

New Reaxys 使用介绍

Reaxys 解决方案咨询师

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提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Elsevier 公司介绍

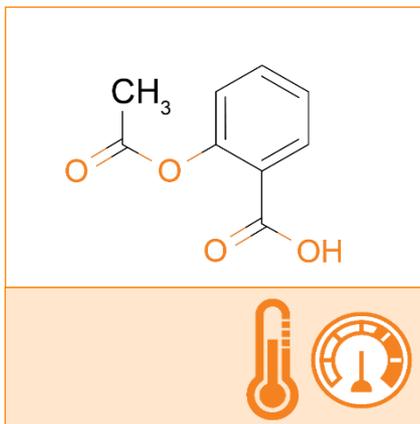
Elsevier于1880年在荷兰成立，成立之初致力于学术期刊杂志的发行和出版，现已发展成为全球最大的科技文献出版社

Elsevier 是一家全球性公司，总部在荷兰阿姆斯特丹，在世界25多个国家雇有7000多名员工，是励德爱思唯尔集团(Reed Elsevier)的成员。



Galileo's last and greatest work, published in 1638 by Elsevir, Discorsi e Dimostrazioni Matematiche is considered the first important discussion of modern physics.

什么是Reaxys?



>105 M 物质记录
>500 M 实验数据
物理的, 化学的, 光谱
数据, 生态学, 生物活
性数据

Chemistry fundamentals



>42 M 反应记录
以及这些反应的条件,
溶剂, 催化剂, 收率,
反应中心, 反应类型


Linked
to



>54 M 文献记录
>16,000 期刊, 专利
涉及有机化学, 材料化学,
生物医药, 地球科学, 工
程等多种领域

**Uses across
disciplines**

Reaxys 收录的文献范围和涉及学科分类

Reaxys总共收录16,098 种期刊

- 涵盖与化学相关16个学科领域
- 农业及生命科学
- 生物化学, 分子生物学
- 化学工程Chemical Engineering
- 化学Chemistry
- 牙科学Dentistry
- 宇宙科学Earth and Planetary Science
- 能源Energy
- 工程Engineering
- 环境Environmental Science
- 免疫学及微生物学Immunology and Microbiology
- 材料科学Materials Science
- 药学Medicine
- 神经系统科学Neuroscience
- 药理学、毒理学Pharmacology, Toxicology and Pharmaceutics
- 物理学和天文学Physics and Astronomy
- 兽医学Veterinary

其中包括化学最核心期刊426种 (其中收录ACS旗下化学最核心期刊31种)

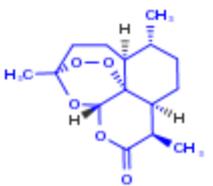
化学相关专利 (76年以来的世界, 美国, 欧洲), 2010年以来的所有日本, 韩国以及2015年以后所有的中国, 中国台湾

对于较早文献的收录比较好, 最早的一篇文章可以追溯到1771年

查看具体的生物数据

231 Substances out of 2,394 Documents, containing 1,199 Reactions, 65 Targets

0 Limit To Exclude Export

1
 

Reaxys ID: 4194670
C15H22O5 282.337 4194670 63968-64-9

[Identification](#)
[Druglikeness](#)
Bioactivity (All)

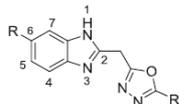
[Physical Data - 375](#)
[Spectra - 102](#)
[Other Data - 213](#)

^ Bioactivity (All)

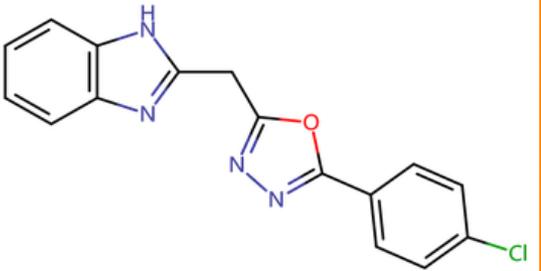
- ✓ In vitro: Efficacy - 1,358
- ✓ In vivo: Animal Model - 135
- ✓ Metabolism - 160
- ✓ Pharmacokinetic - 98
- ✓ Toxicity/Safety Pharmacology

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Population	Route of administration	Dose	Dosing regimen	Reference
	metabolic stability	active			mouse		administration	mg/kg		Acquaah-Mensah, George K.; Rich, Stephen M. - Journal of Ethnopharmacology, 2014, vol. 153, # 3, p. 732 - 736 Full Text Cited 15 times Details Abstract
	Vd ss/F		1363	L	Human	Healthy	oral administration	500 mg	Single	Simonsson, Ulrika S. H.; Jansson, Britt; Hai, Trinh Ngoc; Huong, Dinh Xuan; Tybring, Gunnel; Ashton, Michael - Clinical Pharmacology and Therapeutics, 2003, vol. 74, # 1, p. 32 - 43 Full Text Cited 68 times Details Abstract
	Vd ss/F		967	L	Human	Healthy	oral administration	500 mg	Single	Simonsson, Ulrika S. H.; Jansson, Britt; Hai, Trinh Ngoc; Huong, Dinh Xuan; Tybring, Gunnel; Ashton, Michael - Clinical Pharmacology and Therapeutics, 2003, vol. 74, # 1, p. 32 - 43 Full Text Cited 68 times Details Abstract
	AUC		1696	ng.h/mL	Human	Healthy	oral administration	500 mg	Single	Simonsson, Ulrika S. H.; Jansson, Britt; Hai, Trinh Ngoc; Huong, Dinh Xuan; Tybring, Gunnel; Ashton, Michael - Clinical Pharmacology and Therapeutics, 2003, vol. 74, # 1, p. 32 - 43 Full Text Cited 68 times Details Abstract

文献中的生物活性数据形式



Comp.	R	R'	IC ₅₀ (μM) ^{a,b}						
			EGFR	erbB2	MCF7	HaCaT	MDA-MB231	HepG2	A549
7a	H	4-Cl-C ₆ H ₄ -	0.061	0.63	5.0	9.5	14.5	32.5	15.3
7b	H	2,4-Cl ₂ -C ₆ H ₃ -	3.7	4.7	7.0	23.2	25.9	52.7	52.6
7c	H	C ₆ H ₅ -CH ₂ -	25.0	36.9	26.3	75.3	29.8	51.2	61.4
7d	H	C ₆ H ₅ -	31.8	40.0	59.0	57.5	50.4	65.4	64.7
7e	H	C ₆ H ₅ -O-CH ₂ -	45.3	52.4	32.4	61.0	35.5	45.2	42.5
7f	H	4-OH-C ₆ H ₄ -	>100	ND	32.7	65.9	35.6	85.3	ND
7g	H	2-Cl-C ₆ H ₄ -	4.5	6.5	22.3	25.3	21.2	63.7	>100
7h	H	2-CH ₃ -C ₆ H ₄ -	30.7	46.8	52.2	64.7	69.8	100	ND
7i	H	4-CH ₃ -C ₆ H ₄ -	>100	ND	24.6	62.1	62.1	62.1	ND
7j	H	2,3-(OCH ₃) ₂ -C ₆ H ₃ -	61.0	>100	35.2	62.1	62.1	62.1	ND
7k	H	2-Thiophene	>100	ND	56.3	62.1	62.1	62.1	ND
7l	H	2-Furan	>100	ND	56.3	62.1	62.1	62.1	ND
7m	H	(C ₆ H ₅) ₂ -CH ₂ -	45.0	57.5	42.8	62.1	62.1	62.1	ND
7n	H	4-OCH ₃ -C ₆ H ₄ -	0.096	0.91	2.5	62.1	62.1	62.1	ND
7o	H	2-Pyridinyl	>100	ND	75.9	62.1	62.1	62.1	ND



专利中表达实施例化合物，与多个靶点的IC50构效关系

文献通过图表的形式表达一些列结构构在EGFR, erbB2以及不同的5种细胞系上的IC50构效关系

[0056] The results are shown in the following table, which presents IC₅₀ in μM. S-adenosyl homocysteine (SAH) and sinefungin (SIN) are controls:

	SAH	Sinefungin	Example 100	Example 101	Example 102	Example 103	Example 104
G9a	6.66	18.86					>50
GLP1	5.03	32.02					>50
SET7/9	>100	1.14					>50
SET8	>100	>100					>50
SETD2	2.94	28.44					45
PRMT1(100nm, RGG)	8.59	1.034					>50
PRMT3	39.5	28.17					>50
SUV39H2	0.63	4.58					>50
CARM1 ^a	1.90	0.44	0.045	0.370	0.108	0.870	0.3
CARM1 ^b							0.05
SMYD2-FL	~50	0.22					>50
SMYD3							>50
SETDB1-FL	0.95	8					

Reaxys中的生物活性数据呈现形式

The screenshot displays the Reaxys interface for a heatmap of biological activity data. The main area shows a grid of activity scores for various substances across 17 targets. The top navigation bar includes options like 'Limit To', 'Exclude', 'Export', 'Settings', 'Navigator', and 'Legend'. A sidebar on the left lists targets, with 'Epidermal growth factor receptor' highlighted. A text box on the left indicates that the data can be converted to 'structural formula' and exported as 'SMILES'.

1 Documents with 38 Substances, 42 Reactions, 17 Targets

Substances	Targets	Histone-ly... SUV39H2	Histone-lysin... specific	Histone-ly... se SMYD1	Probable hist... rase 1.3	Histone-lys... se SETD2	Histone-ly... se EHMT1	Histone-ly... se EHMT2	Protein argini... ferase 1	Probable prot... ferase 3	N-lysine ... se SMYD2	Histone-lys... se SETD7	Histone-ly... se ASH2	Protein argini... ferase 8	Probable hist... rase 1.4	Histone-ly... se SMYD3	Histone-lysi... erase 2A	Histone-ar... se CARM1
S-(5'-adeno... cysteine		6.2	6	6	5.7	5.5	5.3	5.1	5	4.4	4.3	4	4					
sinefungin		5.3	5.1	5.1	6.3	4.5	4.4	4.7	5.9	4.5	6.6	5.9	4					
27475498																		5
27475499																		5
27475501		4.3			6.5	4.3	4.3	4.3	4.3	4.3	4.3	4.3	4.3	4.3	7.3	4.3	5.3	5.5
31517920					7.3													5
31517921					6.4													5.5
31517922					6.9													5.5
31517923					6													5.5

可转换成
'结构式'
且可导出
'smile式'

提纲

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Reaxys索引的内容—文献内容

The screenshot shows a multi-column layout of a scientific article. The left column contains the title, authors (Zhenyun Miao, Chuanqun Sheng, Wannian Zhang, Haitao Ji, Jing Shao, Luecheng You, Liang Zhang, Min Yao, and Jianzhong Chao), and their affiliations. The middle and right columns contain chemical structures, reaction schemes, and text. A table of contents is visible at the bottom of the page, listing sections like Introduction, Experimental, and Discussion.

Reaxys提炼了文献的书目信息, 摘要, 题录, 并用不同角度的索引词对文献内容进行描述。

bibliographic

→

Manual [digital] Indexing

→

New homocamptothecins: Synthesis, antitumor activity, and molecular modeling Cited 23 times
 Miao, Zhenyun; Sheng, Chuanqun; Zhang, Wannian; Ji, Haitao; Zhang, Jing; Shao, Luecheng; You, Liang; Zhang, Min; Yao, Jianzhong; Chao, Xiaoyin - *Bioorganic and Medicinal Chemistry*, 2008, vol. 16, # 3, p. 1493 - 1510

Abstract
 Homocamptothecins (hCPTs) represent a class of new emerging antitumor agents, which contains a seven-membered β-hydroxylactone in place of the conventional six-membered α-hydroxylactone (E ring) of camptothecins. Some novel 7-substituted hCPTs were designed and synthesized based on a newly developed synthetic route which couples ring A with ring C, E and D. Most of the synthesized compounds exhibit very high cytotoxic activity on tumor cell line A549. Some compounds, such as 9b, 9l, and 9y, show broad in vitro antitumor spectrum and are more potent than topotecan. Three-dimensional quantitative structure-activity relationship (3D-QSAR) methods, CoMFA and CoMSIA, were applied to explain the structure-activity relationship (SAR) of the synthesized compounds. Furthermore, molecular docking was used to clarify the binding mode of the synthesized compounds to human DNA topoisomerase I. The important hydrophobic, base-pair stacking, and hydrogen-bonding interactions were observed between the hCPT derivatives and their receptor. The results from molecular modeling will guide the design of novel hCPTs with higher antitumor activity.

