical prop... 2,266
chemical transformati... 2,124
physico chemical analy... 2,123
quantum chemical calcul... 596

View more

Manually processed content only

1 Hybridized S cathode with N719 dye for a photo-assisted charging Li-S battery
Li, Jingfa; Ren, Changwei; Zhang, Linbiao; Jiang, Wenhao; Liu, Hongmin; Su, Jing; Li, Min [Journal of Energy Chemistry, 2022, vol. 65, p. 205 - 209]
Abstract Index Terms Full Text
Abstract hit: {...An integrated battery system, which integrates solar power and rechargeable battery in the...}
Index Terms hit: {...Hybridized cathode, Intergrated battery, Lithium-sulfur...}

2 Intagliated Cu substrate containing multifunctional lithiophilic trenches for Li metal anodes
Park, Sunwoo; Ahn, Kihyeon; Lim, Hyung-Kyu; Jin, Hyoung-Joon; Han, Seungyong; Yun, Young Soo [Chemical Engineering Journal, 2022, vol. 428]
Abstract Index Terms Substances 4 Full Text
Index Terms hit: {...Lithium metal anode, Lithium metal battery, Lithium metals...}

3 A new flame-retardant polymer electrolyte with enhanced Li-ion conductivity for safe lithium-sulfur batteries
Li, Hongping; Kuai, Yixi; Yang, Jun; Hirano, Shin-ichi; Nuli, Yanna; Wang, Jiulin [Journal of Energy Chemistry, 2022, vol. 65, p. 616 - 622]
Abstract Index Terms Substances 4 Full Text
Abstract hit: {...fireproof quasi-solid-state battery system....}
Index Terms hit: {...Lithium-ion conductivity, Lithium-sulfur battery, Polymer electrolyte...}

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

全文链接，如果是OA或者学校已经订购可以直接打开

Feedback

ELSEVIER

关键词检索时的麻烦问题

- 获取与低温润滑剂相关的文献 “Low temperature lubricant”

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

Search for Low temperature lubricant

Search Reaxys

Low temperature lubricant × Find >

Target Name, e.g. Polo-like kinase 1

AND

 Draw

因为对输入的关键词不做任何控制，所以给出来的结果会存在一定程度上的不准确。

 ² Influence of the amphiphilic molecule on high-density polyethylene crystallization
Zhu, Chaoqun; Zhang, Yao; Zhou, Xiaochen; Kong, Fanming; Jiang, Guodong [Journal of Thermal Analysis and Calorimetry, 2022, vol. 147, # 6, p. 4151 - 4164]
[Abstract](#) [Index Terms](#) [Full Text](#)

Abstract

The influence of organic additives on crystallization of polyolefins has not been paid enough attention due to the low dosage, but it may have a significant impact on the properties of polyolefins. In the paper, the organic amphiphilic molecules were introduced into high-density polyethylene (HDPE) through melt blending, and compared with neat HDPE. It is mainly discussed for the following aspects including analysis of crystal structure and morphology using wide-angle X-ray diffraction (WAXD) and polarized optical microscopy (POM), respectively; analysis of crystallinity, crystal rate, crystal growth and crystallization enthalpy, using the differential scanning calorimetry (DSC). The research indicates that the organic amphiphilic molecules may act as an internal lubricant. On the one hand, HDPE molecular chains are easy to fall off from crystal lattices, resulting in lagging crystallization peak, simultaneously reducing the interaction between HDPE molecules should induce the lower activation energy (ΔE_m) to increase the crystallinity of HDPE. On the other hand, the amphiphilic molecules should be exclude from HDPE crystal to the amorphous area due to poor compatibility; thus, the HDPE/amphiphilic molecules blends, similar to neat HDPE, conduct homogeneous nucleation, and the growth of monocrystal performs the tendency of the zero-dimension to the two-dimension with increase in temperature of isothermal crystallization and decreasing cooling rate of non-isothermal crystallization. It is hoped that through these studies, people will pay more attention to the impact of organic additives on the performance of HDPE. Graphic abstract: [Figure not available: see fulltext.]

Case 2: 关键词检索时词语的控制

- 获取与低温润滑剂相关的文献 “Low temperature lubricant”
 - Low Temperature以词组的形式存在，Reaxys中用引号解决
 - Lubricant可能存在多种形式的词根，Reaxys中用通配符解决
 - Low Temperature与Lubricant之间的距离在一定数量的单词内（好比<7），Reaxys中用Query Builder解决

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

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

Search fields

Fields Forms History

Reaxys ^

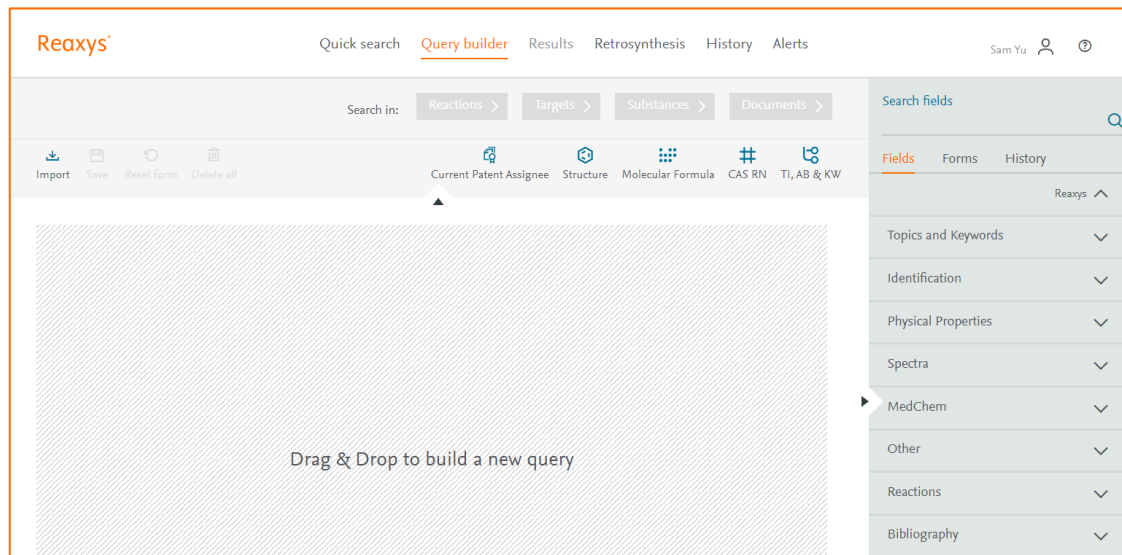
Topics and Keywords v

Identification v

Physical Properties v

Spectra v

Reaxys中的Query Builder是一种高级的组合检索模式



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

Reaxys中检索策略

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

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

◇ Titles, Abstracts & K... is ▾ "Low temperature" ³

⁵ NEAR ⁷ ◇ Titles, Abstracts & K... is ▾ Lubrican* ⁴

OR
AND
NOT
• NEAR
NEXT
PROXIMITY

设定步骤:

- 选择字段: 在Topic and Keywords中选择题录, 摘要, 关键词 (1,2)
- 输入条件: 输入关键词(3,4), 通配符*表示任意
- 确定关系: 选择两个词之间的关系, Near没有前后次序, Next有前后次序, 只有选择Near和Next的时候, 才可能出现数字的选项

Search fields

Fields Forms History

Reaxys ^

Topics and Keywords ¹ ^

◇ Substance Properties & Comments

◇ Reaction Data & Conditions

◇ Titles, Abstracts & Keywords ²

◇ All Keywords

Identification ▾

Physical Properties ▾

Spectra ▾

文献检索的结果

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

1.16 K Filters

Limit to > Exclude >

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

☐ Manually processed content only

1,160 Documents with 249 Substances, 39 Reactions, 0 Targets

☐ 0 Limit To Exclude Export

Publication Year > > Heatmap

☐ 1 No title
Current Patent Assignee: 25TH STATE RESEARCH INSTITUTE OF CHEMMOTOLOGY OF RUSSIAN DEFENSE MINISTRY - RU2763855, 2022, C1
Patent Family Members: RU2763855 C1
[Abstract](#) > [Bibliographic Info](#) > [Full Text](#) >

Abstract hit: {...assessing the low-temperature properties of grease lubricants (GL), for heavily loaded sliding friction...}

☐ 2 Investigation of tribological characteristics of nickel alloy-based solid-lubricating composites at elevated temperatures under vacuum [Cited 2 times](#)
[Zhen, Jinming](#); [Cheng, Jun](#); [Tan, Hui](#); [Sun, Qichun](#); [Zhu, Shengyu](#); [Yang, Jun](#); [Liu, Weimin](#) [Friction, 2021, vol. 9, # 5, p. 990 - 1001]
[Abstract](#) > [Index Terms](#) > [Full Text](#) >

Index Terms hit: {...Graphite, Low temperature testing, Nickel alloys...}

☐ 3 Liquid-repellent and self-repairing lubricant-grafted surfaces constructed by thiol-ene click chemistry using activated hollow silica as the lubricant reservoir [Cited 7 times](#)
[Yu, Mengnan](#); [Liu, Mingming](#); [Zhang, Liping](#); [Li, Min](#); [Hou, Yuanyuan](#); [Wang, Dong](#); [Fu, Shaohai](#) [Journal of Colloid and Interface Science, 2021, vol. 586, p. 279 - 291]
[Abstract](#) > [Index Terms](#) > [Substances](#) 6 > [Full Text](#) >

Index Terms hit: {...Directional migration, High/low temperature, Hollow mesoporous silica...}

ELSEVIER

Agenda

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

Case 3: Reaxys中化合物理化性质的快速获取

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

Tips:
快速获取某个化合物溶解性数据。

Content Overview | Latest update: 16. March 2022 >

248M

58M

95M

31M

42M

 Substances

 Reactions

 Documents

 Patents

 Bioactivities

Reaxys中的结果

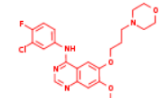
Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Results for solubility of gefitinib

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

1



gefitinib
 $C_{22}H_{24}N_4ClFO_3$ 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

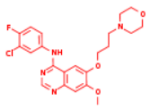
Hit Data - 6
 Solubility (MCS) - 6 hits out of 6

