

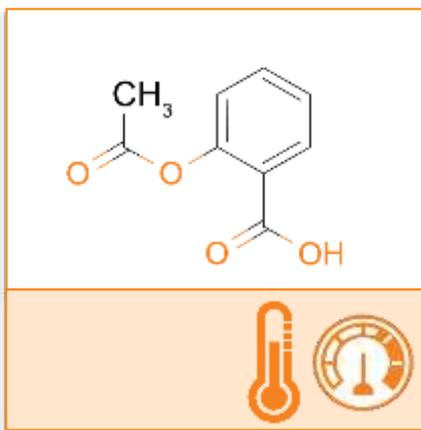
Reaxys使用 反应检索技巧



提纲

- Reaxys的基本介绍和数据索引
- Reaxys最新更新
- Reaxys中的检索
 - Reaxys中结构面板高级应用
 - Reaxys中的高级反应检索
 - Reaxys中的合成计划设计
- Reaxys检索小结

什么是Reaxys?



>110 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



>47M 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

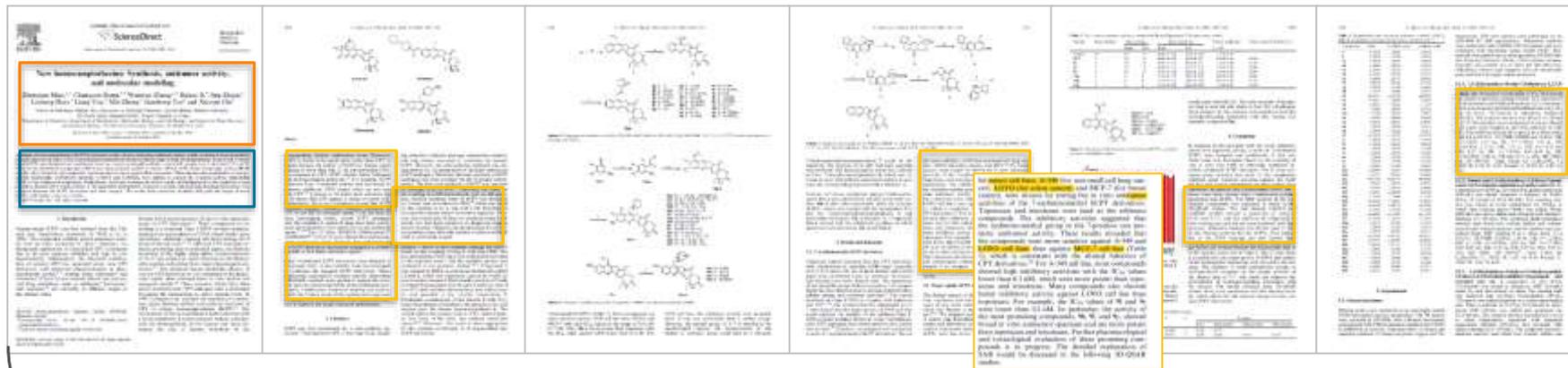

Linked
to



>57 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



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 homocamptothecin: Synthesis, antitumor activity, and molecular modeling Cited 23 times

Miao, Zhenyuan; Sheng, Chunqiang; Zhang, Wannian; Ji, Haitao; Zhang, Jing; Song, Luosheng; You, Liang; Zhang, Min; Yao, Jianhong; Che, Xiaoyin - *Bioorganic and Medicinal Chemistry*, 2008, vol. 16, # 3, p. 1493 - 1510

Abstract [^](#) [Index Terms](#) [^](#) [Substances \(28\)](#) [v](#) [Reactions \(28\)](#) [v](#) [Full Text \(7\)](#)

Abstract

Homocamptothecins (hCPTs) represent a class of new emerging antitumor agents, which contains a seven-membered β -hydroxy lactone in place of the conventional six-membered β -hydroxy lactone ring (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, 9f, and 9j, 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

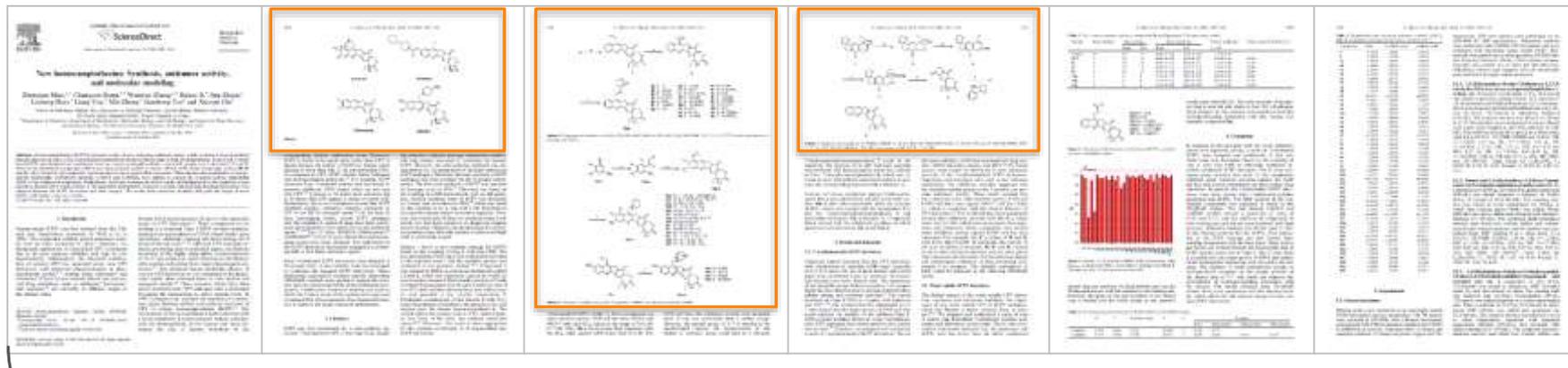
EMTREE drug terms: 10-methyl-11-chloro-7-(pyridiniummethyl)homocamptothecin chloride, 7-(2-bromophenyl)iminomethyl-methoxyphenyl)iminomethyl)homocamptothecin, 7-(2-methylphenyl)iminomethyl)homocamptothecin, 7-(2,4-dichlorophenyl)iminomethyl)homocamptothecin, 7-(3-chloro-4-fluorophenyl)iminomethyl)homocamptothecin, 7-(3-chloro-4-fluorophenyl)iminomethyl)homocamptothecin, 7-(3-methylphenyl)iminomethyl)homocamptothecin, 7-(3,4-dichlorophenyl)iminomethyl)homocamptothecin, 7-(3,5-dichlorophenyl)iminomethyl)homocamptothecin, 7-(3,5-dimethylphenyl)iminomethyl)homocamptothecin, 7-(4-cyanophenyl)iminomethyl)homocamptothecin, 7-(4-methylphenyl)iminomethyl)homocamptothecin, antineoplastic agent, camptothecin derivative, irinotecan, topotecan, unclassified d