Index terms
 EMTREE drug term: 10 methyl 11 chloro 7 (pyridiniummethyl)homocamptothecin chloride, 7 (2 bromophenyl)iminomethyl methoxyphenyl)iminomethylhomocamptothecin, 7 (2 methylphenyl)iminomethylhomocamptothecin, 7 (2,4 dichlorophenyl)dichlorophenyl)iminomethylhomocamptothecin, 7 (3 chloro 4 fluorophenyl)iminomethylhomocamptothecin, 7 (3 chloro 4 fluorophenyl)iminomethylhomocamptothecin, 7 (3 methylphenyl)iminomethylhomocamptothecin, 7 (3,4 dichlorophenyl)dimethylphenyl)iminomethylhomocamptothecin, 7 (3,5 dichlorophenyl)iminomethylhomocamptothecin, 7 (3,5 dimethylphenyl)chlorophenyl)iminomethylhomocamptothecin, 7 (4 cyanophenyl)iminomethylhomocamptothecin, 7 (4 methylphenyl)iminomethylhomocamptothecin, antineoplastic agent, camptothecin derivative, irinotecan, topotecan, unclassified d
 EMTREE medical term: animal experiment, animal model, antineoplastic activity, article, colon cancer, comparative molecule protein binding, drug structure, drug synthesis, human, human cell, hydrogen bond, hydrophobicity, male, molecular dock imaging, tumor cell
 Author keyword: 3D molecular modeling, camptothecins, Molecular docking
 Reaxys Index Terms: camptothecin, hydrophobic surface

Reaxys索引的内容—结构与反应

New homocyclic products Synthesis, antimicrobial activity, and molecular modeling.

Zhenqun Mao,¹ Chensun Song,¹ Wanzun Zhang,¹ Huihui Li,² Jing Zhang,¹ Lisheng Shao,¹ Liang Yu,¹ Min Zhang,¹ Jianrong Yao,¹ and Xiyun Che¹

¹ School of Chemistry, Henan Polytechnic University, Kaifeng, Henan, 455000, China; ² School of Chemistry, Henan Polytechnic University, Kaifeng, Henan, 455000, China

1. Introduction

Homocyclic DNA intercalators (HDI) are a structural class of DNA intercalators. They are composed of the binding of a aromatic 1,2,3,4-tetrahydropyridine (THP) ring to a nucleoside. The structure of HDI is similar to that of the natural DNA base pair. The HDI structure is similar to that of the natural DNA base pair. The HDI structure is similar to that of the natural DNA base pair.

2. Synthesis and antimicrobial activity

The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP). The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP). The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP).

3. Conclusion

The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP). The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP). The synthesis of HDI was carried out from the starting material, 1,2,3,4-tetrahydropyridine (THP).

Reaxys的反应记录，抽提了所有相关的数据，包括收率，催化剂，溶剂，反应类型等

Quick search
Query builder
Results
Synthesis planner
History

Markus Bussen
👤
🔔
🔍

Plan 1

Import Save Export

Undo Redo

1

2

82%

2

3a

89%

3

3b

89%

4

73%

1

5

Reaxys索引的内容——文献中的数据

The collage displays various scientific articles with highlighted sections:

- ScienceDirect Article 1:** "New homocyclic synthesis, antimicrobial activity, and molecular modeling". Authors: Zhenhua Ma, Chaoan Song, Waimin Zhang, Haike Ji, Jing Zhang. Includes chemical structures and a table of antimicrobial activity.
- ScienceDirect Article 2:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 3:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 4:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 5:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 6:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 7:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 8:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 9:** "Synthesis of novel...". Includes chemical structures and a table of properties.
- ScienceDirect Article 10:** "Synthesis of novel...". Includes chemical structures and a table of properties.

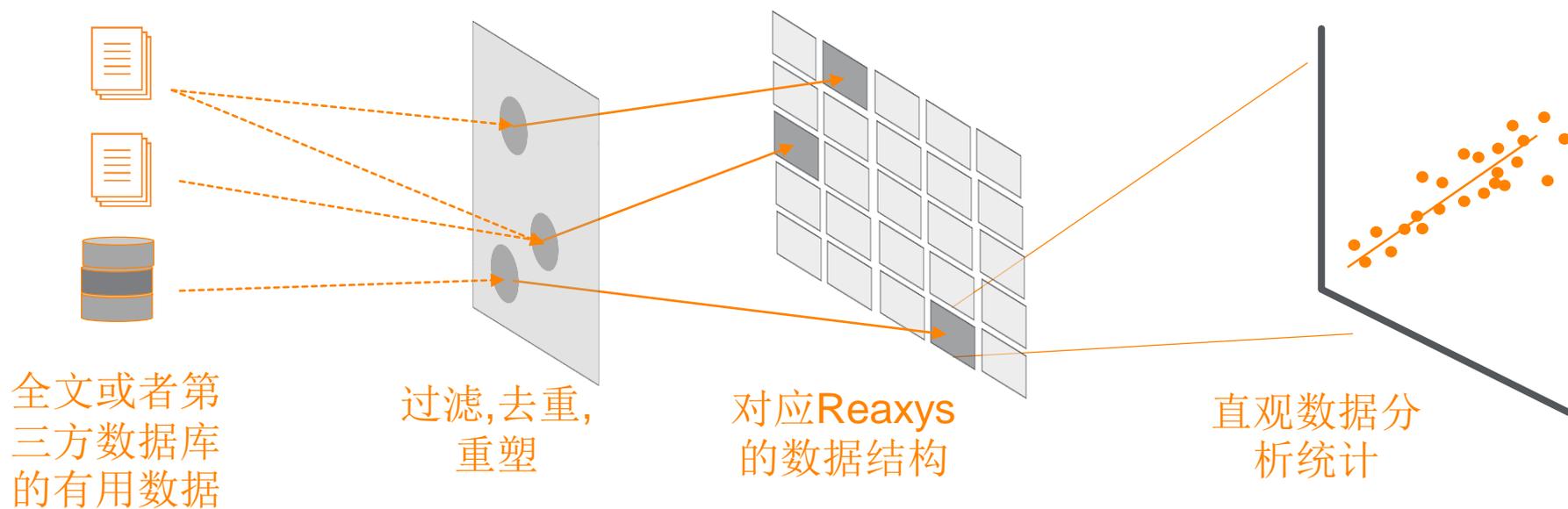
Reaxys的物性记录，抽提了超过500中不同的物性实验数据，生物活性数据，环境数据，以及谱图数据等等

The Reaxys interface shows the following details for 'camptothecin':

- Filters and Analysis:** By Structure (1), Measurement pX, Highest Clinical Phases, Targets, Parameters, Substance Classes, Molecular Weight, Availability, Availability in other databases, Available Data, Document Type, Publication Year.
- Search Results:** camptothecin, C₂₀H₁₆N₂O₄, 348.358, 6075662, 7689-03-4.
- Properties:** Identification, Bioactivity (All), Spectra - 139, Preparations - 221, Druglikeness, Physical Data - 132, Other Data - 1,527, Reactions - 1,112, Targets - 142, Documents - 3,556.
- Property List:**
 - Identification
 - Druglikeness
 - Bioactivity (All)
 - Physical Data - 132
 - Spectra - 139
 - Other Data - 1,527

Arrows from the property list point to corresponding data in the collage of literature pages above.

Reaxys旨在弹指之间传递关键信息



重在索引文献中的有用信息

提纲

- Reaxys中的内容和数据索引介绍
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 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

New Reaxys的界面

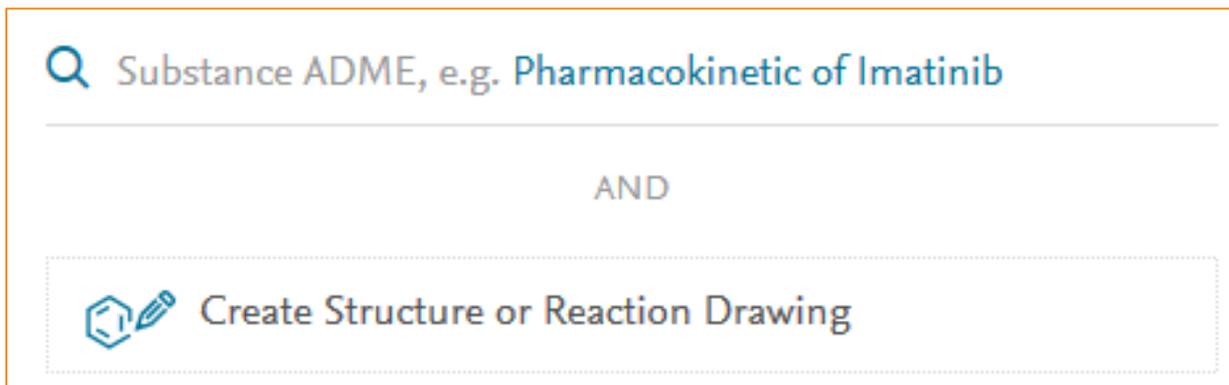
- [Http://new.reaxys.com](http://new.reaxys.com)

Quick Search

Query Builder

The screenshot displays the Reaxys web interface. At the top left is the Reaxys logo. The navigation bar includes 'Quick search' (highlighted), 'Query builder', 'Results', 'Synthesis planner', and 'History'. On the right side of the navigation bar, there is a user profile 'Sam Yu' and icons for a person, a bell, and a question mark. Below the navigation bar, there is a search area with the text 'Search substances, reactions, documents and bioactivity data' and a subtext 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich'. An 'Import' button with a download icon is on the left. The main search area contains a search bar with the text 'Reactions, e.g. phosphorylation'. Below the search bar, the word 'AND' is centered. At the bottom of the search area, there is a dashed box containing a pencil icon and the text 'Create Structure or Reaction Drawing'.

Reaxys的检索方式—Quick Search



Q Substance ADME, e.g. Pharmacokinetic of Imatinib

AND

 Create Structure or Reaction Drawing

Quick Search中可以使用的的方式:

1. 物质名称, Gefitinib
2. 反应名称, Wittig Reaction
3. 物质理化性质, Solubility of Gefitinib
4. 物质的谱图, NMR of Gefitinib
5. 分子式, C₂₂H₂₄ClFN₄O₃
6. 反应类型, Substitution
7. 关键词, nano fiber
8. 反应结构, 物质结构

Reaxys的检索方式—Query Builder

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder' (underlined), 'Results', 'Synthesis planner', and 'History' are in the center. A 'Sign in' link and a help icon are on the right. Below the navigation bar, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all' on the left, and 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index' in the center. A search bar with a 'Search' button and a dropdown arrow is on the right. The main area is a large grid with the text 'Drag & Drop to build a new query'. On the right side, there is a sidebar with a search bar labeled 'Find search fields and forms'. Below this, there are tabs for 'Fields', 'Forms', and 'History'. The 'Fields' tab is selected and highlighted with an orange box. An arrow points from the 'Fields' tab to a list of search fields: 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. Each field has a dropdown arrow on its right side.

Query Builder模块下，Fields中可以选择不同类型的字段进行自由组合检索

Reaxys中的字段检索

Tips:

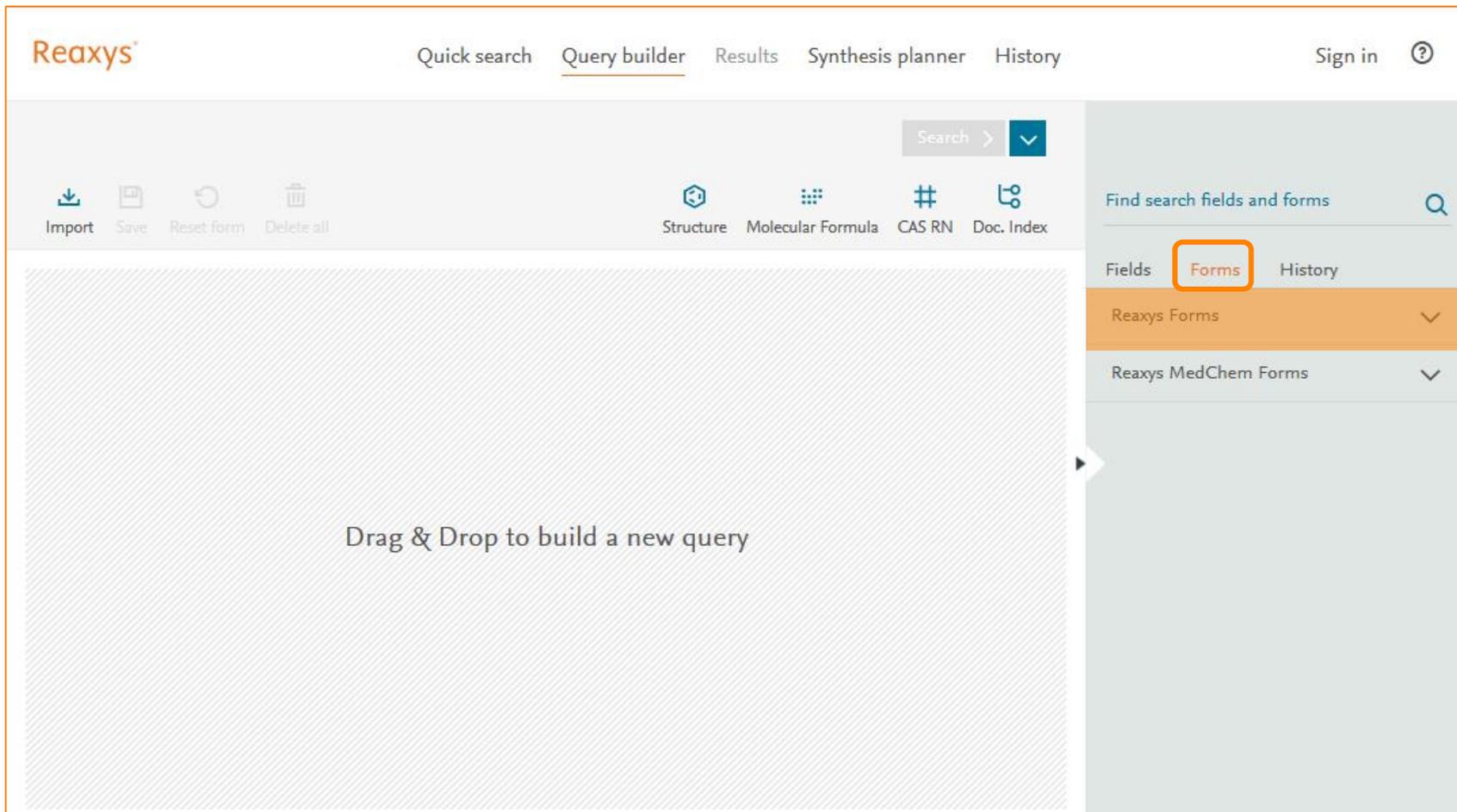
Reaxys提供8种不同的分类，每种分类中拥有和这种分类相关的多种字段，可以依据这些字段自由组合进行检索

