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Reaxys中化学和药学相关信息的获取 和应用

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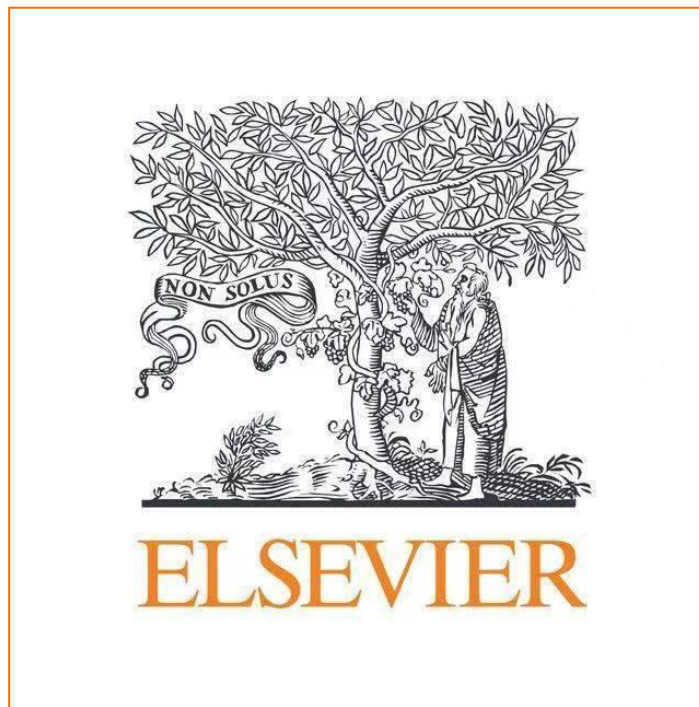
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Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- Q&A

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105专利机构专利

WPO, USPO, EPO [≈ mid 70's >]

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

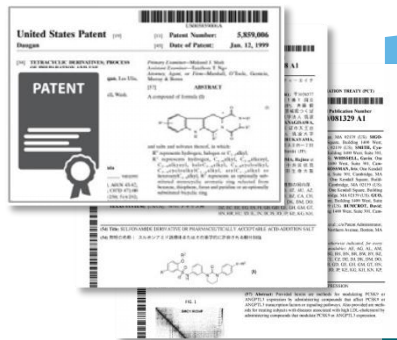
38万书的章节

Beilstein, Gmelin,....

16,300 期刊
(journals, books and patents)



Reaxys数据库全面强化---药学相关专利内容



参考文献

- 105 专利局
- 170 IPC 分类

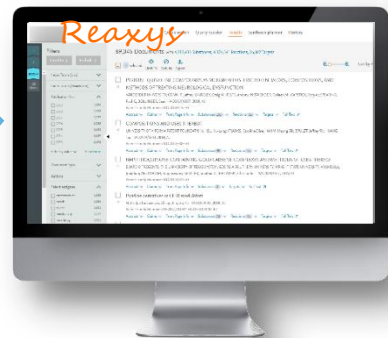
靶点

- 主要专利局
- 7 IPC 分类

2000 - 2022

化合物结构

- 主要专利局
- 170 IPC 分类



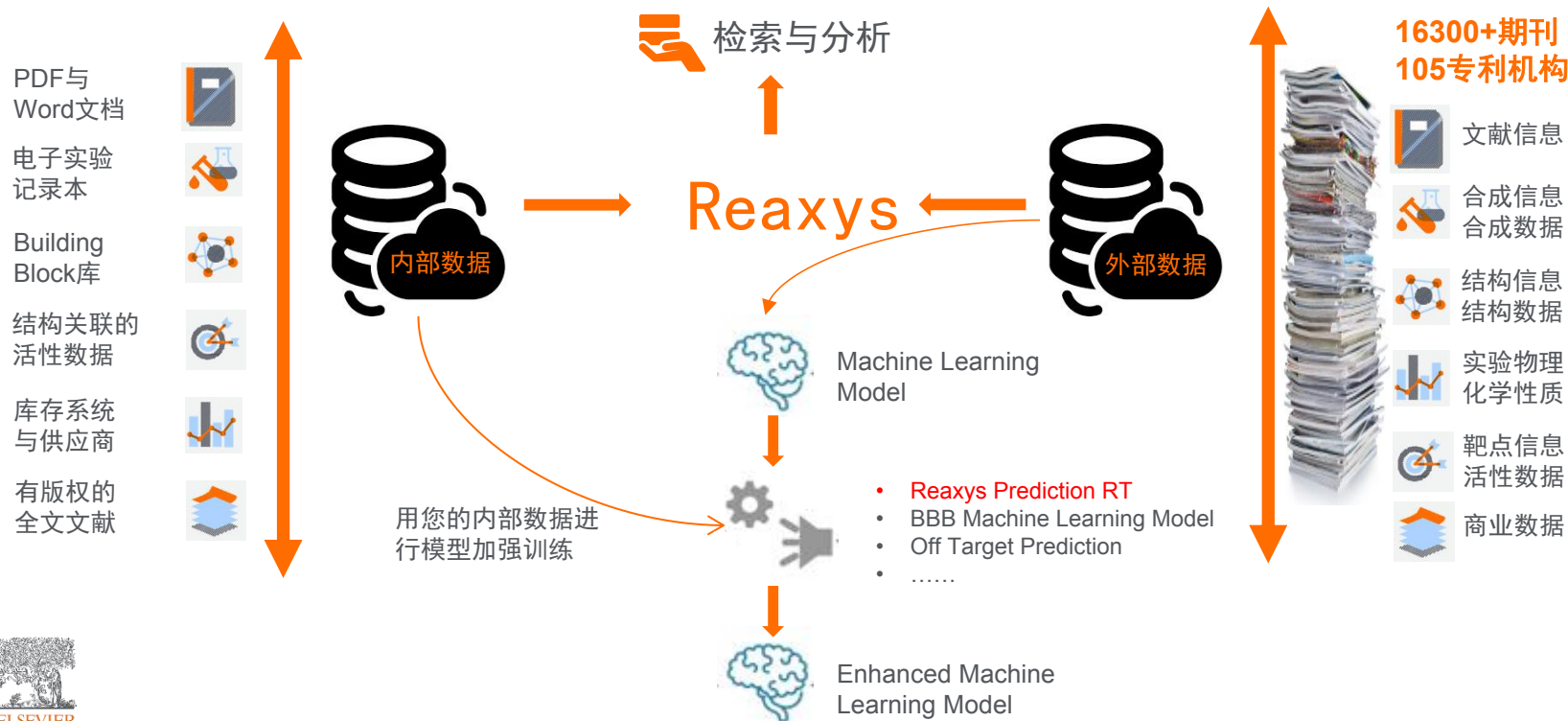
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3. 改进化合物提取技术(NER+I2S)，尽可能全面抓取小分子化合物，降低漏检风险
4. 从专利‘发明描述及claim’内容索引专利，可以便捷进行：靶点，蛋白名，制剂，工艺等专利检索（独有）
5. 从技术领域分类检索专利，专利公开5-7天，自动推送给用户，如：适应症，结构式描述等技术领域推送（独有）
6. 强化专利分类功能，快速分类专利局，权益人，溯源专利权益变更，溯源家族专利等（独有）

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从一篇常见的药物化学文献看科研工作者的信息数据关注点

Chemical Research in Toxicology

Tetrahydrofuran

Support Information

Iron(II)-catalyzed synthesis of multi-substituted imidazoles via [3+2] cycloaddition reaction of nitroolefins and *N*-aryl benzamides

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ARTICLE INFO

ABSTRACT

1. Introduction

Imidazole and its derivatives is a large important heterocyclic ring system, which is widely used in many fields of chemistry, biology, medicine and material science. In the past few decades, a large number of imidazole derivatives have been synthesized and used in various fields. In this paper, we report a novel and efficient synthesis of multi-substituted imidazoles via [3+2] cycloaddition reaction of nitroolefins and *N*-aryl benzamides.

Keywords: Iron(II)-catalyzed synthesis of multi-substituted imidazoles via [3+2] cycloaddition reaction of nitroolefins and *N*-aryl benzamides.

4.1. Synthesis of 3aa

The synthesis of 3aa was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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).

4.2. General procedure of the reaction between nitroolefins and benzamides

The general procedure of the reaction between nitroolefins and benzamides was as follows: A round bottom flask equipped with stirrer was 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 product.

4.3. Synthesis of 3ak

The synthesis of 3ak was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3ak as light yellow solid (90% yield).

4.4. Synthesis of 3am

The synthesis of 3am was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3am as light yellow solid (90% yield).

4.5. Synthesis of 3an

The synthesis of 3an was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3an as light yellow solid (90% yield).

4.6. Synthesis of 3ao

The synthesis of 3ao was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3ao as light yellow solid (90% yield).

4.7. Synthesis of 3ap

The synthesis of 3ap was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3ap as light yellow solid (90% yield).

4.8. Synthesis of 3aq

The synthesis of 3aq was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3aq as light yellow solid (90% yield).

4.9. Synthesis of 3ar

The synthesis of 3ar was carried out according to the general procedure. The reaction mixture was stirred for 4 h at 90 °C. After cooling to room temperature, the reaction mixture was added with 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 3ar as light yellow solid (90% yield).

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。

Table 1
Optimization of the reaction condition^a

合成线路

Reaction scheme showing the synthesis of 3aa from 1a and 2a using a catalyst and ligand in a solvent at 90 °C for 4 hours.

- 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

4.1.11. 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.

化合物性质数据

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



Reaxys中的所有数据源自期刊与专利报导

European Journal of Medicinal Chemistry

Articles 1-10

Research paper

Anti-hepatitis C virus activity and QSAR study of certain thiazolidinone and thiazolidinone derivatives as potential NS5B polymerase inhibitors

Chuanxi S. Hanan^{1,2}, Huihui H. Cheng^{1,2}, Enlai Z. Mohamed¹, Taghaly A. Omar¹

1. Medicinal Chemistry Department, Faculty of Pharmacy, Assiut University, Assiut 68134, Egypt; 2. Medicinal Chemistry Department, Faculty of Pharmacy, Assiut University, Assiut 68134, Egypt

ARTICLE INFO

ABSTRACT

The thiazolidinone derivatives were synthesized and evaluated for their anti-hepatitis C virus (HCV) activity. The results showed that the thiazolidinone derivatives were active against HCV. The QSAR study was performed to study the relationship between the chemical structure and the anti-HCV activity. The results showed that the thiazolidinone derivatives with a certain structure were more active than others. The results also showed that the thiazolidinone derivatives with a certain structure were more active than others.

Keywords and introduction: HCV, anti-hepatitis C virus, NS5B polymerase inhibitors, QSAR study, thiazolidinone derivatives.

1. Introduction

HCV is a RNA virus that replicates in liver cells. The infection leads to chronic hepatitis C, which is a leading cause of liver disease. The HCV genome is a single strand of RNA. The HCV proteinase is a key enzyme in the replication of the virus. The thiazolidinone derivatives were synthesized and evaluated for their anti-HCV activity. The results showed that the thiazolidinone derivatives were active against HCV. The QSAR study was performed to study the relationship between the chemical structure and the anti-HCV activity. The results showed that the thiazolidinone derivatives with a certain structure were more active than others. The results also showed that the thiazolidinone derivatives with a certain structure were more active than others.

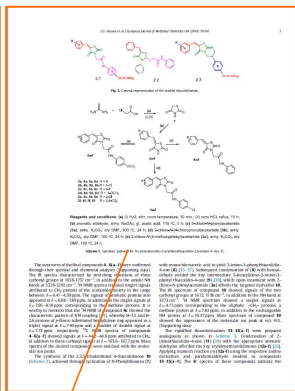


Table 1

NS5B polymerase (GT1a) inhibitory concentrations (IC₅₀ μM) and HCV anti-viral activity (EC₅₀ μM) values of the tested compounds and VCH-759.