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 Journal of the Indian Chemical Society, 2022, vol. 99, # 1, art. no. 100260 Full Text > Details > Abstract >
					soluble in water, pH dependent water solubility	Alany, Raid G.; Fletcher, John; Khoder, Mouhamad; Mustafa, Wessam W. AAPS PharmSciTech, 2022, vol. 23, # 1, art. no. 48 Full Text > Details > Abstract >
					freely soluble in DMSO, THF and PEG-400, sparingly soluble in 2-butanol and slightly soluble in 1-butanol, IPA, ethanol, methanol, EG and PG	Alanazi, Abdulhadi; Alshehri, Sultan; Altamimi, Mohammad; Shakeel, Fayaz Journal of Molecular Liquids, 2020, vol. 299, art. no. 112211 Full Text > Cited 44 times > Details > Abstract >
					soluble in water and 1-octanol	Wu, Kuen-Da; Chen, Grace Shihyui; Liu, Jia-Rong; Hsieh, Chen-En; Chern, Ji-Wang ACS Medicinal Chemistry Letters, 2019, vol. 10, # 1, p. 22-26 Full Text > Cited 6 times > Details > Abstract >
0.00982	In pure solvent	25	water	supporting information		Wang, Xin-Xin; Tian, Fei-Yang; Liu, Ming; Chen, Kai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu Tetrahedron, 2019, vol. 75, # 37, art. no. 130488 Full Text > Cited 2 times > Details > Abstract >
0.0021	In pure solvent	20	water			Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Wei; Dong, Xiaochun Bioorganic and Medicinal Chemistry Letters, 2013, vol. 23, # 19, p. 5385-5388 Full Text > Cited 28 times > Details > Abstract >

Reaxys中化合物更多的理化性质


1

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

直接获取化合物的理化性质或者谱图数据

[Spectra - 89](#)

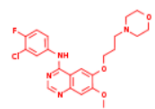
- ✓ NMR Spectroscopy - 47
- ✓ IR Spectroscopy - 9
- ✓ Mass Spectrometry - 19
- ✓ [UV/VIS Spectroscopy - 11](#)
- ✓ Raman Spectroscopy - 1
- ✓ Fluorescence Spectroscopy - 2

[Physical Data - 123](#)

- ✓ Melting Point - 28
- ✓ Density - 1
- ✓ Association (MCS) - 12
- ✓ Chromatographic Data - 8
- ✓ Conformation - 1
- ✓ Crystal Phase - 9
- ✓ Crystal Property Description - 27
- ✓ Crystal System - 2
- ✓ Dissociation Exponent - 3
- ✓ Further Information - 1
- ✓ Interatomic Distances and Angles - 3
- ✓ Partition octan-1-ol/water (MCS) - 14
- ✓ Solubility (MCS) - 6
- ✓ Space Group - 8

Reaxys中化合物的生物活性数据（需要RMC模块）

RMC是Reaxys药物化学模块，文献与专利中的活性数据全部收录在其中。


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

Bioactivity (All)

- In vitro: Efficacy - 5843
- In vivo: Animal Model - 838
- Metabolism - 349
- Pharmacokinetic - 816
- Toxicity/Safety Pharmacology - 2366

In vitro Efficacy - 5843

Quantitative Results

pK	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Bioassay	Dose	Effect	Concomitants	Reference
10.4	K _i (inhibition constant)		0.028	nM		Inhibitor	Epidermal growth factor receptor (L858R)Wild				enzyme inhibitor		Argyrou, Argyrides; Deig, Peter; Zhai, Xiang[Biochemistry, 2020, 144]
10.2	K _i (inhibition constant) (Apparent)		0.07	nM			EGFR (T746-A750del) [human]Wild	Trichoplusia ni baculovirus infected	Enzymology inhibition			Marker: [33P]ATP; CoEnzyme: Mg-ATP	Gilmer, Tona M; Cable, Louann; Ruznak, David; Spehar, Glenn; G Woldu, Ermas; (...) Shewchuk, I research, 2008, vol. 68, # 2, p. 5; Full Text > Cited 60 times >
10.2	K _i (inhibition constant)	=	0.07	nM		Radioligand (ligand)	Epidermal growth factor						Gilmer, Tona M; Cable, Louann; Ruznak, David; Spehar, Glenn; G

Pharmacokinetic - 816

Quantitative Results

pK	Parameter	Value (quant)	Biological Species	(Clinical) findings / disease	Route of administration	Dose	2...	Reference
3.37	concentration (parameter)	0.03	mouse		intraperitoneal administration	25 mg/kg		Agarwal, Sagar; Sane, Ramolo; Gallardo, Jose L; Ohlfest, John R; Elmquist, William F; [Journal of Pharmacology and Experimental Therapeutics, 2010, vol. 334, # 1, p. 147 - 155] Full Text > Cited 183 times > Details > Abstract >
4.39	concentration (parameter)	0.18	human	breast cancer	oral administration	250 mg		McKillop, David; Partridge, Elizabeth A; Kemp, John V; Spence, Mike P; Kendrew, Jane; Barnett, Sharon; Wood, Philippa G; (...) Guillaud, Nicolas; Stephens, Trevor C; [Molecular Cancer Therapeutics, 2005, vol. 4, # 4, p. 641 - 649] Full Text > Cited 106 times > Details > Abstract >
4.37	concentration (parameter) (Plasma)	0.43 - 1.29	human		oral administration			Tamura, Shinichi; Hosoi, Hajime; Kuwahara, Yasumichi; Kikuchi, Ken; Otake, Osamu; Izumi, Moriatsu; Tsuchiya, Kunihiko; Iehara, Tomoko; Gotoh, Takahiro; Sugimoto, Tohru [Biochemical and Biophysical Research Communications, 2007, vol. 358, # 1, p. 226 - 232] Full Text > Cited 29 times > Details > Abstract >

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 displays the Reaxys Query Builder interface. At the top, navigation tabs include 'Quick search', 'Query builder' (selected), 'Results', 'Synthesis planner', and 'History'. On the right, there are links for 'Register >' and 'Sign in ?'. Below the navigation, a 'Search in:' section contains buttons for 'Reactions >', 'Targets >', 'Substances >' (selected), and 'Documents >'. A toolbar with icons for 'Import', 'Save', 'Reset form', and 'Delete all' is located below the search in section. To the right of the toolbar, there are icons for 'Structure', 'Molecular Formula' (selected), 'CAS RN', and 'TI, AB & KW'. The main query builder area shows a table with columns for field selection, logical operators, and field names. The first row is 'Molecular Formula' with the operator 'is'. The second row is 'Catalyst Investigation' with the operator 'AND'. Below the 'Catalyst Investigation' row, there are several sub-rows for specific fields: 'Investigated characteristic(s)', 'Specification of catalysis', 'Classification of catalysis', 'Type of reaction', and 'Co-catalyst/co-substrate name'. On the right side of the interface, there is a 'Search fields' panel with a search bar containing 'catalyst'. Below the search bar, there are expandable sections for 'Catalyst Investigation' and 'Reagent/Catalyst'. An orange arrow points from the 'Molecular Formula' icon in the top navigation bar to the 'Molecular Formula' field in the query builder. Another orange arrow points from the 'Catalyst Investigation' field in the query builder to the 'Catalyst Investigation' section in the search fields panel.

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 ◇ 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

Search fields
Q catalyst

Catalyst Investigation

Reagent/Catalyst

Reaxys ^

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

条件的输入

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

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula contains ▼ Fe

AND

◇ Catalyst Investigation

☐ Find any Hide fields ^

is ▼ Investigated characteristic(s)

is ▼ stereoselective catalysis

is ▼ Classification of catalysis

is ▼ Type of reaction

is ▼ Co-catalyst/co-substrate name

Step3: 进行物质检索

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

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

Specification of catalysis 1

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

最后的结果

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

311 Filters

Limit to > Exclude >

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

0 selected Limit To Exclude Export Preparations

Sort by No of References ↓

Grid Heatmap

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

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

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

Hit Data - 2

Catalyst Investigation - 2 hits out of 25

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: 获取含C的在低温具有导电性能的化合物

- 获取在零下250摄氏度下，含有C的，且电导率 $>10000\text{s/cm}$ 的化合物
- Query Builder下联合Electrical Data与分子式进行检索

The screenshot displays the Reaxys Query Builder interface. At the top, navigation tabs include 'Quick search', 'Query builder' (selected), 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user 'Sam Yu' is logged in. Below the navigation bar, there are buttons for 'Import', 'Save', 'Reset form', and 'Delete all'. The 'Search in:' section has tabs for 'Reactions', 'Targets', 'Substances', and 'Documents'. The 'Molecular Formula' tab is selected and highlighted with a red box. The 'Search fields' dropdown on the right shows 'electrical' entered. The main query builder area shows two conditions connected by 'AND':

- Molecular Formula** contains **Molecular Formula**
- Electrical Data** is **Description (Electrical Data)**, **= Electric Conductivity, S/cm**, **= Temperature of Electric Conductivity, °C**, and **= Critical Superconductivity Temperature, °C**

An orange arrow points from the 'Electrical Data' field in the query builder to the 'Electrical Data' and 'Electrical Data (MCS)' options in the 'Search fields' dropdown, which are also highlighted with a red box.

设定条件

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

Search in: Reactions > Targets > Substances > Documents >

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

◇ Molecular Formula contains ▼ C

AND

◇ Electrical Data ☐ Find any Hide fields ^

is ▼ Description (Electrical Data)

>= ▼ 10000

<= ▼ -250

= ▼ Critical Superconductivity Temperature, °C

Search fields Fields Forms History Reaxys ^ Topics and Keywords Identification Physical Properties Spectra MedChem Other

输入条件

最后的结果

Reaxys®

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

Sam Yu

30

Query

Filters

Limit to > Exclude >

By Structure >

Measurement pX >

Highest Clinical Phases >

Targets >

Parameters >

Substance Classes >

Molecular Weight >

Number of Fragments >

Availability >

Availability in other databases >

Available Data >

Document Type >

Publication Year >

Patent Assignee >

LogP >

0 selected

Limit To Exclude Export Preparations

Sort by No of References ↓

Grid Heatmap

2

CTa

tantalum carbide

TaC_{1.0} 192.959 16507128

Hit Data - 3

Identification

Druglikeness

Spectra - 16

Physical Data - 278

Other Data - 20

Preparations - 57 >

Reactions - 133 >

Documents - 384 >

Hit Data - 3

Electrical Data - 3 hits out of 26

3

CB₂Ni₂Y

yttrium nickel borocarbide

Y(NiB)₂C 239.919 16214287

Hit Data - 3

Identification

Druglikeness

Spectra - 35

Physical Data - 201

Other Data - 17

Preparations - 4 >

Reactions - 18 >

Documents - 250 >

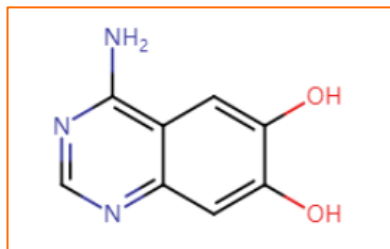
Hit Data - 3

Electrical Data - 3 hits out of 89

Feedback

Case 6: 骨架化合物活性获取（需要RMC模块）

- 获取包含下面骨架，且在EGFR-T790M上有活性，且有ic50报道的化合物
- 类似视频操作：<https://www.bilibili.com/video/bv1pK411G7rX>



The screenshot displays the Reaxys Query builder interface. The top navigation bar includes links for Quick search, Query builder, Results, Synthesis planner, History, and Alerts. The user is logged in as Sam Yu. The search criteria are defined in the 'Structure' field, which contains the chemical structure of the quinazolin-2-amine derivative. The search criteria are also defined in the 'Target Name' and 'Measurement Parameter' fields.