Basic Indexes		^
◇	Substance Basic Index	☰ ⋮
◇	Reaction Basic Index	⋮
◇	Document Basic Index	⋮

Identification		^
◇	Chemical Name	☰ ⋮
◇	Element Symbols	☰ ⋮
◇	Molecular Formula	☰ ⋮
◇	Molecular Weight	☰ ⋮
◇	Preferred CAS Registry Number	⋮
◇	CAS Registry Number	☰ ⋮
◇	Bioactivity Presence	⋮
◇	Catalyst Investigation	⋮
◇	Charge	☰ ⋮
◇	Chemical Name Segment	☰ ⋮
◇	Derivative	⋮
◇	Druglikeness	⋮
◇	Element Counts	☰ ⋮

Physical Properties		^
◇	Melting Point	⋮
◇	Boiling Point	⋮
◇	Sublimation	⋮
◇	Refractive Index	⋮
◇	Density	⋮
◇	Adsorption	⋮
◇	Association	⋮
◇	Autoignition	⋮
◇	Azeotropes	⋮
◇	Boundary Surface Phenomena	⋮
◇	Chromatographic Data	⋮
◇	Bulk Viscosity	⋮
◇	Circular Dichroism	⋮

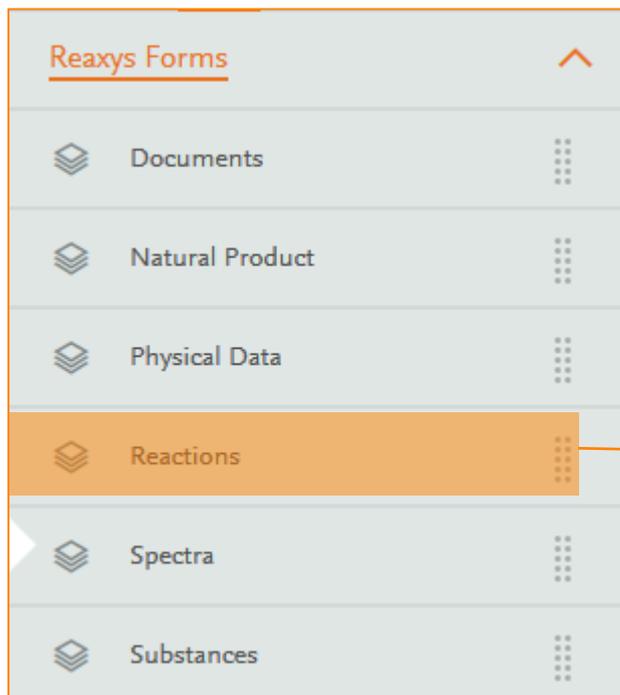
Reaxys检索方式—Query Builder Forms



The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation tabs for 'Quick search', 'Query builder' (which is underlined), 'Results', 'Synthesis planner', and 'History' are in the center. On the far right, there are 'Sign in' and a help icon. Below the navigation, a toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all'. To the right of these are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. A search bar with a dropdown arrow is also present. The main workspace is a large grey area with a diagonal line pattern and the text 'Drag & Drop to build a new query'. On the right side, there is a sidebar with a search bar labeled 'Find search fields and forms'. Below this are three tabs: 'Fields', 'Forms' (which is highlighted with an orange border), and 'History'. Under the 'Forms' tab, there are two expandable sections: 'Reaxys Forms' and 'Reaxys MedChem Forms', both with downward-pointing chevrons.

Query Builder模块下，Forms中Reaxys的预设模块检索

Reaxys Form中的预设模块



A screenshot of the Reactions form in Reaxys. The form is titled "Reactions" and contains several sections, each with a dropdown menu and a search field. The sections are: Structure (with a "Create Structure / Reaction Drawing" button), Yield (with a dropdown set to "Yield"), Solvent (with a dropdown set to "Solvent"), Reagent/Catalyst (with a dropdown set to "Reagent/Catalyst"), Time (Reaction Details) (with a dropdown set to "Time (Reaction Details)"), Temperature (Reaction Details) (with a dropdown set to "Temperature (Reaction Details)"), Pressure (Reaction Details), Torr (with a dropdown set to "Pressure (Reaction Details), Torr"), and Reaction Type (with a dropdown set to "Reaction Type"). Each section is separated by an "AND" connector.

反应结构

反应收率

反应溶剂

试剂催化剂

反应时间

反应温度

反应压力

反应类型

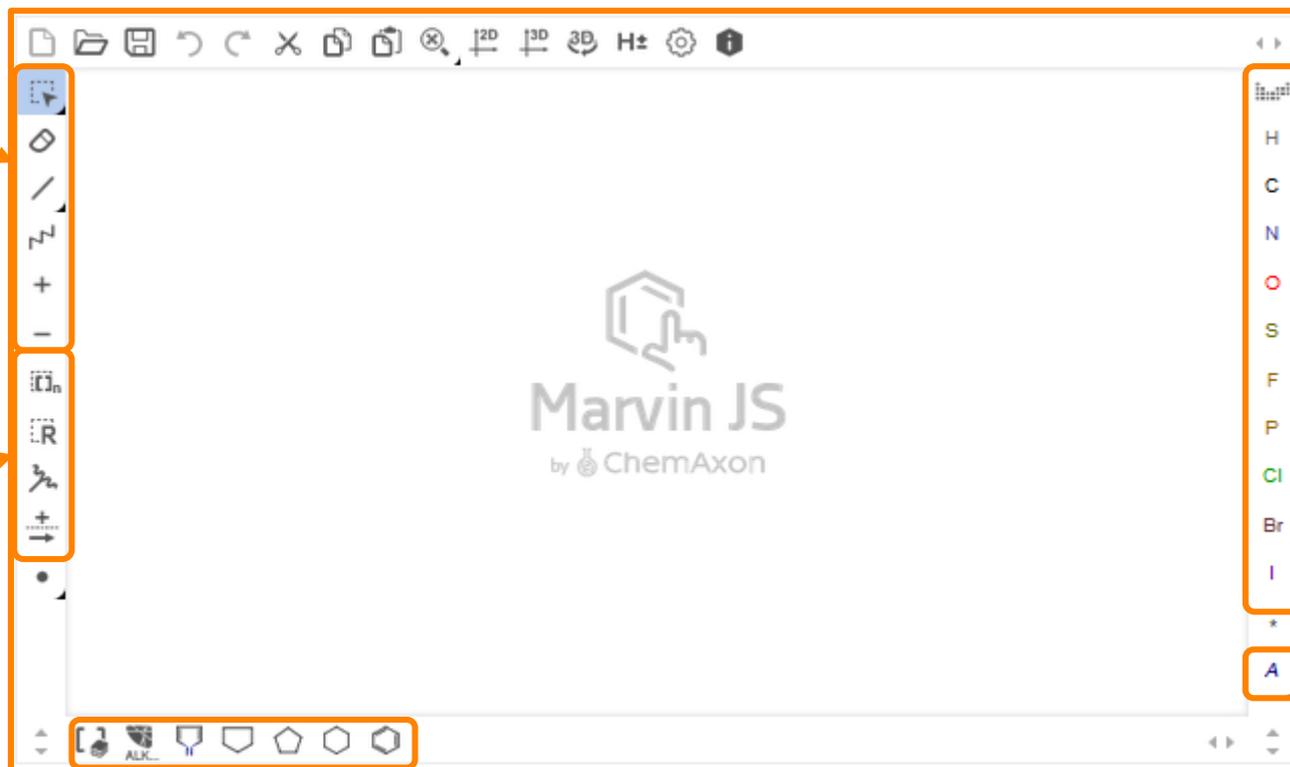
提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Reaxys中Marvin JS结构编辑器使用

选择工具，
橡皮，键
定义，链，
正负电子

重复基团，
R基团，R
基团链接
端，反应
定义工具



元素周期
表以及常
用原子

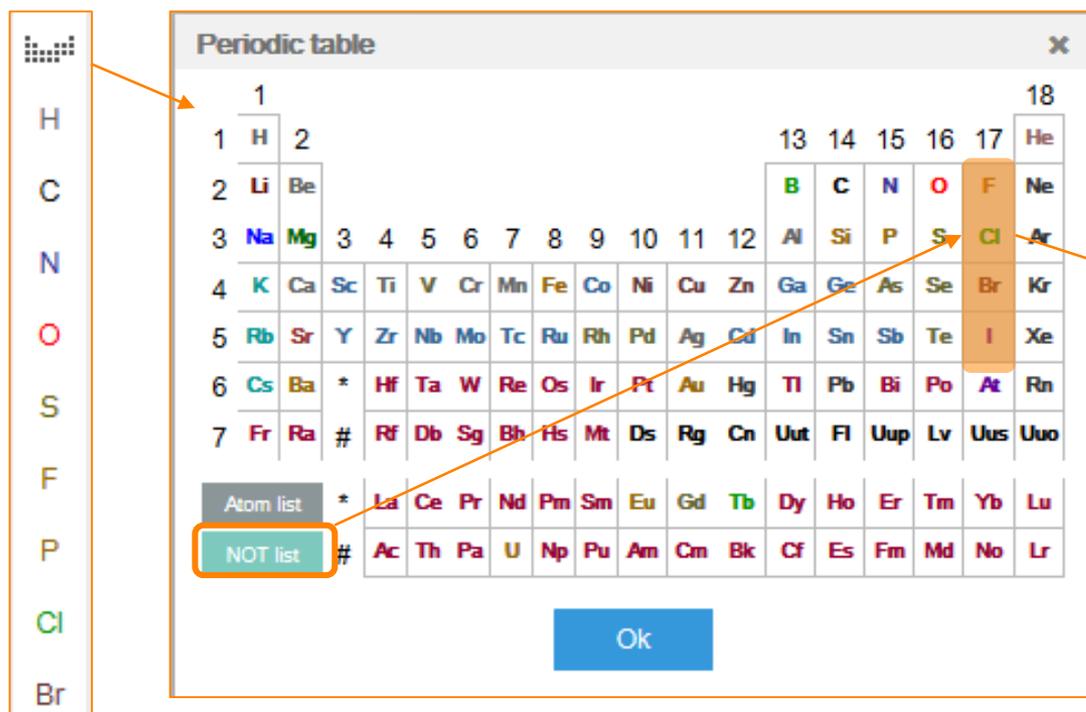
A:
原子属性
定义工具

常见的环，官能团，Reaxys的
Generic Group 定义

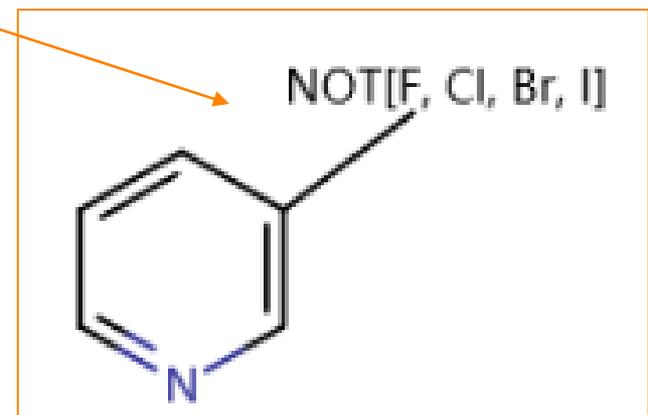
Ctrl+Alt+C=复制，Ctrl+V=
黏贴

结构定义案例1—Not List的应用

- 案例:
 - 定义某位点上不能发生F, Cl, Br, I取代

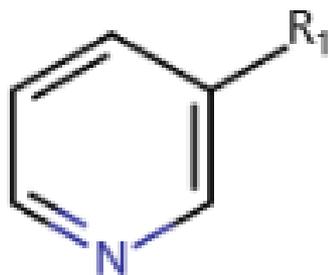


The screenshot shows a software interface for defining a 'NOT list' in a chemical structure. On the left, a vertical list of atoms is shown: H, C, N, O, S, F, P, Cl, Br. The main window is titled 'Periodic table' and displays a standard periodic table. A box labeled 'NOT list' is highlighted in orange, and an arrow points from it to the 'Atom list' section. The 'Atom list' section contains a list of atoms: La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu. The 'NOT list' section is currently empty. An 'Ok' button is visible at the bottom of the window.