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

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4e	2-Cl	H	0.035	3.80
4f	2,4(Cl) ₂	H	0.44	10.78
5a	H	4-Cl	0.14	16.70
5b	4-Cl	4-Cl	0.21	7.80

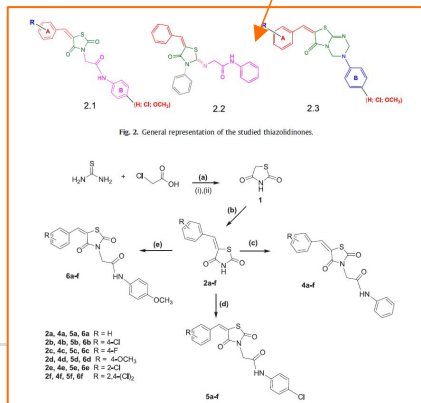


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一篇全文以及Support Information中有大量的数据，科研人员如果要获取，需要花费多的时间去阅读全文。

Reaxys对这篇全文的提炼—概览

1 Iron(III)-catalyzed synthesis of multi-substituted imidazoles via [3+2] cycloaddition reaction of nitroolefins and N-aryl benzamides 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 benzamides 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 terms: 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]benzotrile • 5-methyl-2-phenyl-1,4-di(4-tolyl)-1H-imidazole • alkene derivative • benzamide derivative • ferric ion • imidazole derivative • ligand • nitroolefin derivative • unclassified drug

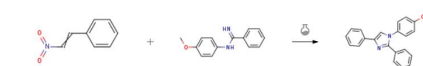
EMTREE medical terms: article • atmosphere • catalysis • catalyst • cycloaddition • drug structure • drug synthesis • green chemistry • priority journal • reaction optimization • solvent effect • substitution reaction

Author keyword: Benzamides • 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


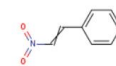
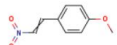

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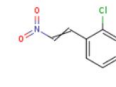
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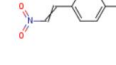
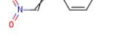
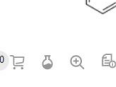
11 Hits 3 Conditions Find Similar Reaction ID: 35243549

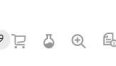


Conditions	Yield	Reference
With iron(III) chloride in N,N-dimethyl-formamide at 90°C; for 4h; Green chemistry; regioselective reaction; Experimental Procedure <input type="checkbox"/>	85%	Liu, Xiang; Wang, Dong; Chen, Baohua [Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text <input type="checkbox"/>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




+ Show all conditions 1 hit out of 1

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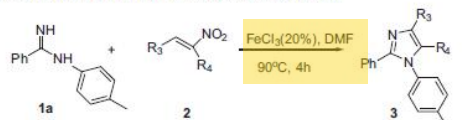
7

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

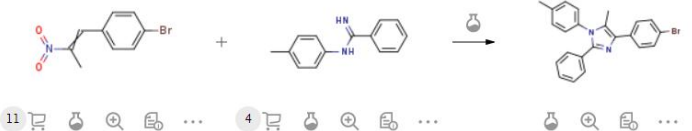


Entry	R ₃	R ₄	Product	Yield ^b (%)
1	H	H	3aa	82
2	4-CH ₃	H	3ab	60
3	4-CH ₃ O	H	3ac	51
4	4-F	H	3ad	61
5	4-Cl	H	3ae	68
6	2-Cl	H	3af	55
7	4-CF ₃	H	3ag	50
8	2,4-DiCH ₃ O	H	3ah	53
9	H	CH ₃	3ai	47
10	4-CH ₃ O	CH ₃	3aj	35
11	4-Br	CH ₃	3ak	41
12	4-Cl	CH ₃	3al	45
13	4-CN	CH ₃	3am	56

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.

21



11 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
C₂₂H₁₉N₂Br 403.321 24040362 1462876-22-7

Hit Data - 6
Identification

Druglikeness
Physical Data - 2

Spectra - 3

^ 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

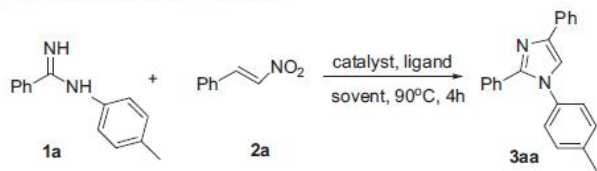
white

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对全文中的化合物生物活性的提炼(所有活性数据在RMC模块中)

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

^ In vitro: Efficacy - 2

Quantitative Results Show/Hide columns v

pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Effect	Reference
7.46	IC50	0.035	µM	Hepatitis C virus subtype 1a	Inhibitor	NS5B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus];Wild		anti-HCV	Hassan, Ghaneya S.; Georger, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details > Abstract >
5.42	EC50	3.8	µM		Inhibitor	NS5B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus];Wild	Huh-7.5 cell line	anti-HCV	Hassan, Ghaneya S.; Georger, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details > Abstract >

Table 2

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

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

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

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

^ Toxicity/Safety Pharmacology - 2

Quantitative Results Show/Hide columns v

pX	Parameter	Value (quant)	Unit	Cell	Effect	Reference
3.99	CC50 (cytotoxic concentration)	102.77	µM	THLE-2 cell line	Cytotoxic	Hassan, Ghaneya S.; Georger, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details > Abstract >
3.79	CC50 (cytotoxic concentration)	161.37	µM	RPTEC/TERT1 cell line	Cytotoxic	Hassan, Ghaneya S.; Georger, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[European Journal of Medicinal Chemistry, 2019, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details > Abstract >

Reaxys将文献中报道的科学数据进行了抽提, 归纳, 标准化

^ **Bioactivity (All)**

- ✓ In vitro: Efficacy - 5709
- ✓ In vivo: Animal Model - 817
- ✓ Metabolism - 345
- ✓ Pharmacokinetic - 816
- ✓ Toxicity/Safety Pharmacology - 2045

Conditions	Yield	Reference
Stage #1: 7-methoxy-4-(2-morpholino)propyl-2,4-dihydroquinazolin-4-one With thionyl chloride; N,N-dimethyl-formamide for 1h; Reflux	84%	Shanghai Tiansi International Pharmaceutical Co., Ltd.; Li Xian-jun; Li Jian-hui; Ma Xia; Chi Wang-hou; Sun Li; Liu Hai; (...) Zhai Zhijun; Li Jianjun CN103533065, 2017, B
Stage #2: 3-chloro-4-fluorophenylamine In isopropyl alcohol for 1h; Reflux		Location in patent: Paragraph 0166; 0167; 0168; 0169 Full Text > Details > Abstract >
With potassium carbonate In isopropyl alcohol at 80 - 85°C; for 1h; Experimental Procedure >	82%	Chongqing Laimei Longju Pharmaceutical Co., Ltd.; Wen Hai-ying; Ren Shao-xu; Xie-fang; Tang Qun-lan; Yang Sheng-li CN107998863, 2017, A Location in patent: Paragraph 0053-0054 Full Text > Details > Abstract >

10,992 Documents with 74,211 Substances, 79,080 Reactions, 2,355 Targets

Reaxys - 10,992

Limit To Exclude Export

Publication Year > > > Heatmap

1 Bcr-abl tyrosine kinase inhibitors as candidates for the treatment of covid-19: Molecular docking, pharmacophore modeling, admet studies
Atia, Mohamed S.; Hassaballah, Mohammed Y.; Negida, Ahmad; Sebahi, Mahmoud M.; Zedan, Noha I. (Biointerface Research in Applied Chemistry, 2022, vol. 12, # 3, p. 3357 - 3371)
Abstract > Index Terms > Substances (1) > Full Text >
Hit Substances (3) >

2 Etiologic Role of Kinases in the Progression of Human Cancers and Its Targeting Strategies
Das, Sanjoy; Bhattacharya, Birendra; Das, Biplob; Sinha, Bibek; Jamatia, Taison; Paul, Kishan (Indian Journal of Surgical Oncology, 2021, vol. 12, p. 34 - 45)
Abstract > Index Terms > Substances (5) > Full Text >
Hit Substances (3) >

3 Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer
Karuppusamy, Ramanaathar; Venkappapilla, Shriniv; Mohan, Sanyal; Shin, Woong-Hae; Khara, Dhanu (Seminars in Cancer Biology, 2021, vol. 68, p. 84 - 92)
Abstract > Index Terms > Substances (48) > Full Text >
Hit Substances (3) >

gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Identification Physical Data - 113 >

Druglikeness Spectra - 71 >

Bioactivity (All) Other Data - 4,344 >

Preparations - 83 >

Reactions - 154 >

Targets - 1,156 >

Documents - 10,992 >

Reaxys从文献中提炼出来的内容

文献记录:

>111 million
17000+期刊
105专利机构的专利
38万书的章节

化合物记录:

>177 million
期刊, 专利, 商品
2022年开始回溯98
家专利机构2000年
以来专利中的物质
及反应

化学反应记录:

>65.0 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:

> 1.0 Billion
化合物实验数据,
并提炼实验数据检
测条件

生物活性记录:

> 45.6 million数据
> 40,700靶点
> 8.6 million化合物
化合物在不同生物
体内活性数据

Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- 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

Reaxys®

Quick search Query builder Results Retrosynthesis History Register > Sign in

Search substances, reactions, documents and bioactivity data
in Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances

Search Reaxys

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

AND

Draw

Content Overview | Latest update: 16. March 2022 >

248M 58M 95M 31M 42M

Substances Reactions Documents Patents Bioactivities

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

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'. The user 'Sam Yu' is logged in. Below the navigation bar, a search bar is labeled 'Search Reaxys' and contains the text 'Substance Properties, e.g. solubility of vitamin D3'. A 'Find >' button is to the right of the search bar. Below the search bar, the text 'AND' is displayed, followed by a 'Draw' button with a chemical structure icon. At the bottom of the interface, there is a 'Content Overview' section with the text 'Latest update: 16. March 2022 >' and five statistics: '248M Substances', '58M Reactions', '95M Documents', '31M Patents', and '42M Bioactivities'. Two orange callout boxes are present: one on the left pointing to the search bar 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), and one on the right pointing to the 'Draw' 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 reactions containing these structures can be entered for search).

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

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

Content Overview | Latest update: 16. March 2022 >

248M 58M 95M 31M 42M

Substances Reactions Documents Patents Bioactivities

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

Reaxys的登录界面-模块检索界面

The screenshot displays the Reaxys Query Builder interface. At the top left is the Reaxys logo. The navigation bar includes 'Quick search', 'Query builder' (highlighted), 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user 'Jason Zhao' is logged in, indicated by a profile icon and a question mark. Below the navigation bar is a search area with 'Search in:' and four filters: 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar contains 'Import', 'Save', 'Reset form', and 'Delete all' buttons. A central area is labeled 'Drag & Drop to build a new query'. A right-hand sidebar titled 'Search fields' is open, showing a list of search categories: 'Fields', 'Forms', and 'History'. The 'Fields' section is expanded, listing: 'Reaxys', 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. A red box highlights the 'Current Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW' options in the toolbar.

Case 1: 关键词检索—千金藤素 Covid-19

- Cepharanthine Covid-19

The screenshot shows the Reaxys search interface. At the top, there are navigation tabs: [Quick search](#), [Query builder](#), [Results](#), [Retrosynthesis](#), [History](#), and [Alerts](#). Below this is a search bar with the text "Search for Cepharanthine Covid-19". Underneath the search bar, it says "Search Reaxys" and shows the input "Cepharanthine Covid-19" with a "Find >" button. Below the search bar, there is a section for "Substance Properties, e.g. solubility of vitamin D3" with an "AND" operator and a "Draw" button. At the bottom, there is a "Content Overview" section with the text "Latest update: 03. June 2022 >". Below this, there are five categories with their respective counts: "257M Substances", "58M Reactions", "97M Documents", "32M Patents", and "42M Bioactivities".

Quick search Query builder Results Retrosynthesis History Alerts

Search for Cepharanthine Covid-19

Search Reaxys

Cepharanthine Covid-19 Find >

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

Draw

Content Overview | Latest update: 03. June 2022 >

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

Reaxys中的检索结果

Results for **Cepharanthine Covid-19** New Edit

72	Documents	Titles, Abstracts, Keywords : "Cepharanthine", covid 19 <small>Edit in Query Builder</small> <small>Create Alert</small>	Preview Results View Results
27	Substances	Structure : as drawn <small>Edit in Query Builder</small> <small>Create Alert</small>	Preview Results View Results
921	Documents	Titles, Abstracts, Keywords : "Cepharanthine" <small>Edit in Query Builder</small> <small>Create Alert</small>	Preview Results View Results
241,484	Documents	Titles, Abstracts, Keywords : covid 19 <small>Edit in Query Builder</small> <small>Create Alert</small>	Preview Results View Results
1	Commercial Substances	Structure : as drawn <small>Edit in Query Builder</small> <small>Create Alert</small>	Preview Results View Results

72 Documents with 609 Substances, 0 Reactions, 7 Targets

0 selected Limit To Exclude Export Sort by Public

1 **Trace Minerals, Vitamins and Nutraceuticals in Prevention and Treatment of COVID-19** Cited 3 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

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

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

2 **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

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...}

3 **Vibrational spectroscopic characterization and structural investigations of Cepharanthine, a natural alkaloid** Cited 2 times
Akyuz, Sevim; Celik, Sefa; Ozel, Aysen E. [Journal of Molecular Structure, 2022, vol. 1258, art. no. 132693]
Abstract Index Terms Substances 4 Full Text

Abstract hit: {...Cepharanthine, a natural alkaloid obtained from the Stephania cepharantha Hayata plant,...}

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 (ReaxTree)
- Manually processed content only

Reaxys中对于文献检索结果的分析

The screenshot displays the Reaxys search results analysis interface. On the left is a sidebar with a 'Filters' section containing 93 items. The main area shows four expanded filter panels: 'Publication Year', 'Document Type', 'Current Patent Assignee', and 'Journal Title'. A fifth panel, 'Index Terms (List)', is also visible at the bottom right. The 'Publication Year' panel shows counts for 2022 (7), 2021 (36), and 2020 (28). The 'Document Type' panel lists categories like 'review' (33), 'article' (32), 'patent' (3), 'note' (1), 'letter' (1), and 'editorial' (1). The 'Current Patent Assignee' panel lists 'rigel pharmaceuticals inc' (1), 'kowa company, ltd' (1), 'institut pasteur' (1), and '(no entry given)' (68). The 'Journal Title' panel lists 'frontiers in pharmacology' (7), 'pharmacological reports' (4), 'pharmaceuticals' (3), 'molecules' (2), 'journal of medical virology' (2), 'current pharmaceutical d...' (2), and 'current medicinal chemistry' (2). The 'Index Terms (List)' panel shows a list of terms such as 'agent' (33), 'antiviral' (29), 'occurrence' (22), 'nature' (22), 'in' (22), 'toxicity' (16), 'drug' (16), 'property' (15), 'pharmacokinetics' (15), 'structure' (14), and 'pharmacological' (14). The interface includes navigation elements like 'Limit to' and 'Exclude' buttons, a 'Go to page' field, and a 'Filter by value' dropdown.

