

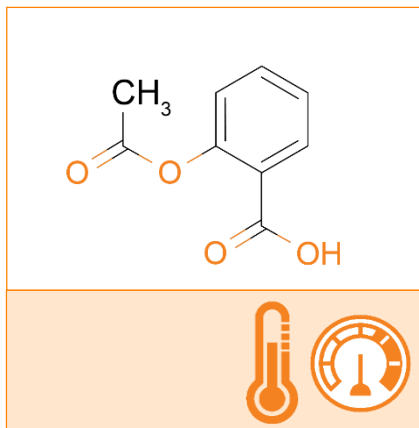
New Reaxys 使用介绍

Reaxys 解决方案咨询师
俞靓

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

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 (Zhennan Mao, Changqun Sheng, Wanzhi Zhang, Haitao Ji, Jing Zhang, Luecheng Shao, Liang You, Min Zhang, Heshou Yao, and Xiaolin Che), 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.

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, Zhenyan; Sheng, Chunqun; Zhang, Wannian; Ji, Haitao; Zhang, Jing; Shao, Luecheng; You, Liang; Zhang, Min; Yao, Jianzhong; Che, Xiaolin - *Biorganic and Medicinal Chemistry*, 2008, vol. 16, # 3, p. 1493 - 1510

[Abstract](#) [Index Terms](#) [Substances](#) 124 [Reactions](#) 78 [Full Text](#) 71

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 **tumor cell line** camptothecins, Molecular docking

Reaxys Index Terms: hydrophobic surface

Reaxys索引的内容—文献中的数据

The collage displays various scientific articles with highlighted sections:

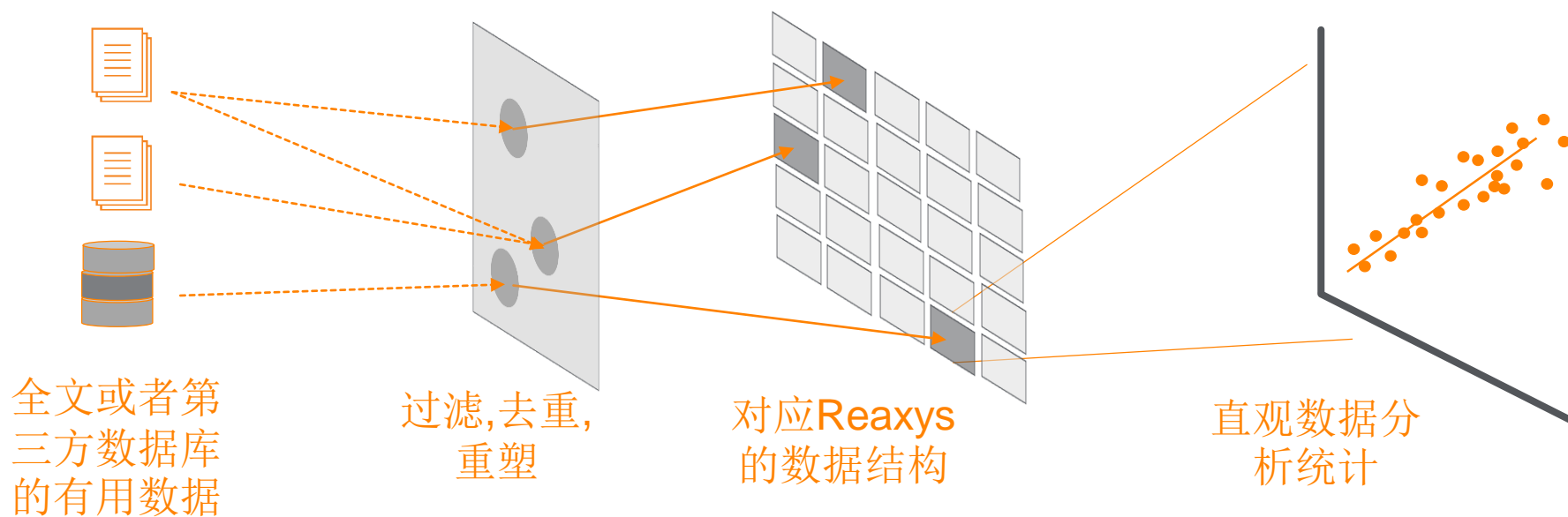
- ScienceDirect Article 1:** "New homocyclic synthesis, antimicrobial activity, and molecular modeling" by Zhenhua Mao, Chuanxin Song, Waimin Zhang, Haike Ji, Jing Zhang, Kailiang Shao, Lina Yao, Xin Zhang, Fenghua Yao, and Xiaoyan Cao. It features chemical structures and a table of antimicrobial activity.
- ScienceDirect Article 2:** "Synthesis of novel...". It shows a chemical reaction scheme and a table of results.
- ScienceDirect Article 3:** "Synthesis of novel...". It includes a chemical structure and a table of data.
- ScienceDirect Article 4:** "Synthesis of novel...". It features a chemical structure and a table of results.
- ScienceDirect Article 5:** "Synthesis of novel...". It shows a chemical reaction scheme and a table of results.
- ScienceDirect Article 6:** "Synthesis of novel...". It includes a chemical structure and a table of data.
- ScienceDirect Article 7:** "Synthesis of novel...". It features a chemical structure and a table of results.
- ScienceDirect Article 8:** "Synthesis of novel...". It shows a chemical reaction scheme and a table of results.
- ScienceDirect Article 9:** "Synthesis of novel...". It includes a chemical structure and a table of data.
- ScienceDirect Article 10:** "Synthesis of novel...". It features a chemical structure and a table of results.

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 screenshot shows the Reaxys search results for 'camptothecin' (C₂₀H₁₆N₂O₄). The interface includes:

- Filters and Analysis:** A sidebar with dropdown menus for By Structure (1), Measurement pX, Highest Clinical Phases, Targets, Parameters, Substance Classes, Molecular Weight, Availability, Availability in other databases, Available Data, Document Type, and Publication Year.
- Results:** A main area showing the chemical structure of camptothecin and a list of properties:
 - Identification
 - Druglikeness
 - Bioactivity (All)
 - Physical Data - 132
 - Spectra - 139
 - Other Data - 1,527
 - Targets - 142
 - Documents - 3,556
- Document Preview:** A preview of the document for camptothecin, showing a list of properties:
 - Identification
 - Druglikeness
 - Bioactivity (All)
 - Physical Data - 132
 - Spectra - 139
 - Other Data - 1,527

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

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 - 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

New Reaxys的界面

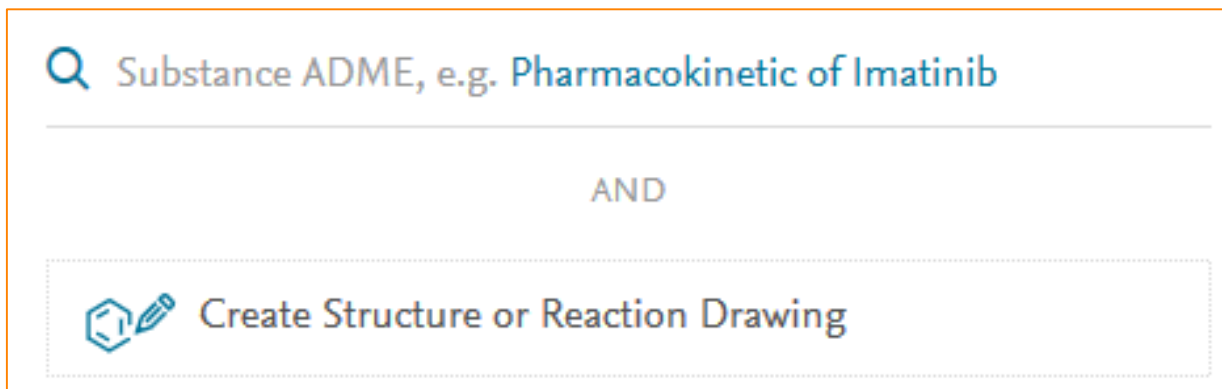
- [Http://new.reaxys.com](http://new.reaxys.com)

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' (highlighted), '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 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'. There is an 'Import' button with a download icon. The main search area contains a search bar with the text 'Reactions, e.g. phosphorylation'. Below the search bar is an 'AND' operator. At the bottom of the search area 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, Immunology Oncology
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 tabs for 'Quick search', 'Query builder' (which is selected), 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there is a 'Sign in' button and a help icon. Below the navigation, a toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all'. Another set of icons includes 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. A search bar with a 'Search' button and a dropdown arrow is positioned above a large, light-blue grid area. The grid area contains the text 'Drag & Drop to build a new query'. On the right side of the interface, there is a sidebar with a search bar labeled 'Find search fields and forms'. Below this, there are three tabs: 'Fields', 'Forms', and 'History'. The 'Fields' tab is selected and highlighted with an orange box. An orange arrow points from the 'Fields' tab to a list of search fields. The list includes 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography', each with a downward-pointing arrow.