Search in: Reactions > Targets > Substances > Documents >

Structure Molecular Formula CAS RN TI, AB & KW

On all atoms

Target Name is t790m

Measurement Parameter is ic50

Search fields: Fields Forms History

Reaxys > Topics and Keywords > Identification > Physical Properties > Spectra > MedChem > Other > Reactions > Bibliography > PubChem > Commercial Substances >

检索策略的构建

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Search fields

Fields Forms History

Topics and Keywords

Tips: 手动添加, 结构, Target, Parameter 的字段

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Structure

Create Structure / Reaction Drawing

AND Target Name is Target Name/ Uniprot ID/ PDB ID/ Reaxys Target ID

AND Measurement Parameter is Measurement Parameter

Search fields

target

Reaxys ^

Target Name

Substance Action on Target

Target Nature

Target Mutant/Chimera Details

Target Transfection

Keywords

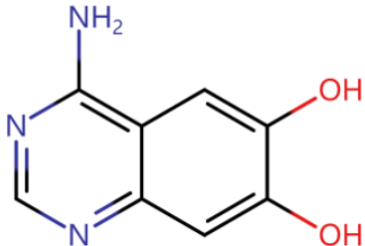
条件的输入

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

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

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

◇ Structure



On all atoms

AND ◇ Target Name is ▼ T790m

AND ◇ Measurement Parameter is ▼ ic50

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
- Commercial Substances v

最后的结果

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

106 Substances out of 76 Documents, containing 843 Reactions, 50 Targets

Reaxys - 106

Limit To Exclude Export Preparations No of References Grid Heatmap

Filters

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

1

gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 194475-25-7

Identification
Druglikeness
Bioactivity (Hit Data)
Bioactivity (All)

pX	Parameter	Value (quant)	Unit	Action on target	Target	Cell	Bioassay	Dose	Effect	Concomitants	Reference
7.64	IC50	0.023	μM	Inhibitor	Epidermal growth factor receptor (T790M);Wild	cell line			antineoplastic agent		Abbass, Safinaz E. S.; Allam, Heba Abdelrasheer Aly, Enayat E.; El Kerdawy, Ahmed M.; Farouk, Ahmed K. B. A. W.; Rashwan, Essam [Biochemistry, 2020, vol. 98] Full Text Details Abstract

2

vandetanib
C₂₂H₂₄N₄O₂BrF 475.361 9161676

Identification
Druglikeness
Bioactivity (Hit Data)
Bioactivity (All)

pX	Parameter	Value (quant)	Unit	Action on target	Target	Cell	Bioassay	Dose	Effect	Concomitants	Reference
6.43	IC50	369.2	nM	Inhibitor	Epidermal growth factor receptor (L858R/T790M)/C7975;Wild				antineoplastic agent		Li, Qiannan; Zhang, Tao; Li, Shiliang; Tong, Linjiang; Li, Junyu; Su, Zhicheng; Feng, Fang; (...) Xie, Hua; Xu, Yufang [ACS Medicinal Chemistry Letters, 2019, vol. 10, # 6, p. 869 - 873] Full Text Cited 3 times Details Abstract

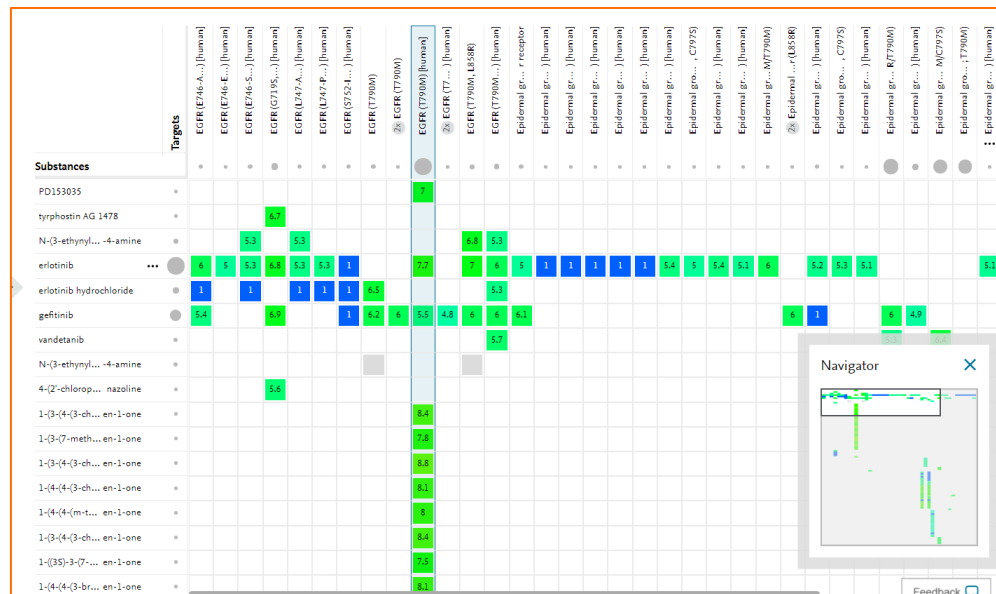
3

erlotinib
C₂₂H₂₃N₃O₄ 393.442 8798958 1

Identification
Druglikeness
Bioactivity (Hit Data)
Bioactivity (All)

pX	Parameter	Value (quant)	Unit	Action on target	Target	Cell	Bioassay	Dose	Effect	Concomitants	Reference
7.7	IC50	20 - 200	nM	Inhibitor	EGFR (T790M) [human];Wild			1-10 μM		Substrate: ATP	Yuhan Corporation; Suh, Byung-Chul; Salgaonkar, Paresh Devidas; Lee, Jaekyoo; Koh, Jong Sung; Song, Ho-Juhn; Lee, In Yong; (...) Kim, Jung-Ho; Kim, Se-Won - US2016/102076, 2016, A1 Full Text Details Abstract

Feedback



Case 7: 快速筛选对特定靶点有活性的化合物（需要RMC模块）

- 获取文献中报道的对“RNA依赖的RNA聚合酶（RdRp）”有活性报道的化合物
- 希望这些化合物的IC50在um级别

The screenshot displays the Reaxys Query Builder interface. At the top, navigation tabs include 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History'. On the right, there are 'Register' and 'Sign in' buttons. Below the navigation, a 'Search in:' section contains four buttons: 'Reactions', 'Targets', 'Substances' (highlighted with an orange box), and 'Documents'. A toolbar below this includes 'Import', 'Save', 'Reset form', and 'Delete all' icons, followed by icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main query area shows a search for 'Target Name is rdrp'. Below this, a group of conditions is defined: 'Group 1' contains 'Measurement Parameter is ic50|' and 'Measurement pX >= 6'. A 'Tips' box on the right provides guidance on using the 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

Target Name is rdrp

AND

Group 1 Ungroup

Measurement Parameter is ic50|

AND Measurement pX >= 6

Search fields Q PX

Reaxys ^

Measurement pX

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

Reaxys中的结果

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

554 Filters

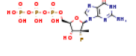
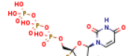
Limit to > Exclude >

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

554 Substances out of 13 Documents, containing 759 Reactions, 7 Targets

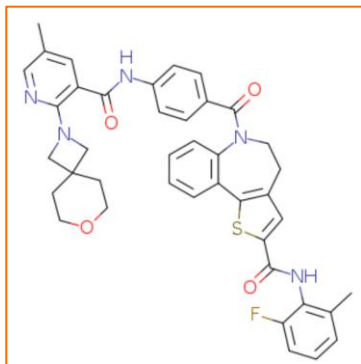
0 selected Limit To Exclude Export Preparations

Sort by No of References ↓ Grid Heatmap

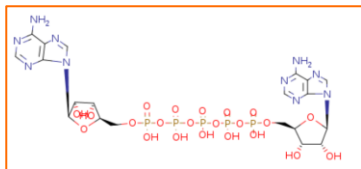
	p1,p5-di(adenosine 5'-)-pentaphosphate C ₂₀ H ₂₉ N ₁₀ O ₂₂ P ₅ 916.373 604343 41708-91-2	Identification Druglikeness Bioactivity (Hit Data)	Bioactivity (All) Physical Data - 1 Spectra - 1	Other Data - 28	Preparations - 4 Reactions - 7 Targets - 35 Documents - 77
	2'-deoxy-2'-alpha-fluoro-2'-beta-C-methylguanosine-5'-triphosphate C ₁₁ H ₁₇ N ₅ O ₁₃ P ₃ 539.201 12162768	Identification Druglikeness Bioactivity (Hit Data)	Bioactivity (All)	Spectra - 4	Preparations - 3 Reactions - 3 Targets - 11 Documents - 10
	Reaxys ID: 27022205 C ₁₁ H ₁₄ FN ₂ O ₁₅ P ₃ 526.156 27022205 1613590-42-3	Identification Druglikeness Bioactivity (Hit Data)	Bioactivity (All)	Spectra - 9	Preparations - 18 Reactions - 18 Feedback