Filters (93 items)

- 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

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

Filter by value v

Document Type

<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

<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 v

Journal Title

<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 v View more

Index Terms (List)

Clear selected X Sort by Occurrence v X

<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 v

Document Type v

Authors/Inventors v

Current Patent Assignee v

Patent Office v

Journal Title v

Substance Classes v

Reaction Classes v

Index Terms (List) v

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) 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

Click the arrow to expand the level.

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](#)

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 3CL^{PRO} and TMPRSS-2 using molecular docking software. CEP displayed strong binding interactions-8.5 and-7.4 Kcal/mol. 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.

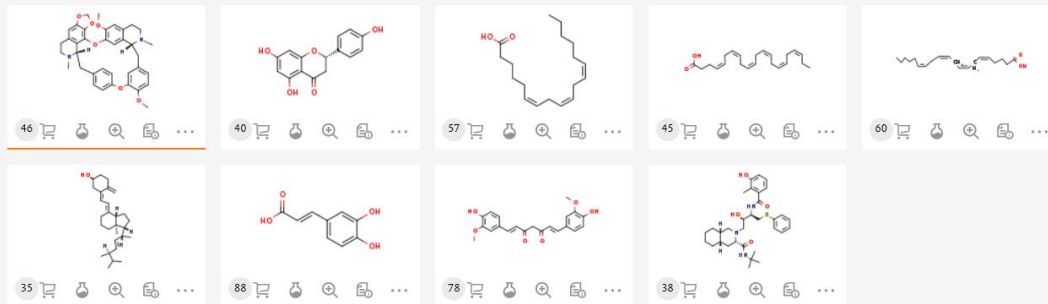
Index Terms

Author keyword: 3CL^{PRO} • Cepharanthine • COVID-19 • Molecular docking
Reaxys Index Terms: Hydrogen bond • IC₅₀ • LD50 • Permeability • Pi-pi
reference in nature • pharmacokinetics • reactivity • toxicity

全文链接，如果是OA或者学校已经订购可以直接打开

Cepharanthine (CEP) exhibits antiviral activity in SARS-CoV at 9.5 µg/mL IC₅₀ level.

Substances



+ Show All Available 3

Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- Q&A

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'. To the right of the search bar is a 'Find >' button. Below the search bar, there is a suggestion: 'Substance Properties, e.g. solubility of vitamin D3' with 'AND' below it. A 'Draw' button with a chemical structure icon is also present. At the bottom of the interface, there is a 'Content Overview' section with the text 'Latest update: 16. March 2022 >'. Below this, five categories are listed with their respective counts: '248M Substances', '58M Reactions', '95M Documents', '31M Patents', and '42M Bioactivities'. The background features a pattern of light blue hexagons.

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

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 Physical Data - 123 Preparations - 85
 Identification Spectra - 89 Reactions - 164
 Druglikeness Other Data - 4,498 Targets - 1,170
 Bioactivity (All) Documents - 12,124

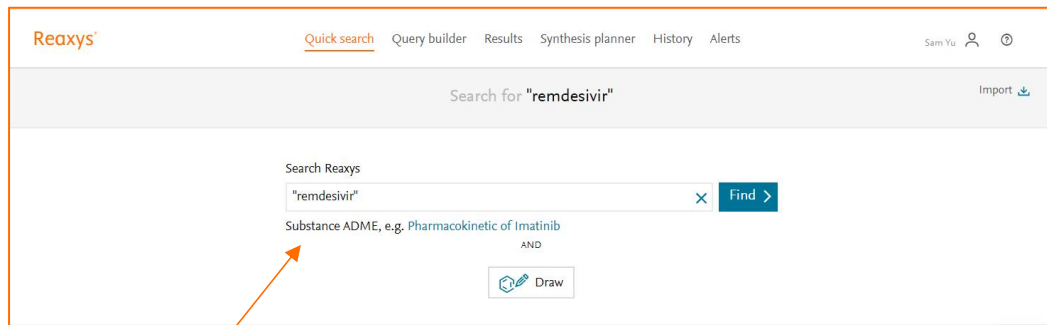
Hit Data - 6
 Solubility (MCS) - 6 hits out of 6

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	Alamy, Raid G.; Fletcher, John; Khoder, Mouhamad; Mustafa, Wesam W. JAAPS 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; Shaheeh, Fayez 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 Shihyuy; 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
0.009832	in pure solvent	25	water	supporting information		Wang, Xin-Xin; Tian, Fei-Yang; Liu, Ming; Chen, Kai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu Tetrahedron, 2019, vol. 75, # 37, art. no. 130488 Full Text Cited 2 times Details Abstract
0.0021	in pure solvent	20	water			Zhao, Feng; Lin, Zhaojun; 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

Case 3: 快速获取化合物的活性数据—Remdesivir



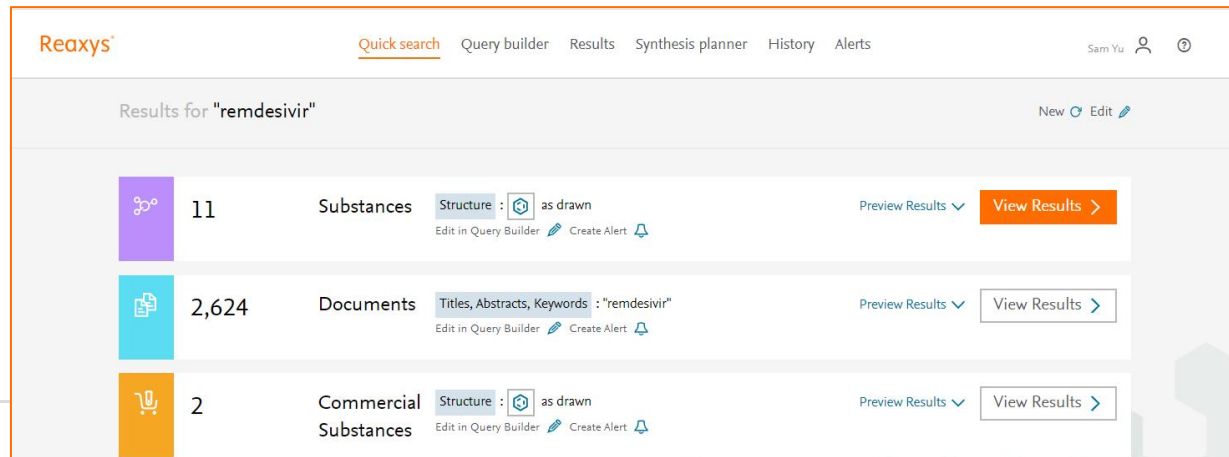
Reaxys[®] Quick search Query builder Results Synthesis planner History Alerts Sam Yu

Search for "remdesivir" Import

Search Reaxys
"remdesivir" Find >

Substance ADME, e.g. Pharmacokinetic of Imatinib
AND
Draw

直接输入Remdesivir
进行检索



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

Results for "remdesivir" New Edit

11	Substances	Structure : as drawn Edit in Query Builder Create Alert	Preview Results View Results >
2,624	Documents	Titles, Abstracts, Keywords : "remdesivir" Edit in Query Builder Create Alert	Preview Results View Results >
2	Commercial Substances	Structure : as drawn Edit in Query Builder Create Alert	Preview Results View Results >

Reaxys中的结果（含结构分身，盐，混合物等）

11 Substances

out of 25 Documents, containing 53 Reactions, 0 Targets

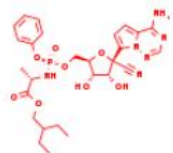
Reaxys - 11

Limit To Exclude Export Preparations

No of References

Grid Heatmap


1



(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 Physical Data - 15 Preparations - 43 >
Druglikeness Spectra - 19 Reactions - 44 >
Bioactivity (All) Other Data - 34 Documents - 25 >

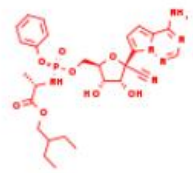





2



(S)-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 dichloromethane solvate monohydrate
C₂₇H₃₅N₆O₈P*CH₂Cl₂*H₂O 705.532 30969697

Identification Documents - 1 >
Druglikeness
Physical Data - 5

Reaxys中生物活性数据

1







(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 Physical Data - 15 Preparations - 43 >

Druglikeness Spectra - 19 Reactions - 44 >

Bioactivity (All) Other Data - 34 Documents - 25 >

^ Bioactivity (All)

- ✓ In vitro: Efficacy - 56
- ✓ In vivo: Animal Model - 47
- ✓ Metabolism - 13
- ✓ Pharmacokinetic - 86
- ✓ Toxicity/Safety Pharmacology - 10

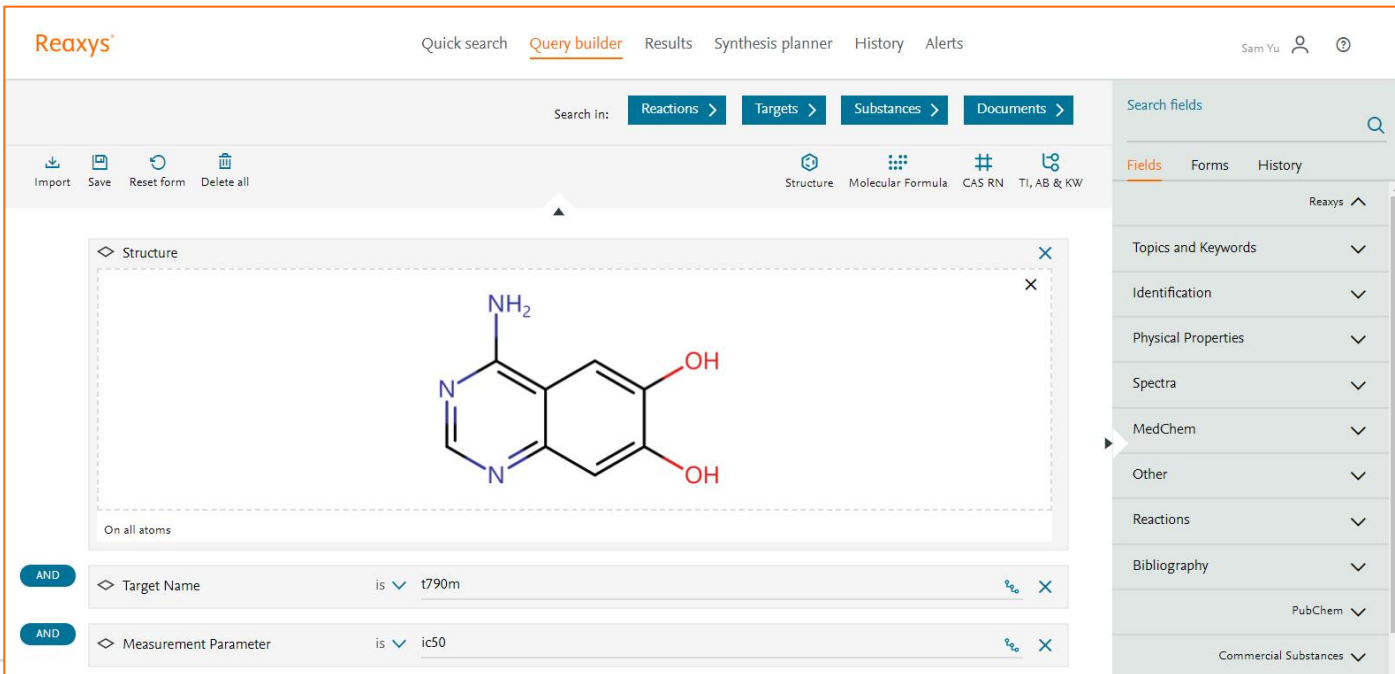
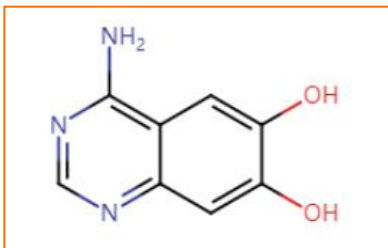
^ In vitro: Efficacy - 56

Quantitative Results Show/Hide columns v

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Cell	Dose	Effect	Reference
8.8	decrease rate (Viral titre)	Active			human	airway epithelium cell	0.0016 - 10 μM	antiviral agent	Agostini, Maria L.; Andres, Erica L.; Sims, Amy C.; Graham, Rachel L.; Sheahan, Timothy P.; Lu, Xiaotao; Smith, Everett Clinton; (...) Baric, Ralph S.; Denison, Mark R. <i>mBio</i> , 2018, vol. 9, # 2, art. no. E00221-18] Full Text Cited 30 times Details Abstract
8	IC50		0.01	μM		Calu-3 cell line		antiviral agent	Gilead Sciences, Inc.; Clarke, Michael O' Neil Hanrahan; Feng, Joy Yang; Jordan, Robert; Mackman, Richard L.; Ray, Adrian S.; Siegel, Dustin - <i>US2017/71964</i> , 2017, A1 Full Text Details Abstract

Case 4: 骨架化合物活性获取

- 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



The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs for "Quick search", "Query builder" (selected), "Results", "Synthesis planner", "History", and "Alerts". The user "Sam Yu" is logged in. Below the navigation, there are search filters for "Reactions", "Targets", "Substances", and "Documents". The main workspace is divided into two sections: "Structure" and "Query".