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:

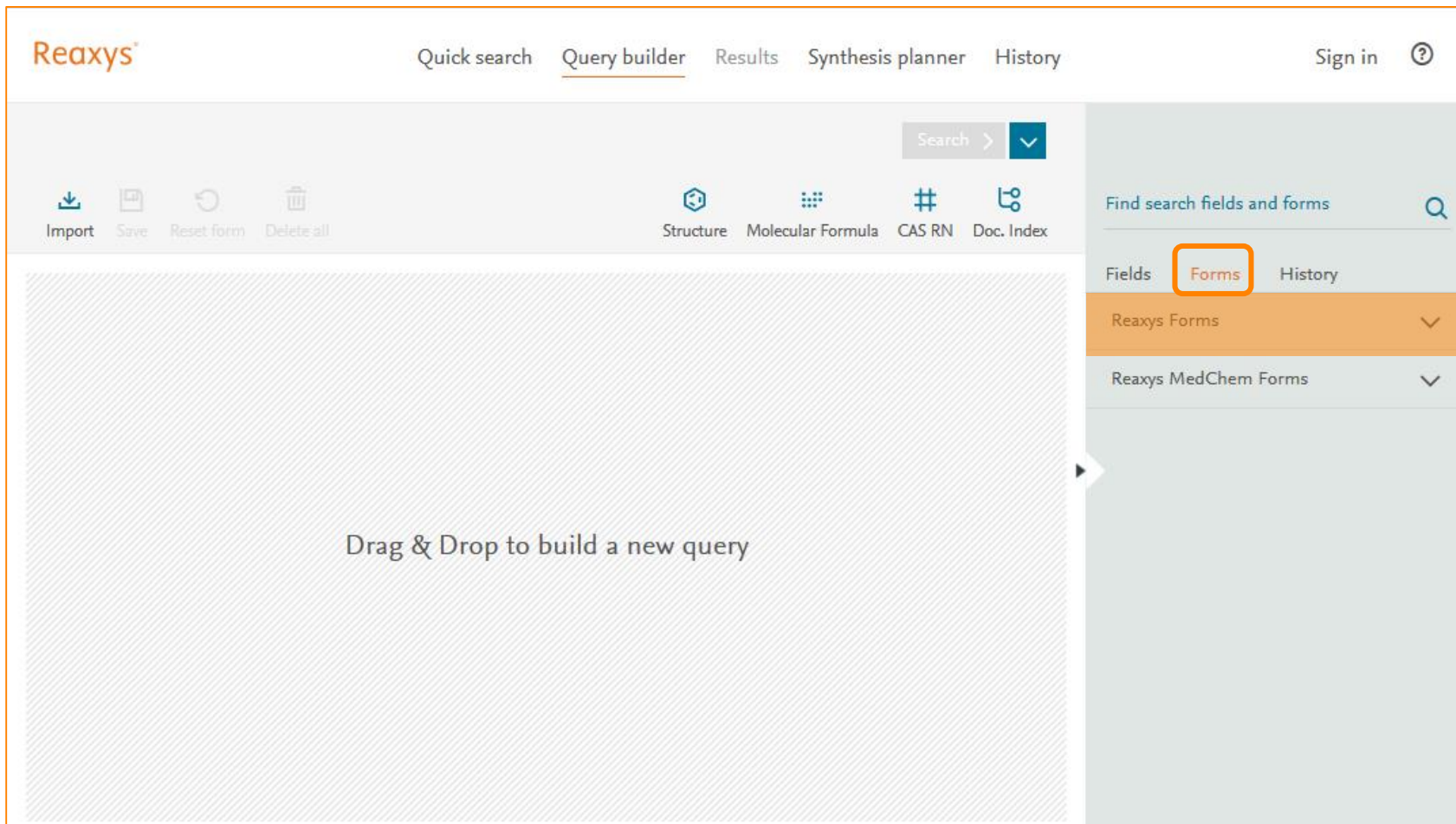
Reaxys提供8种不同的分类，每种分类中拥有和这种分类相关的多种字段，可以依据这些字段自由组合进行检索

<u>Basic Indexes</u>		^
◇	Substance Basic Index	☰ ⋮
◇	Reaction Basic Index	⋮
◇	Document Basic Index	⋮

<u>Identification</u>		^
◇	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	☰ ⋮