EMTREE medical terms: animal experiment, animal model, antineoplastic activity, article, colon cancer, comparative molecule binding, drug structure, drug synthesis, human, human cell, hydrogen bond, hydrophobicity, male, molecular docking, tumor cell

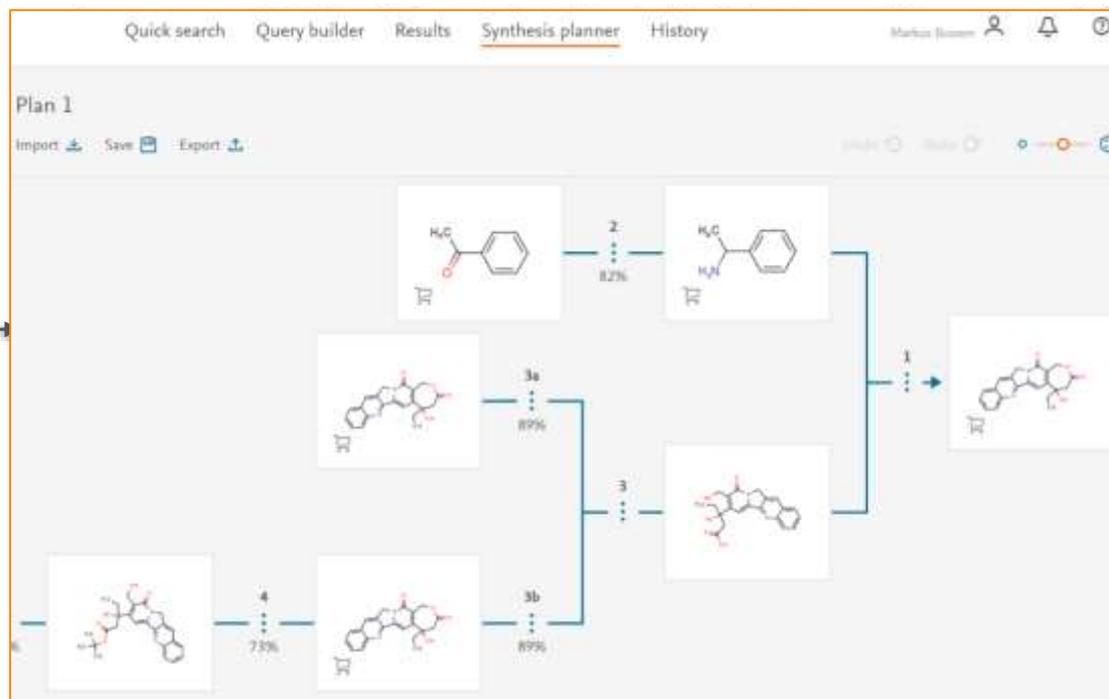
Author keyword: 3D **tumor cell line** camptothecins, Molecular docking