The "Structure" section contains a dashed box with the chemical structure of 2-aminophenanthroline-6,8-diol. Below it, the text "On all atoms" is visible. The "Query" section contains two criteria:

- Target Name is t790m
- Measurement Parameter is ic50

The right sidebar shows search fields and a list of categories: Fields, Forms, History, Reaxys, Topics and Keywords, Identification, Physical Properties, Spectra, MedChem, Other, Reactions, Bibliography, PubChem, and Commercial Substances.

检索策略的构建

The screenshot shows the Reaxys Query builder interface. At the top, there are navigation tabs: "Quick search", "Query builder" (selected), "Results", "Synthesis planner", "History", and "Alerts". The user name "Sam Yu" is visible in the top right. Below the navigation, there is a "Search in:" section with buttons for "Reactions", "Targets", "Substances", and "Documents". A "Search fields" dropdown menu is open, showing options like "Fields", "Forms", "History", and "Topics and Keywords". The "Structure" icon is highlighted with an orange arrow pointing to it.

Tips:
手动添加，结构，
Target, Parameter
的字段

The screenshot shows the Reaxys Query builder interface with a constructed search query. The "Search in:" section now includes "Reactions", "Targets", "Substances", and "Documents". The "Search fields" dropdown menu is open, and the search term "target" is entered. The query is built using the following criteria:

- Structure (with a "Create Structure / Reaction Drawing" button)
- AND Target Name is Target Name/ Uniprot ID/ PDB ID/ Reaxys Target ID
- AND Measurement Parameter is Measurement Parameter

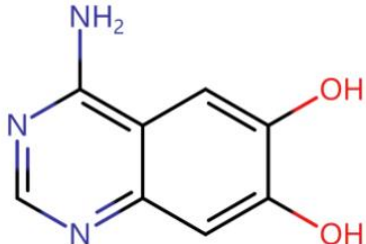
The right sidebar shows a list of search fields: Target Name, Substance Action on Target, Target Nature, Target Mutant/Chimera Details, Target Transfection, and Keywords.

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  X

On all atoms

AND ◇ Target Name is T790m X

AND ◇ Measurement Parameter is ic50 X

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

Limit to > Exclude > 0 Limit To Exclude Export Preparations No of References Grid Heatmap

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

Available Data

Document Type

Publication Year

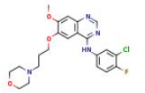
Patent Assignee

LogP

H Bond Donors

H Bond Acceptors

1

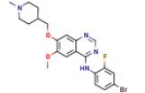


gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 194475-25-7

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 Abdelrasheeh Aly, Enayat E.; El Kerdawy, Ahmed M.; Farouk, Ahmed K. B. A. W.; Rashwan, Essam [Biochemistry, 2020, vol. 98] Full Text Details Abstract

2

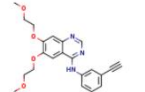


vandetanib
C₂₂H₂₄N₄O₂BrF 475.361 9161676

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);Wild				antineoplastic agent		Li, Qiannan; Zhang, Tao; Li, Shiliang; Tong, Linjiang; Li, Junyu; Su, Zhicheng; Feng, Fang; (...) Xie, Hui; 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
7.77	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 5: 如何用Reaxys快速筛选对“冠状病毒”有活性的化合物

- 获取文献中报道的对“RNA依赖的RNA聚合酶（RdRp）”有活性报道的化合物
- 希望这些化合物的IC50在um级别
- 视频操作：<https://www.bilibili.com/video/bv1pK411G7rX>

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (highlighted), Results, Synthesis planner, and History. On the right, there are buttons for Register and Sign in. Below the navigation, there is a search bar with 'Search in:' and four dropdown menus: Reactions, Targets, Substances (highlighted with an orange box), and Documents. 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, CAS RN, and TI, AB & KW. The main query builder area contains three criteria: 1. Target Name is rdp. 2. Measurement Parameter is ic50. 3. Measurement pX is >= 6. A 'Tips' box on the right contains the text: 'Tips: 利用Query Builder构建靶点, 检测参数, 以及参数大小的检索式'.

Reaxys中的结果

Reaxys

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

1,20 K Query

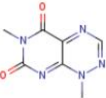
Filters

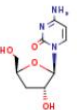
Limit to > Exclude >

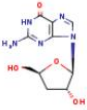
1,204 Substances out of 33 Documents, containing 2,896 Reactions, 6 Targets

0 Limit To Exclude Export Preparations No of References ↓ Grid Heatmap

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

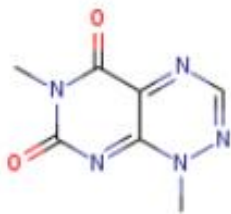
1  **toxoflavin**
C₇H₇N₅O₂ 193.165 21014 84-82-2
Identification Physical Data - 22 Preparations - 19 >
Druglikeness Spectra - 29 Reactions - 23 >
Bioactivity (Hit Data) Other Data - 3 Targets - 27 >
Bioactivity (All) Documents - 124 >

2  **3'-deoxycytidine**
C₈H₁₃N₃O₄ 227.22 616742 7057-33-2
Identification Bioactivity (All) Preparations - 54 >
Druglikeness Physical Data - 15 Reactions - 92 >
Bioactivity (Hit Data) Spectra - 31 Targets - 10 >
Documents - 44 >

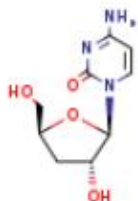
3  **3'-deoxyguanosine**
C₁₀H₁₃N₅O₄ 267.244 561508 3608-58-0
Identification Bioactivity (All) Preparations - 20 >
Druglikeness Physical Data - 12 Reactions - 55 >
Targets - 6 >

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的时间，可以通过各自的Hit Data查看具体数据

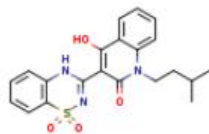
Reaxys中的结果



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



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



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

利用HeatMap看结构与靶点关系

Reaxys

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

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

Limit To Exclude Export Preparations No of References Grid Heatmap

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

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

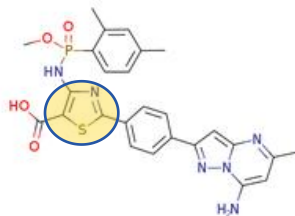
3 C10H13N5O4 **3'-deoxyguanosine** 267.244 561508 3608-58-0
Identification Bioactivity (All) Preparations - 20 >
Druglikeness Physical Data - 12 Reactions - 55 >



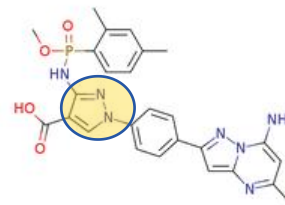
利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

一些非常有意思的结构

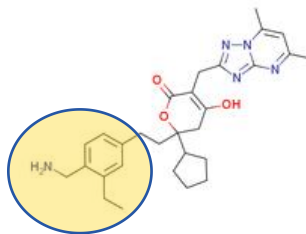
RNA-dependent RNA polymerase	
Substances	Targets
5-thiazolec... ylamine]	9.5
(E)-N-(4-(... fonamide	9.5
IDX17119	9.4
20673525	9.3
5-thiazolec... lamine]	9.1
20673509	9.1
20673467	9.1
29885944	9
27259279	9
6-cyclope... an-2-one	9
(6R)-6-cy... an-2-one	9
6-cyclope... an-2-one	9
6-cyclope... an-2-one	9
6-cyclope... an-2-one	9
N-(4-(3-(t... fonamide	8.9
5-[2-(4-flu... boxamide	8.7
(1aR,12b... boxamide	8.7
20673500	8.7
N-[4-(2-(2... cetamide	8.7
6-cyclope... an-2-one	8.7
6-cyclope... an-2-one	8.7
N-(2-(4-(2... cetamide	8.7
6-cyclope... an-2-one	8.7



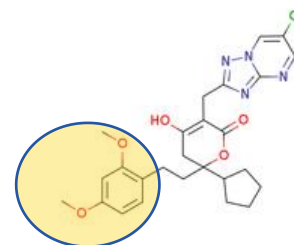
PX=9.5



PX=9.4



PX=8.0



PX=7.7

Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- Q&A

CASE 6: SAR分析与全新化合物设计

- 案例背景：
 - 我们知道SCD1缺陷型小鼠可以明显抵抗肥胖及其相关胰岛素抵抗的发生
 - SCD有两种亚型，SCD1在脂肪组织中表达，SCD5在大脑中表达
 - 因此开发一种有效的SCD1抑制剂以最小限度地抑制SCD5对项目的成功至关重要
- 检索困难点：
 - Selectivity Profile需要进行数值的输入，但是在这个案例中没有要求
 - 如何获悉哪些片段是有积极或者负面的活性影响的

获取SCD1[Human]上有活性的化合物

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Retrosynthesis, History, and Alerts. The user is identified as Sam Yu. The search criteria are defined in two rows:

- Row 1: Target Name is Target Name/ Uniprot ID/ PDB ID/ Reaxys Target ID
- Row 2: Substance Action on T... is Substance Action on Target

The search is connected by an AND operator. A sidebar on the right shows search fields: substance, Substance Properties & Comments, Substance Action on Target, and Substance Effect.

检索策略的构建：

1: Target Name

2: Substance Action on Target

检索条件的输入1

Reaxys Quick search Query builder Results Retrosynthesis History Alerts

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all

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

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

AND Substance Action on T... is Substance Action on Target

Target Name/ Uniprot ID/ PDB ID/ ... 3715 is Q SCD1

Category	Count
Targets	22,409,153
Defined target classes	19,659,174
binding protein	3,528,094
protein binding protein	2,230,613
WD40 repeat	23,415
DENN domain and WD repeat-containing protein SCD1 (SCD1)	19
WD40-repeat-containing domain	20,392
DENN domain and WD repeat-containing protein SCD1 (SCD1)	19
WD40-repeat-containing domain superfamily	41,633
DENN domain and WD repeat-containing protein SCD1 (SCD1)	19
WD40/YVTN repeat-like-containing domain superfamily	162,836

Selected search items:

DENN domai... ein SCD1 Scytalone dehydratase Acyl-CoA desaturase 1

Clear selected x Transfer >

输入SCD1进行靶点的扩展

检索条件的输入2

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

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

Import Save Reset form Delete all

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

Target Name is DENN domain and WD repeat-containing protein SCD1;Scytalone dehydrogenase

AND Substance Action on T... is Substance Action on Target

获取在SCD1上有, inhibitor, Inactivator, blocker, antagonist作用的化合物

Substance Action on Target 4



Search

<input type="checkbox"/>	activator	119,457
<input type="checkbox"/>	agonist	957,487
<input type="checkbox"/>	allosteric modulator	153,863
<input checked="" type="checkbox"/>	antagonist	974,820
<input checked="" type="checkbox"/>	blocker	165,289
<input checked="" type="checkbox"/>	inactivator	4,264
<input checked="" type="checkbox"/>	inhibitor	12,206,478
<input type="checkbox"/>	inverse agonist	19,585
<input type="checkbox"/>	irreversible antagonist	3
<input type="checkbox"/>	irreversible inhibitor	83
<input type="checkbox"/>	modulator	306,378
<input type="checkbox"/>	opener	19,050

1 of 2 | Go to page >












Clear selected x Transfer >

物质检索的结果









Reaxys® Quick search Query builder **Results** Retrosynthesis History Alerts Sam Yu   3

2.27 K Filters

Limit to > Exclude >

By Structure 
Measurement pX 
Targets 
Parameters 
Substance Classes 
Molecular Weight 
Number of Fragments 
Availability 
Availability in other databases 
Available Data 
Document Type 




2,275 Substances out of 26 Documents, containing 3,393 Reactions, 9 Targets

 0      No of References  Grid 

Limit To Exclude Export Preparations




1-hexadecylcarboxylic acid
C₁₆H₃₁O₂H 256.429 607489 57-10-3

Identification Physical Data - 1,272 Preparations - 224 >
Druglikeness Spectra - 378 Reactions - 3,980 >
Bioactivity (Hit Data) Other Data - 1,356 Targets - 217 >
Bioactivity (All) Documents - 44,316 >

93    ...