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

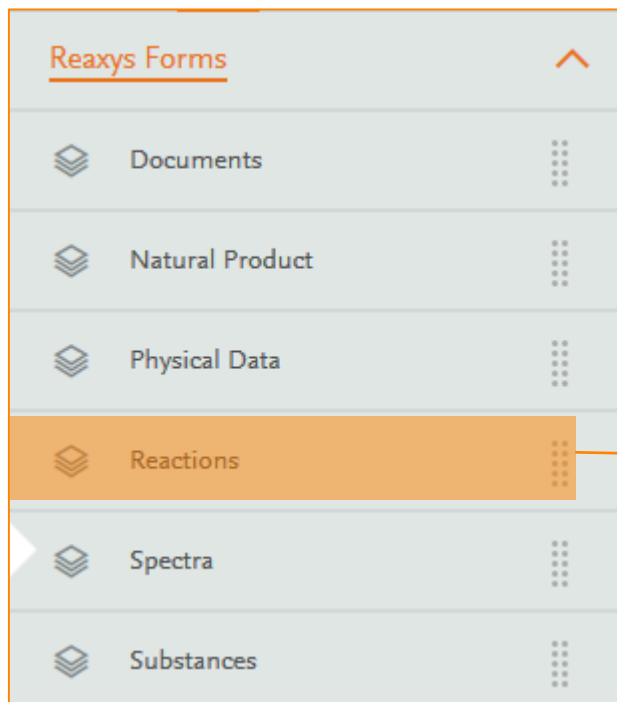
Reaxys检索方式—Query Builder Forms



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

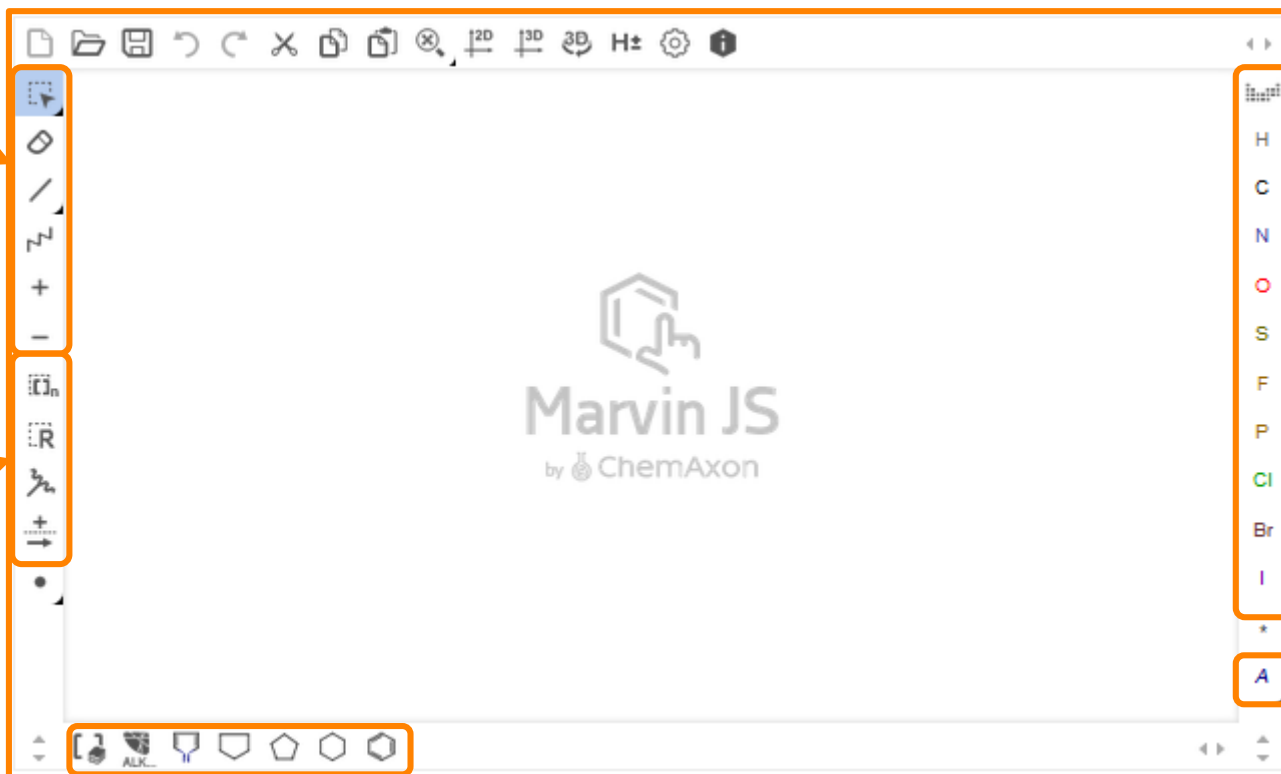
提纲

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 - 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



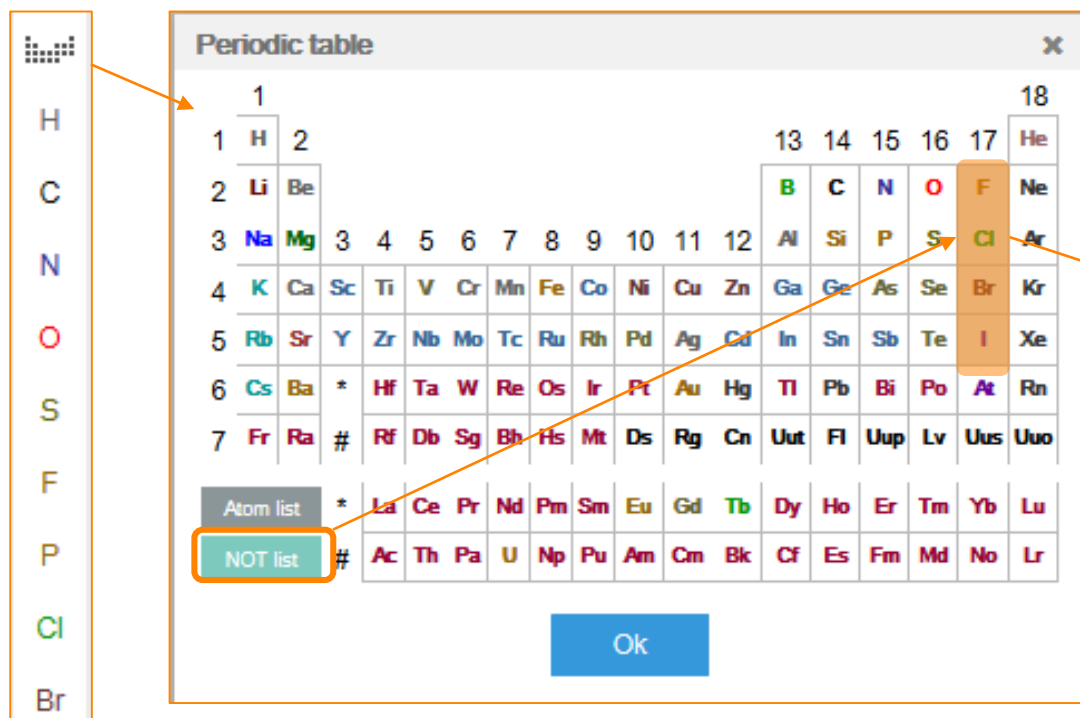
元素周期
表以及常
用原子

A:
原子属性
定义工具

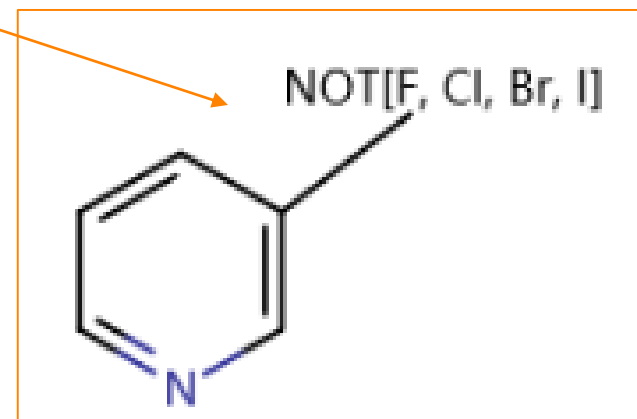
常见的环，官能团，Reaxys的
Generic Group定义

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

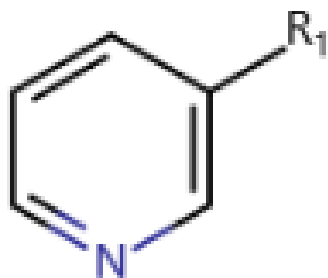


The screenshot shows a software interface for defining a 'NOT list' of atoms. On the left, a vertical list contains the atoms H, C, N, O, S, F, P, Cl, and Br. The main window, titled 'Periodic table', displays a periodic table with a column of atoms (F, Cl, Br, I) highlighted in orange. A 'NOT list' box is highlighted in green, and an arrow points from it to the highlighted column in the periodic table. An 'Atom list' box is also visible, containing the same vertical list of atoms. An 'Ok' button is at the bottom.