Reaxys Index Terms: hydrophobic surface

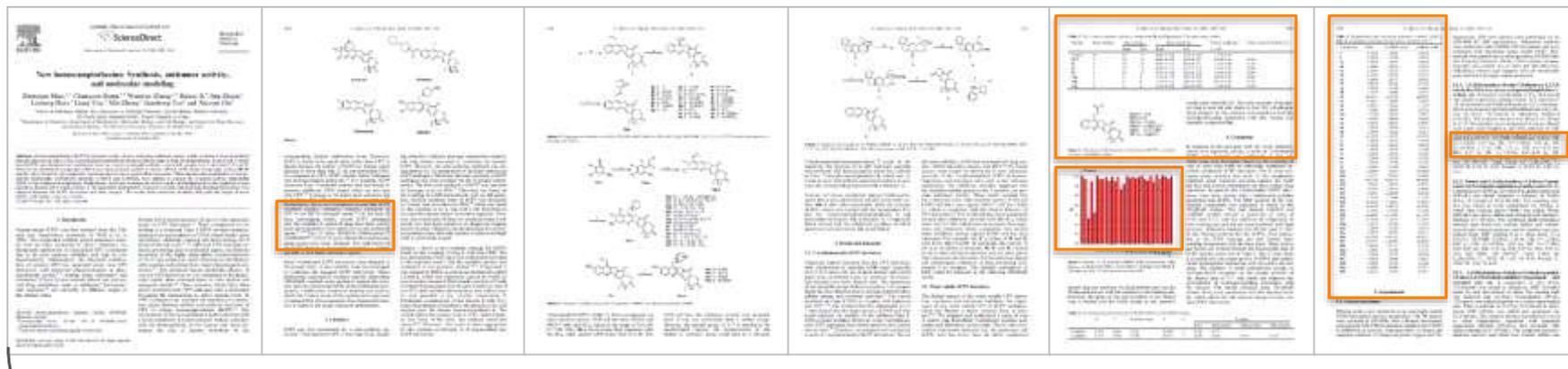
Reaxys索引的内容—结构与反应



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



Reaxys索引的内容—文献中的数据



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

Reaxys Quick search Query builder Results Synthesis planner History Marvin Basic

Filters and Analysis

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

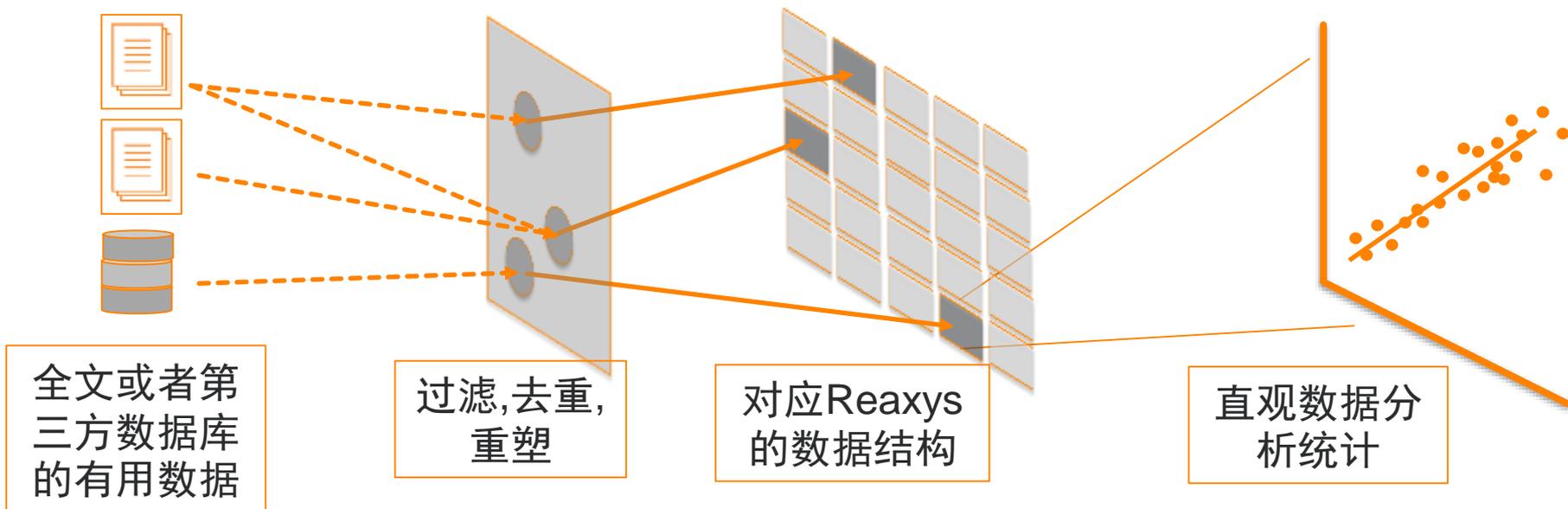
camptothecin
 $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_4$ 148.358 607362 7MF-03-4

Identification Bioactivity (All) Spectra - 139 Preparations - 221
Druglikeness Physical Data - 132 Other Data - 1,527 Reactions - 1,312
Targets - 142
Documents - 3,556

camptothecin

- 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

- Reaxys的基本介绍和数据索引
- Reaxys最新更新
- Reaxys中的检索
 - Reaxys中结构面板高级应用
 - Reaxys中的高级反应检索
 - Reaxys中的合成计划设计
- Reaxys检索小结

20180702更新主要内容

- 关键词检索的Auto Suggest
- 优化检索结果集界面
- 新增Chemdraw JS结构面板
- Query Builder使用教程的加入
- Marvin JS结构面板，使用教程的加入

关键词检索的Auto Suggest

- Quick Search中输入Key Word检索，会自动弹出建议的词语。
- 使用建议词语检索，可以自动添加一些相关概念，用于获得全面结果

The image illustrates the auto-suggest functionality in the Reaxys search interface. It is divided into two main sections:

Top Section (Search Reaxys): Shows a search bar with the input "suzuki". Below the search bar, a dropdown menu lists suggested search terms under the heading "Concepts". The terms are: "suzuki", "suzuki (kyodai) nitration", "suzuki coupling", "suzuki cross coupling", "suzuki reaction", "suzuki synthesis", "suzuki-miyaura", "suzuki-miyaura coupling", "suzuki-miyaura reaction", and "suzuki-miyaura synthesis". An orange arrow points from the underlined "suzuki reaction" term to the search bar in the bottom section.

Bottom Section (Search Reaxys): Shows the search bar with the input "suzuki reaction". Below the search bar, the word "AND" is displayed. At the bottom, there is a dashed box containing a chemical drawing tool icon (a hexagon with a pencil) and the text "Create Structure or Reaction Drawing".

优化检索结果集界面

- 预览结果界面优化
- 当前界面可直接返回Quick Search界面，进行检索式修改

直接当前页面返回Quick Search页面进行检索式修改

The screenshot shows the Reaxys search results page for 'suzuki reaction'. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A 'Register' button and 'Sign in' link are on the right. Below the navigation, there are 'New' and 'Edit' icons. The main content area displays two result categories: 'Reactions' (3,500 results) and 'Documents' (22,448 results). Each category has a 'View Results' button and a 'Create Alert' button. An orange arrow points to the 'Edit' icon in the top left, and another orange arrow points to the 'Documents' result type icon.

Result Type	Count	Condition	Actions
Reactions	3,500	Condition : suzuki reaction	Edit in Query Builder, Create Alert, Preview Results, View Results
Documents	22,448	Titles, Abstracts, Keywords : suzuki reaction	Edit in Query Builder, Create Alert, Preview Results, View Results

新增结果类型图标，对结果类型的呈现更为直观

反应结果集检索结果

Reaxys® Quick search Query builder ^{new} Results Synthesis planner History Register > Sign in ?

3,500 Filters and Analysis 3,500 Reactions out of 4,438 Documents containing 5,369 Substances, 853 Targets

By Structure 0 Limit To Exclude Export Syn-Plan No of References ↓

Yield Reaction ID: 4033276

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability 50 Hits 1,299 Conditions Find Similar >