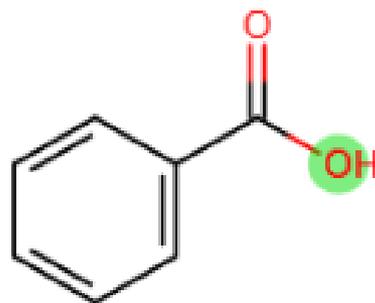


自定义R基团

- 案例
 - 定义一个结构A
 - R1分别是下面的这些结构，结构中绿色原子与A结构相连接

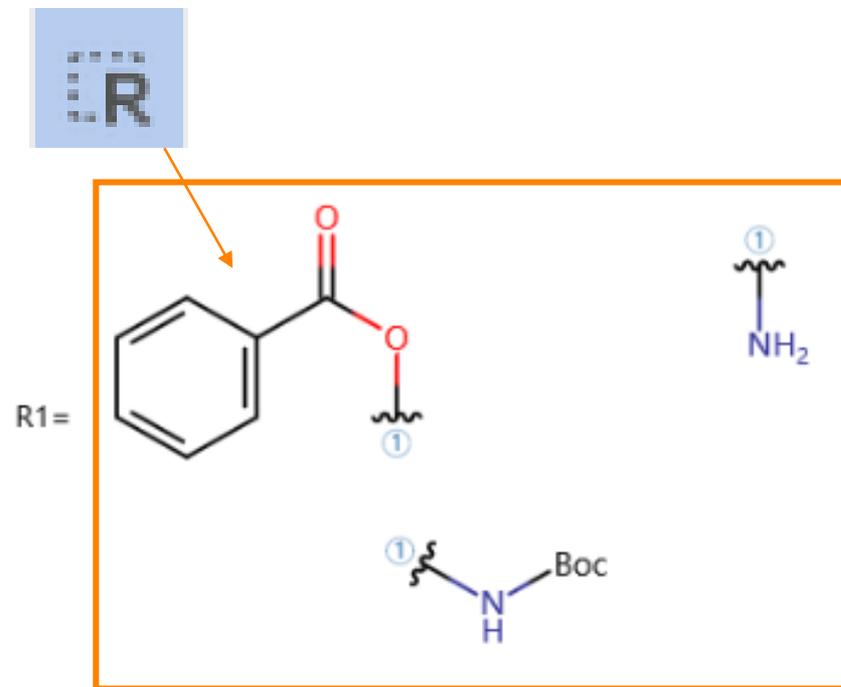
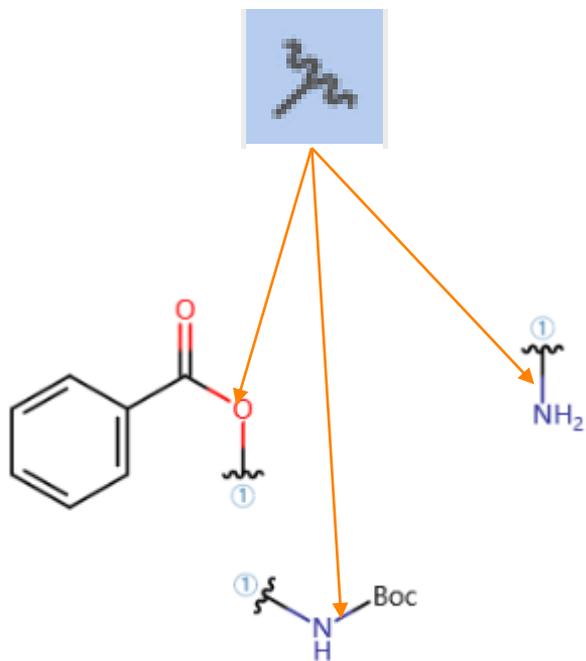


A



绘制方法

- 定义步骤：
 - 使用R基团末端定义工具定义绿色原子
 - 使用R基团定义工具，选择全部片段，即可完成R1的定义



提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Case Study 1—结构检索物质

The screenshot shows the Reaxys 'Structure editor' interface. At the top, there are navigation tabs: 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A dialog box titled 'Create structure template from name' is open, with a search input field containing 'Gefitinib' and a search icon. The background shows a blank structure editor workspace with a toolbar on the left and the 'Marvin JS by ChemAxon' logo in the center.

This screenshot shows the Reaxys interface with the chemical structure of Gefitinib displayed in the structure editor. The structure is a complex molecule with a piperazine ring, a propyl chain, and a quinazolinone core with a 4-chloro-3-fluorophenyl group. On the right side, there is a search options panel titled 'Search this structure as:' with radio buttons for 'As drawn' (selected), 'As substructure', and 'Similar'. Below this is an 'Include' section with checkboxes for various options: Tautomers, Stereo, Additional ring closures, Related Markush, Salts, Mixtures, Isotopes, Charges, and Radicals. At the bottom right, there is a 'Feedback' button. At the bottom of the editor, there are buttons for 'Clear', 'Cancel', and 'Transfer to query'.

Reaxys可以直接通过物质名称直接导入结构

New Reaxys给出的结果

The screenshot displays the Reaxys search results interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, the user name 'Sam Yu' is shown along with icons for a profile, notifications, and help. Below the navigation bar, there are 'New' and 'Edit' buttons on the left, and 'Results for' followed by a chemical structure icon in the center. The main content area lists three search results:

Count	Category	Structure	Preview Results	View Results
222	Substances	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results ▾	View Results >
1,038	Targets	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results ▾	View Results >
194	Substances	Structure : average similarity; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes,	Preview Results ▾	View Results >

A 'Feedback' button with a speech bubble icon is located at the bottom right of the page.

New Reaxys中的结果集

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

222 Filters and Analysis

222 Substances out of 2,879 Documents, containing 133 Reactions, 1,038 Targets Reaxys - 222

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes

0 Limit To Exclude Export No of References ↓ Heatmap

1

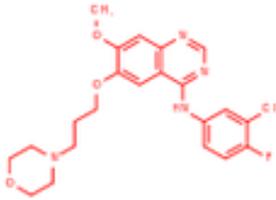
gefitinib
C₂₂H₂₄ClFN₄O₃ 446.909 8949523 184475-35-2

Identification	Physical Data - 52	Preparations - 53 >
Druglikeness	Spectra - 43	Reactions - 83 >
Bioactivity (All)	Other Data - 2,446	Targets - 1,027 >
		Documents - 2,861 >

Tips:

1. 每一个结构结果中，存在的理化性质数据可以直接打开，且可以直接看到对应文献的出处，
2. 物质对应的文献，可以进行进一步的分析，筛选

New Reaxys中的物质理化性质



gefitinib

C₂₂H₂₄ClFN₄O₃ 446.909 8949523 184475-35-2

Identification

Druglikeness

Bioactivity (All)

Physical Data - 52

Spectra - 43

Other Data - 2,446

Preparations - 53 >

Reactions - 83 >

Targets - 1,027 >

Documents - 2,861 >

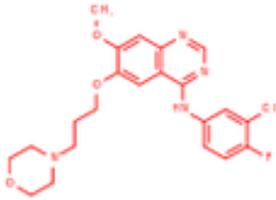
^ Physical Data - 52

- ∨ Melting Point - 17
- ∨ Chromatographic Data - 4
- ∨ Conformation - 1
- ∨ Crystal Phase - 5
- ∨ Crystal Property Description - 10

^ Crystal Property Description - 10

Colour & Other Properties	Location	Reference
white	Paragraph 0126; 0133	shanghai tianci shengwu gu Biological Engineering Co., Ltd.; Pu; Li, Jianzhi; +5 others - CN105218476, 2016, A Full Text ↗ Show details >
white	Paragraph 0038	Southwest University of Science and Technology; WANG, CHUANFANG; +2 others - CN105399688, 2016, A Full Text ↗ Show details >
white	Paragraph 0037	CSPC Zhongqi Pharmaceutical Technology(Shijiazhuang)Co., Ltd.; CSPC Ouyi Pharmaceutical Co., Ltd; Zhang, Yanqiao; +4 others - CN103319422, 2016, B Full Text ↗ Show details >

New Reaxys中的谱图



gefitinib
 $C_{22}H_{24}ClFN_4O_3$ 446.909 8949523 184475-35-2

Identification
 Druglikeness
 Bioactivity (All)

Physical Data - 52
 Spectra - 43
 Other Data - 2,446

^ Spectra - 43

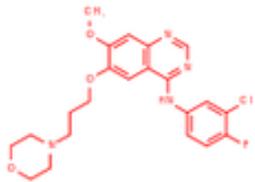
- ∨ NMR Spectroscopy - 27
- ∨ IR Spectroscopy - 4
- ∨ Mass Spectrometry - 7
- ∨ UV/VIS Spectroscopy - 4
- ∨ Raman Spectroscopy - 1

Tips:

Reaxys直接摘录原文中的NMR谱图描述，并提供原文中的位置

¹H NMR (400 MHz, d₆-DMSO) 9.44 (5, 1H), 8.50 (5, 1H), 8.12 (dd, J = 6.9, 2.7 Hz, 1H), 7.80 (m, 2H), 7.44 (t, 1H), 7.20 (5, 1H), 4.18 (t, J = 6.7 Hz, 2H), 3.94 (5, 3H), 3.59 (t, J = 4.4 Hz, 4H), 2.49 (t, J = 6.9 Hz, 2H), 2.41 (bs, 4H), 2.00 (m, 2H).	Paragraph 0035	SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1 Full Text ↗ Show details >
¹³C NMR (100 MHz, d₆-DMSO) 156.48, 154.94, 153.57 (J = 241 Hz), 153.05, 148.74, 147.43, 137.33 (J = 3 Hz), 123.91, 122.77 (J = 7 Hz), 119.19 (J = 19 Hz), 116.90 (J = 21 Hz), 109.26, 107.72, 103.14, 67.59, 66.43, 56.31, 55.35, 53.73, 26.13.	Paragraph 0035	SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1 Full Text ↗ Show details >

Reaxys中的分析文献的获取



gefitinib
C22H24ClFN4O3 446.909 8949523 184475-35-2

Identification	Physical Data - 52	Preparations - 53 >
Druglikeness	Spectra - 43	Reactions - 83 >
Bioactivity (All)	Other Data - 2,446	Targets - 1,027 >
		Documents - 2,861 >

Tips:

获得文献后，
 可以通过
 Reaxys的文献
 过滤工具对
 文献进行后
 处理

Reaxys
Quick search Query builder Results Synthesis planner History
Sam Yu   

2,861

222

- Filters and Analysis
- Index Terms (List) v
- Index Terms (ReaxysTree) v
- Publication Year v
- Document Type v
- Authors v
- Patent Assignee v
- Journal Title v
- Substance Classes v
- Reaction Classes v

2,861 Documents with 67 Substances, 41,978 Reactions, 1,594 Targets

0 Limit To Exclude Export

Reaxys - 2,861 v

Relevance v Heatmap 

- Oxindole derivatives
¹ Zeneca Limited - US6265411, 2001, B1
 Patent Family Members: GB9707800 D0; ZA9703844 B; WO1997/42187 A1; AU2647597 A; EP912557 A1; ...
Abstract v Front Page Info v Substances 279 v Reactions 182 v Targets v Full Text ↗
- Oxindolylquinazoline derivatives as angiogenesis inhibitors
² Zeneca Limited - US6294532, 2001, B1
 Patent Family Members: WO1999/10349 A1; AU8816298 A; EP1005470 A1; JP2001/514182 A; US6294532 B1; ...
Abstract v Front Page Info v Substances 135 v Reactions 81 v Full Text ↗
- Use of tyrosine kinase inhibitors for the treatment of inflammatory processes
³ Boehringer Ingelheim Pharma GmbH and Co. KG - US2003/149062, 2003, A1
 Patent Family Members: DE10204462 A1; US2003/149062 A1; CA2472282 A1; WO2003/66060 A2; ...