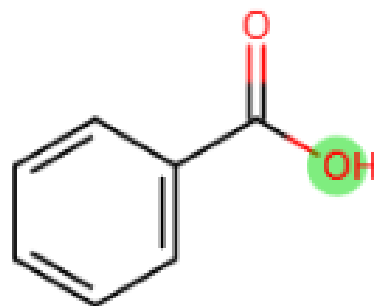


自定义R基团

- 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

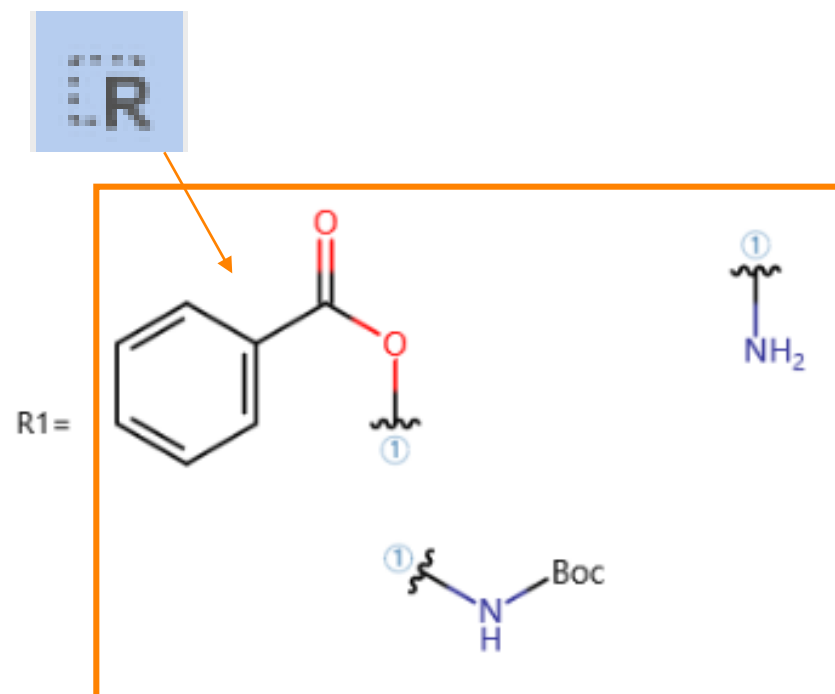
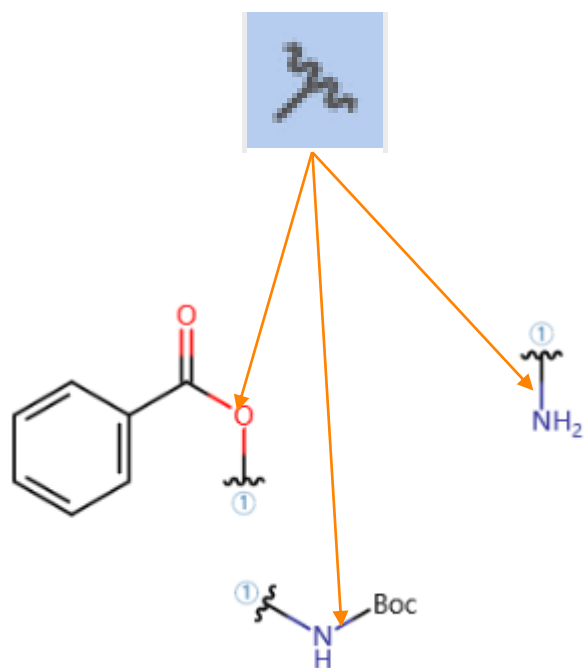


A



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

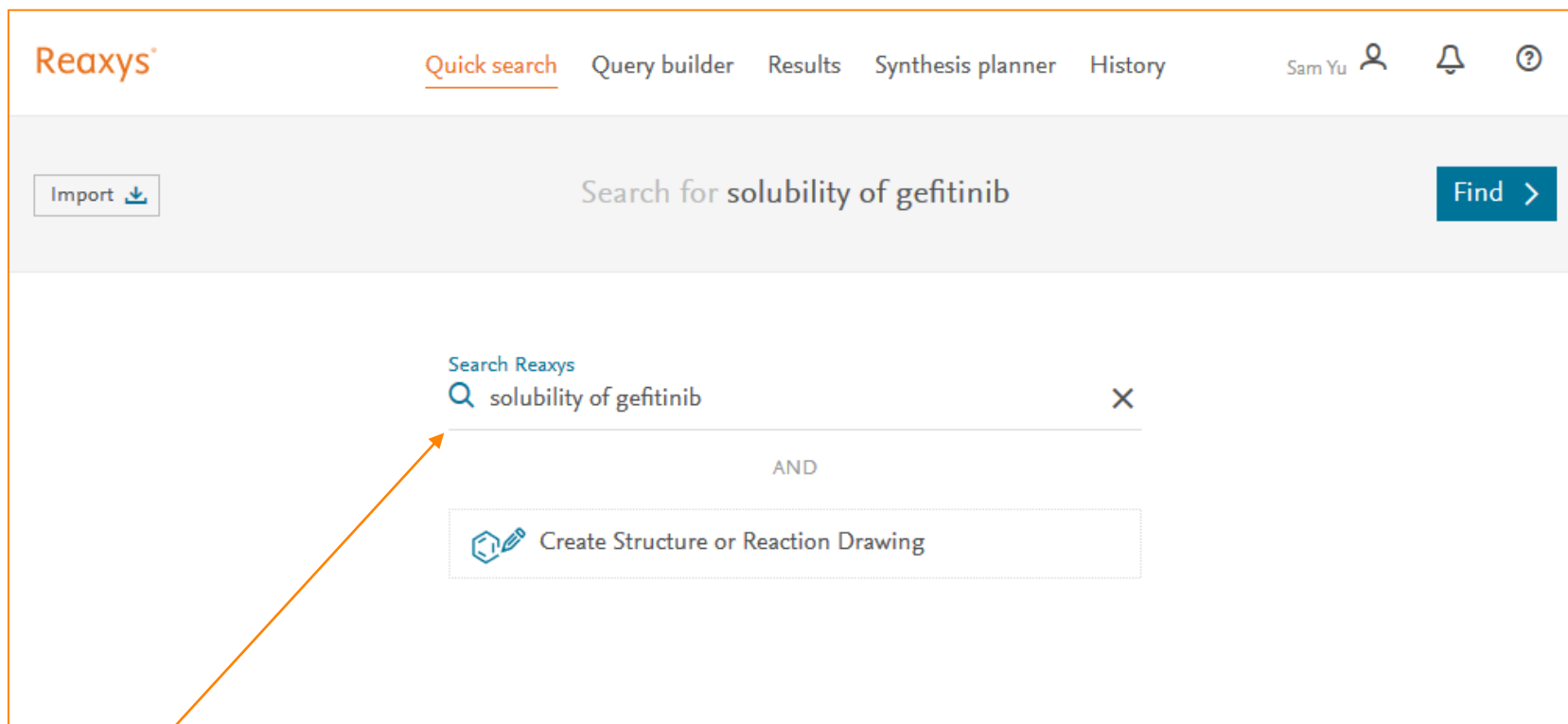


提纲

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Case Study 1—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 is a user profile for 'Sam Yu', a notification bell, and a help icon. Below the navigation bar, there is an 'Import' button with a download icon. The main search area contains the text 'Search for solubility of gefitinib' and a 'Find >' button. Below this, a search box shows 'Search Reaxys' with a magnifying glass icon and the text 'solubility of gefitinib'. Below the search box, the word 'AND' is displayed. 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

Reaxys直接给出结果

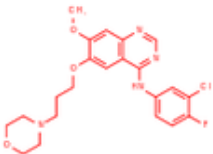
The screenshot shows the Reaxys search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, the user name 'Sam Yu' is displayed along with icons for a profile, notifications,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


Count	Category	Criteria	Preview Results	View Results
1	Substances	Structure :  as drawn AND Property : solubility	Preview Results ▾	View Results >
96	Documents	Titles, Abstract, Keywords : solubility, gefitinib	Preview Results ▾	View Results >
277,479	Documents	Titles, Abstract, Keywords : solubility	Preview Results ▾	View Results >

The 'View Results >' button for the first result is highlighted with an orange border.

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 2—结构检索物质

The screenshot shows the Reaxys interface with the 'Structure editor' active. A dialog box titled 'Create structure template from name' is open, prompting the user to 'Enter a chemical name, CAS-RN, InChiKey or SMILES'. The input field contains 'Gefitinib' and a search icon is visible. The background shows the 'Marvin JS by ChemAxon' logo and various editing tools.

This screenshot shows the chemical structure of Gefitinib rendered in the Reaxys interface. The structure is a complex molecule featuring a quinazolinone core with a piperidine ring, a methoxy group, and a 4-chloro-3-fluorophenyl group. On the right side, a search options panel is visible, titled 'Search this structure as:'. It includes radio buttons for 'As drawn' (selected), 'As substructure', and 'Similar'. Below this, there is an 'Include' section with checkboxes for 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. 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'.

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 page. 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 are 'New' and 'Edit' buttons on the left, and 'Results for' followed by a chemical structure icon in the center. The main content area shows 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

Limit To Exclude Export No of References Heatmap

1

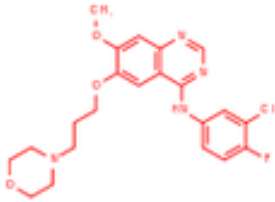
gefitinib
C₂₂H₂₄ClFN₄O₃ 446.909 8949523 184475-35-2

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 >

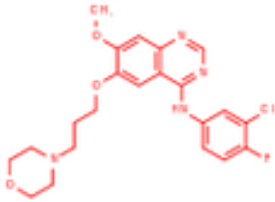
^ Physical Data - 52

- ∨ 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
C₂₂H₂₄ClFN₄O₃ 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

<p><u>1H NMR (400 MHz, d6-DMSO)</u> 0 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).</p>	Paragraph 0035	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1</p> <p>Full Text ↗ Show details ></p>
<p><u>13C NMR (100 MHz, d6-DMSO)</u> 0 156.48, 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.</p>	Paragraph 0035	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1</p> <p>Full Text ↗ Show details ></p>

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 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 lines for the rings and red for the 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

<input type="checkbox"/>	Functional Group Classification	<input checked="" type="checkbox"/>	2,471
<input type="checkbox"/>	Richter Classification	<input checked="" type="checkbox"/>	2,471
<input type="checkbox"/>	Ring Classification	<input checked="" type="checkbox"/>	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 links: 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 orange arrow points from the search box to the first result in the table below.