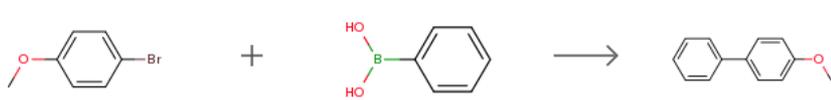
Reactant Availability

Reaction Classes

Document Type

Publication Year

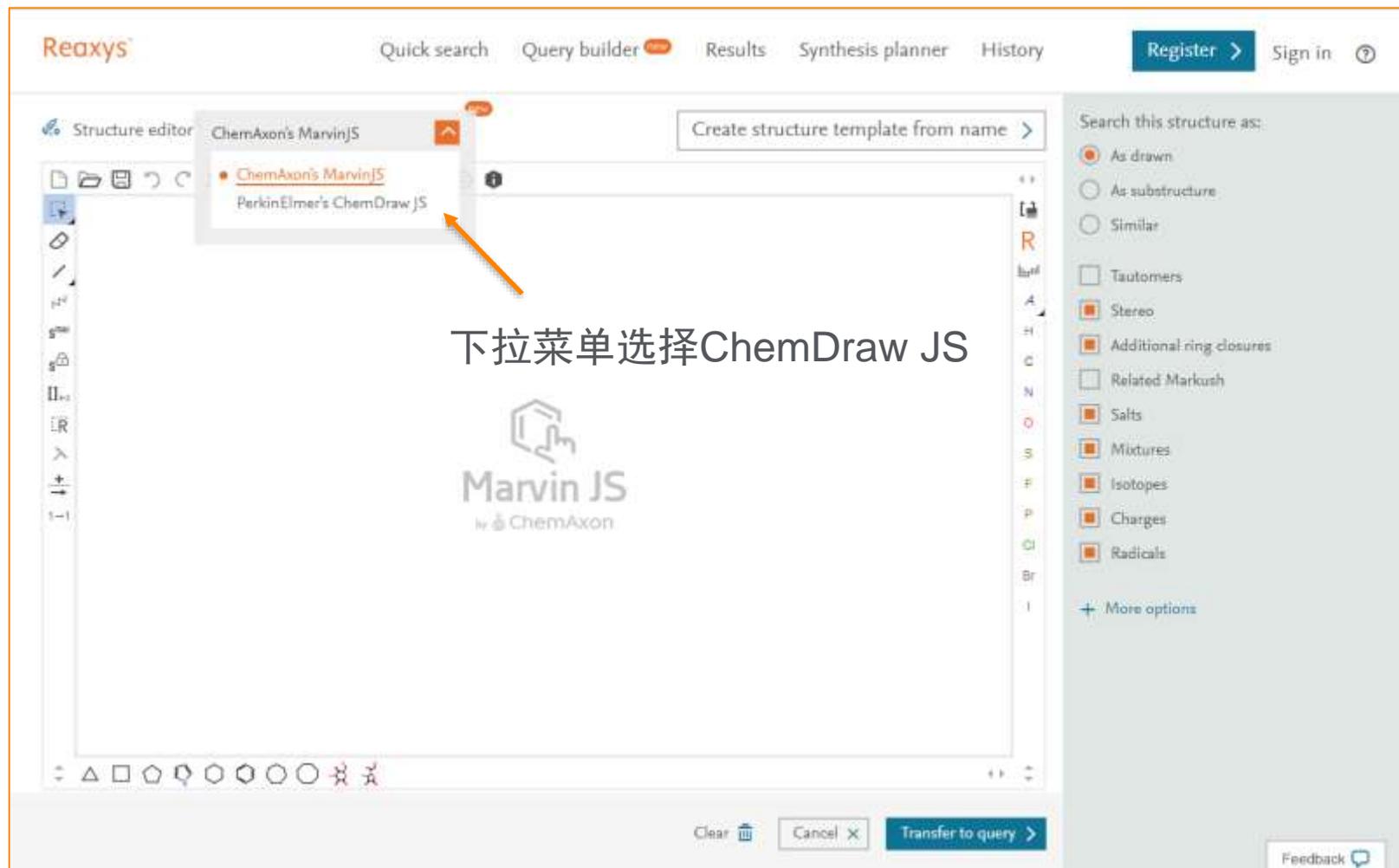
Single step reactions only



Yield	Conditions	References
100%	With [PdCl ₂ (2-ethyl-2-oxazoline) ₂]; potassium carbonate In toluene at 110°C; for 3h; Suzuki reaction;	Gossage, Robert A.; Jenkins, Hilary A.; Yadav, Paras N. - Tetrahedron Letters, 2004, vol. 45, # 41, p. 7689 - 7691 Full Text ↗ Cited 78 times ↗ Details > Abstract >
99%	With 1,8-diazabicyclo[5.4.0]undec-7-ene; palladium diacetate In ethanol; water at 20 - 150°C; microwave irradiation; Suzuki reaction;	Chanthavong, Florine; Leadbeater, Nicholas E. - Tetrahedron Letters, 2006, vol. 47, # 12, p. 1909 - 1912 Full Text ↗ Cited 45 times ↗ Details > Abstract >
99%	With sodium carbonate; polystyrene-supported N-heterocyclic carbene-Pd catalyst In N,N-dimethyl-formamide at 20°C; for 24h; Suzuki reaction;	Kang, Tairan; Feng, Qiang; Luo, Meiming - Synlett, 2005, # 15, p. 2305 - 2308 Full Text ↗ Cited 66 times ↗ Details > Abstract >

新增Chemdraw JS结构面板

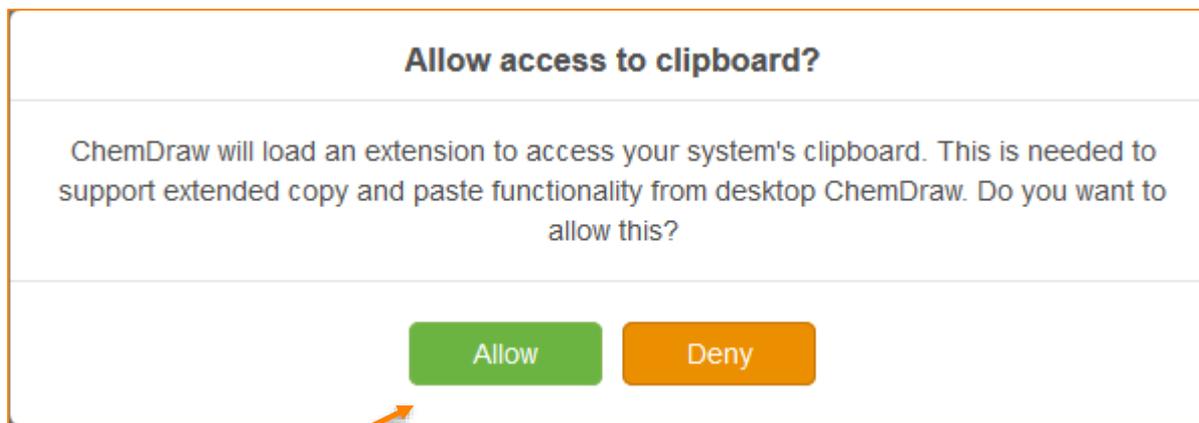
- 结构面板进入后，可以选择Chemdraw JS结构面板



The screenshot displays the Reaxys web interface. At the top, there are navigation links: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". On the right, there are buttons for "Register" and "Sign in". The main area is the "Structure editor", which has a dropdown menu open. The dropdown menu lists two options: "ChemAxon's MarvinJS" (selected) and "PerkinElmer's ChemDraw JS". An orange arrow points to the "PerkinElmer's ChemDraw JS" option. Below the dropdown, the text "下拉菜单选择ChemDraw JS" is written. The main editor area shows the "Marvin JS by ChemAxon" logo. On the right side, there is a "Search this structure as:" panel with various search options like "As drawn", "As substructure", "Similar", "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", "Radicals", and "More options". At the bottom, there are buttons for "Clear", "Cancel", and "Transfer to query".