[1-(2-aminoethyl)-3-aminopropyl]trimethoxysilane
(CH₃O)₃Si(CH₂)₃NHC₂H₄NH₂ 222.36 636230 1760-24-3

Identification Physical Data - 20 Preparations - 4 >
Druglikeness Spectra - 43 Reactions - 136 >
Bioactivity (Hit Data) Other Data - 7 Targets - 7 >
Bioactivity (All) Documents - 1,783 >

77    ...

靶点分析，获取涉及“人”的靶点

选择Acyl-CoA desaturase 1 [human]:Wild，确保与人相关。

Reaxys[®]

2.27 K

Filters

Limit to > Exclude >

By Structure

Measurement pX

Targets 1

- acyl-coa desaturase 1 [... 2,126
- acyl-coa desaturase 1 [mo... 58
- scytalone dehydratase [m... 55
- scytalone dehydratase [rice] 24
- acyl-coa desaturase 1 8
- scytalone dehydratase [rat] 7
- denn domain and wd repe... 5
- stearoyl-coa desaturase 5 [... 2
- acyl-coa desaturase 1 [bovine] 2
- (no entry given) 2,180

Filter by value

2,126 Substances out of 13 Documents, containing 2,817 Reactions, 1 Targets

0 Limit To Exclude Export Preparations

No of References ↓ Grid Heatmap

1

sodium palmitate

$\text{Na}^{(1+)} * \text{CH}_3(\text{CH}_2)_{14} \text{CO}_2^{(1-)} = \text{CH}_3(\text{CH}_2)_{14} \text{CO}_2 \text{Na}$ 278.411 3575882 408-35-5

Identification Physical Data - 123

Druglikeness Spectra - 14

Bioactivity (Hit Data) Other Data - 30

Bioactivity (All)

Preparations - 6 >

Reactions - 85 >

Targets - 8 >

Documents - 639 >

2

sterculic acid

$\text{C}_{19}\text{H}_{34}\text{O}_2$ 294.478 1880442 738-87-4

Identification Physical Data - 16

Druglikeness Spectra - 10

Bioactivity (Hit Data) Other Data - 7

Bioactivity (All)

Preparations - 4 >

Reactions - 7 >

Targets - 4 >

Documents - 173 >

相同的步骤获取SCD5[Human]上有活性的化合物

Reaxys

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

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

Import Save Reset form Delete all

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

Target Name is [%](#) [X](#)

AND

Substance Action on T... is [%](#) [X](#)

Filters

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

By Structure [v](#)

Measurement pX [v](#)

Targets 1 [^](#)

- stearoyl-coa desaturase 5 2,520
- stearoyl-coa desaturase 5 86
- stearoyl-coa desaturase 5 [rat] 8
- stearoyl-coa desaturase 5 [... 2
- (no entry given) 2,589

Filter by value [v](#)

2,520 Substances

out of 24 Documents, containing 3,328 Reactions, 1 Targets

0 [Limit To](#) [Exclude](#) [Export](#) [Preparations](#) [No of References](#) [v](#) [Grid](#) [Heatmap](#)

1

CN(C)C(=O)c1ccc(NC(=O)N2CCOC(c3ccc(Cl)cc3)C2)c1

A939572
C₂₀H₂₂ClN₃O₃ 387.866 18848670 1032229-33-6

Identification Physical Data - 1 Preparations - 1 [>](#)
Druglikeness Spectra - 2 Reactions - 1 [>](#)
Bioactivity (Hit Data) Other Data - 37 Targets - 9 [>](#)
Bioactivity (All) Documents - 31 [>](#)

2

C1=NC2=C(N1)N=CN=C2N3CCOC(c4ccc(F)cc4)C3

MF-438
C₁₉H₁₈F₃N₅OS 421.446 12652434 [Retrieve CAS RN](#)

Identification Physical Data - 1 Preparations - 1 [>](#)
Druglikeness Spectra - 2 Reactions - 1 [>](#)
Bioactivity (Hit Data) Other Data - 42 Targets - 12 [>](#)
Bioactivity (All) Documents - 24 [>](#)

利用Query Builder获取两个结果集的交集

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected and highlighted with an orange box. Below the navigation bar, the 'Search in:' section includes buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all', along with search filters for 'Current Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main search area shows two query boxes: the first contains '2,520 Substances' and the second contains '2,126 Substances', with an 'AND' button between them. Green arrows point from the '2,520 Substances' box to the 'History' tab in the right sidebar, and from the '2,126 Substances' box to the '2,126 Substances' entry in the 'Recent' list. The 'History' tab is also highlighted with an orange box. The sidebar shows a list of recent searches, including '2,520 Substances', '2,520 Substances', '2,588 Substances', and '2,126 Substances'.

最后的检索结果

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

2,067 Substances out of 109 Documents, containing 2,605 Reactions, 5 Targets

Limit To Exclude Export Preparations No of References Grid Heatmap

By Structure Measurement pX Targets Parameters Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases Available Data Document Type

A939572
C20H22ClN3O3 387.866 18848670 1032229-33-6
Identification Physical Data - 1 Preparations - 1 >
Druglikeness Spectra - 2 Reactions - 1 >
Bioactivity (All) Other Data - 37 Targets - 9 >
Documents - 31 >

MF-438
C19H18F3N4OS 421.446 12652434 Retrieve CAS RN
Identification Physical Data - 1 Preparations - 1 >
Druglikeness Spectra - 2 Reactions - 1 >
Bioactivity (All) Other Data - 42 Targets - 12 >
Documents - 24 >

Heatmap settings

Value of X-axis **Targets**

Value of Y-axis **Substances**

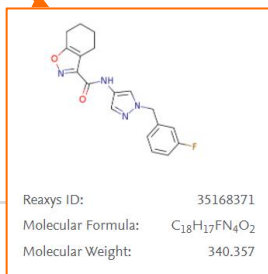
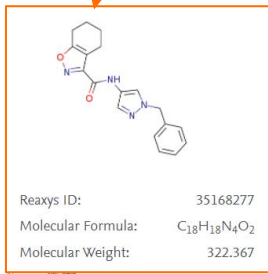
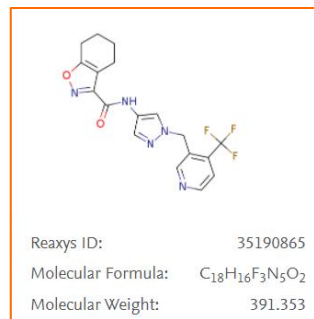
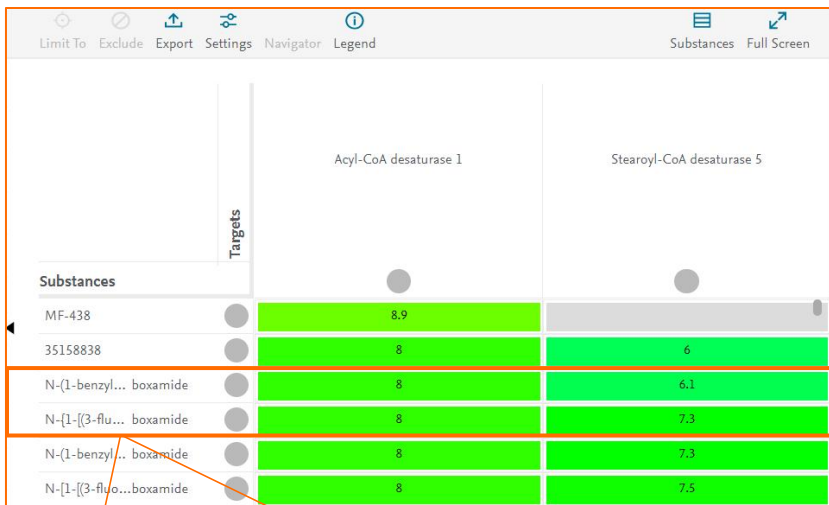
Value of Cells **Maximum of pX**

Show substances Names Structure drawing

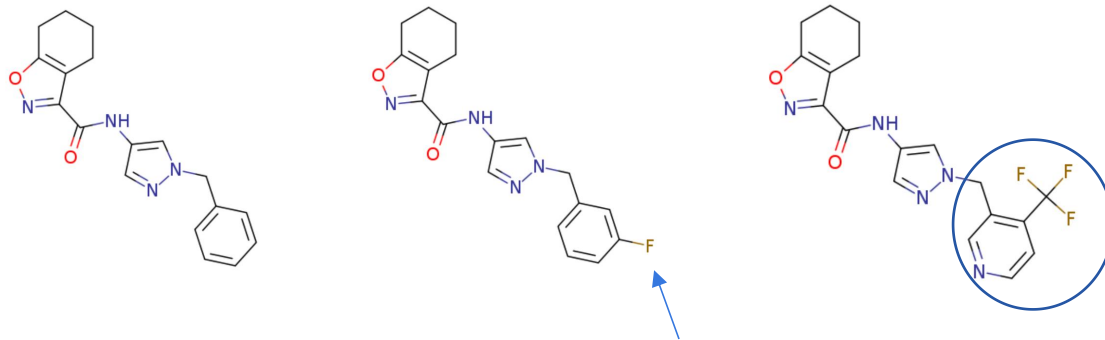
Display mode Normal Full Screen

Always show settings Apply >

Heat Map结果

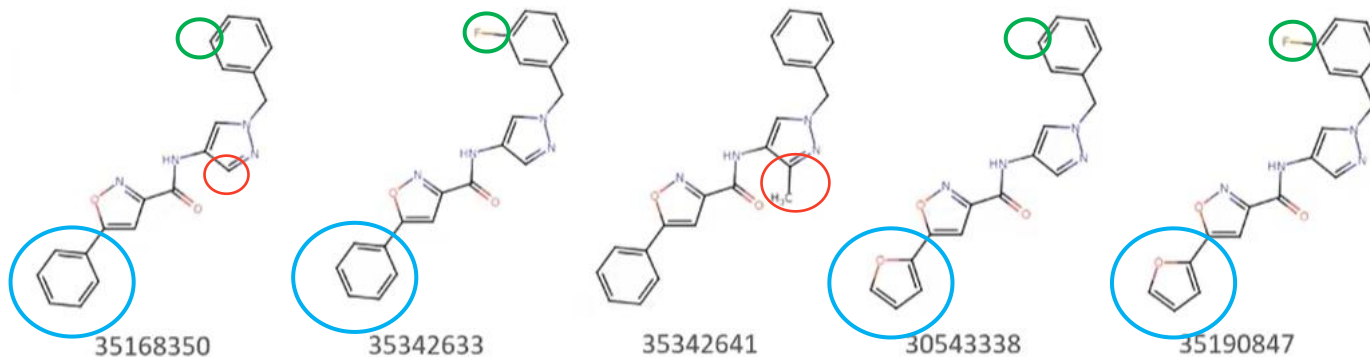


SAR分析数据



	PX		
SCD1	8.0	8.0	4.6
SCD5	6.15	7.3	6.3

SAR深度分析



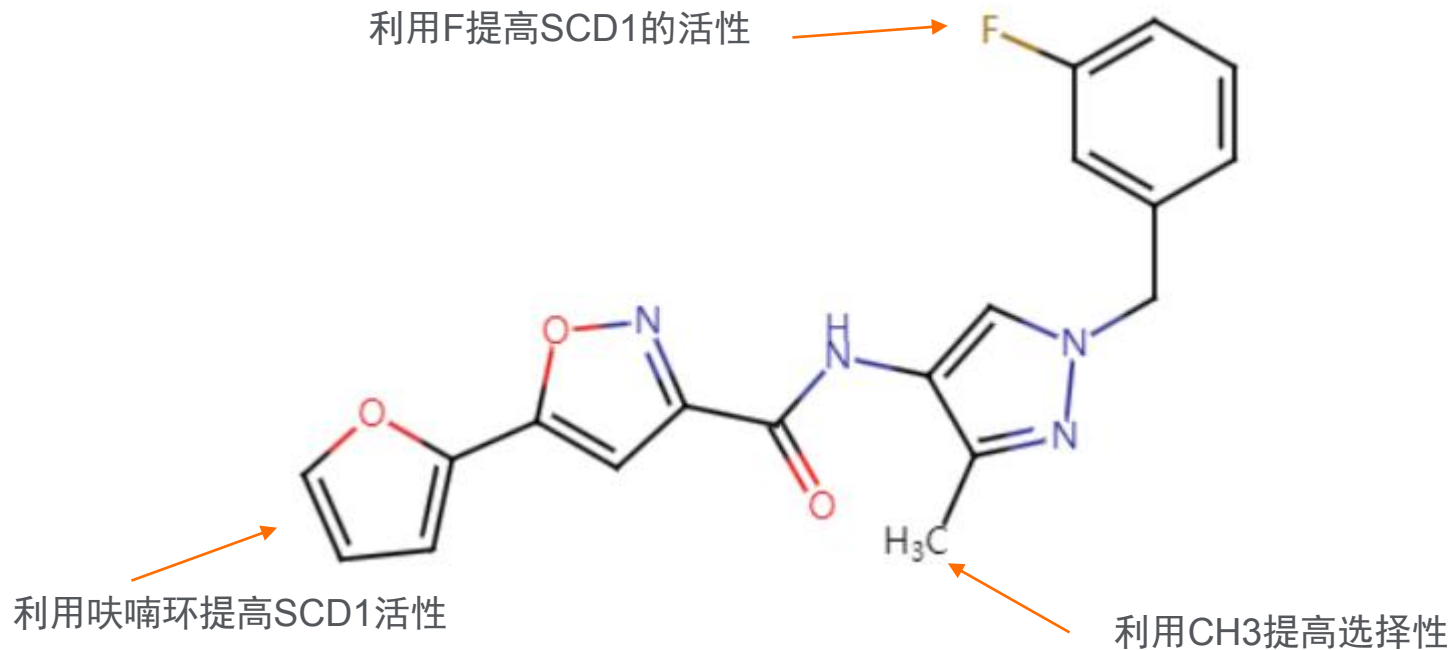
	PX				
SCD1	6.3	7.1	5.7	7	8
SCD5	7	1	1	7.1	7.5