Count	Category	Filters	Actions
70	Reactions	Product(s) : as drawn	Preview Results <input type="button" value="View Results >"/>
896	Documents	Titles, Abstracts, Keywords : synthesis, 3-hydroxy-indole	Preview Results <input type="button" value="View Results >"/>
8,268,579	Documents	Titles, Abstracts, Keywords : synthesis	Preview Results <input type="button" value="View Results >"/>
2,670	Documents	Titles, Abstracts, Keywords : 3-hydroxy-indole	Preview Results <input type="button" value="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

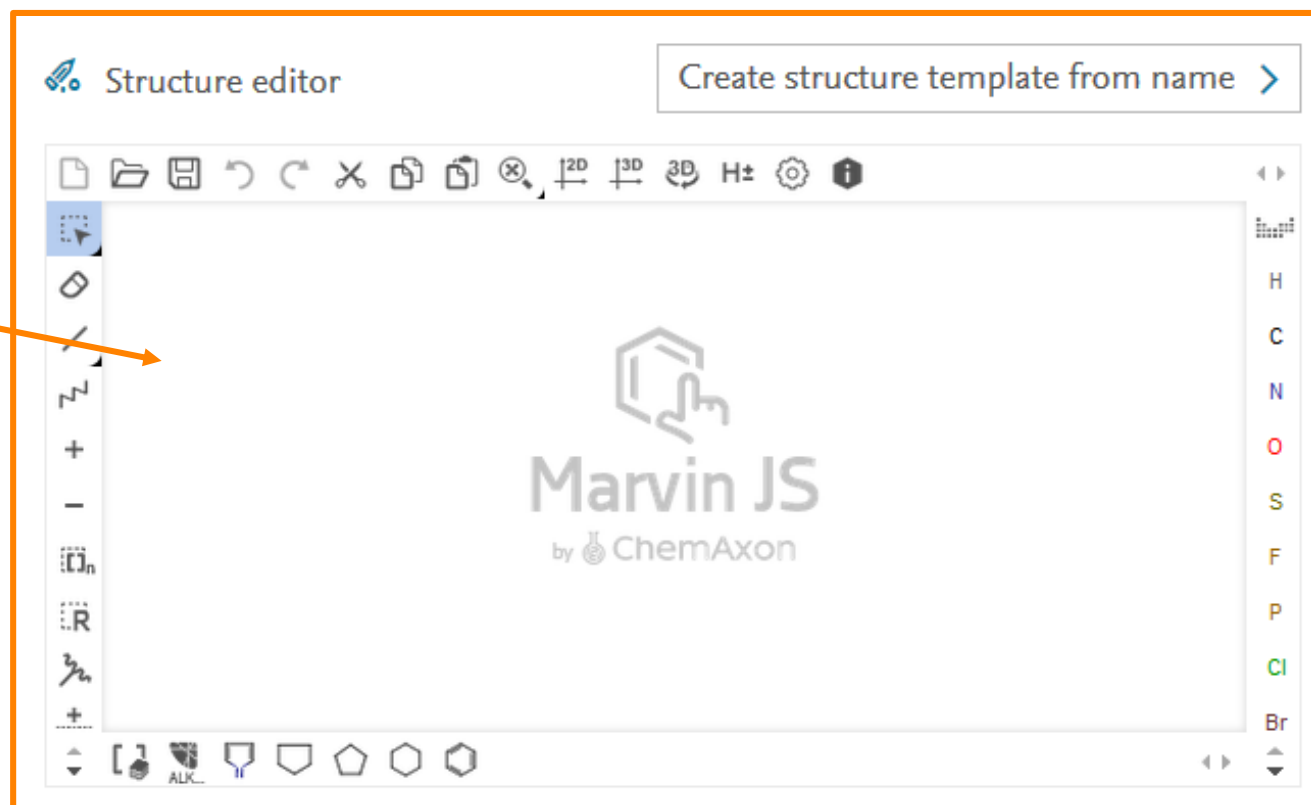
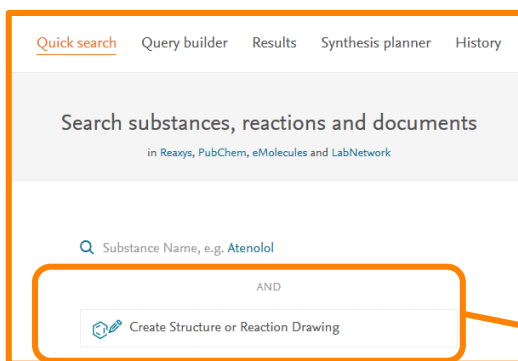
2 Conditions ▾ Find Similar >

Reaction ID: 387961
11

2 Conditions ▾ Find Similar >

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

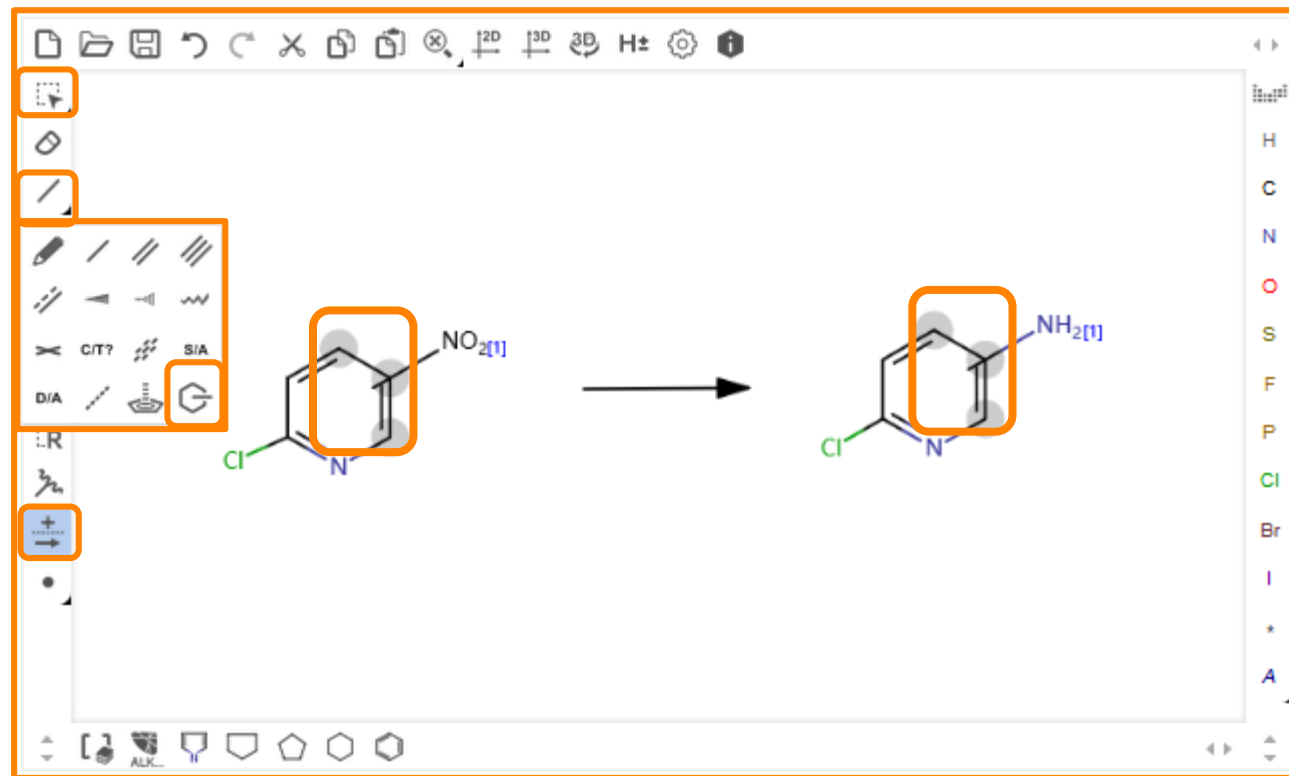
结构的定义

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

3: 用反应定义工具, 指定反应前后NO₂到NH₂的变化



检索功能的选择和检索

The screenshot displays a chemical structure editor window. The main workspace shows a reaction between 2-chloro-5-nitropyridine and 2-chloro-5-aminopyridine. The left structure is 2-chloro-5-nitropyridine, and the right structure is 2-chloro-5-aminopyridine. An arrow points from the left structure to the right structure. The interface includes a toolbar with various editing tools, a search panel on the right, and a bottom bar with buttons for 'Clear', 'Cancel', and 'Transfer to query'.