Chemdraw JS结构面板

- 初次加载Chemdraw JS需要从网上下载插件，依据网速关系会耗费不等时间
- 加载成功后，提示是否允许访问粘帖版，用于直接从Chemdraw复制结构



点击Allow

Chemdraw JS结构面板

- Chemdraw JS结构面板

The screenshot displays the Reaxys Structure editor interface. At the top, there is a navigation bar with options: Quick search, Query builder (with a 'NEW' badge), Results, Synthesis planner, and History. On the right side of the navigation bar are buttons for Register > and Sign in (with a help icon). Below the navigation bar, the main workspace is titled 'Structure editor' and 'PerkinElmer's ChemDraw JS'. A search box contains the text 'Create structure template from name >'. The central area is a large white canvas for drawing chemical structures, with a toolbar above it containing various drawing tools. On the right side, there is a sidebar with search options: 'Search this structure as:' followed by radio buttons for 'As drawn' (selected), 'As substructure', and 'Similar'. Below these are checkboxes for 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom of the sidebar is a '+ More options' link. In the bottom right corner of the main workspace, there is a small icon representing a plugin. An orange arrow points from the text '可以按教程安装Copy Paste插件' to this icon. At the bottom of the interface, there are buttons for 'Clear' (with a trash icon), 'Cancel' (with an 'X' icon), and 'Transfer to query' (with a right arrow icon). A 'Feedback' button with a speech bubble icon is located in the bottom right corner.

可以按教程安装Copy Paste插件

Query Builder使用教程的加入

- 进入Query Builder可以看到Query Builder的使用步骤

The screenshot displays the Reaxys web interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder' (highlighted with a red 'new' badge), 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there are 'Register' and 'Sign in' buttons. Below the navigation bar, a search bar is present with a 'Search in:' dropdown menu showing options for 'Reactions', 'Targets', 'Substances', and 'Documents'. A central pop-up window titled 'Searching with Query Builder' is overlaid on the main content area. The pop-up contains the following text: 'Understanding the simple rules for working with fields, forms and search history makes it even easier to create complex queries.' Below this text is a link 'Guide to Query Builder' and a blue button labeled 'Take the Tour >'. The main content area below the pop-up features the text 'Drag & Drop to build a new query'. On the right side of the interface, there is a sidebar with a search box 'Find search fields and forms' and a list of categories: 'Fields', 'Forms', and 'History'. Under 'Fields', there are several expandable sections: 'Reaxys', 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. At the bottom of the sidebar, there are sections for 'PubChem' and 'eMolecules'.

Query Builder使用教程的加入

介绍不同部分的使用方法

Searching with Query Builder ×

Understanding the simple rules for working with fields, forms and search history makes it even easier to create complex queries.

[Guide to Query Builder](#)

[Take the Tour >](#)

Results Synthesis planner History

[Register >](#) [Sign in](#) ?

Find search fields and forms 🔍

[Fields](#) [Forms](#) [History](#)

Reaxys ^

Basic Indexes ∨

Identification ∨

Using Fields ×

Reaxys offers hundreds of search fields to help you quickly get precise answers. Click Reaxys or one of the integrated databases to see the available search fields. Click MedChem to show the fields specific to medicinal chemistry.

[Guide to Query Builder](#)

[Next >](#)

Marvin JS结构面板，使用教程的加入

- Marvin JS结构面板使用教程

The screenshot displays the Reaxys Marvin JS interface. At the top, there are navigation links: 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. On the right, there are buttons for 'Register' and 'Sign in'. The main area is titled 'Structure editor' and 'ChemAxon's MarvinJS'. A 'Create structure template from name' search bar is visible. On the left, there is a vertical toolbar with various editing tools. On the right, there is a search filter panel with options like 'As drawn', 'As substructure', 'Similar', 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. A modal window titled 'Marvin JS' is open, listing updates: '1. Lock Atoms', '2. Maximum Substitution', '3. Atom-Atom Mapping (reactions)', '4. Edit abbreviated groups & Reaxys group generics using keyboard', and '5. Bond tool updated'. Below the list, it states: 'The new MarvinJS version will make structure query generation much easier and faster'. A blue button labeled 'Take the tour >' is highlighted with an orange arrow. Another orange arrow points to the 'Marvin JS ChemAxon' logo in the bottom right of the modal. The text '点击进入教程' (Click to enter the tutorial) is written in Chinese next to the second arrow. At the bottom of the interface, there are buttons for 'Clear', 'Cancel', and 'Transfer to query', along with a 'Feedback' button.

Marvin JS结构面板，使用教程的加入

Lock Atoms



You can perform a substructure search and simultaneously lock substitutions on one or more atoms in your structure.

1. Click the new "Lock Atom" tool
2. Click the atom of choice
3. (S*) will appear on the atom
4. Select the Substructure option in the right hand panel: On All Atoms radio button
5. Click on 'Transfer to query' button and then the Find button

Structure editor new

Search this structure as:

- As drawn
- As substructure
 - On all atoms: 4
 - On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures

Transfer to query >

Cancel Back Next >

Maximum Substitution



"Substitution count" refers to the desired total number of non-hydrogen substituents on an atom. The retrieved hits will contain any number of substituents.

1. Click the new "Smax" tool (maximum substitution count)
 2. Click the atom of choice
 3. S6 will appear on the atom
 4. Select the As Drawn radio button to retrieve hits with the designated substitution count on the atom of choice only
 5. Click on Transfer to query button and then Find button
- S6 is a placeholder for maximum substitution count. More specific substitution counts can be set via the atom properties.