Index Term Reaxys Tree的应用

Reaxys通过Index Term Reaxys Tree的方式，将文献进行精确分类，帮助大家快速定位所需分析文献。

Index Terms (List) ∨

Index Terms (ReaxysTree) ∧

- physico chemical properties 1,065
- chemical transformations 1,042
- physico chemical analysis methods 350
- quantum chemical calculation methods

+ More

Index Terms (ReaxysTree) ×

- 📁 Index Terms (ReaxysTree) 3,004
- 📁 physico chemical properties 1,129
- 📁 chemical transformations 1,105
- 📁 physico chemical analysis methods 374
- 📁 quantum chemical calculation methods 31

物理化学分析方法

Clear selected × Limit To Exclude

物理化学分析方法中的细节性分类

Index Terms (ReaxysTree) ×

> > <input type="checkbox"/> chemical transformations		<input type="checkbox"/>	1,105
✓ > > <input type="checkbox"/> physico chemical analysis methods		<input type="checkbox"/>	374
> > <input checked="" type="checkbox"/> spectroscopical analysis	谱图分析方法	<input type="checkbox"/>	180
> > <input checked="" type="checkbox"/> separation method	分离方法	<input type="checkbox"/>	163
> > <input type="checkbox"/> microscopy		<input type="checkbox"/>	78
> > <input type="checkbox"/> quantitative analysis		<input type="checkbox"/>	18
> > <input type="checkbox"/> elemental analysis		<input type="checkbox"/>	16
> > <input checked="" type="checkbox"/> thermal analysis	热力学分析	<input type="checkbox"/>	13
> > <input checked="" type="checkbox"/> crystal structure determination	晶型结构鉴定	<input type="checkbox"/>	12
> > <input type="checkbox"/> electro analytical method		<input type="checkbox"/>	3
<input type="checkbox"/> qualitative analysis		<input type="checkbox"/>	14
> > <input type="checkbox"/> quantum chemical calculation methods		<input type="checkbox"/>	31

Clear selected × Limit To > Exclude >

Case Study 2—快速获得物质的理化性质

- 检索吉非替尼的溶解性数据

The screenshot displays the Reaxys search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there are user profile icons for 'Sam Yu', a notification bell, and a help icon. Below the navigation bar, there is a search bar with the text 'Search for solubility of gefitinib' and a 'Find >' button. An 'Import' button with a download icon is on the left. Below the search bar, a search box contains the text 'Search Reaxys' and 'solubility of gefitinib' with a magnifying glass icon and a close 'X' icon. Below the search box, the word 'AND' is centered. At the bottom, there is a button with a pencil icon and the text 'Create Structure or Reaction Drawing'. An orange arrow points from the bottom left towards the search box.

直接用自然语言在输入，solubility of gefitinib，检索

组合检索

Reaxys®

Quick search Query builder Results Synthesis planner History

Peng Wu

Import

Search for solubility AND

Find

Search Reaxys

solubility

AND

As drawn

Feedback

REAXYS® Version 1

Detailed description: The image shows a screenshot of the Reaxys search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, the user's name 'Peng Wu' and icons for profile, notifications, and help are visible. Below the navigation bar is a search bar containing the text 'Search for solubility AND' followed by a structure icon. To the right of the search bar is a 'Find' button. Below the search bar, a search results window is open, showing 'Search Reaxys' and 'solubility'. Below this, a dashed box contains a chemical structure with the label 'AND' above it. The structure is a complex molecule consisting of a piperazine ring connected via a propyl chain to a benzimidazole core. The benzimidazole core has a methoxy group (-OCH3) at the 6-position and an NH group at the 2-position, which is further connected to a 3-chloro-4-fluorophenyl ring. The structure is labeled 'As drawn' at the bottom. In the bottom left corner, there is a 'REAXYS® Version 1' logo, and in the bottom right corner, there is a 'Feedback' button with a speech bubble icon.

Reaxys直接给出结果

The screenshot shows the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The user 'Peng Wu' is logged in. The search results are for 'solubility AND' and are displayed in a list format. The first result is highlighted with a blue vertical bar on the left. The 'View Results' button for the first result is circled in orange.

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

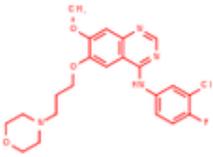
Results for solubility AND

New Edit

Count	Category	Structure / Property	Preview Results	View Results
1	Substances	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals, no separate fragments AND Property : solubility	Preview Results	View Results
241	Substances	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals, no separate fragments	Preview Results	View Results
311,871	Substances	Property : solubility	Preview Results	View Results

Feedback

最后的结果

1 
gefitinib
C22H24ClFN4O3 446.909 8949523 184475-35-2

[Hit Data - 1](#) [Bioactivity \(All\)](#) [Other Data - 2,446](#) [Preparations - 53 >](#)
[Identification](#) [Physical Data - 52](#) [Reactions - 83 >](#)
[Druglikeness](#) [Spectra - 43](#) [Targets - 1,027 >](#)
[Documents - 2,861 >](#)

[^ Hit Data - 1](#)
[v Solubility \(MCS\) - 1 hits out of 1](#)

[^ Solubility \(MCS\) - 1 hits out of 1](#) [Show/Hide columns v](#)

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Reference
0.0021	in pure solvent	20	water	Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Weili; Dong, Xiaochun - Bioorganic and Medicinal Chemistry Letters, 2013, vol. 23, # 19, p. 5385 - 5388 Full Text ↗ Cited 16 times ↗ Details > Abstract >

Hit Data直接给出具体的实验数据，以及检测条件和全文链接

Case Study 3—母核结构检索

- 检索包含以下母核的结构

The screenshot displays the Reaxys software interface. At the top, there are navigation tabs: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". The user's name "Sam Yu" and notification icons are visible in the top right. The main area is the "Structure editor", which contains a chemical structure of a fused bicyclic system: a pyrimidine ring fused to a 2-pyridone ring. The structure is rendered with blue nitrogen atoms and a red carbonyl group. To the right of the editor is a search configuration panel titled "Search this structure as:". It includes several options: "As drawn" (radio button), "As substructure" (radio button, highlighted in orange), "Similar" (radio button), "Tautomers" (checkbox), "Stereo" (checkbox), "Additional ring closures" (checkbox), "Related Markush" (checkbox), "Salts" (checkbox), "Mixtures" (checkbox), "Isotopes" (checkbox), "Charges" (checkbox), and "Radicals" (checkbox). A "+ More options" link is at the bottom of the panel. At the bottom of the interface, there are buttons for "Clear", "Cancel", and "Transfer to query".

As Substructure检索结果

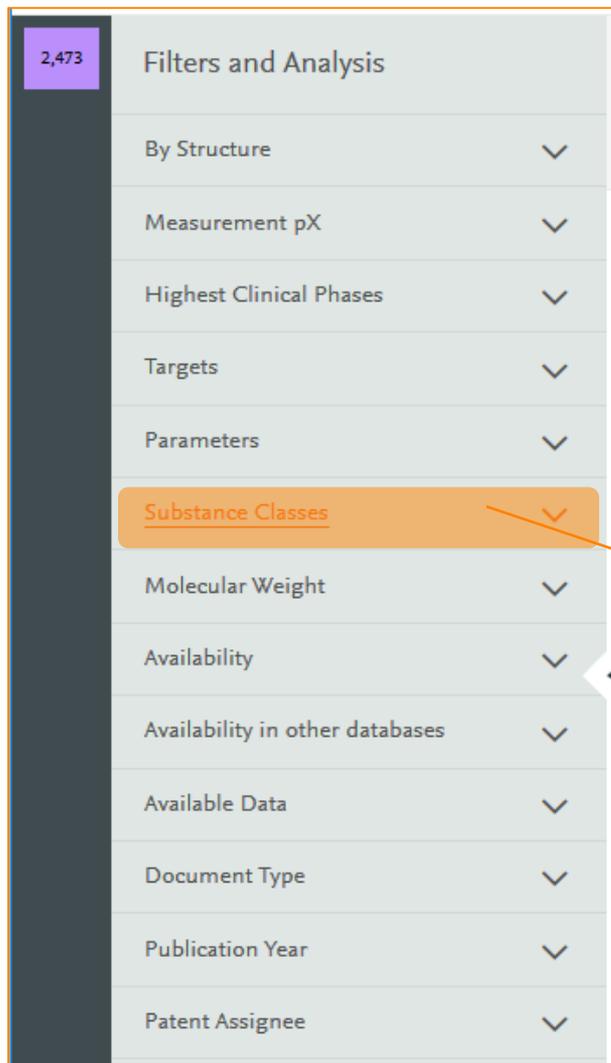
Reaxys® Quick search Query builder Results Synthesis planner History Sam Yu

2,473 Filters and Analysis 2,473 Substances out of 462 Documents, containing 3,611 Reactions, 215 Targets Reaxys - 2,473

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

<input type="checkbox"/>	1		pipedimic acid C ₁₄ H ₁₇ N ₅ O ₃ 303.321 626575 51940-44-4	Identification Druglikeness	Bioactivity (All) Physical Data - 23	Spectra - 34 Other Data - 25	Preparations - 7 > Reactions - 124 > Targets - 12 > Documents - 242 >
<input type="checkbox"/>	2		piromidic acid C ₁₄ H ₁₆ N ₄ O ₃ 288.306 625004 19562-30-2	Identification Druglikeness	Bioactivity (All) Physical Data - 8	Spectra - 2 Other Data - 17	Preparations - 1 > Reactions - 7 > Targets - 5 > Documents - 85 >
<input type="checkbox"/>	3		4-amino-8H-pyrido[2,3-d]pyrimidin-5-one C ₇ H ₆ N ₄ O 162.151 8902253 306960-30-5	Identification Druglikeness	Bioactivity (All) Physical Data - 1	Spectra - 3	Preparations - 4 > Reactions - 83 > Targets - 1 > Documents - 14 >

Reaxys中的筛选过程



2,473

Filters and Analysis

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

结构的筛选工具，Substance Class帮助了解结构中的特殊片段



Substance Classes

- Functional Group Classification 2,471
- Richter Classification 2,471
- Ring Classification 2,471

+ More

Reaxys中的结构分析

Substance Classes

Substance Classes	2,473
Functional Group Classification	2,471
Richter Classification	2,471
Ring Classification	2,471

环系分类

Ring Classification

6-membered rings	
9-18-membered rings	
5-membered rings	997
3-membered rings	
4-membered rings	
bridged ring systems	
8-membered rings	
7-membered rings	
macrocycles (18+ rings)	

5-membered rings

5-membered rings, fused systems	599
5-membered rings, substituted	586
cyclopentane and derivatives	489
cyclopentene and derivatives	431
pyrrolidine and derivatives	265
tetrahydrofuran and derivatives	101
thiazolidine and derivatives	67
5-membered rings, disubstituted	63
2,3-dihydro-1,3-thiazole and derivatives	61
furan and derivatives	44
pyrazole and derivatives	37

不同的5元环系

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Case Study 4 关键词检索反应

- Synthesis of 3-hydroxy-indole

The screenshot displays the Reaxys search interface. At the top, there are navigation options: Quick search, Query builder, Results, Synthesis planner, and History. A search bar contains the text "Search for synthesis of 3-hydroxy-indole" with a "Find" button. Below the search bar, a search box shows "Search Reaxys" and "synthesis of 3-hydroxy-indole". An arrow points from this search box to the first result in the table below.

Count	Category	Filters	Actions
70	Reactions	Product(s) : as drawn	Preview Results View Results
896	Documents	Titles, Abstracts, Keywords : synthesis, 3-hydroxy-indole	Preview Results View Results
8,268,579	Documents	Titles, Abstracts, Keywords : synthesis	Preview Results View Results
2,670	Documents	Titles, Abstracts, Keywords : 3-hydroxy-indole	Preview Results View Results