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

Reaxys中的结果



pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	(Clinical) findings / disease	Cell	Dose	Effect	Reference
6.97	IC50 (AUC viral load (Log ₁₀ PFU/ml *Day))	108	nM	human	Inhibitor	RNA-directed RNA polymerase L:Wild	lung cancer	Small airway epithelial cell	28-700 nM	antivirus agent	Brookes, Daniel W; Coates, Matthew; Allen, Heather; Daly, Leah; Constant, Samuel; Huang, Song; Hows, Mark; (...) Rapeport, Garth; Ito, Kazuhiro[British Journal of Pharmacology, 2018, vol. 175, # 12, p. 2520 - 2534] Full Text ↗ Cited 13 times ↗ Details > Abstract >
6.81	IC50 (AUC viral load (Log ₁₀ PFU/ml *Day))	154	nM	human	Inhibitor	RNA-directed RNA polymerase L:Wild	lung cancer	Bronchial airway epithelial cell	28-700 nM	antivirus agent	Brookes, Daniel W; Coates, Matthew; Allen, Heather; Daly, Leah; Constant, Samuel; Huang, Song; Hows, Mark; (...) Rapeport, Garth; Ito, Kazuhiro[British Journal of Pharmacology, 2018, vol. 175, # 12, p. 2520 - 2534] Full Text ↗ Cited 13 times ↗ Details > Abstract >



Reaxys将全文中的活性数据提炼出来，并进行标准化处理。

pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	Effect	Reference
7.05	IC50 (with extended primer)	0.09	μM	Influenza A virus (A/Puerto Rico/8/1934(H1N1))	Inhibitor	RNA-directed RNA polymerase [Influenza A virus]:Wild + No given title	anti-influenza virus agent	Bhat, Rakesh; Kumar D, Jagadeesh; Landi, Abdolamir; Pagadala, Nataraj Sekhar[Medicinal Chemistry Research, 2020] Full Text ↗ Details > Abstract >

利用HeatMap看结构与靶点关系

Reaxys

Quick search Query builder Results Synthesis planner History Alerts

554 Substances out of 13 Documents, containing 759 Reactions, 7 Targets

Limit to Exclude selected Limit to Exclude Export Preparations

Sort by No. of References

Grid Heatmap

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

pⁱp^o-d(adenosine 5'-pentaphosphate)
C₂₀H₂₉N₁₀O₁₂P₅ 956.373 604.343 41708.91-2

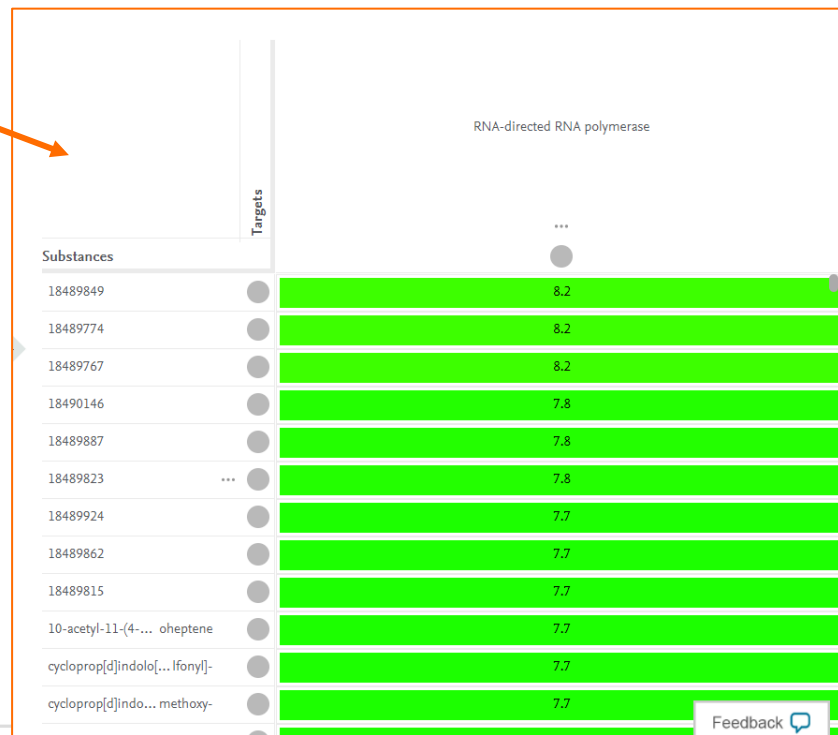
Identification Bioactivity (All) Other Data - 28 Preparations - 4
Druglikeness Physical Data - 1 Reactions - 7
Bioactivity (Hit Data) Spectra - 1 Targets - 35 Documents - 77

2'-deoxy-2'-α-fluoro-2'-β-C-methylguanosine-5'-triphosphate
C₁₁H₁₂FN₂O₁₂P₃ 539.265 12162768

Identification Bioactivity (Hit Data) Spectra - 4 Preparations - 3
Druglikeness Bioactivity (All) Reactions - 3
Targets - 11 Documents - 10

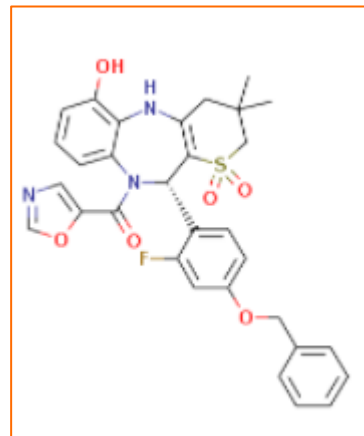
Reaxys ID: 27022205
C₁₁H₁₄N₂O₁₂P₃ 536.154 27022205 1613590-42-3

Identification Bioactivity (Hit Data) Spectra - 9 Preparations - 18
Druglikeness Bioactivity (All) Reactions - 18
Feedback

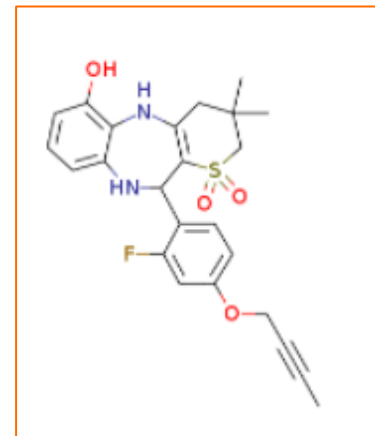


利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

一些非常有意思的结构



PX=8.2



PX=6.9

Case 8: 双靶点活性化合物的获取（需要RMC模块）

- PI3K和mTOR双抑制剂，且活性都在nM级别化合物

视频操作链接: <https://www.bilibili.com/video/BV1vK4y1Z7fr>

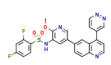
The screenshot displays the Reaxys Query Builder interface. At the top, navigation tabs include 'Quick search', 'Query builder' (selected), 'Results', 'Synthesis planner', and 'History'. On the right, there are 'Register >' and 'Sign in' buttons. Below the navigation, a 'Search in:' section has buttons for 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. A toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all'. Another toolbar shows 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main area features a 'Selectivity Profile' panel with two query blocks. The first block is for 'PI3K' with a 'Measurement pX' of '>= 9'. The second block is for 'mTOR' with a 'Measurement pX' of '>= 9'. A right-hand sidebar titled 'Search fields and forms' lists various search criteria: 'Fields', 'Forms' (selected), and 'History'. Under 'Forms', there are expandable sections for 'Reaxys Forms' and 'Reaxys MedChem Forms'. The 'Reaxys MedChem Forms' section is expanded, showing a list of search fields: 'Affinity on target', 'Cell proliferation: inhibition', 'Selectivity Profile', 'Animal models: Tumor xenografts', 'Bioavailability', 'Volume of distribution', and 'Absorption (Cmax, Cavg)'.

双靶点活性化合物

96 Substances out of 47 Documents, containing 148 Reactions, 17 Targets

☐ 0 selected [Limit To](#) [Exclude](#) [Export](#) [Preparations](#)

☐ 1

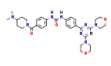


GSK2126458
C₂₈H₁₇F₂N₅O₃S 505.504 20875369 1086062-66-9

[Identification](#)
[Druglikeness](#)
[Bioactivity \(Hit Data\)](#)

[Bioactivity \(All\)](#)
[Physical Data - 3](#)
[Spectra - 3](#)

☐ 2



PKI-587
C₃₂H₄₁N₅O₄ 615.735 19641026 1197160-78

[Identification](#)
[Druglikeness](#)
[Bioactivity \(Hit Data\)](#)

Substances Exit Full Screen			
Limit To Exclude Export Settings Navigator Legend			
		Targets	
		Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	Serine/threonine-protein kinase mTOR
Substances i			
GSK2126458		10.7	11.7
1-(trans-4-hy...in-2-one		9.8	9.4
1-[(2Z)-2-[(2...thylurea		9.7	9
N-[2-(dimet...enzamide		9.7	9.1
(Z)-N-(2-(di...enzamide		9.7	9.5
(Z)-N-(2-(di...oacetate		9.7	9.5
1-(4-[[3-(dime...yl]urea		9.6	9
24438406		9.6	9
N-[2-(dimet...enzamide		9.5	9

Case 9: 寻找在特定靶点上存在变构调节的分子

- 传统Adenosine A1 receptor激动剂由于正构位点保守性造成选择性差而无法进入临床，因此，在具有特异性的A1R变构位点上发现激动剂就存在巨大的潜力

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 (highlighted), Results, Retrosynthesis, History, and Alerts are on the right. Below this is a search bar with a 'Search in:' dropdown and four buttons: Reactions, Targets, Substances, and Documents. A toolbar contains icons for Import, Save, Reset form, and Delete all. On the right side of the toolbar are icons for Patent Assignee, Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main query area shows two conditions: 'Substance Action on T...' is 'allosteric modulator' and 'Target Name' is 'Adenosine A1 receptor'. The conditions are linked by an 'AND' button. Each condition has a dropdown arrow on the left and a search icon on the right.