Structure editor

Create structure template from name >

Search this structure as:

- As drawn
- As substructure
- Similar

Include

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

+ More options

Clear Cancel **Transfer to query** >

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 反应条件筛选

- 检索包含以下核心结构的反应，并对条件进行筛选

The screenshot shows the Reaxys interface with a chemical reaction: benzaldehyde (left) reacting to form benzyl alcohol (right). The structure editor is active, and the search options panel is open. The search options include:

- Search this structure as:
 - As drawn
 - As substructure (selected)
 - On all atoms (selected)
 - On heteroatoms
 - Similar
- Tautomers
- Stereo
- Additional ring closures (selected)
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals
- More options

The Atom query properties panel is also open, showing a grid of query options:

.H+	.h+	.v+	.X+
.H-	.h-	.v-	.X-
.R+	.r+	.rb+	.s+
.R-	.r-	.rb-	.s-
.u	.a/A	.rb*	.s*

Below the grid, there is a search bar containing the query: `A Q M X AH QH MH XH ? query prop.`

亚结构检索，用于检索核心结构

Tips:
Additional Ring Closures用于保护环系，在进行亚结构检索时，不发生稠环

Tips:
S*的定义是在进行亚结构检索时没有取代

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

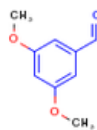
Limit To

Exclude

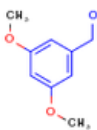
Export

○ ○ ○
Reaxys Ranking ↓

Reaction ID: 305004
1



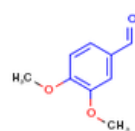
→



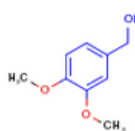
🛒
35 Conditions
🛒

Find Similar
>

Reaction ID: 627405
2



→



🛒
🔗
1

同一条反应的不同条件，点开进行对比

Reaxys中的反应呈现形式

- 同底物，同产物的反应归并到一起，有利于科研工作者的评估

Reaction ID: 305004

1

以及原文中的实验过程

Yield	Conditions	References
100%	With sodium tetrahydroborate In methanol at 20°C; for 0.166667h;	De, Subhadip; Chaudhuri, Saikat; Mishra, Sourabh; Mamtani, Himanshu; Bisai, Alakesh - Journal of the Indian Chemical Society, 2013, vol. 90, # 10, p. 1871 - 1884 Full Text ↗ Details > Abstract >
100%	With sodium tetrahydroborate In methanol at 20°C; for 1h;	Parihar, Swati; Kumar, Amit; Chaturvedi, Amit K; Sachan, Naresh Kumar; Luqman, Suaib; Changkija, Bendangla; Manohar, Murl; (...) Konwar, Rituraj; Negi, Arvind S. - Journal of Steroid Biochemistry and Molecular Biology, 2013, vol. 137, p. 332 - 344 Full Text ↗ Cited 16 times ↗ Details > Abstract >
100%	With sodium tetrahydroborate In ethanol at 20°C; for 0.5h; Inert atmosphere;	Desroches, Justine; Champagne, Pier Alexandre; Benhassine, Yasmine; Paquin, Jean-Francois - Organic and Biomolecular Chemistry, 2015, vol. 13, # 8, p. 2243 - 2246 Full Text ↗ Cited 5 times ↗ Details > Abstract >

Experimental Procedure ▾

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	<input type="checkbox"/>	10,545
> active center	非均相催化	<input type="checkbox"/>	9,335
> heterogeneous		<input type="checkbox"/>	322
> organism / enzymes	生物催化	<input type="checkbox"/>	62

Clear selected ✕

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

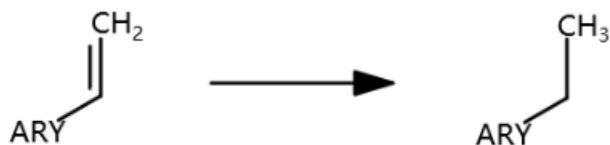
sodium tetrahydroborate

sodium borohydride powder

sodium cyanoborohydride

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 >

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 the navigation, there are utility buttons: "Import", "Save", "Reset form", and "Delete all". To the right, there are search options: "Search Documents" (with a dropdown arrow), "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 indicates the reaction. Below the reaction, there is a text box labeled "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. 133, # 9, 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 study
Hoshi, Konoka; Tahara, Atsushi; Sunada, Yusuke; Tsunoda, Takanori; Yoshizawa, Kazunari; Nagashima, Hideo - Bulletin of Chemical Society of Japan, 2013, vol. 86, # 12, p. 2585-2592
Abstract ▾ Index Terms ▾ Substances (1) ▾
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

74 Filters and Analysis

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

Reaction Classes ^

<input type="checkbox"/>	reduction	<input type="checkbox"/>	65
<input type="checkbox"/>	substitution	<input type="checkbox"/>	16
<input type="checkbox"/>	addition	<input type="checkbox"/>	12
<input type="checkbox"/>	oxidation	<input type="checkbox"/>	9
<input type="checkbox"/>	rearrangement	<input type="checkbox"/>	9
<input type="checkbox"/>	condensation	<input type="checkbox"/>	9
<input type="checkbox"/>	C-C bond formation	<input type="checkbox"/>	7
<input type="checkbox"/>	hydrolysis	<input type="checkbox"/>	6
<input type="checkbox"/>	reductive ...	<input type="checkbox"/>	4
<input type="checkbox"/>	addition/elimination	<input type="checkbox"/>	3
<input type="checkbox"/>	cyclization	<input type="checkbox"/>	2
<input type="checkbox"/>	ring opening	<input type="checkbox"/>	1
<input type="checkbox"/>	dehydration	<input type="checkbox"/>	1
<input type="checkbox"/>	oxidation/substitution	<input type="checkbox"/>	1
<input type="checkbox"/>	oxidative...	<input type="checkbox"/>	1
<input type="checkbox"/>	addition/substitution	<input type="checkbox"/>	1
<input type="checkbox"/>	ring closure	<input type="checkbox"/>	1

+ More

Reaction Classes可以利用反应中心的类型进行筛选

Reaction Classes x

Reaction Classes	<input type="checkbox"/>	74
> reduction	<input type="checkbox"/>	65
> substitution	<input type="checkbox"/>	16
> addition	<input type="checkbox"/>	12
> oxidation	<input type="checkbox"/>	9
> rearrangement	<input type="checkbox"/>	9
> condensation	<input type="checkbox"/>	9
> C-C bond formation	<input type="checkbox"/>	7
> hydrolysis	<input type="checkbox"/>	6
> reductive ...	<input type="checkbox"/>	4
> addition/elimination	<input type="checkbox"/>	3
> cyclization	<input type="checkbox"/>	2

Clear selected x

Limit To > Exclude >

Reaxys抽提出文献中所有的反应类型，帮助做进一步的筛选

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 Physical Data - 66 Preparations - 65 >
Druglikeness Spectra - 52 Reactions - 98 >
Bioactivity (All) Other Data - 2,500 Targets - 1,032 >
Documents - 3,345 >