Reaxys中的智能解析直接将短语转换成反应式

Reaxys中的结果

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

70 Filters and Analysis

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

Single step reactions only

70 Reactions out of 82 Documents containing 54 Substances, 71 Targets

0 Limit To Exclude Export Product Availability

Reaction ID: 354985
10

Cc1ccc2nc3ccccc3o2 → Oc1ccc2c(c1)c[nH]2 + O=C1Nc2ccccc2N1

2 Conditions Find Similar

Reaction ID: 387961
11

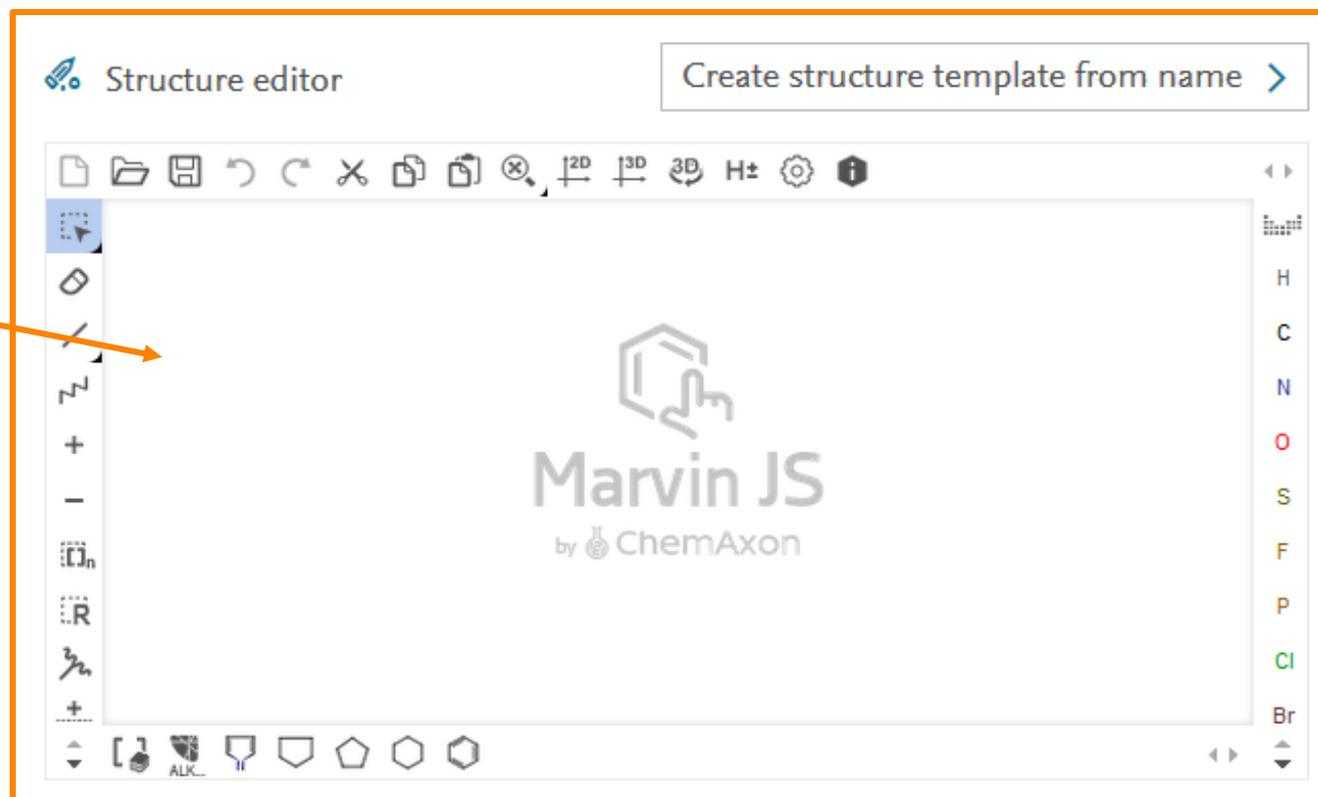
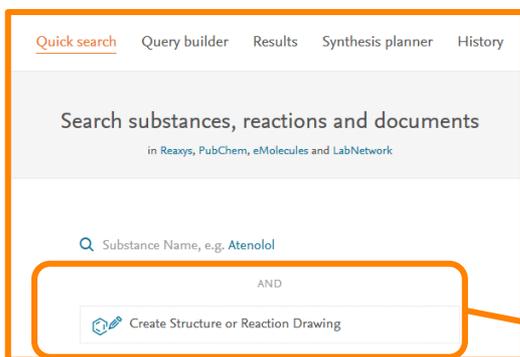
OCCNC(=O)c1ccccc1 → Oc1ccc2c(c1)c[nH]2

2 Conditions Find Similar

相同反应的‘所有报道的反应条件’收集在一起，便于查看和筛选

Case Study 5 基本反应结构检索

- 检索以下的反应
 - 吡啶环2, 3, 4位上存在一个硝基还原成氨基
 - 吡啶环6位上存在一个Cl



检索Tips:

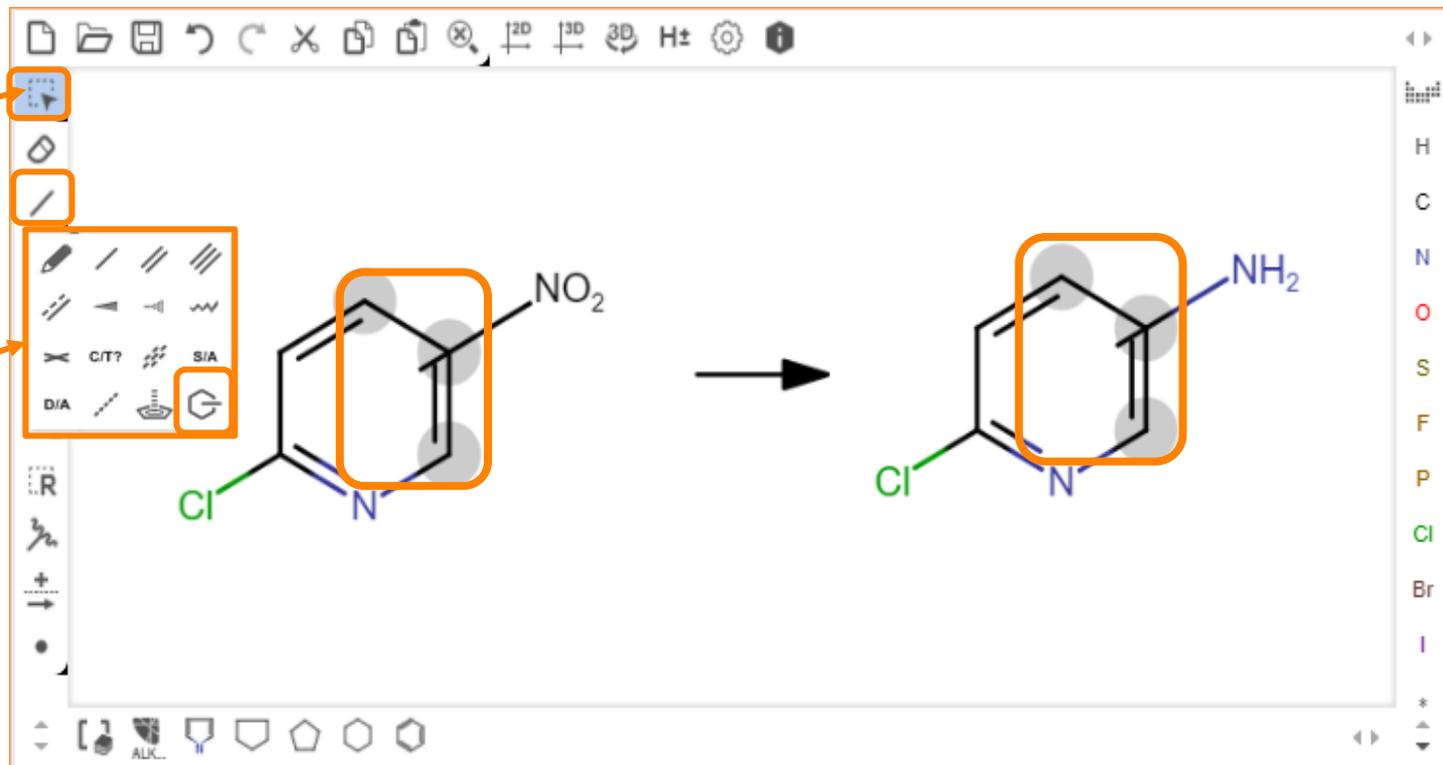
在Quick Search界面启动Marvin JS结构编辑器，进行结构编辑

结构的定义

结构绘制步骤:

1: 用套索选择工具选择吡啶上的3个C原子

2: 用链工具中的不定位取代键将吡啶和NO₂, NH₂相接



检索功能的选择和检索

The screenshot displays a chemical structure editor window. The main workspace shows a chemical reaction: 2-chloro-5-nitropyridine (left) reacts to form 2-chloro-5-aminopyridine (right). The interface includes a toolbar on the left with various drawing tools, a top menu bar with 'Structure editor' and 'Create structure template from name', and a right-hand panel titled 'Search this structure as:'. This panel contains several search options, with 'As drawn' selected and highlighted by an orange box. Below the main workspace, there are buttons for 'Clear', 'Cancel', and 'Transfer to query', with the latter also highlighted by an orange box.

检索Tips:

- 1: As Drawn, 和所画结构完全一致的反应
- 2: Substructure, 亚结构反应检索, 会展开所有H, 可以设定所有原子开放还是杂原子开放

最终的结果

Reaxys

Quick search Query builder Results Synthesis planner History

Sam Yu

7 Filters and Analysis

By Structure

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Reactant Availability

Reaction Classes

Document Type

< Back to Results Preview

7 Reactions out of 37 Documents containing 11 Substances

0 selected: Limit To Exclude Export

Reaxys Ranking

1

Clc1cc([N+](=O)[O-])cnc1>>Clc1cc(N)ncn1

Show All Details Find Similar Reactions

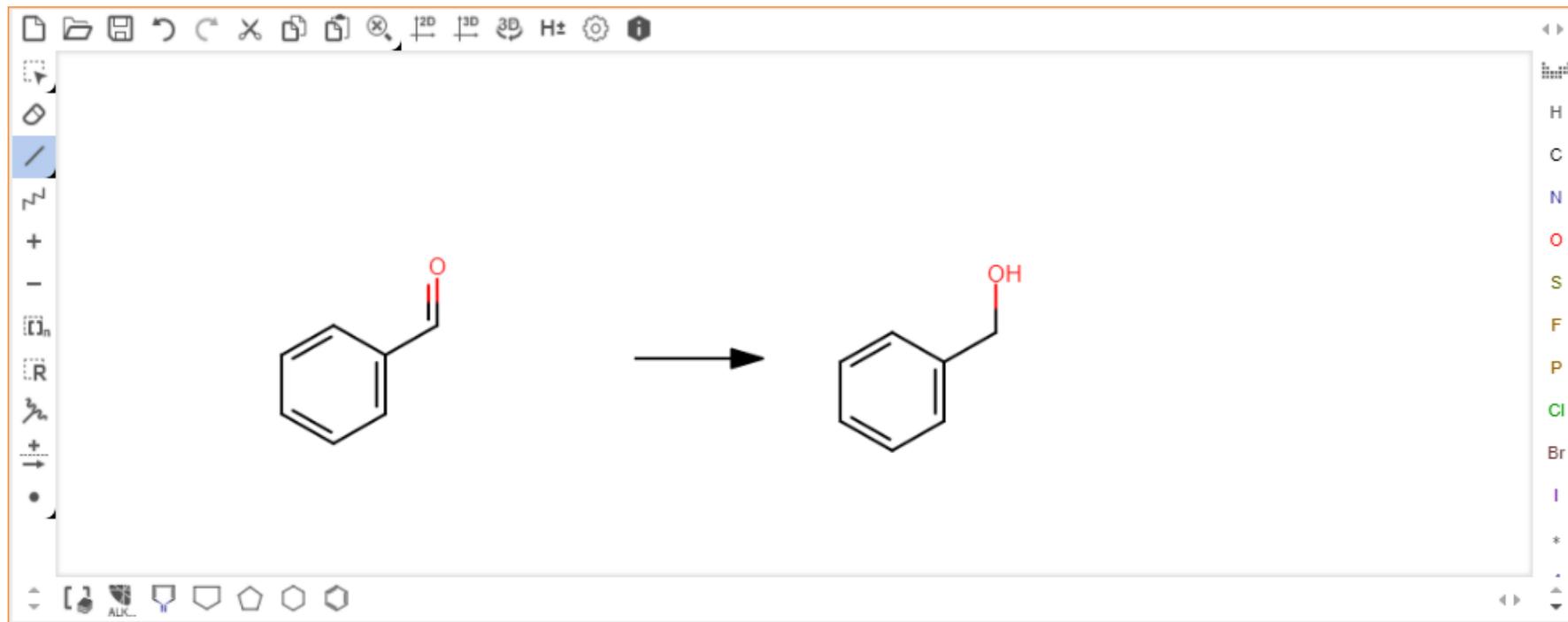
Yield Conditions

Tips:

检索到结果后，可以通过旁边的工具进行筛选

Case Study 5 特定位点反应条件检索及其条件筛选

- 参与反应的分子结构太复杂
- 参与反应的分子结构太新颖
- 需要选择性反应条件，如，选择性还原，氧化，脱保护基等



干扰反应产生

The image shows a chemical structure editor interface. The main workspace displays a chemical reaction: benzaldehyde (a benzene ring with a formyl group, O=Cc1ccccc1) on the left, followed by a right-pointing arrow, and benzyl alcohol (a benzene ring with a hydroxymethyl group, OCCc1ccccc1) on the right. The oxygen and hydroxyl groups are highlighted in red. The interface includes a top toolbar with various editing tools, a search bar at the top right, and a sidebar on the right with search options. The sidebar options are: 'As drawn', 'As substructure' (selected and highlighted with an orange box), 'On all atoms', and 'On heteroatoms'. Below these are checkboxes for 'Similar', 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom of the sidebar is a '+ More options' link. At the bottom of the editor window are buttons for 'Clear', 'Cancel', and 'Transfer to query'.

Substructure, 亚结构反应检索, 会随机开放‘隐藏H’的取代, 可以设定所有原子开放还是杂原子开放

检索结果

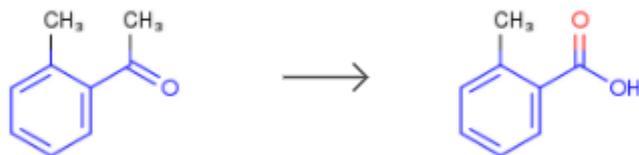
2,525,540 Reactions

Reaction Query :  substructure; included: only absolute stereo, salts, mixtures, isotopes, charges, radicals

Preview Results ▾

[View Results >](#) Reaction ID: 4919673

1

 1 Reaction ID: 167693

2

  1 Reaction ID: 297405

3

  1  1

11 Conditions ^ Find Similar >

反应条件限定

- 检索包含以下结构的反应，并对条件进行筛选

The screenshot shows a chemical structure editor with a reaction scheme: benzaldehyde (left) → benzyl alcohol (right). The carbonyl oxygen in benzaldehyde and the hydroxyl oxygen in benzyl alcohol are both labeled with a blue '(S*)' and a '[i]' in a box. An orange arrow points from the '(S*)' label in benzaldehyde to the '(S*)' label in benzyl alcohol. The search panel on the right has 'As substructure' selected, with 'On all atoms' also selected. The 'Additional ring closures' checkbox is unchecked. The atom query properties dialog at the bottom shows a grid of query options, with '.s*' circled in orange. A small 'query prop.' dialog is also visible over the grid.