有变构调节研究的化合物

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Sam Yu

1,204 Substances out of 44 Documents, containing 4,173 Reactions, 5 Targets

☐ 0 selected

Sort by No of References Grid

Filters

Limit to > Exclude >

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

Available Data

Document Type

Publication Year

Patent Assignee

LogP

1

Reaxys ID: 8626983

C₁₃H₁₁NO₅ 261.368 8626983 Retrieve CAS RN

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Preparations - 2 >

Reactions - 2 >

Targets - 1 >

Documents - 1 >

2

Reaxys ID: 8635048

C₁₄H₁₂INOS 369.226 8635048 Retrieve CAS RN

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Preparations - 2 >

Reactions - 2 >

Targets - 1 >

Documents - 1 >

3

Reaxys ID: 8651630

C₂₂H₁₉IN₂O₃S 518.375 8651630 304018-35-7

Identification

Druglikeness

Preparations - 2 >

Reactions - 2 >

Targets - 1 >

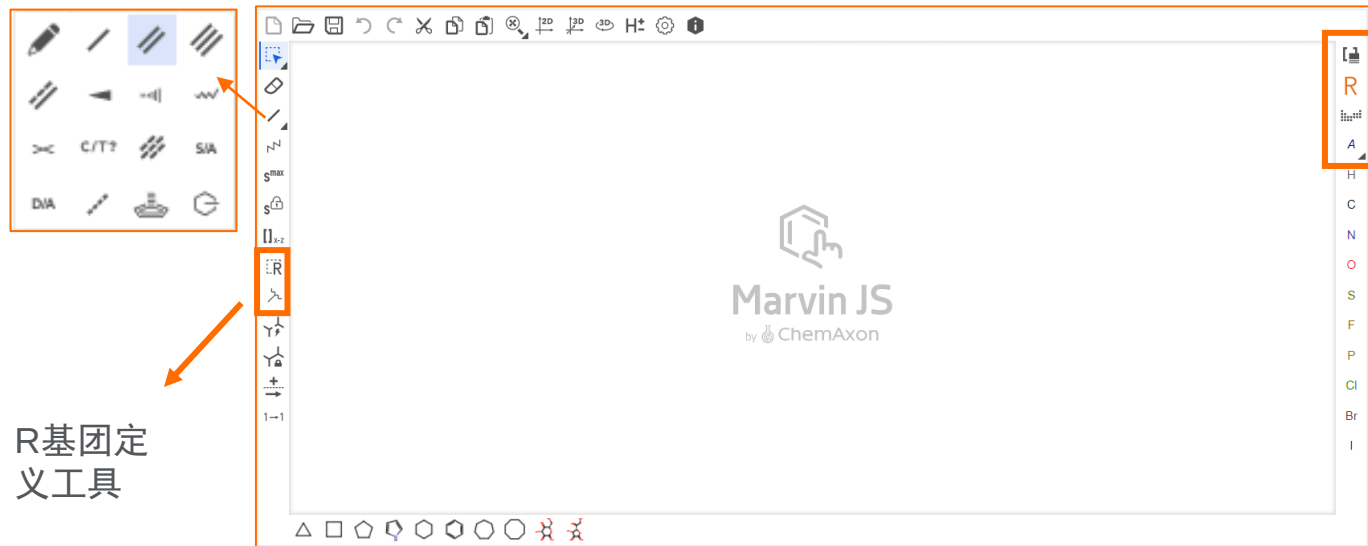
Documents - 1 >

Feedback

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中的科技文献检索与分析
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A

Reaxys中的结构面板

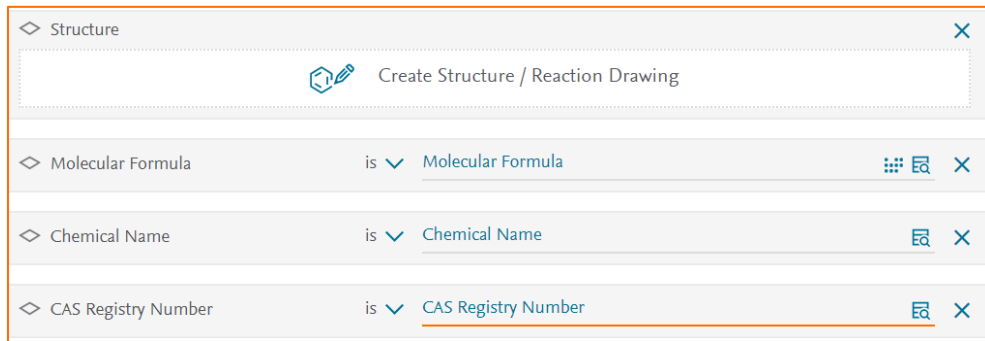
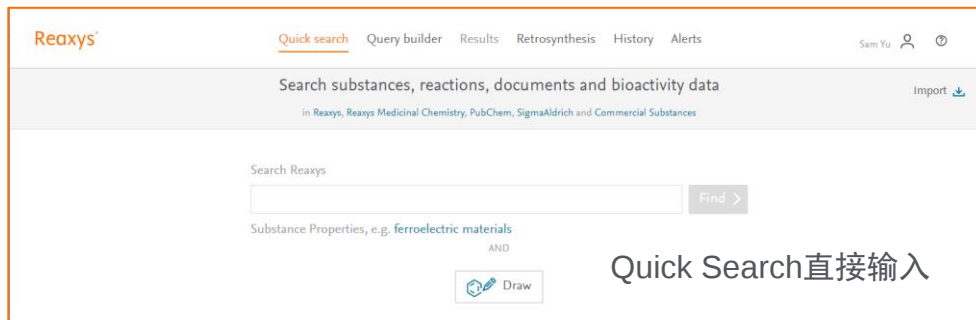


一些常见的功能使用视频

常用功能	视频链接	
最基本功能	https://www.bilibili.com/video/BV13i4y177wV	基础结构面板使用
不定位键	https://www.bilibili.com/video/BV1LK411P7nW	
通用/缩写官能团	https://www.bilibili.com/video/BV1PV41117J6	
原子列表与列表非	https://www.bilibili.com/video/BV1Ay4y1z7a5	
R基团定义	https://www.bilibili.com/video/BV1654y1r7be	
原子锁定与环锁定	https://www.bilibili.com/video/BV175411V77h	
G Group与通用原子	https://www.bilibili.com/video/BV1fy4y1B7LU	
原子属性列表	https://www.bilibili.com/video/BV1uD4y1R7K2	
盐，自由基，同位素	https://www.bilibili.com/video/BV1Rr4y1c7AL	
反应定义基本操作	https://www.bilibili.com/video/BV19r4y1w7Z5	基础反应功能使用
反应条件的定义	https://www.bilibili.com/video/BV1Af4y1q7xk	
合成计划的制作	https://www.bilibili.com/video/BV1oL411u7yP	
机理性文献查询	https://www.bilibili.com/video/BV1pK4y1E7Qx	

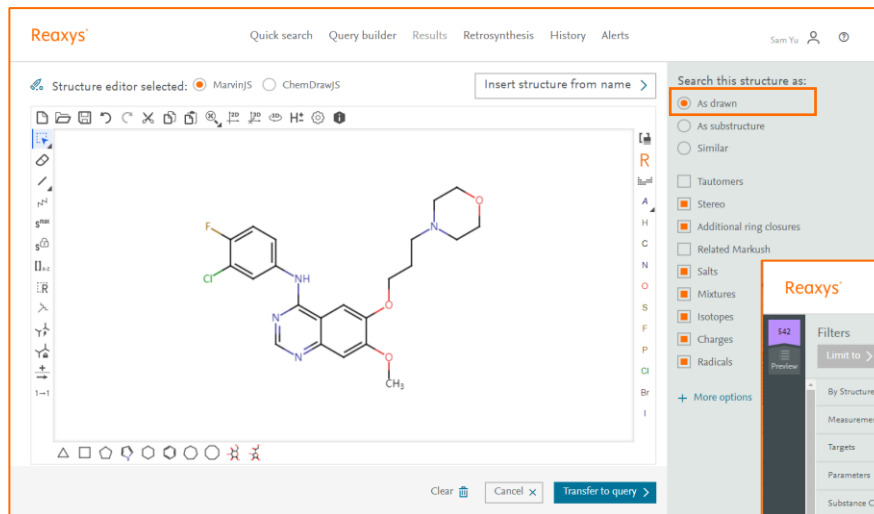
Reaxys中的结构获取物质的常用方法小结

- 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



Query Builder选择不同字段

CASE 10: Reaxys中具体化合物的获取



结构面板中绘制具体化合物，同时使用As Drawn进行检索，即可获取具体化合物，包括盐，同位素，配合物，混合物等

Reaxys

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

Sam Yu

542 Substances out of 12,159 Documents, containing 216 Reactions, 1,214 Targets

Reaxys - 542

0 selected Limit To Exclude Export Preparations

Sort by No of References

Grid Heatmap

Filters

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

1

2

3

gefitinib

C22H24N4ClO3 446.909 8949523 184475-35-2

Identification Bioactivity (All) Spectra - 89

Druglikeness Physical Data - 123 Other Data - 4,498

Preparations - 85

Reactions - 164

Targets - 1,170

Documents - 12,124

Reaxys ID: 28938758

28938758

mixture (composition partially given)