Synthesize **Autoplan**

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

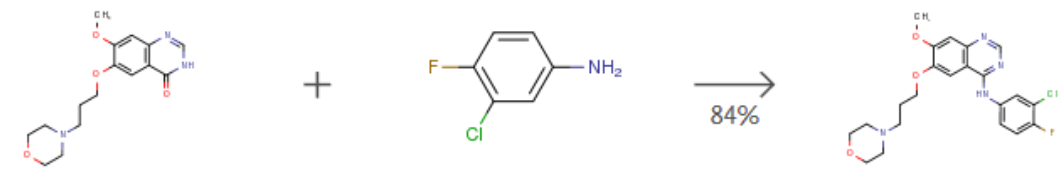
Synthesis Plan—添加感兴趣的反应

- 可以添加多条反应在一个Plan中，用于比较

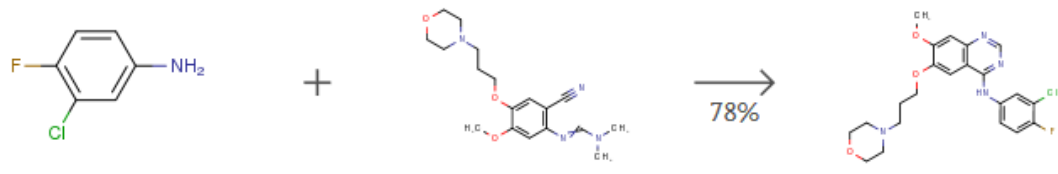
Add preparation - 64 ×

Preparation

1

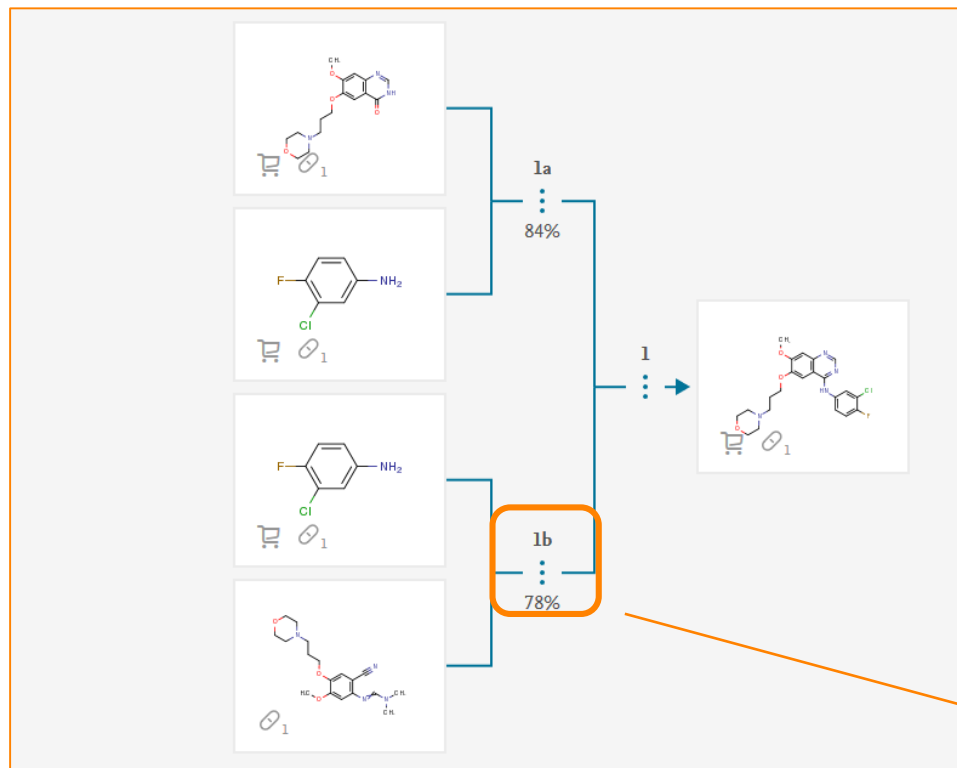


2



+ Load more Cancel × Add 2 to plan >

添加好的结果界面



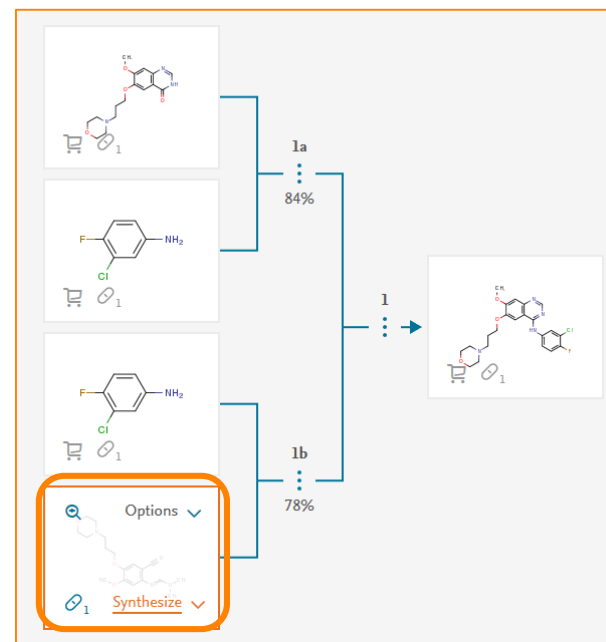
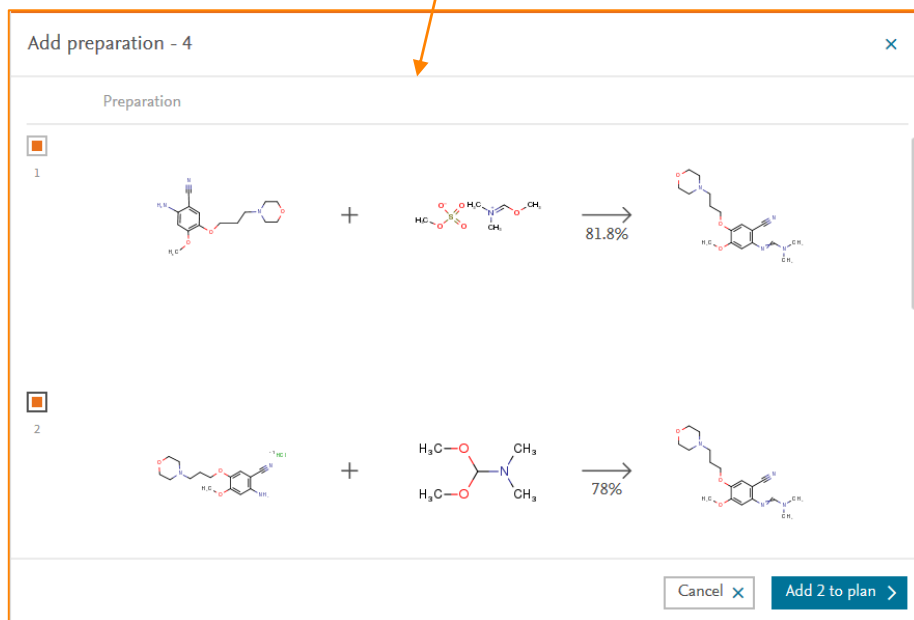
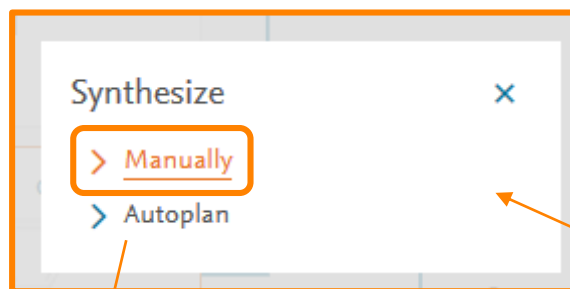
Preparation - 1b		
Yield	Conditions	Reference
78%	With acetic acid at 130°C; for 3h; Temperature; Experimental Procedure ▼	Guangzhou Baiyunshan Pharmaceutical Group Co., Ltd. Baiyunshan Pharmaceutical Zong Factory; Chen Mao; Zhu Shaoxuan; Huang Xiaoguang - CN104072426, 2017, B Location in patent: Paragraph 0050; 0051; 0052; 0053; 0054; 0055 Full Text ↗ Details > Abstract >
71.19%	With acetic acid In 5,5-dimethyl-1,3-cyclohexadiene at 135°C; Experimental Procedure ▼	Shaanxi Normal University; Li, Baolin; Ren, Yufei; Wang, Liu-chang; Jia, Yucui; Ding, Siyi; Wang, Wei - CN103539702, 2016, B Location in patent: Paragraph 0094-0096 Full Text ↗ Details > Abstract >
70%	With acetic acid at 125 - 130°C; for 3h;	- Organic Process Research and Development, 2007, vol. 11, # 5, p. 813 - 816 Full Text ↗ Cited 51 times ↗ Details > Abstract >