1: F的对SCD1的影响可能是积极的

2: 苯环换成呋喃环对SCD1的影响也是积极的

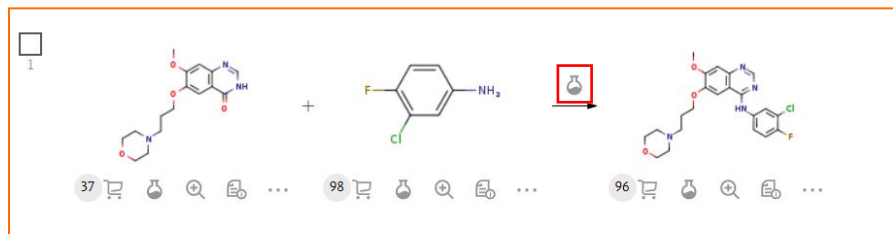
3: 结构中甲基对于靶点的选择性存在积极作用

设计新的结构并合成（该结构Reaxys中不存在）



Case 7: 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

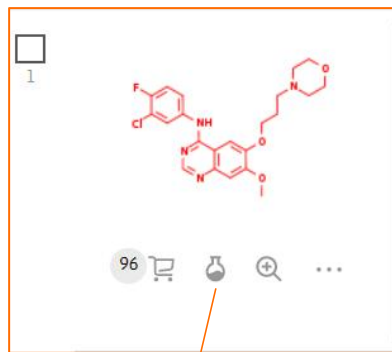


Quick search Query builder Results **Retrosynthesis** History Alerts

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

Always show screen before creating plan

Create Plans >

AI逆合成预测

编辑条件

Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- 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

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

Marvin JS ChemAxon

Clear Cancel Transfer to query >

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	

Case 5: Reaxys中快速获取化学合成路线

如何最快获取一个目标结构的合成路线

The screenshot displays the Reaxys software interface. At the top, the navigation bar includes "Quick search", "Query builder", "Results", "Retrosynthesis", "History", and "Alerts". The user's name "Peng Wu" is visible in the top right corner. The main workspace is titled "Structure editor selected: Marvins J S" and "ChemDraw J S". A search bar contains the text "Insert structure from name >". The central canvas shows a complex chemical structure with the text "Ctrl+alt+c" overlaid. The structure consists of a thiazole ring substituted with a methyl group, connected via a methylene group to a nitrogen atom. This nitrogen is part of an amide chain that includes a chiral center with two methyl groups, another amide group, a chiral center with a hydroxyl group, and a benzyl group, which is further connected to another amide group and a thiazole ring. The bottom of the interface has buttons for "Clear", "Cancel", and "Transfer to query". On the right side, there is a search options panel with the following sections:

- Search this structure as:**
 - As drawn
 - As substructure
 - Similar
- 对所画结构及其衍生物进行定义**
- 对所画结构的各种异构体进行定义**
 - Tautomers
 - Stereo
 - Additional ring closures
 - Related Markush
 - Salts
 - Mixtures
 - Isotopes
 - Charges
 - Radicals
- 更多功能, 如碎片融合**
 - [+ More options](#)

At the bottom left, the Elsevier logo is visible.

Reaxys中一次性获取所有信息



1

ritonavir

C₃₇H₄₈N₆O₅S₂ 720.957 7680098 155213-67-5


Identification Bioactivity (All) Spectra - 36

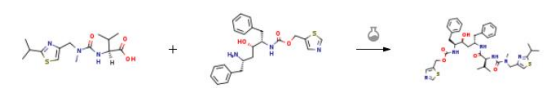
Druglikeness Physical Data - 77 Other Data - 1,414









获取合成计划

获取最后一步的合成方法








- Preparations - 19 >
- Reactions - 47 >
- Targets - 352 >
- Documents - 9,096 >

85    ...

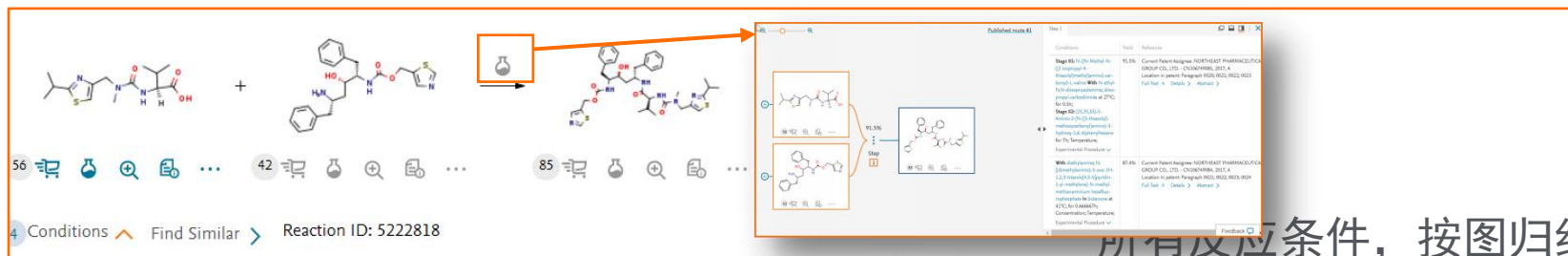


50     ... 42     ... 85     ...

4 Conditions  Find Similar  Reaction ID: 5222818

Conditions	Yield	Reference
Stage #1: N-((N-Methyl-N-(2-isopropyl-4-thiazolyl)methyl)amino)-carbonyl-L-valine With N-ethyl-N,N-disopropylamine; diisopropylcarbodiimide at 27°C; for 0.5h; Stage #2: (2S,3S,5S)-5-Amino-2-(N-((5-thiazolyl)-methoxycarbonyl)amino)-3-hydroxy-1,6-diphenylhexane for 7h; Temperature; Experimental Procedure 	91.5%	Current Patent Assignee: NORTHEAST PHARMACEUTICAL GROUP CO., LTD. - CN106749085, 2017, A Location in patent: Paragraph 0020; 0021; 0022; 0023 Full Text  Details  Abstract 
With diethylamine; N-((dimethylamino)-3-oxo-1H-1,2,3-triazolo[4,5-b]pyridin-1-yl-methylene)-N-methylmethanaminium hexafluorophosphate In butanone at 41°C; for 0.666667h; Concentration; Temperature; Experimental Procedure 	87.4%	Current Patent Assignee: NORTHEAST PHARMACEUTICAL GROUP CO., LTD. - CN106749084, 2017, A Location in patent: Paragraph 0021; 0022; 0023; 0024 Full Text  Details  Abstract 
With N-ethyl-N-(3-diethylaminopropyl)-carbodiimide; 1-hydroxybenzotriazol-hydrate In tetrahydrofuran for 16h; Ambient temperature; Yield given;		Kempf, Dale J.; Sharn, Hing L.; Marsh, Kennan C.; Flentge, Charles A.; Betebenner, David; Green, Brian E.; McDonald, Edith; (...) Plattner, Jacob J.; Norbeck, Daniel W. [Journal of Medicinal Chemistry, 1998, vol. 41, # 4, p. 602 - 617] Full Text  Cited 181 times  Details  Abstract 

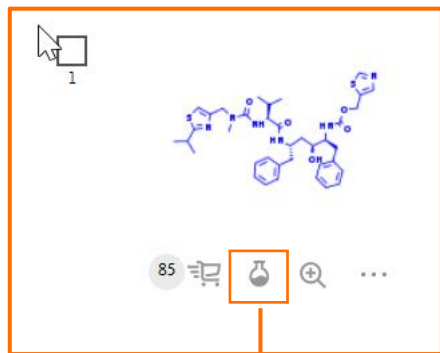
所有关键信息都会进行归纳整理



4 Conditions ^ Find Similar > Reaction ID: 5222818

Conditions	Yield	Reference
<p>Stage #1: N-((N-Methyl-N-((2-isopropyl-4-thiazolyl)methyl)amino)-carbonyl)-L-valine With N-ethyl-N,N-diisopropylamine; diisopropylcarbodiimide at 27°C; for 0.5h;</p> <p>Stage #2: (2S,3S,5S)-5-Amino-2-N-((5-thiazolyl)-methoxycarbonyl)amino)-3-hydroxy-1,6-diphenylhexane for 7h; Temperature;</p> <p>Experimental Procedure v</p>	91.5%	<p>Current Patent Assignee: NORTHEAST PHARMACEUTICAL GROUP CO., LTD. - CN106749085, 2017, A</p> <p>Location in patent: Paragraph 0020; 0021; 0022; 0023</p> <p>Full Text ↗ Details > Abstract ></p>
<p>With diethylamine; N-[(dimethylamino)-3-oxo-1H-1,2,3-triazolo[4,5-b]pyridin-1-yl-methylene]-N-methylmethanaminium hexafluorophosphate In butanone at 41°C; for 0.666667h; Concentration; Temperature;</p> <p>Experimental Procedure v</p>	87.4%	<p>Current Patent Assignee: NORTHEAST PHARMACEUTICAL GROUP CO., LTD. - CN106749084, 2017, A</p> <p>Location in patent: Paragraph 0021; 0022; 0023; 0024</p> <p>Full Text ↗ Details > Abstract ></p>
<p>With N-ethyl-N'-(3-diethylaminopropyl)-carbodiimide; 1-hydroxybenzotriazol-hydrate In tetrahydrofuran for 16h; Ambient temperature; Yield given;</p>		<p>Kempf, Dale J.; Sham, Hing L.; Marsh, Kennan C.; Flentge, Charles A.; Betebenner, David; Green, Brian E.; McDonald, Edith; (...) Plattner, Jacob J.; Norbeck, Daniel W.</p> <p>Journal of Medicinal Chemistry, 1998, vol. 41, # 4, p. 602 - 617</p> <p>Full Text ↗ Cited 181 times ↗ Details > Abstract ></p>

所有反应条件，按图归纳
便于比较筛选条件



Synthesize

- > Find preparations
- > Create retrosynthesis plans

Parameters

<input type="checkbox"/> Predicted <i>i</i>	<input type="checkbox"/> Published <i>i</i>
20 full routes (up to)	5 full routes (up to)
3 identical reaction steps per project (up to)	5 branches per step (up to)
3 identical building blocks per project (up to)	5 steps per route (up to)
10 min processing time	Don't Stop at commercial building blocks
STD SIAL LN EM U2 U5 T1 RSM3 RSM4 RSM5 building blocks	50% yield per step (assumed, if not published)