Identification Targets - 2

Bioactivity (All) Documents - 8

Gefitinib hydrochloride

C22H24ClFN4O3*ClH 483.37 14998854 184475-55-6

Identification Bioactivity (All) Spectra - 1

Druglikeness Physical Data - 1

Preparations - 1

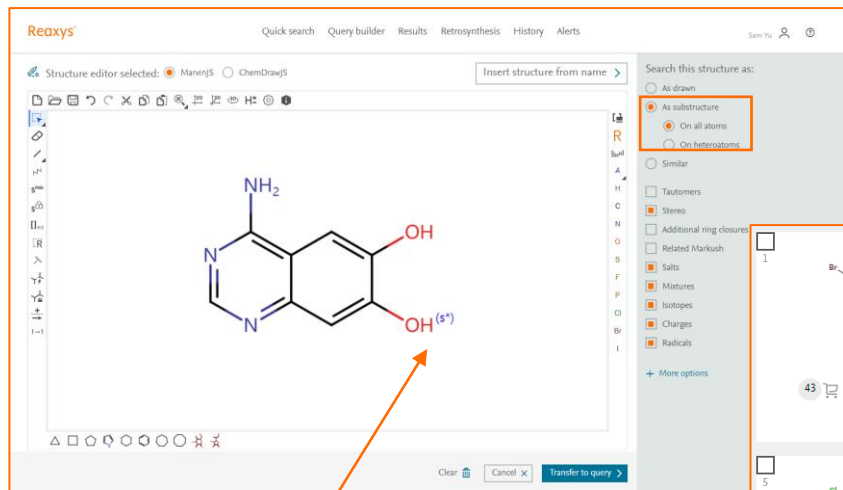
Reactions - 2

Targets - 3

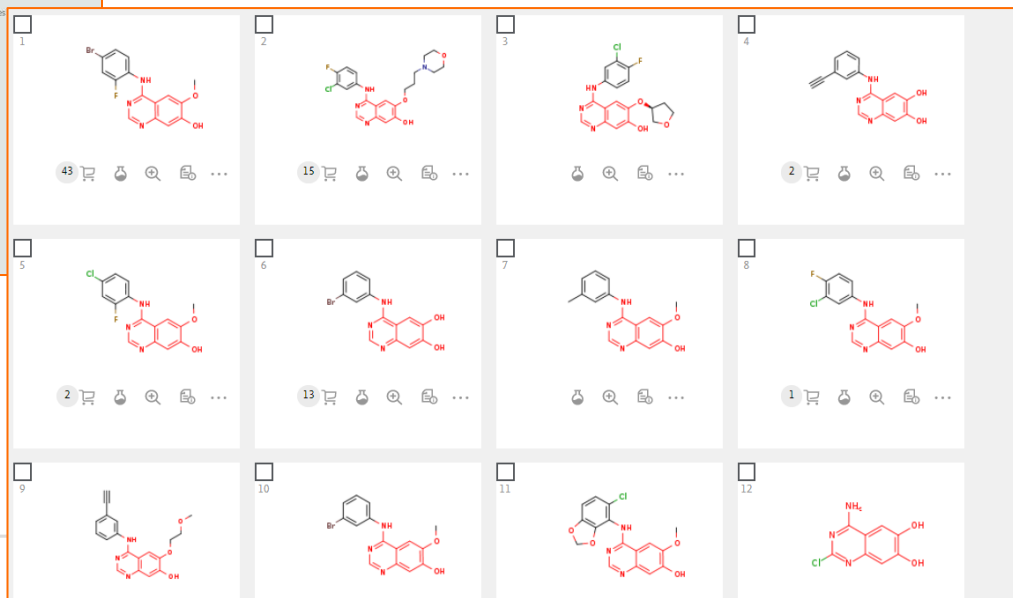
Documents - 7

Feedback

CASE 11: Reaxys中骨架化合物的获取



结构面板中绘制具体或通式结构，同时使用As Substructure进行检索，即可获得包含这个骨架的化合物。



标记这个位点上不允许有取代

Case 12: Reaxys中最简单的反应定义与筛选

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

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

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

Search this structure as:

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

+ More options

原子匹配与原子锁定

Reaxys中的结果

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

11,06 K Filters

Limit to > Exclude >

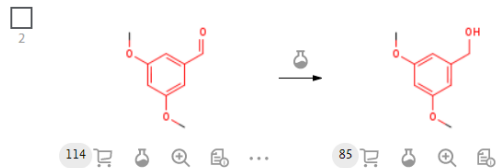
By Structure 
Yield 
Reagent/Catalyst 
Solvent 
Catalyst Classes 
Solvent Classes 
Product Availability 
Reactant Availability 
Reaction Classes 
Document Type 
Publication Year 

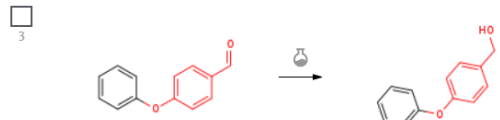
☐ Single step reactions only
☐ Experimental procedure only

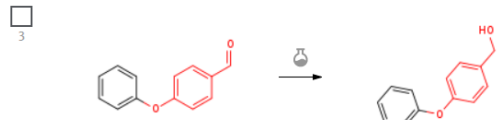
11,063 Reactions out of 7,929 Documents, containing 14,783 Substances, 2,966 Targets

 0    Show Conditions

Reaxys Ranking   

1  79  63 Conditions  Find Similar > Reaction ID: 2407606

2  114 Conditions  Find Similar > Reaction ID: 305004

3  38 Conditions  Find Similar > Reaction ID: 305004

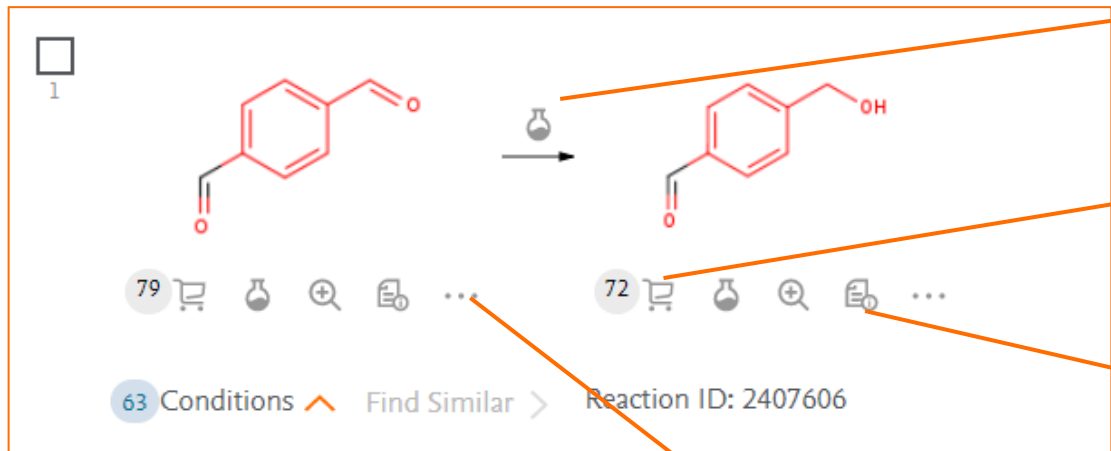
Show/Hide Conditions, 选择显示/隐藏条件

43 Conditions  Find Similar > Reaction ID: 2407606

Conditions	Yield	Reference
With sodium tetrahydroborate in tetrahydrofuran; ethanol at 0°C; for 7h;	97%	Bahn, Yong-Sun; Cheong, Eunji; Choi, Ji Won; Hwang, Hayoung; Kim, Byungsun; Kim, Myeon Jeong; Kim, Jun Woo; [et al] Seo, Seon Hee; Yoon, Seul Ki <i>Journal of Medicinal Chemistry</i> , 2021 Full Text  Details 
With formic acid; [R5-C5H5]Ru(K)-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 <i>Journal of Organometallic Chemistry</i> , 2009, vol. 694, # 22, p. 3643 - 3652 Full Text  Cited 22 times  Details 
With bis[15-cyclopentadienyl]hafnium dihydride in isopropyl alcohol at 80°C; for 8h;	91%	Nakano, Tatsuya; Umano, Shigetoshi; Kino, Yoshiyuki; Yasutaka, Osamu; Masaya <i>Journal of Organic Chemistry</i> , 1988, vol. 53, # 16, p. 3752 - 3757 Full Text  Cited 48 times  Details 

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

☐ >95 - 100 924

☐ >90 - 95 835

☐ >85 - 90 614

☐ >80 - 85 456

☐ >75 - 80 375

☐ >70 - 75 287

☐ >65 - 70 223

Filter by value ▾ View more

Document Type

☐ article 7,543

☐ patent 3,181

☐ review 68

☐ conference paper 44

☐ letter 11

☐ short survey 4

☐ note 4

View more

Reagent/Catalyst

☐ sodium tetrahydroborate 7,079

☐ methanol 1,387

☐ potassium carbonate 1,236

☐ water 690

☐ lithium aluminium tetrahydride 639

☐ hydrogen 620

☐ hydrogenchloride 599

Filter by value ▾ View more

Publication Year

☐ 2020 393

☐ 2019 788

☐ 2018 834

☐ 2017 780

☐ 2016 921

☐ 2015 829

☐ 2014 755

Filter by value ▾ View more

Solvent

☐ methanol 4,014

☐ tetrahydrofuran 3,375

☐ ethanol 2,025

☐ water 1,395

☐ dichloromethane 1,268

☐ n,n-dimethyl-formamide 1,105

☐ toluene 515

Filter by value ▾ View more

Tips:

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

Reaxys中的一些特殊筛选工具—溶剂分类

Solvent Classes ^

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

[View more](#)

Solvent Classes X

▼ Solvent Classes

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

Clear selected X

Limit to > Exclude >

Reaxys中的一些特殊筛选工具—催化剂分类

Catalyst Classes ^

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

[View more](#)

Catalyst Classes X

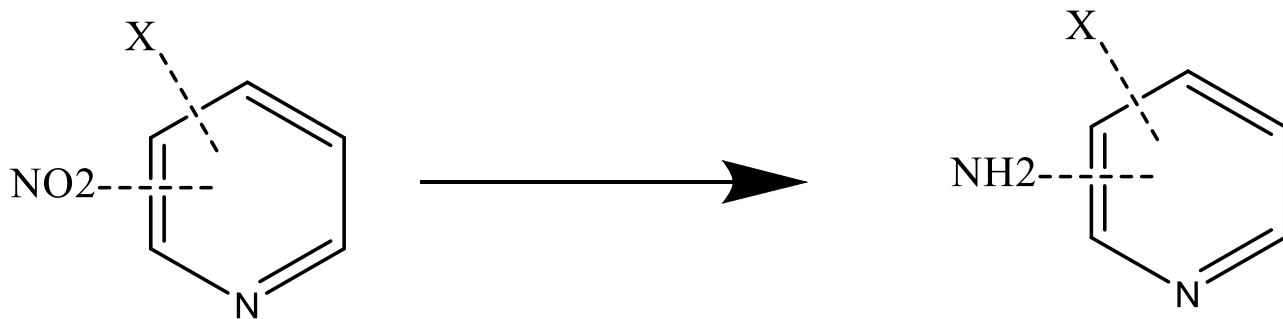
- ▼ Catalyst Classes 10,112
 - ▼ active center 8,926
 - > B 7,587
 - > Al 956
 - > Pd 803
 - ▼ Cu 288
 - ☐ copper(I) iodide 160
 - ☐ copper 40
 - ☐ copper(II) oxide 35
 - ☐ copper(I) chloride 13
 - ☐ copper diacetate 11
 - ☐ copper oxide-chromium oxide 10