Structure editor new

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Suffix

Transfer to query >

Cancel Back Next >

提供了一些常见的功能的使用方法

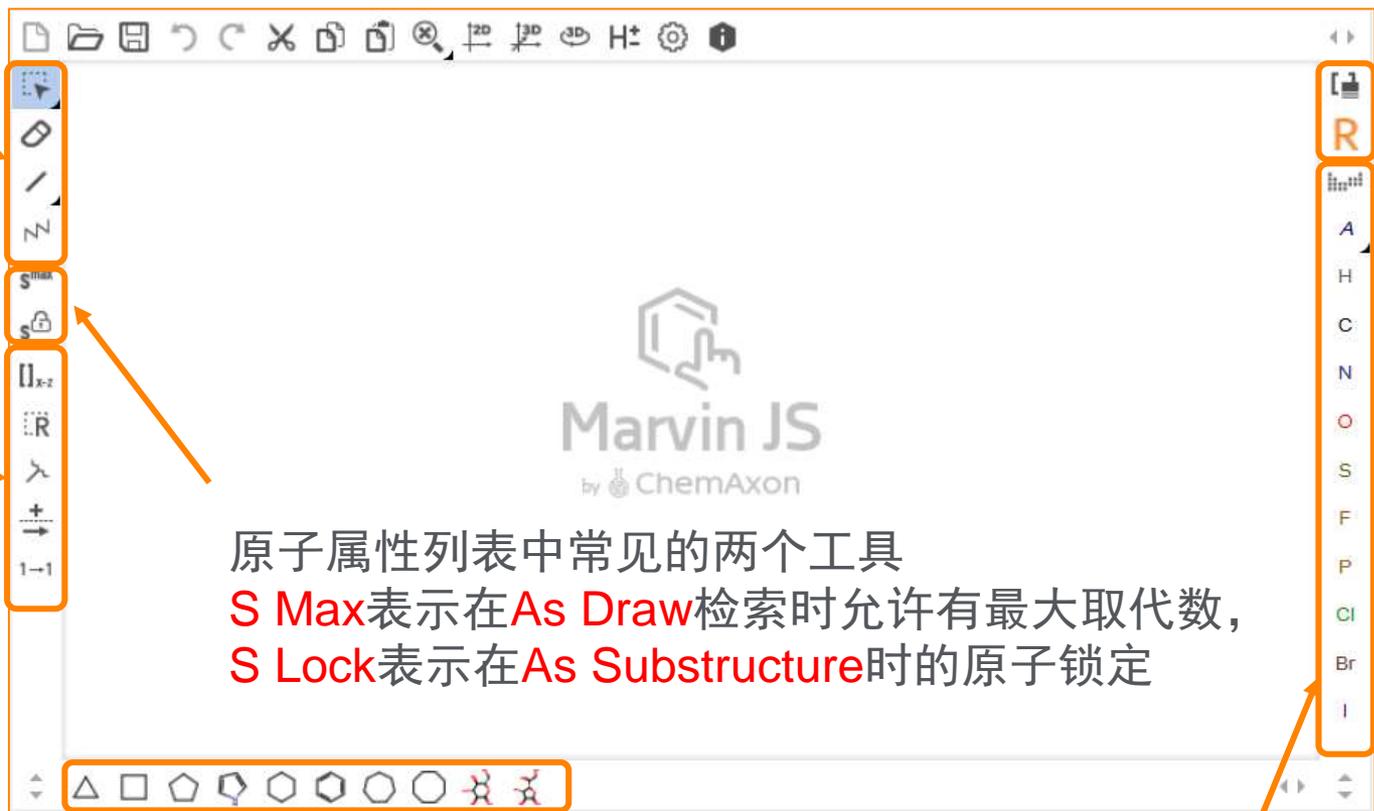
提纲

- Reaxys的基本介绍和数据索引
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 - Reaxys中的高级反应检索
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- 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，

重复基团，
R基团，
R基团链
接端，反
应定义工
具，原子
匹配工具



原子属性列表中常见的两个工具

S Max表示在**As Draw**检索时允许有最大取代数，
S Lock表示在**As Substructure**时的原子锁定

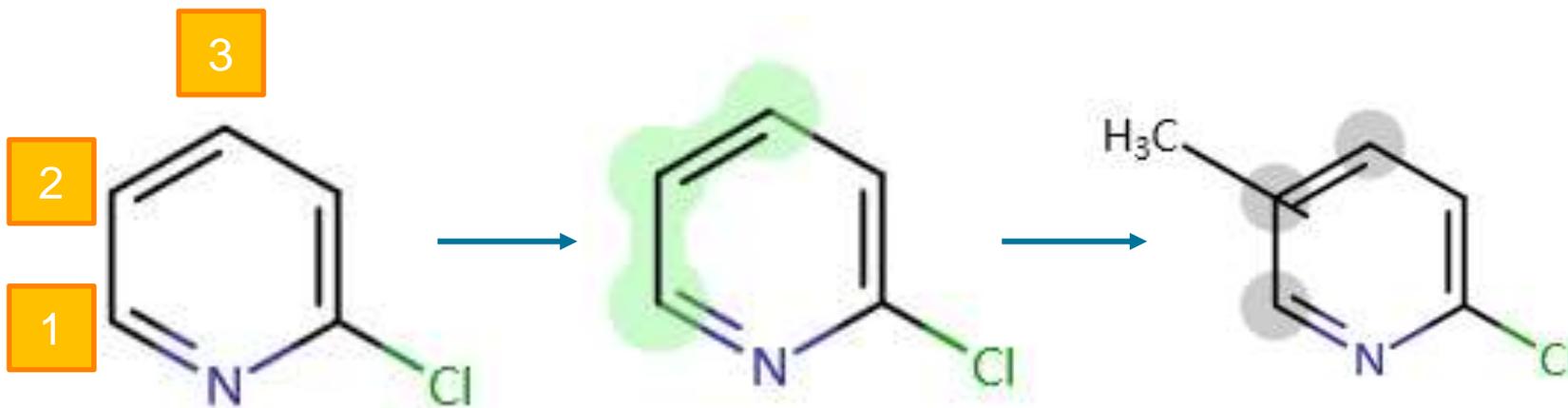
缩写官
能团，
通用官
能团定
义，

常见的环， 常见的糖分子模板

元素周期表以及常用原子，
A:原子属性定义工具

不定位取代键的使用

- 不定位取代键：
 - 在选定的原子上进行基团的链接
 - 可以使用在链上，也可以使用在环上



绘制要求:

希望1, 2, 3C上存在一个NH₂

绘制步骤:

1. 用选择工具选择1, 2, 3号C原子,
2. 添加不定位取代, 系统默认添加CH₃
3. 将CH₃换成NH₂

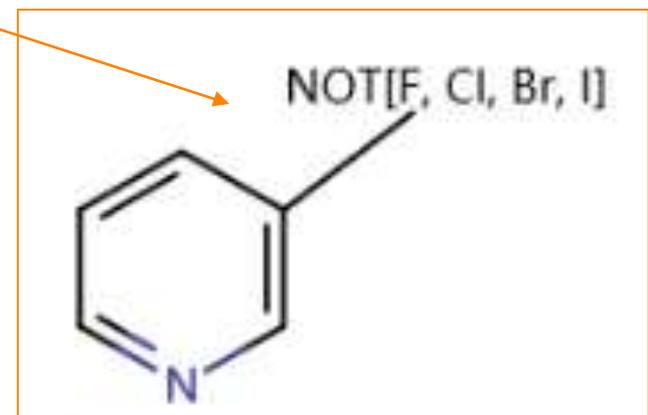
Not List的应用

- 案例:
 - 定义某位点上不能发生F, Cl, Br, I取代

Periodic table

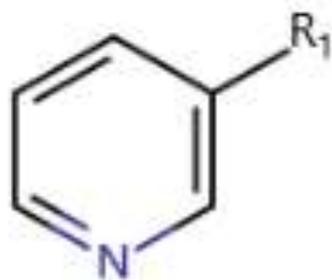
1																	18	
1	H	2											13	14	15	16	17	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	#	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
Atom list			*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
NOT list			#	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Ok