- 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

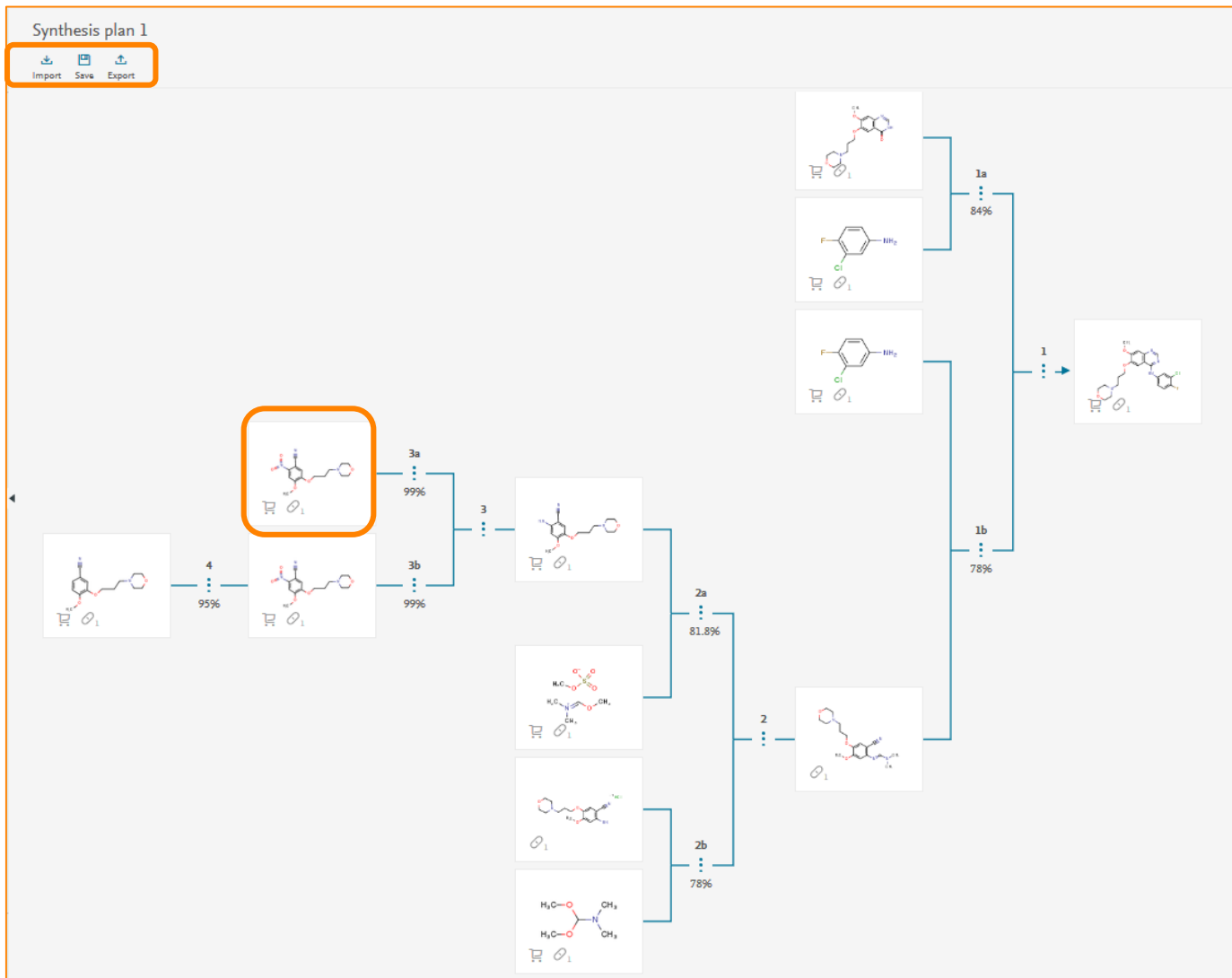
继续的扩充反应路线



Tips:

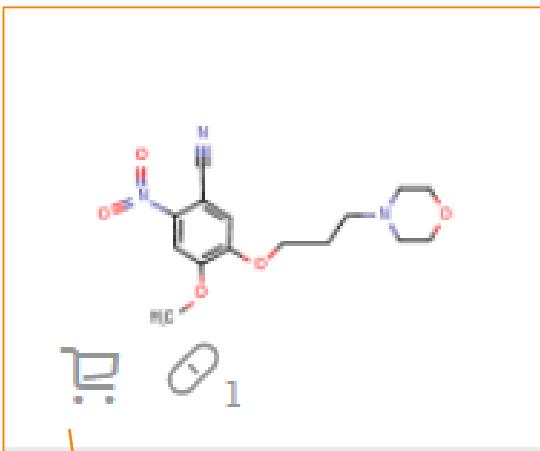
在Synthesis Plan上可以对任意一个物质进行同样的Synthesis的操作，可以将更多的反应添加进来

最后的结果



可以对Synthesis Plan进行导入，导出或者保存等操作。

获得物质的商业信息



Substance Availability ✕

- Accelrys' ACD
- 100g \$462 eMolecules
- Sigma Aldrich
- Labnetwork

| | 关键词搜索

4-methoxy-5-(3-morpholin-4-ylpropoxy)-2-nitrobenzonitrile

查看大图

览博网化合物ID: LN01377940

CAS: 675126-26-8

MDL: MFCD1110476

分子式: C15H19N3O5

分子量: 321.329

Log P: 暂无

重原子个数: 23

同位素原子数: 暂无

SMILES: COC1=C(C=C(C#N)C(=C1)[N+]=O)[O-]OCCCN2CCOCC2

InChI 编码: FYCDMKYKSPHRFW-UHFFFAOYSA-N

InChI: InChI=1S/C15H19N3O5/c1-21-4-10-13(18(19)20)12(11-16)9-15(14)23-6-2-3-17-4-7-22-8-5-17/h9-10H,2-8H2,1H3

氢键受体数: 5

氢键给体数: 0

旋转键数: 7

共显示 19 个结果

产品名称	供应商	排名	基价	纯度 (大于等于)	库存	展开全部
Benzonitrile,4-methoxy-5-(3-(4-morpholinyl)propoxy)-2-nitro-	北京飞龙瑞南药有限公司	★★★★★	¥407.14 (10g)	98%	无现货	- 展开
4-Methoxy-5-(3-morpholin-4-yl-propoxy)-2-nitro-benzonitrile	药明康德 (物流库房)	★★★★★	询盘	95%	491.84g - CN-SH 129g - CN-TJ	- 展开
2-Amino-4-methoxy-5-(3-morpholinopropoxy)benzonitrile	青垦科瑞希医药技术有限公司	★★★★★	询盘	99%	无现货	- 展开
2-nitro-4-methoxy-5-(3-morpholinopropoxy)benzonitrile	萨惠化学技术(上海)有限公司	★★★★★	¥237.00 (5g)	98%	无现货	- 展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile	上海泰恒科技股份有限公司	★★★★★	¥80.00 (1g)	98%	2g - CN	- 展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile	上海泰恒科技股份有限公司	★★★★★	¥270.00 (5g)	98%	20g - CN	- 展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile	上海泰恒科技股份有限公司	★★★★★	¥880.00 (25g)	98%	175g - CN	- 展开

提纲

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 - 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，跨学科的精确答案
- **New Reaxys**中的结构面板，能够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



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