Clear selected X

Limit to > Exclude >

Case 13: 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

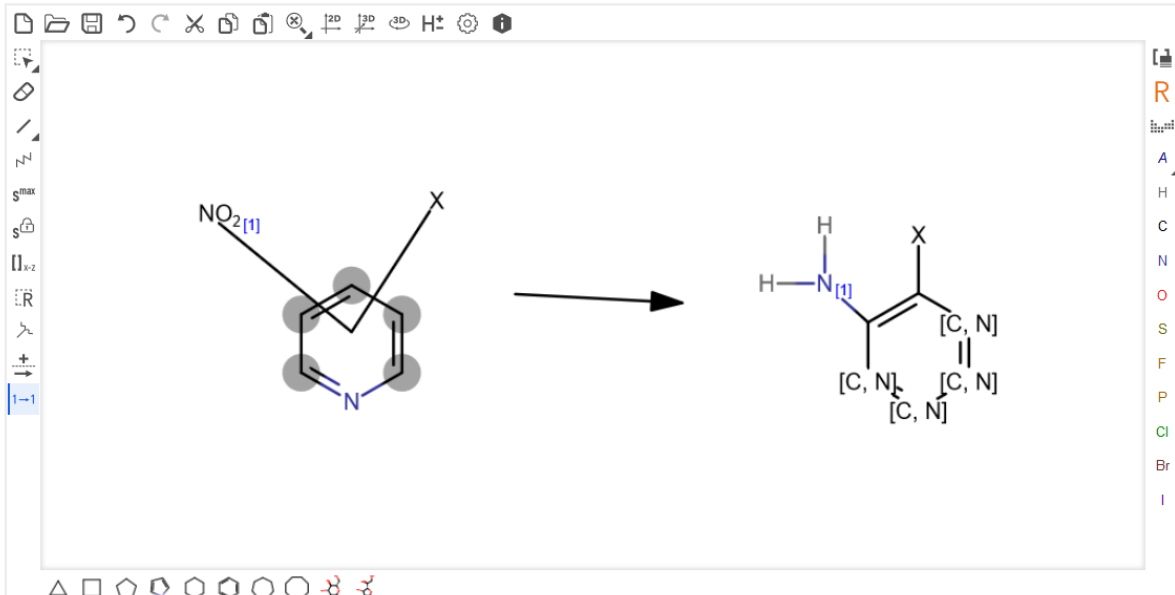
Reaxys®

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 X Transfer to query >

最后的结果

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

624 Filters

Limit to > Exclude >

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

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

0 selected Limit To Exclude Export Syn-Plan Show Conditions

1

2

3

6 Conditions Find Similar > Reaction ID: 149845

7 Conditions Find Similar > Reaction ID: 22895930

1

Conditions Find Similar > Reaction ID: 149845

Conditions	Yield	Reference
With hydrogen in methanol at 20°C, for 2h; Experimental Procedure >	96%	LIFESCI PHARMACEUTICALS, INC., MCDONALD, Andrew, QIAN, Shawn WO2017/1936, 2017, A2 Location in patent: Paragraph 00159 Full Text > Details > Abstract >
With hydrogen, nickel in ethanol at 20°C, under 760.051 Torr, for 4h; Experimental Procedure >	95%	UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC. WO2007/47793, 2007, A2 Location in patent: Page/Page column 87 Full Text > Details > Abstract >
With iron, acetic acid Erwärmen des Reaktionsgemisches mit HgCl ₂ und Zink.		Talik, Plazek [Roczniki Chemii, 1956, vol. 30, p. 1139,1145.][Chem.Abstr., <1957> 12089] Full Text > Details >

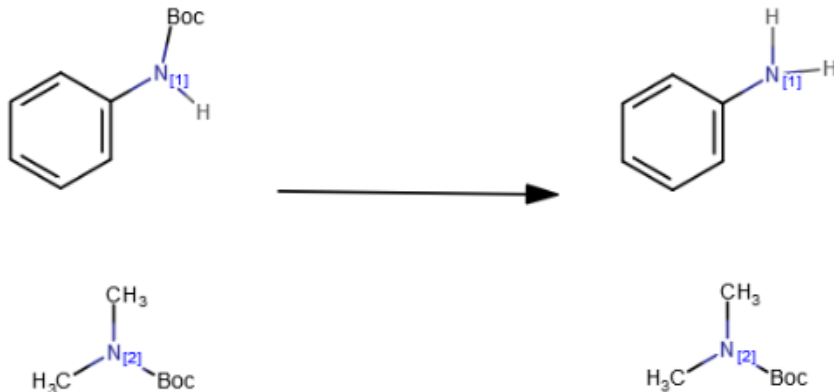
Experimental Procedure

4-Amino-2-chloro-3-nitropyridine (6.0 g, 34.57 mmol) in 150 mL of ethanol was hydrogenated over Raney nickel catalyst (6.0 g wet) for 4h at room temperature under 1.0 atm of H₂ atmosphere. After addition of 4.0 g of celite to the solution, the mixture was stirred vigorously and filtered over celite pad. The filtrate was concentrated and purified with silica gel column chromatography (CH₂Cl₂:MeOH = 20:1 v/v) to give 2-Chloro-3,4-diaminopyridine (4.72 g, 32.84 mmol) in 95% yield. ¹H-NMR (DMSO, 500 MHz) δ 7.31 (d, J = 5.0, 1H), 6.45 (d, J = 5.0, 1H), 5.79 (s, 2H), 4.68 (s, 2H); ¹³C-NMR (DMSO, 125 MHz) δ 143.41, 138.03, 135.61, 126.66, 108.73, 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 14: 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

Clear Cancel Transfer to query >

Reaxys可以直接设定这些片段在一个结构中

☐ Ignore Atom Mappings

☒ Keep fragments

☐ Separate ☒ Together

Reaxys中结果

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

12 Filters

Limit to > Exclude >

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

0 Limit To Exclude Export Syn-Plan Show Conditions

By Structure ▾

Yield ▾

Reagent/Catalyst ▾

Solvent ▾

Catalyst Classes ▾

Solvent Classes ▾

Product Availability ▾

Reactant Availability ▾

Reaction Classes ▾

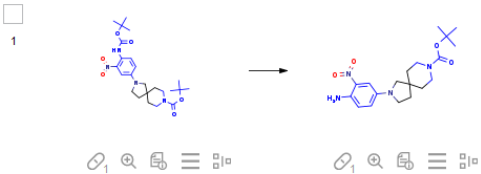
Document Type ▾

Publication Year ▾

☐ Single step reactions only

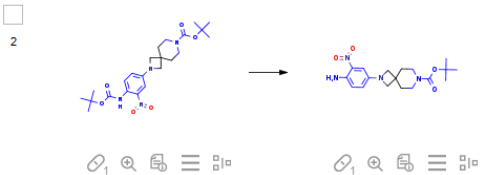
☐ Experimental procedure only

1



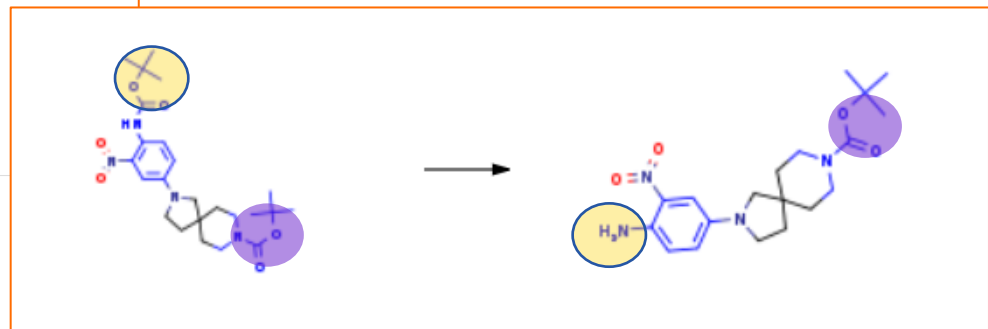
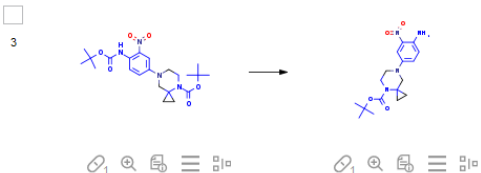
1 Conditions Find Similar > Reaction ID: 51038227

2



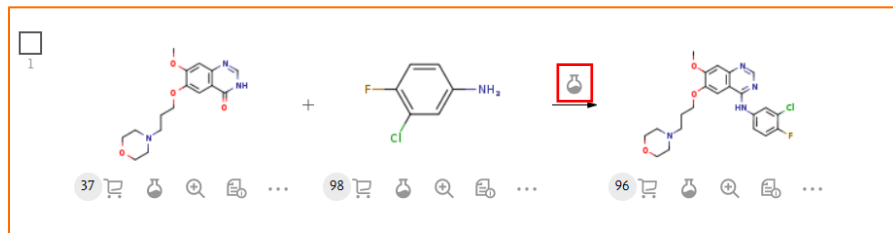
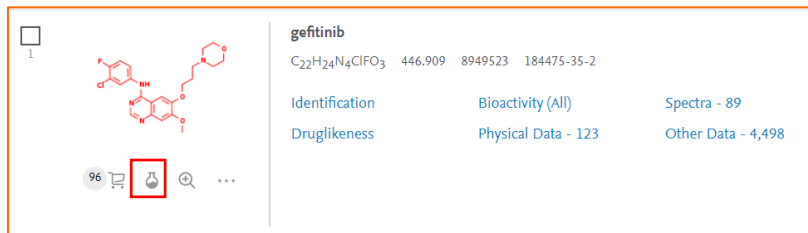
1 Conditions Find Similar > Reaction ID: 51038186

3



Case 15: 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

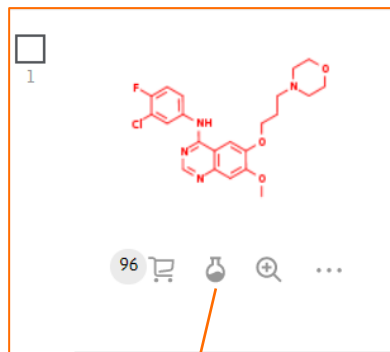


Quick search Query builder Results **Retrosynthesis** History Alerts

视频操作过程:

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

从具体物质出发的合成计划制作



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

☒ 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

目前学校没有开通AI模块

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  给几条，给全部还是只给最后一步？

☐ Last step only

Branches per step: 5  设定最大分支，最大步数

Max. number of steps: 5 

Stop searching if building block is commercially available ☐ Yes ☒ No 底物是否可购买

Assumed yield for reactions without a given yield

0%  100% 每一步收率

Published Route 5

View >

Edit

Published Route 81

Published Route 82

Published Route 83

Tree view >

Table view >

Preview

Feedback

Export Legend

Hide conditions **Tree view** Table view

Rotate Fit view Copy route

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 v	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 >

↔

✕

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

Feedback

Agenda

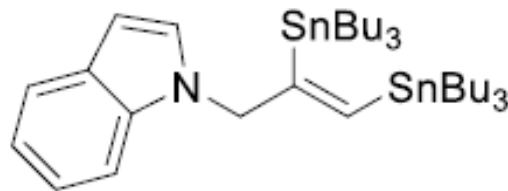
- Reaxys介绍与内容
 - Reaxys介绍
 - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
 - Reaxys中的科技文献检索与分析
 - Reaxys中物质理化性质数据的查询与反向物质获取
 - Reaxys中结构面板与物质结构和反应数据的获取
 - Reaxys中的实用小案例
- Q&A

Case 16: 化合物的文献定位

这是一篇常见的化学文献，包含：

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

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



视频操作过程：

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

Chem

Article

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

Wen-Yong Huang, Guo-Qing Wang, Wen-Hao Li, ..., Hai-Tao Tang, Ying-Ming Pan, Yun-Jie Ding

htang@pku.edu.cn (H.-T.T.), pengyimin@pku.edu.cn (Y.-M.P.), dy@pku.edu.cn (Y.-J.D.)