亚结构开放
'H'取代

关闭'允许环取代'
减少稠环化合物

'原子映射' 标定反应前后 '相同原子位置'

'S*' 用于锁定 'H'，使其不发生取代

Reaxys中的结果

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

16,067 Filters and Analysis

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

16,067 Reactions out of 7,886 Documents containing 19,034 Substances, 2,499 Targets

0 Limit To Exclude Export Reaxys Ranking

Reaction ID: 305004
1

35 Conditions Find Similar >

Reaction ID: 627405
2

1

同一条反应的不同条件，点开进行对比

通过碎片结构筛选

By Structure ^

 Create Structure Drawing

Yield v

Reagent/Catalyst v

Solvent v

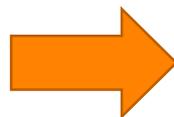
Catalyst Classes v

Solvent Classes v

Product Availability v

Reactant Availability v

Reaction Classes v

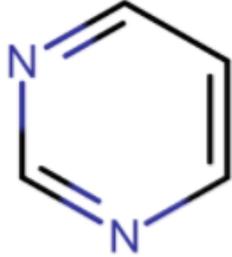


Filters and Analysis

Limit to > Exclude >

By Structure ^

pyrimidine x



On all atoms

Yield v

Reagent/Catalyst v

Solvent v

Catalyst Classes v

Tip:

通过结构
筛选时：
1. 画好结
构
2. 检索逻
辑选择
'亚结构'

筛选结果

114

16,230

114 Reactions

out of 57 Documents containing 185 Substances, 43 Targets

Limit To Exclude Export

0

Reaction ID: 24813606

1

→

2 Conditions Find Similar

Yield	Conditions	
100%	With sodium tetrahydroborate In methanol; dichloromethane at 20°C; for 0.166667h;	AVENTIS PHARMACEUTICALS INC. - WO2006/44732, 2006, A2 Location in patent: Page/Page column 94 Full Text Details Abstract
100%	With sodium tetrahydroborate In methanol; dichloromethane at 20°C; for 0.166667h;	SANOPI-AVENTIS U.S. LLC - WO2008/39882, 2008, A1 Location in patent: Page/Page column 93

更多的筛选条件

16,067

Filters and Analysis

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

Yield

<input type="checkbox"/> >95 - 100		996
<input type="checkbox"/> >90 - 95		861
<input type="checkbox"/> >85 - 90		616
<input type="checkbox"/> >80 - 85		444
<input type="checkbox"/> >75 - 80		390
<input type="checkbox"/> >70 - 75		277
<input type="checkbox"/> >65 - 70		228

Solvent

<input type="checkbox"/> methanol		4,183
<input type="checkbox"/> tetrahydrofuran		3,554
<input type="checkbox"/> ethanol		2,200
<input type="checkbox"/> water		1,418
<input type="checkbox"/> dichloromethane		1,281
<input type="checkbox"/> n,n-dimethylformamide		961
<input type="checkbox"/> toluene		512
+ More		

Reaxys提供多种反应条件
过滤工具

Reagent/Catalyst

<input type="checkbox"/> sodium tetrahydroborate		7,140
<input type="checkbox"/> potassium carbonate		1,072
<input type="checkbox"/> methanol		997
<input type="checkbox"/> lithium aluminium tetrahydride		861
<input type="checkbox"/> water		758
<input type="checkbox"/> sodium hydroxide		645
<input type="checkbox"/> hydrogen		616
+ More		

类别条件筛选—溶剂类别， 催化剂类别

16,067

Filters and Analysis

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

Single step reactions only

Solvent Classes

<input type="checkbox"/>	Low boiling (<100°C)	13,776
<input type="checkbox"/>	Green	9,921
<input type="checkbox"/>	Protic	9,620
<input type="checkbox"/>	Aprotic apolar	7,865
<input type="checkbox"/>	Aprotic dipolar	7,746
<input type="checkbox"/>	Yellow	7,594
<input type="checkbox"/>	Red	7,513
<input type="checkbox"/>	High boiling (>150°C)	3,250
<input type="checkbox"/>	Middle boiling(100°C - 150°C)	2,379
<input type="checkbox"/>	Inorganic	93

可以通过一些溶剂的类型进行筛选，高沸，中沸，低沸的溶剂，质子溶剂等等

Reaxys中独有的催化剂类别筛选工具

- 催化剂分类工具

Catalyst Classes ✕

✓ Catalyst Classes	活性中心		10,545
> active center	非均相催化		9,335
> heterogeneous			322
> organism / enzymes	生物催化		62

Clear selected ✕

✓ organism / enzymes			62
<input type="checkbox"/> glucose dehydrogenase	葡萄糖脱氢酶		27
<input type="checkbox"/> D-glucose dehydrogenase			15
<input type="checkbox"/> alkaline phosphatase	碱性磷酸酶		10
<input type="checkbox"/> fermenting yeast			9
<input type="checkbox"/> pig testicular 20 β -hydroxysteroid dehydrogenase			8
<input type="checkbox"/> ketoreductase			8
<input type="checkbox"/> Candida antarctica lipase B			4
<input type="checkbox"/> horse liver alcohol dehydrogenase			4
<input type="checkbox"/> Bacillus subtilis glucose dehydrogenase			2
<input type="checkbox"/> equine liver alcohol dehydrogenase			2

活性中心分类

Catalyst Classes

不同的活性中心

硼氢化钠

硼氢化氰钠

Catalyst Class	Count
Catalyst Classes	10,545
active center	9,335
B	7,742
Al	1,204
Pd	803
Cu	277
Fe	262
Zn	167
Si	154
Ni	146
Pt	109
Ru	102

Clear selected X

it To > Exclude >

sodium tris(acetoxy)borohydride

borane-THF

boron tribromide

sodium borodeuteride

sodium tetrahydroborate

sodium borohydride powder

sodium cyanoborohydride

选择性条件检索

Structure editor

Create structure template from name >

Boc

Boc

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

Clear Cancel Transfer to query >

+ More options

Tip:

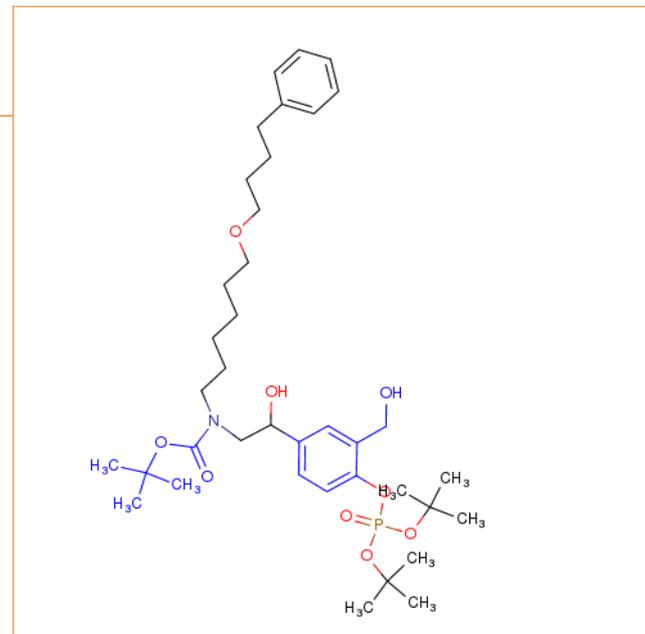
Rx 支持多种碎片画入检索，并可以把‘碎片’融合到一个分子当中。

- Ignore Atom Mappings
- Keep fragments
 - Separate
 - Together

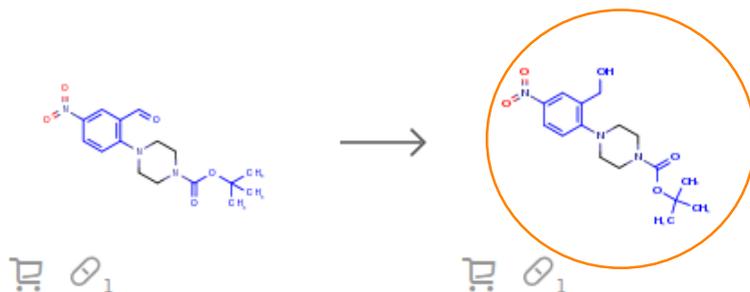
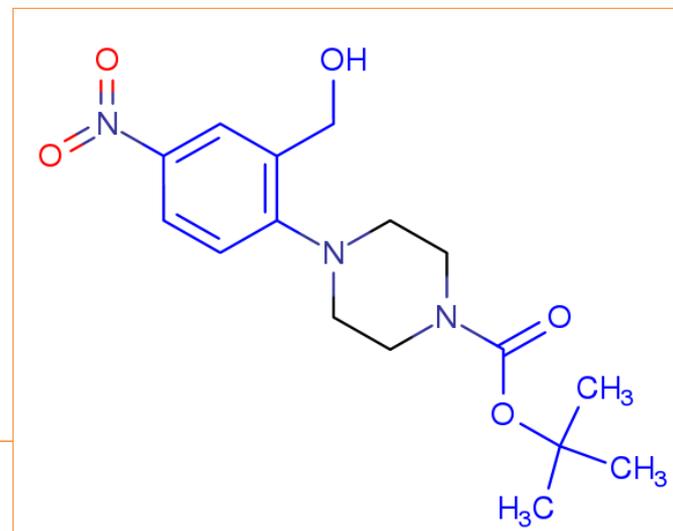
检索结果

 Reaction ID: 25611987

1

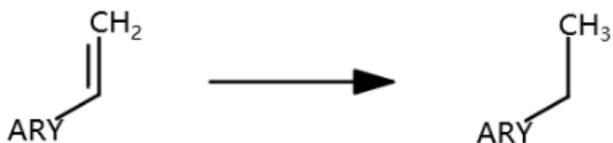
4 Conditions ▼ Find Similar > Reaction ID: 31341750

2

3 Conditions ▲ Find Similar >

Case Study 6 反应组合检索, 关键词联合反应检索

- 检索涉及以下反应机理的文献



通过Query Builder创建组合检索式

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

Search Documents > ▾

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Find search fields and forms 🔍

Fields Forms History

Reaxys ^

Basic Indexes ▾

Identification ▾

Physical Properties ▾

Spectra ▾

MedChem ▾

反应结构的添加

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

Structure editor Create structure template from name >

Structure editor

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

Tips:
S*的定义
原子的匹配

Clear Cancel Transfer to query >

添加关键词后的检索式

The screenshot displays the Reaxys Query builder interface. At the top, there are navigation tabs: "Quick search", "Query builder" (which is selected), "Results", "Synthesis planner", and "History". Below these are utility buttons: "Import", "Save", "Reset form", and "Delete all". On the right side of the top bar, there is a "Search Documents" button with a dropdown arrow. Below the utility buttons are search filters: "Structure", "Molecular Formula", "CAS RN", and "Doc. Index".

The main workspace contains two query components:

- Structure:** A panel titled "Structure" containing a chemical reaction scheme. The reactant is an alkene with an "ARY" group and a "CH₂" group. The product is an alkane with an "ARY" group and a "CH₃" group. An arrow points from the reactant to the product. Below the reaction is a text box containing "On all atoms".
- Document Basic Index:** A panel titled "Document Basic Index" containing the text "is" followed by a dropdown arrow and "Document Basic Index mechanism*".

An orange arrow points from the text "添加机理单词" (Add mechanism words) to the "Document Basic Index" panel.

检索文献

添加机理单词

最后的结果

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

74 Filters and Analysis

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

74 Documents with 2,267 Substances, 2,185 Reactions, 5 Targets

0 Limit To Exclude Export Relevance ↓ Heatmap

1 Metal-free $\text{HB}(\text{C}_6\text{F}_5)_2$ -catalyzed hydrogenation of unfunctionalized olefins and mechanism study of borane-mediated σ -bond metathesis
Wang, Yuwen; Chen, Weiqiang; Lu, Zhenpin; Li, Zhen Hua; Wang, Huadong - Angewandte Chemie - International Edition, 2013, vol. 52, # 29, p. 7496 - 7499, Angew. Chem., 2013, vol. 125, # 29, p. 7644 - 7647,4
Abstract ▾ Index Terms ▾ Substances 26 ▾ Reactions 13 ▾ Full Text ↗
Hit Reactions 1 ▾

2 Supported palladium nanomaterials as catalysts for petroleum chemistry: 2. Kinetics and specific features of the mechanism of selective hydrogenation of olefins by supported palladium nanocatalyst
Berenblyum; Al-Wadhaf; Katsman - Petroleum Chemistry Letters, 2013, vol. 1, # 1, p. 133-139
Abstract ▾ Index Terms ▾ Substances 4 ▾
Hit Reactions 1 ▾

3 α -CAM mechanisms for the hydrogenation of α -olefins by transition metal complexes (M = Fe, Ru, Os): Experimental and theoretical studies
Hoshi, Konoka; Tahara, Atsushi; Sunada, Yusuke; Tsutsui, Masahito; Yoshizawa, Kazunari; Nagashima, Hideo - Bulletin of Chemical Society of Japan, 2013, vol. 86, # 12, p. 1711-1716
Abstract ▾ Index Terms ▾ Substances 4 ▾
Hit Reactions 1 ▾

Hit Reactions

Reaction ID: 39024

Find Similar >

检索到的文献.....