Powered by Edit

AI设计路线

以文献报道为基础设计路线

Always show screen before creating plan

Create Plans >

强大的运算功能，快捷给出不同的合成方案

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

合成计划 Peng Wu

Export Legend

Rotate Fit view Copy route

Project #588502 My Synthesis Projects Draw

拷贝并粘贴到 Chemdraw

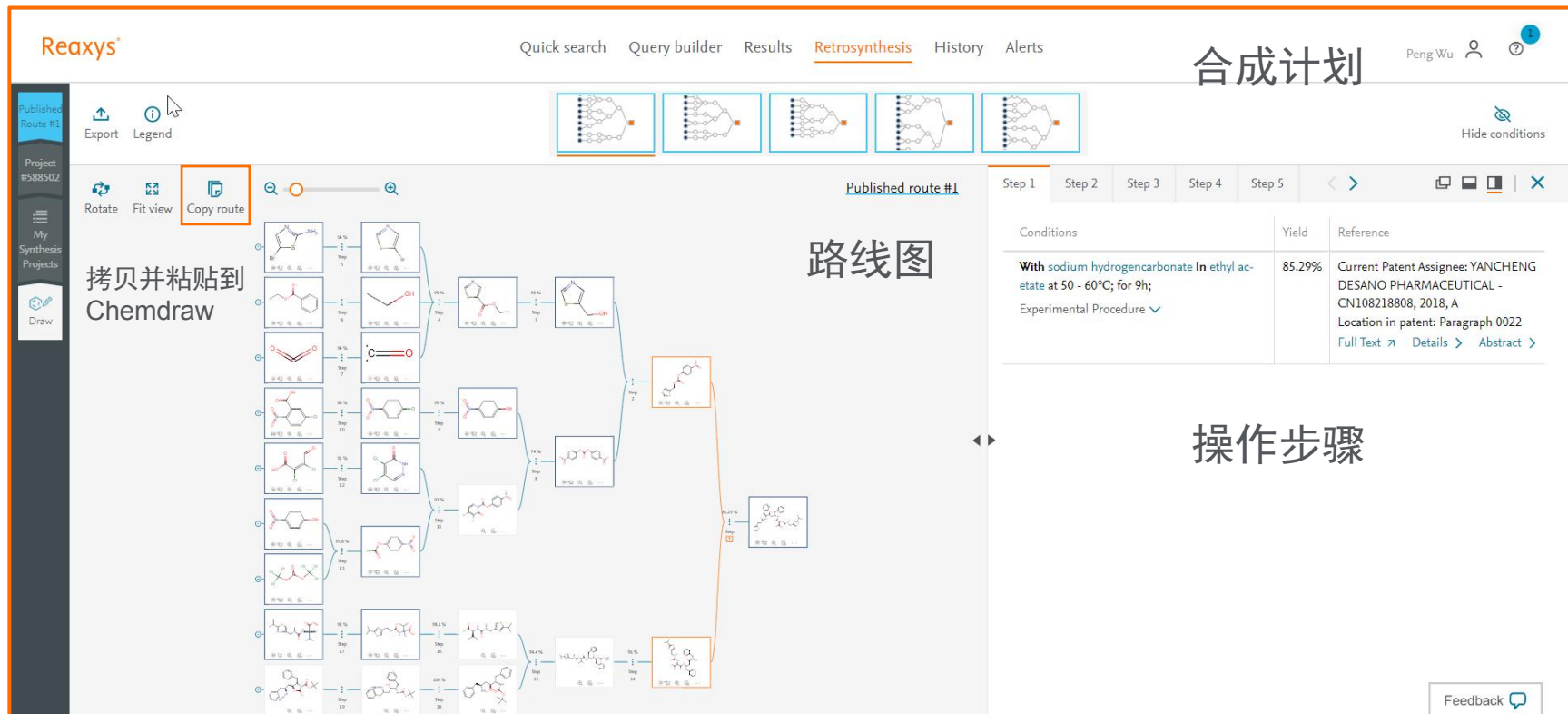
Published route #1

路线图

操作步骤

Conditions	Yield	Reference
With sodium hydrogencarbonate in ethyl acetate at 50 - 60°C; for 9h; Experimental Procedure	85.29%	Current Patent Assignee: YANCHENG DESANO PHARMACEUTICAL - CN108218808, 2018, A Location in patent: Paragraph 0022 Full Text Details Abstract

Feedback



Case 6: Reaxys中最简单的反应定义与筛选

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

The screenshot displays the Reaxys web 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 toolbar. One arrow points to the "1-1" button, and the other points to the "lock" icon (a padlock).

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 >

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

Limit To Exclude Export Show Conditions

Reaxys Ranking >

Show/Hide Conditions, 选择显示/隐藏条件

Reaction 1: O=Cc1ccc(O)cc1 → O=Cc1ccc(O)cc1 (Reaction ID: 2407606)

Reaction 2: COc1cc(O)cc(C=O)c1 → COc1cc(O)cc(O)c1 (Reaction ID: 305004)

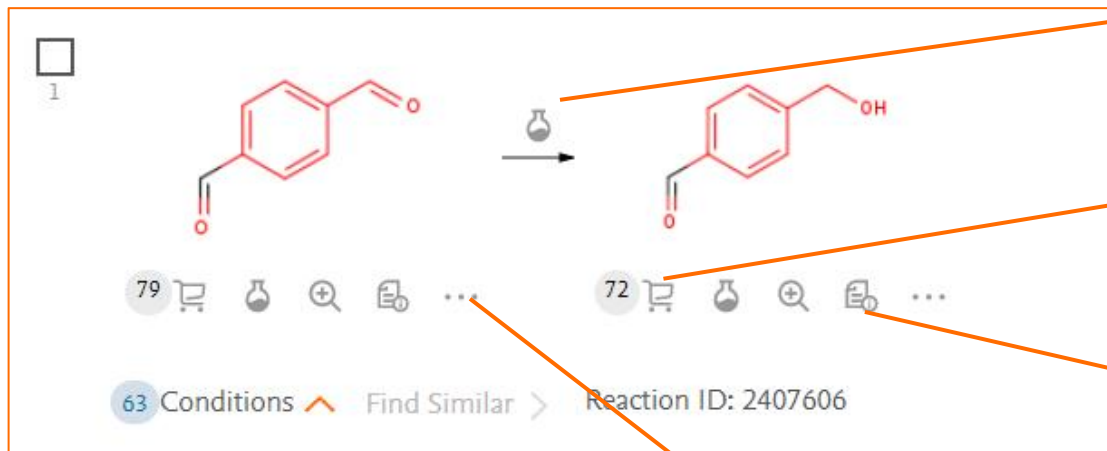
Reaction 3: O=Cc1ccc(Oc2ccccc2)cc1 → O=Cc1ccc(Oc2ccccc2)cc1

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, 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; [(η ⁵ -C ₅ H ₅)Ru](Cl)-P-PPH ₂ (P)/PPH ₃ (C); 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(η ⁵ -cyclopentadienyl)hafnium dihydride in isopropanol at 80°C; for 8h;	91%	Nakano, Tatsuya; Umamo, Shigetoshi; Kino, Yoshio; Ishii, Yasutaka; Ogawa, Masaya [Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757] Full Text > Cited 48 times > Details > Abstract >

Single step reactions only
Experimental procedure only

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](#)

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](#)

Solvent

▾

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

Filter by value ▾ [View more](#)

Document Type

▾

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

[View more](#)

Publication Year

▾

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

Filter by value ▾ [View more](#)

Tips:

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

Reaxys中的一些特殊筛选工具—溶剂分类

The image displays two panels from the Reaxys interface. The left panel shows a list of solvent classes with checkboxes and counts. The right panel shows a detailed view of these classes with expandable arrows and progress indicators.

Solvent Class	Count
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

- ✓ 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 ✕ 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](#)

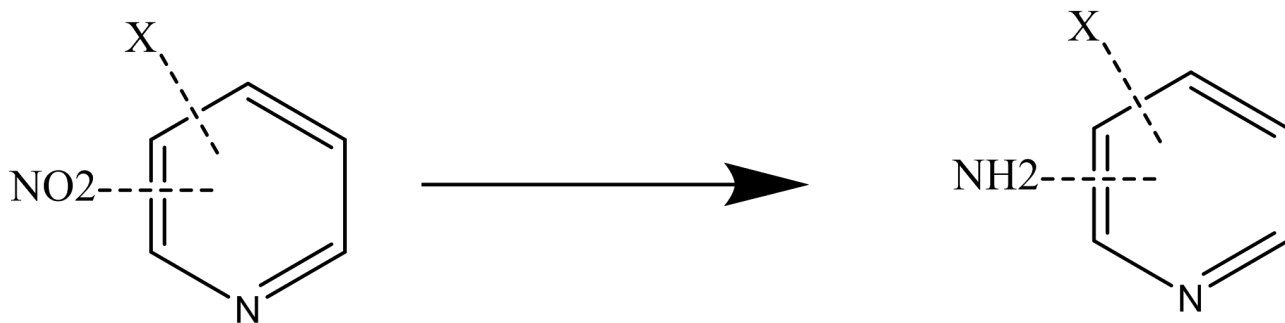
Catalyst Classes ×

- ▼ 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 7: 结构中有特殊需求的反应定义

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



视频操作过程:

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

Reaxys中的结构定义

Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in ⓘ

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Structure editor selected: MarvinJS ChemDrawJS

Search this structure as:

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

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

+ More options

Clear 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  6 Conditions Find Similar > Reaction ID: 149845

2  7 Conditions Find Similar > Reaction ID: 22895930

3 

1 

6 Conditions Find Similar > Reaction ID: 149845

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

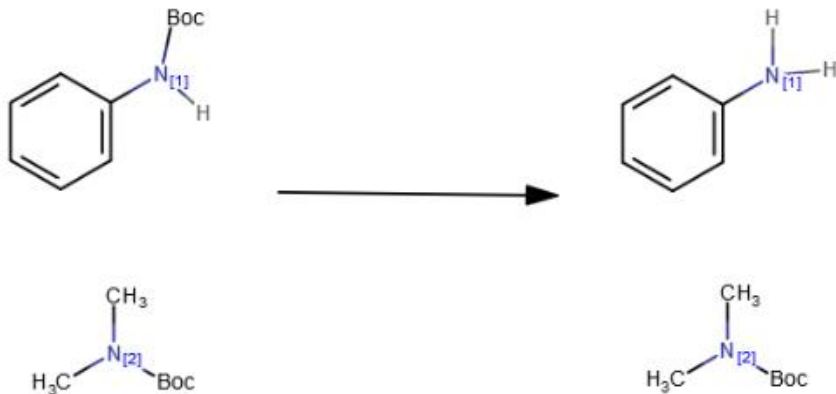
Experimental Procedure

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 8: 选择性氧化还原脱保护反应的定义

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



视频操作过程:

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

Reaxys中的结构定义

Reaxys

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

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Search this structure as:

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

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

+ More options

Ignore Atom Mappings

Keep fragments

- Separate
- Together

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

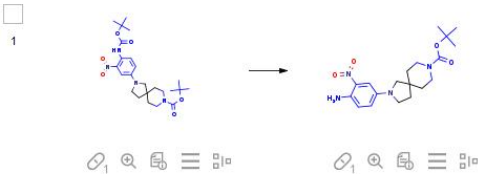
Reaxys[®] Quick search Query builder **Results** Synthesis planner History

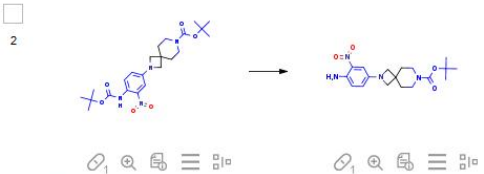
12 Reactions out of 8 Documents containing 22 Substances, 5 Targets

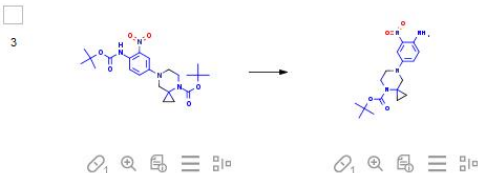
Limit to > Exclude >

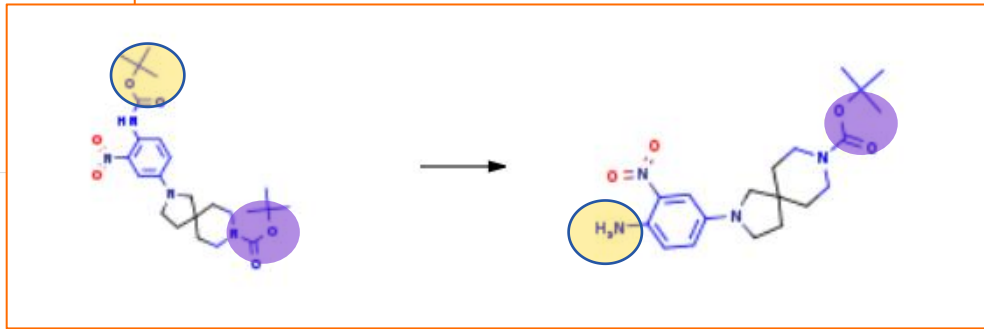
By Structure >
Yield >
Reagent/Catalyst >
Solvent >
Catalyst Classes >
Solvent Classes >
Product Availability >
Reactant Availability >
Reaction Classes >
Document Type >
Publication Year >

Single step reactions only
 Experimental procedure only

1 
1 Conditions Find Similar > Reaction ID: 51038227

2 
1 Conditions Find Similar > Reaction ID: 51038186

3 



Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- Q&A

Reaxys AI逆合成—基于深度神经网络算法的逆合成模型

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

Reaxys Data

- >12.5 M reactions data
- Organic, single step reactions
- Harmonized, curated and AI/ML ready data

Waller Lab – Predictive Retrosynthesis

Game Changer: Scientist Mark Waller first tried with AI-driven Synthesis

Planning chemical synthesis with deep neural networks and symbolic AI

AI in Action: Neural networks learn the art of chemical synthesis

Reaxys empowers cutting edge research at MIT

Connor Coley

ELSP & Elsevier Confidential
09/10/2019

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

Route selection

- Retrosynthesis planning
- Condition recommendation
- Pathway evaluation

Process development

- Identification of expensive times, concentrations
- Module selection

Reaction execution

- Reaction stream synthesis
- Robotic reconfiguration
- Process monitoring

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 in the rules.