HIGHLIGHTS

- Design single-atom-site catalyst based on organic synthesis mechanism
- Utilizing pores, ligands, and SAS for synergistic controlling reaction paths
- A highly selective distannylation of terminal alkynes was achieved

• 21 examples
• Up to 89% yield
• Cheap Sn source
• Recyclable catalyst
• 1.7 with Pd loading SAS
• High Reactivity: TON up to 770
• High Selectivity: Z only, cr up to 100%

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

Huang et al., Chem 6, 200–2313
September 10, 2020 © 2020 Elsevier Inc.
<https://doi.org/10.1016/j.chem.2020.08.020>

Reaxys中的检索

- Query Builder联合化合物结构与文献DOI号

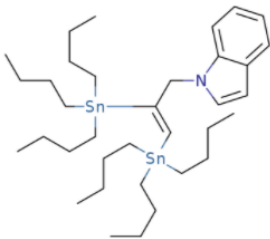
Reaxys[®] Quick search Query builder Results Synthesis planner History Alerts

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Structure ×



As drawn

AND ◇ DOI is 10.1016/j.chempr.2020.06.020

The image shows a screenshot of the Reaxys Query Builder interface. The main window displays a chemical structure of a tin complex, which is a bis(stannylene) compound. It features two tin (Sn) atoms, each bonded to two n-butyl groups and a central carbon atom. This central carbon is part of a five-membered ring that also includes a nitrogen atom (N) and two carbon atoms, one of which is part of a benzene ring. The interface includes a top navigation bar with 'Quick search', 'Query builder' (highlighted), 'Results', 'Synthesis planner', 'History', and 'Alerts'. Below this is a search bar with buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar on the left offers 'Import', 'Save', 'Reset form', and 'Delete all' options. On the right, there are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The chemical structure is shown in a dashed box with a close button (X) in the top right corner. Below the structure, it says 'As drawn'. At the bottom, there is a search criteria bar showing 'AND' followed by '◇ DOI is 10.1016/j.chempr.2020.06.020'.

Reaxys中的结果

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

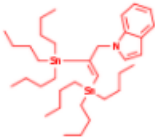
0 selected Limit To Exclude Export Preparations

Reaxys - 1

Grid Heatmap

Sort by No of References

1



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

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

Hit Data - 6

- Substance Label - 1 hits out of 1
- Chromatographic Data - 1 hits out of 1
- Crystal Property Description - 1 hits out of 1
- NMR Spectroscopy - 2 hits out of 2
- Mass Spectrometry - 1 hits out of 1

Hit Data - 6

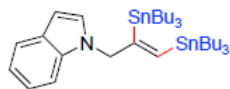
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Label	Reference
3j	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, - 2313]

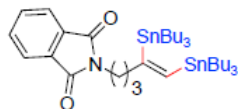
Full Text Details Abstract

全文检索3J定位化合物

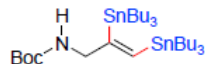
N-containing terminal alkynes



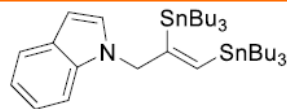
3j 89% (100:1)



3k 58% (25:1)



3n 81% (100:1)



(Z)-1-(2,3-bis(tributylstannyl)allyl)-1H-indole 3j: colorless oil. Petroleum ether as eluent for column chromatography (**3j**, $R_f = 0.75$; **2j**, $R_f = 0.4$, 42% of alkyne was isolated and recovered); ^1H NMR (400 MHz, CDCl_3) $\delta = 7.52$ (1H, d, $J = 7.8$ Hz), 7.15 (1H, d, $J = 8.2$ Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, $J = 3.1$ Hz), 6.46 (1H, s, $J = 168.4$ Hz, 65.5 Hz), 6.40 (1H, d, $J = 3.1$ Hz), 4.78 (2H, d, $J = 1.3$ Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ^{13}C NMR (400 MHz, CDCl_3) $\delta = 160.6, 144.4, 140.1, 139.9, 139.8, 139.7, 139.6, 139.5, 139.4, 139.3, 139.2, 139.1, 139.0, 138.9, 138.8, 138.7, 138.6, 138.5, 138.4, 138.3, 138.2, 138.1, 138.0, 137.9, 137.8, 137.7, 137.6, 137.5, 137.4, 137.3, 137.2, 137.1, 137.0, 136.9, 136.8, 136.7, 136.6, 136.5, 136.4, 136.3, 136.2, 136.1, 136.0, 135.9, 135.8, 135.7, 135.6, 135.5, 135.4, 135.3, 135.2, 135.1, 135.0, 134.9, 134.8, 134.7, 134.6, 134.5, 134.4, 134.3, 134.2, 134.1, 134.0, 133.9, 133.8, 133.7, 133.6, 133.5, 133.4, 133.3, 133.2, 133.1, 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-26.7, -26.8, -26.9, -27.0, -27.1, -27.2, -27.3, -27.4, -27.5, -27.6, -27.7, -27.8, -27.9, -28.0, -28.1, -28.2, -28.3, -28.4, -28.5, -28.6, -28.7, -28.8, -28.9, -29.0, -29.1, -29.2, -29.3, -29.4, -29.5, -29.6, -29.7, -29.8, -29.9, -30.0, -30.1, -30.2, -30.3, -30.4, -30.5, -30.6, -30.7, -30.8, -30.9, -31.0, -31.1, -31.2, -31.3, -31.4, -31.5, -31.6, -31.7, -31.8, -31.9, -32.0, -32.1, -32.2, -32.3, -32.4, -32.5, -32.6, -32.7, -32.8, -32.9, -33.0, -33.1, -33.2, -33.3, -33.4, -33.5, -33.6, -33.7, -33.8, -33.9, -34.0, -34.1, -34.2, -34.3, -34.4, -34.5, -34.6, -34.7, -34.8, -34.9, -35.0, -35.1, -35.2, -35.3, -35.4, -35.5, -35.6, -35.7, -35.8, -35.9, -36.0, -36.1, -36.2, -36.3, -36.4, -36.5, -36.6, -36.7, -36.8, -36.9, -37.0, -37.1, -37.2, -37.3, -37.4, -37.5, -37.6, -37.7, -37.8, -37.9, -38.0, -38.1, -38.2, -38.3, -38.4, -38.5, -38.6, -38.7, -38.8, -38.9, -39.0, -39.1, -39.2, -39.3, -39.4, -39.5, -39.6, -39.7, -39.8, -39.9, -40.0, -40.1, -40.2, -40.3, -40.4, -40.5, -40.6, -40.7, -40.8, -40.9, -41.0, -41.1, -41.2, -41.3, -41.4, -41.5, -41.6, -41.7, -41.8, -41.9, -42.0, -42.1, -42.2, -42.3, -42.4, -42.5, -42.6$

Case 17: 机理性文献的检索

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

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

Search in: Reactions > Targets > Substances > Documents >

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

Structure

On all atoms

AND

Subject Studied is mechanism

Search fields

Fields Forms

Topics and Keyw

Identification

Physical Propert

Spectra

MedChem

Other

Reactions

Bibliography

The screenshot displays the Reaxys Query Builder interface. The main workspace shows a chemical reaction scheme: an alkyne (R₁-C≡C-H) reacting with stannane (Sn-H) to form a trans-stannane (R₁-CH=CH-Sn). The reaction is enclosed in a dashed box labeled 'Structure'. Below this, the 'Subject Studied' field is set to 'is mechanism'. On the right, a sidebar lists search fields: Fields, Forms, Topics and Keyw, Identification, Physical Propert, Spectra, MedChem, Other, Reactions, and Bibliography. An orange arrow points from the reaction scheme in the main workspace to a larger, detailed view of the same reaction scheme on the right side of the image.

最后的结果

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

1 Filters

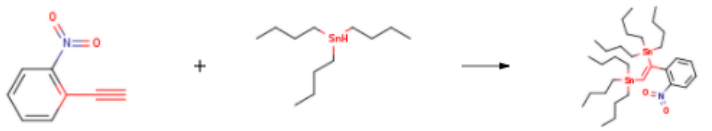
Limit to > Exclude >

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

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

0 Limit To Exclude Export Syn-Plan Hide Conditions

1



1 Hits/Conditions Find Similar > Reaction ID: 54835337

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

1 hit out of 1

Agenda

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

Reaxys小结

- Reaxys从大量文献中摘取和物质性质相关的所有数据，帮助科研人员获得标准化，规范化，格式化的物性数据列表及参考文献
- Reaxys中的Query Builder检索帮助科研人员通过简便的方式，获得精准，跨学科精确答案
- Reaxys中的结构面板，能实现科研人员绝大部分的结构绘制要求，帮助科研人员用最直接的方式获得相应的物质和反应
- Elsevier Life Science线上服务：
 - 关注B站Up主：ELS生命科学，获取所有Elsevier Life Science数据库的使用视频
 - 添加Elsevier Life Science小助手微信号：ELS-LSS，邀请进Elsevier Life Science用户群，获取最新资料分享以及使用Q&A

请就今天的培训
进行问卷调查





Thank you