文献中更多的内容—利用反应中心对文献进行筛选

Reaction Classes可以利用反应中心的类型进行筛选

Reaxys抽提出文献中所有的反应类型，帮助做进一步的筛选

Reaction Class	Count
reduction	65
substitution	16
addition	12
oxidation	9
rearrangement	9
condensation	9
C-C bond formation	7
hydrolysis	6
reductive ...	4
addition/elimination	3
cyclization	2
ring opening	1
dehydration	1
oxidation/substitution	1
oxidative...	1
addition/substitution	1
ring closure	1

更加细节性内容

Reaction Classes ×

▼	📁	Reaction Classes		74
▼	📁	reduction		65
>	📁	C=C double bond	C=C还原	63
>	📁	acetylenes to alkenes		9
>	📁	acetylenes	酮到醇	8
>	📁	ketones to alcohols	醛到醇	8
>	📁	nitro to primary amine		8
>	📁	aldehydes to alcohols		5
>	📁	aldimines		4
>	📁	Ar-CO-C to Ar-CH2-C		3
>	📁	alpha,beta-unsaturated ketones to alcohols		2
>	📁	1,2-diones to 1,2-diols		1

Clear selected ×

▼

📁

C=C double bond

63

- RCH=CH2 to RCH2-CH3 62
- >C=CH2 to >CH-CH3 12
- >C=CH- to >CH-CH2- 8
- RCH=CH- to RCH2-CH2- 8
- >C=C< to >CH-CH< 2

Reduction下的反应类型

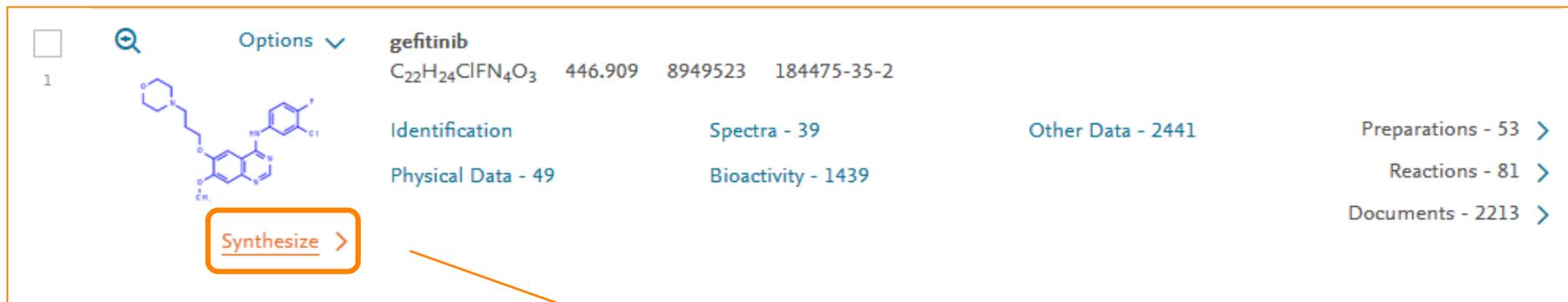
涉及到C=C双键还原的不同反应类型

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Case Study 7 如何利用Reaxys制作合成计划

- 给吉非替尼制定合成计划
 - Step1: 检索到吉非替尼
 - Step2: 导入合成计划



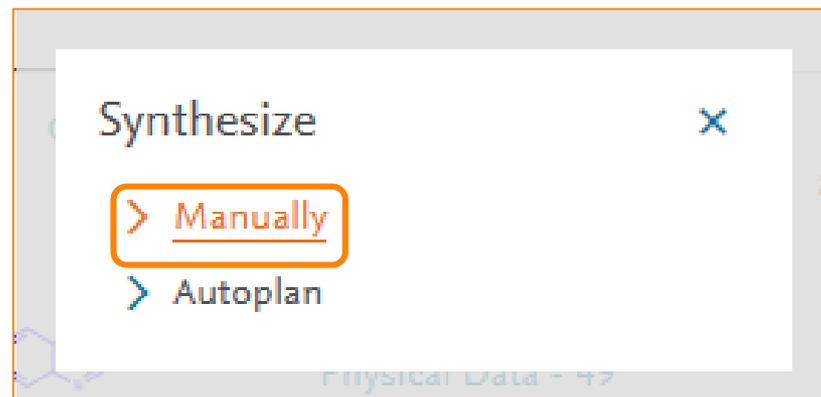
Options ▾ **gefitinib**
C₂₂H₂₄ClFN₄O₃ 446.909 8949523 184475-35-2

Identification Spectra - 39 Other Data - 2441 Preparations - 53 >
Physical Data - 49 Bioactivity - 1439 Reactions - 81 >
Documents - 2213 >

Synthesize >

Tips:

- 1: 通过前述的操作找到物质
- 2: 鼠标悬停在结构上，看到Synthesize
- 3: 点击，打开Synthesis Plan，这里选择手动



Synthesize X

> **Manually**

> Autoplan

Synthesis Plan—添加感兴趣的反应

- 可以添加多条反应在一个Plan中，用于比较

Add preparation - 52 ×

Preparation

1

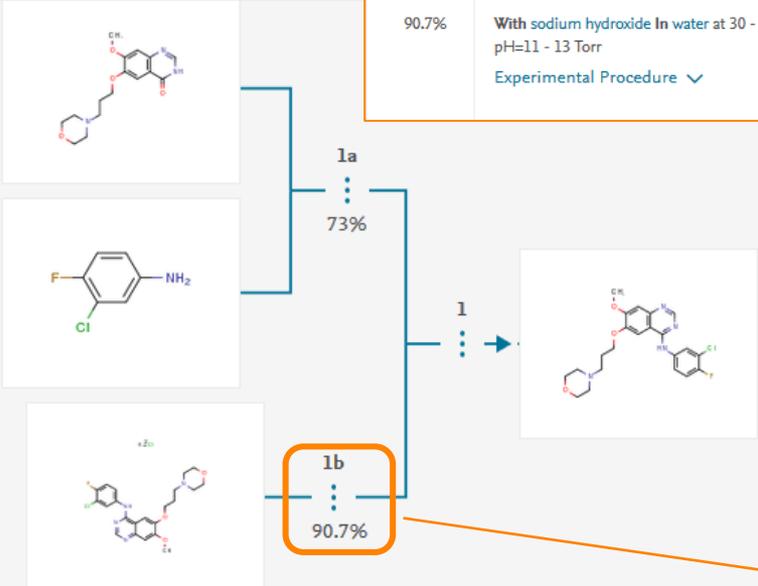
2

[+ Load more](#) [Cancel X](#) [Add 2 to plan >](#)

添加好的结果界面

Synthesis plan 3

Import  Save  Export 



Conditions

Preparation - 1b

Yield	Conditions	Reference
90.7%	With sodium hydroxide in water at 30 - 70°C for 1.5h ; pH=11 - 13 Torr Experimental Procedure 	Jeil Pharm Co., Ltd.; Jung, Uli Sung; Choe, Gyu Hyun; +1 other - KR2015/1936, 2015, A Location in patent: Paragraph 0096; 0097; 0106; 0107 Full Text  Show details 

1b
90.7%

Show conditions 

Hide preparation 

Remove preparation 

Tips:

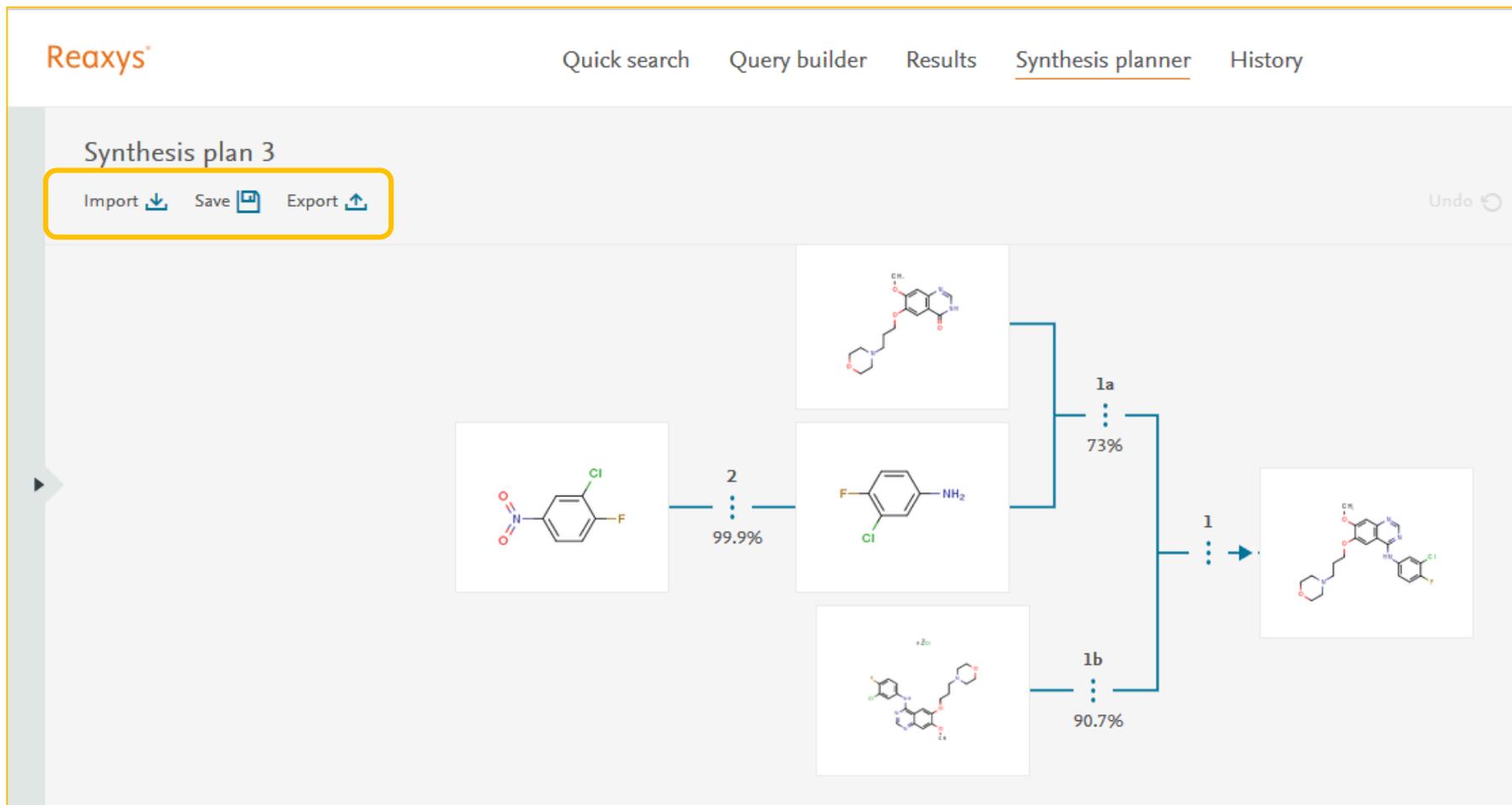
- 1: 通过添加多条反应，可以用来评估反应信息
- 2: 点击虚线的地方，可以查看条件，或者隐藏，移除反应

继续的扩充反应路线

The image displays a software interface for a synthesis plan. The main window, titled "Synthesis plan 3", shows a reaction network. A "Synthesize" dialog box is open, with the "Manually" option selected. An "Add preparation - 4" window is also open, showing two chemical reactions. The reaction network diagram shows a starting material (a benzimidazole derivative) reacting with two different reagents, labeled "1a" (73% yield) and "1b" (90.7% yield), to produce a final product. A "Synthesize" button is highlighted in the diagram, and an arrow points from the "Manually" option in the dialog box to this button. The "Add preparation - 4" window shows two reactions: 1) A reaction with a 99.9% yield, and 2) A reaction with a 90.7% yield. The "Add 1 to plan" button is highlighted in the bottom right of this window.

Tips:
在Synthesis Plan上可以对任意一个物质进行同样的Synthesis的操作，可以将更多的反应添加进来

最后的结果



可以对Synthesis Plan进行导入，导出或者保存等操作。

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
 - Reaxys的基本检索模式
 - 如何利用Reaxys结构面板实现复杂结构定义
 - 如何利用Reaxys进行物质检索和物质分析
 - 如何利用Reaxys进行反应检索和条件筛选
 - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Reaxys中的检索小结

- Reaxys中的物质检索方法
 - Quick Search 物质名称
 - Quick Search 结构检索
 - Query Builder 组合检索
 - Quick Search 理化性质+物质名称/结构
- Reaxys中反应检索方法
 - Quick Search 关键词
 - Quick Search 结构式检索
 - Query Builder 组合检索

Reaxys检索小结

- **New 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
- **New Reaxys**中的**Query Builder**检索帮助科研人员通过简便的方式，获得精准，跨学科的精确定案
- **New 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