ELSP & Elsevier Confidential
09/10/2019

Reaxys data is powering Lapkin Group's research into planning supply chains in the chemical industry that can help to improve sustainability

Algorithm finds the 569 molecules that might drive a waste-free economy

Interview with Professor Alexei Lapkin, University of Cambridge

Which Molecules Are Key for a Sustainable Chemical Industry?

Author: ChemRxiv.org
Published: 27 Jun 2019
Copyright: Wiley InterScience (WILEY) & Co. (WILEY)
Source: Publisher: ChemRxiv

Lapkin group gratefully acknowledges collaboration with RELX Intellectual Properties SA and their technical support, which enabled us to mine Reaxys. Reaxys data were made accessible to our research project via the Elsevier R&D Collaboration Network. Read more in [ChamRxiv](#)

ELSP & Elsevier Confidential
09/10/2019

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

MedChem ELN
AstraZeneca
PharmSci ELN

Reaxys*
Reaxys

AZ ChemistryConnect

AZ Reaction Connect
~20M reactions

LAB

Drug Discovery Project

DMTA cycles

European Laboratory Research & Innovation Group: https://eirig.org/downloads/r119/Clis_Enakvst.pdf

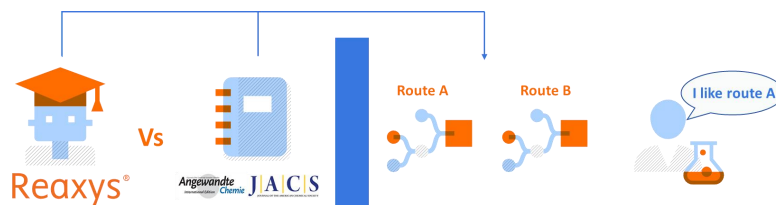
ELSP & Elsevier Confidential
09/10/2019

Elsevier Life Science 逆合成模型的定量评估

Quantitative evaluation against other predictive models and tools for 100 chEMBL molecules.

Retrosynthesis method	% of molecules for which a route was predicted	# of molecules for which a route was predicted using only the indicated method
Reaxys Predictive Retrosyntheses	95%	24
AiZynthFinder	54%	2
ASKCOS	64%	0

Qualitative double-blind test carried out with 45 organic chemists



Experts chose Reaxys predictive retrosynthesis routes 57% of the time versus 43% choosing the literature routes

Reaxys AI使用方法(需要有开通权限)

- 针对具体的化合物进行合成计划制作（可以是已知的，也可以是未知的）
 - 需要自行注册账号才可以用这个功能
 - 全新化合物需要通过Retrosynthesis功能进入

通过结构面板添加结构

Quick search Query builder Results Retrosynthesis History Alerts

Search substances, reactions, documents and bioactivity data
in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances

Search Reaxys

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

Reaxys Quick search Query builder Results Retrosynthesis History Alerts Sam Yu

No.	Date/Time	Project name	Draw new structure	No. of routes
936352	01 Mar 2023 08:28	Project #936352 Delete	 106 Edit	Customized 2 Published 5 View
881253	15 Feb 2023 02:54	Project #881253 Delete	 106 Edit	Customized 2 Predicted 16 Published 5 View

参数设置：概览

The screenshot displays the Reaxys Retrosynthesis interface. At the top, navigation tabs include 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The user 'Peng Wu' is logged in. The main workspace shows the 'Structure editor selected' with 'MarvinJS' chosen. A 'Parameters' panel on the right is expanded to show settings for a 'Predicted' route. The parameters include: 20 full routes (up to), 3 identical reaction steps per project (up to), 3 identical building blocks per project (up to), Standard processing time, and a list of building blocks: STD, SIAL, LN, EM, U2, U5, T1, RSM3, RSM4, RSM5. Below this, it states 'Powered by AI模块' (AI Module). The 'Published' section shows 5 full routes (up to), 5 branches per step (up to), 5 steps per route (up to), and a note: 'Don't Stop at commercial building blocks' and '50% yield per step (assumed, if not published)'. An orange callout box in the center of the workspace contains the text: 'Reaxys-AI设计简洁合理的参数设置，尽可能高效的获得预测路线' (Reaxys-AI designs concise and reasonable parameter settings to efficiently obtain predicted routes). The interface also features a 'Draw' toolbar on the left and 'Clear', 'Cancel', and 'Synthesize' buttons at the bottom.

设计路线数量和长度

不同方案中相同中间体合成方法重复次数

不同方案中相同中间体原料出现重复次数

预测时长

中间体来源库（文献+商业数据库）

Reaxys-AI设计简洁合理的参数设置，尽可能高效的获得预测路线

Parameters

Predicted

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

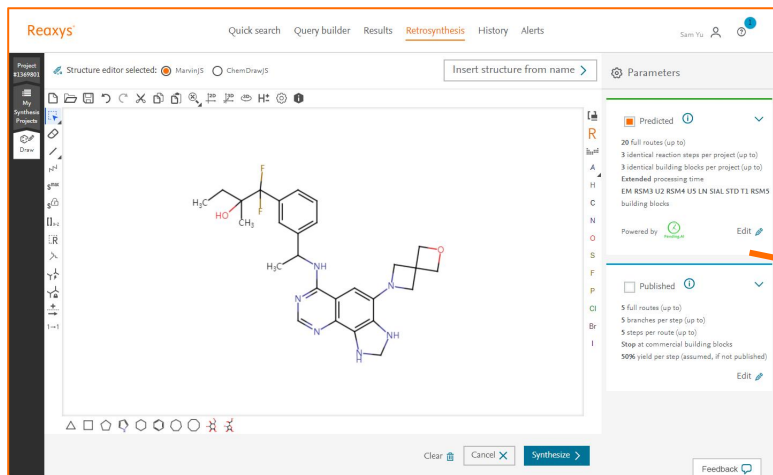
Powered by AI模块

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)

Clear Cancel Synthesize Feedback

参数设置：详细功能设定



1. 预测20条全路线，还是最后一步
2. 多样性设置，相同的步骤最多出现在几条线路中，相同BB最多出现在几条线路中
3. 时长，15min、30min
4. BB源头的设置

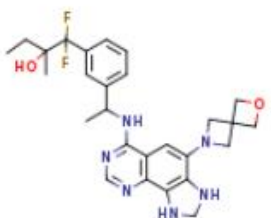
Parameters panel showing settings for Predicted routes, Length and depth of routes, Diversity of routes, and Processing time.

- Predicted
- Length and depth of routes: Full routes: 20, Last step only
- Diversity of routes: Allow 3 identical reaction steps per project, 3 identical building blocks per project
- Processing time: Standard, Extended

Select Building Block Libraries

- Standard Lab Chemicals (STD)
- Sigma Aldrich (SIAL)
- LabNetworks (LN)
- emolecules (EM)
- BBs Under 200 US per gram (U2)
- BBs Under 500 US per gram (U5)
- BBs from Tier 1 supplier (T1)
- Reaxys Starting Materials Occur 3 (RSM3)
- Reaxys Starting Materials Occur 4 (RSM4)
- Reaxys Starting Materials Occur gte 5 (RSM5)


Reaxys AI逆合成后的结果（不同参数设置，结果不一样）



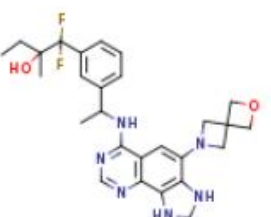
Chemical structure of a complex molecule, featuring a fluorinated phenyl ring, a hydroxyl group, and a piperazine ring system. The structure is shown in a search interface with a magnifying glass icon and a search bar.

Predicted 3

[View >](#)

Edit 


全线路3条



Chemical structure of a complex molecule, featuring a fluorinated phenyl ring, a hydroxyl group, and a piperazine ring system. The structure is shown in a search interface with a magnifying glass icon and a search bar.

Predicted 17

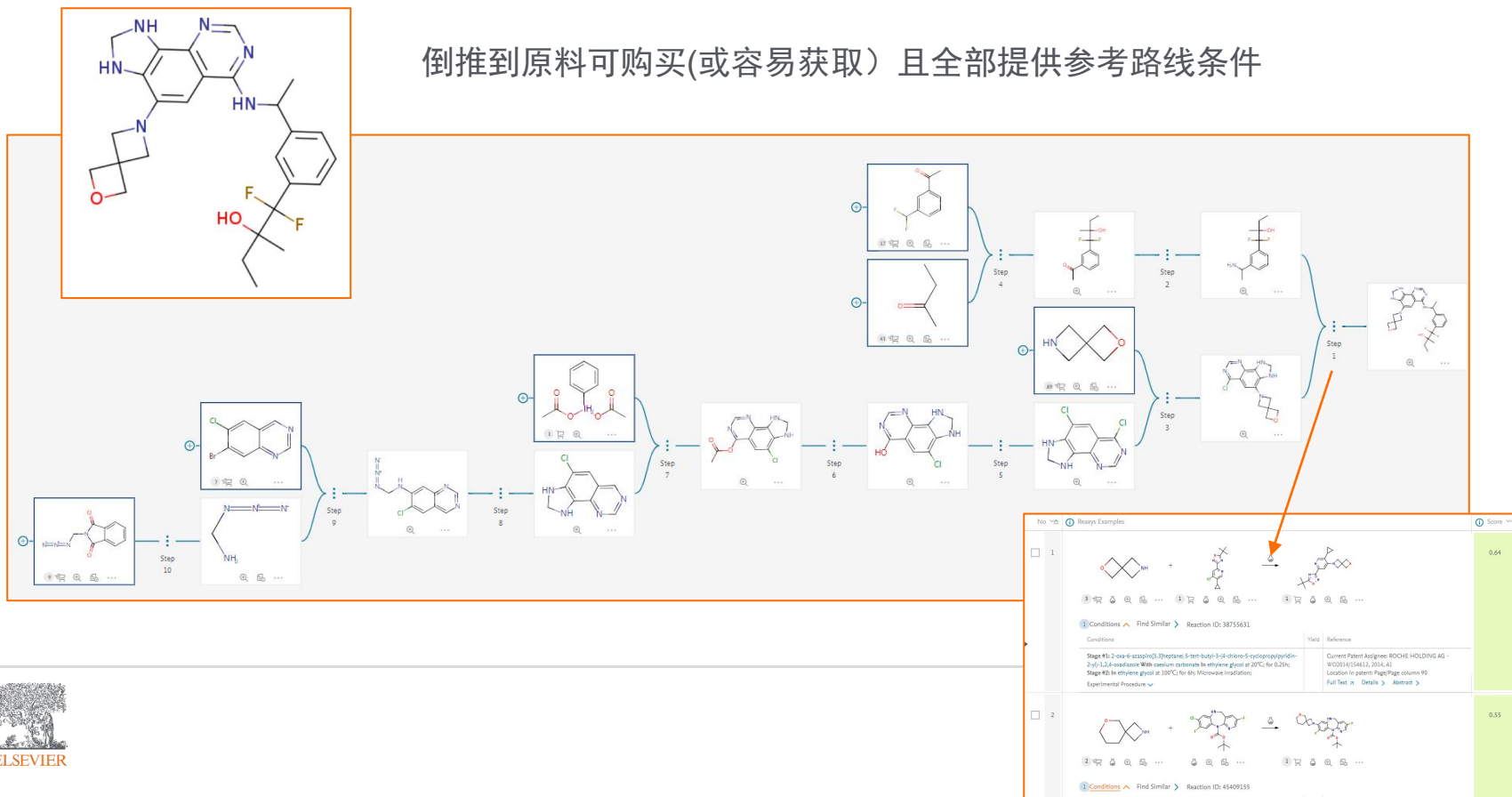
[View >](#)

Edit 

最后一步
17条

一条完整的线路

倒推到原料可购买(或容易获取) 且全部提供参考路线条件



Agenda

- Reaxys的底层逻辑和发展方向
 - Reaxys及其对于科技文献的提炼
- Reaxys中科研数据的获取和应用场景
 - Reaxys中的文献与专利的获取
 - Reaxys中物质理化性质的获取，反向应用，可视化分析
 - Reaxys中化合物活性数据在先导化合物优化方面的应用
 - Reaxys中结构面板与反应数据的获取
 - Reaxys中的AI逆合成模块介绍
- 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
- 多种途径的Elsevier Life Science网络社区服务：
 - B站：ELS生命科学，提供Elsevier Life Science数据库的使用视频
 - 微信群：添加小助手微信号：ELS-LSS，邀请进Elsevier Life Science用户群，最新资料分享以及使用Q&A
 - 微信公众号（非官方）：闲谈化学药学数据获取，检索原理与检索心得分享



欢迎广大师生积极试用数据库！

如果您想推荐该数据库，请扫描以下二维码填写推荐信息。



我校目前开通了Reaxys 数据库的试用。本校师生可在校园网范围内通过网址（asia.reaxys.com 或 www.reaxys.com）访问该数据库。试用期限：2024-5-7 至 2024-6-6。