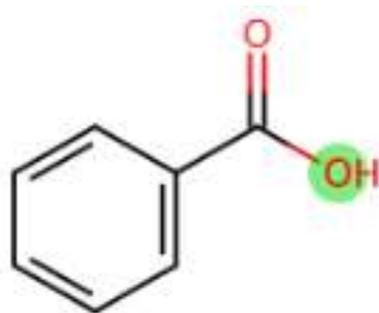


自定义R基团

- 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

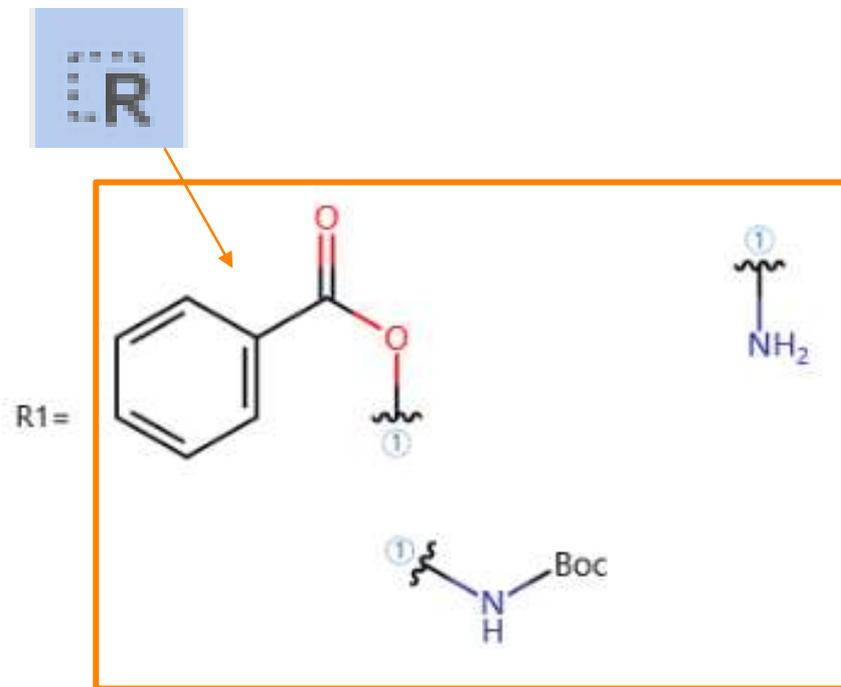
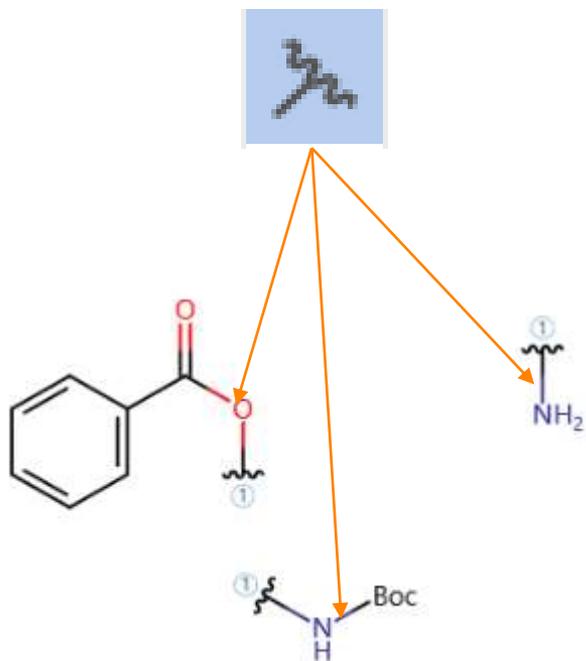


A

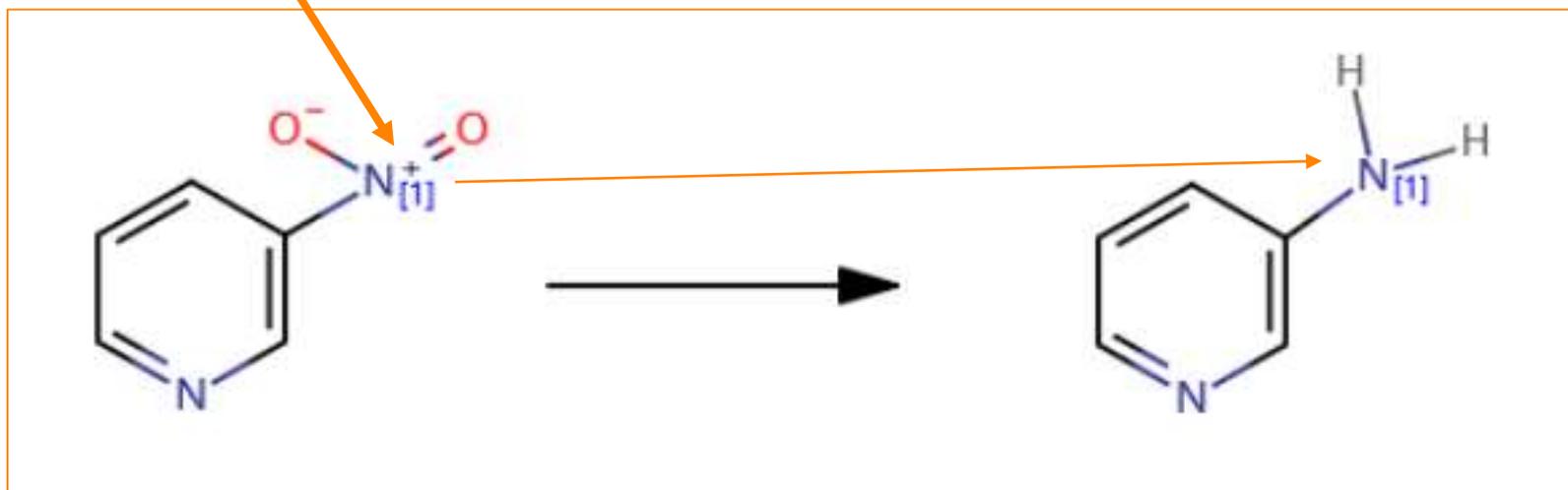
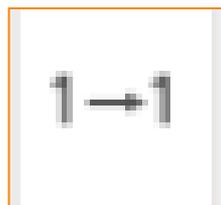


绘制方法

- 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



反应原子标记工具



Tips:

1. 定义反应前后必须匹配的原子
2. 建议将官能团展开后进行匹配
3. 在定义原子匹配时，两工具等效。

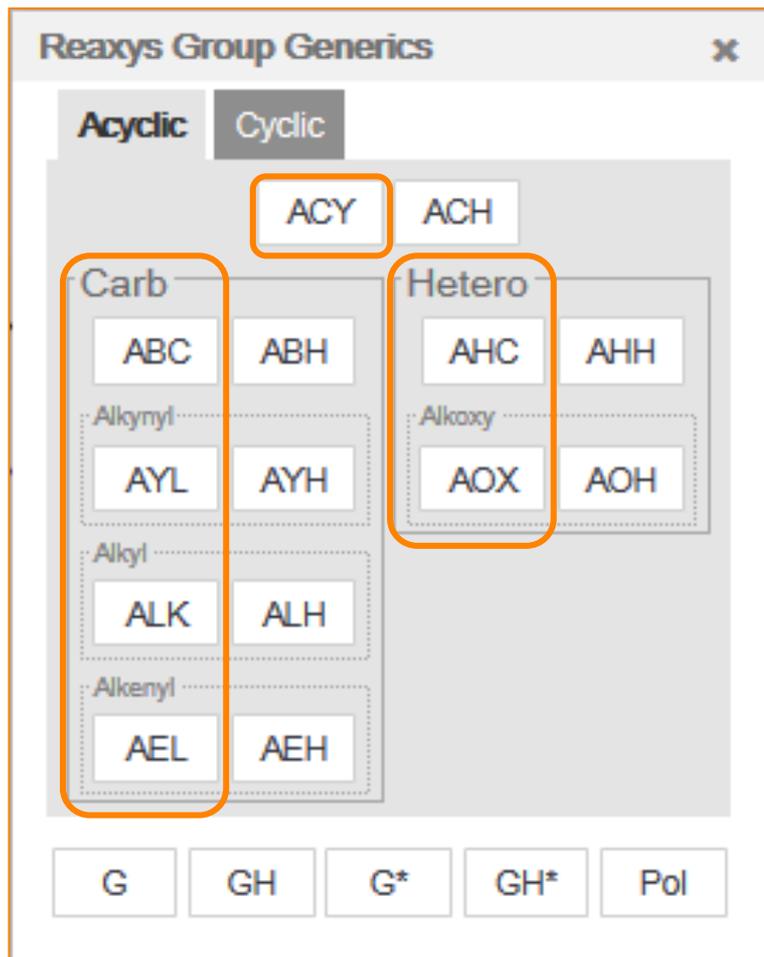
缩写官能团， Reaxys的Generic Group定义

The image displays two dialog boxes from the Reaxys software interface. The top dialog, titled "Abbreviated groups", features a text input field containing "BOC", an "Expand" checkbox, a dropdown menu showing "Boc", and an "Ok" button. The bottom dialog, titled "Reaxys Group Generics", has tabs for "Acyclic" and "Cyclic", with "Acyclic" selected. It contains a grid of buttons for various functional groups: ACY, ACH, ABC, ABH, AHC, AHH, AYL, AYH, AOX, AOX, ALK, ALH, AEL, AEH, G, GH, G*, GH*, and Pol. A separate box on the left contains a bracket icon and a large orange "R", with arrows pointing to the "Abbreviated groups" and "Reaxys Group Generics" dialog boxes respectively.

Tips:

1. Abbreviated Group:提供一些缩写的基团，直接键盘输入即可
2. Reaxys Generic Group: 提供一些通用官能团

Generic Group定义—链的定义



Tips:

ACY: 任意的链

ABC: 任意C链（只含C原子）

AYL: 含有炔基取代的链

ALK: 含有烷基取代的链（饱和链）

AEL: 含有烯基取代的链

AHC: 含有杂原子的链

AOX: 烷氧基

其他带H的分别是，前面对应基团或H

Generic Group定义—环的定义

The screenshot shows the 'Reaxys Group Generics' dialog box with the 'Cyclic' tab selected. The dialog is organized into several sections:

- Acyclic** (unselected)
- Cyclic** (selected):
 - CYC** (highlighted with an orange box)
 - CYH**
 - Carb** (highlighted with an orange box):
 - CBC** (highlighted with an orange box)
 - CBH**
 - Aryl** (dotted border):
 - ARY** (highlighted with an orange box)
 - ARH**
 - Cycloalkyl** (dotted border):
 - CAL** (highlighted with an orange box)
 - CAH**
 - Cycloalkenyl** (dotted border):
 - CEL** (highlighted with an orange box)
 - CEH**
 - Hetero** (highlighted with an orange box):
 - CHC** (highlighted with an orange box)
 - CHH**
 - Heteroaryl** (dotted border):
 - HAR** (highlighted with an orange box)
 - HAH**
 - No carbon** (dotted border):
 - CXX** (highlighted with an orange box)
 - CXH**
- G**
- GH**
- G***
- GH***
- Pol**

Tips:

CYC: 任意的环

CBC: 任意C环（只含C原子）

ARY: 芳香基（只含C原子）

CAL: 环烷基（饱和C环）

CEL: 环烯基（不饱和C环）

CHC: 任意杂环

HAR: 含杂原子的芳香环

CXX: 不含C原子的环

其他带H的分别是，前面对应基团或H

Generic Group定义—G Group定义

G

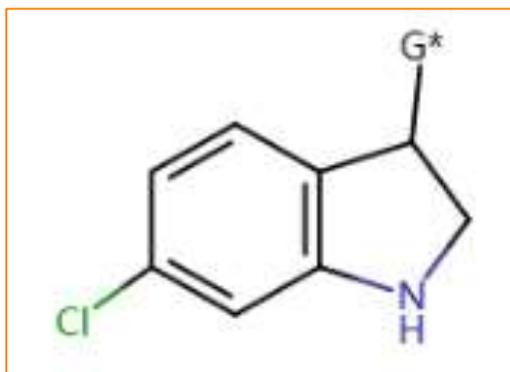
GH

G*

GH*

Tips:

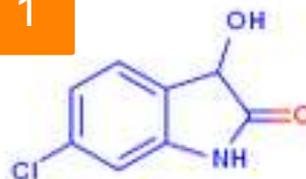
1. G代表的是任意基团，GH表示的是任意基团或H
2. G*和G的区别是，G*所连接的基团允许和母体成环，G不允许成环



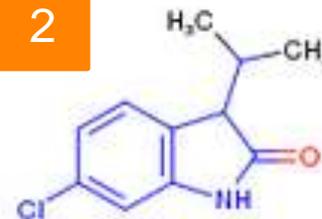
思考:

As Substructure检索这个结构，哪些结构可以被检索出来，如果不是G*，而是G呢？

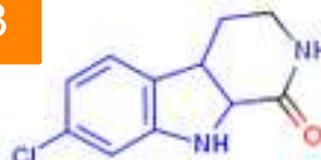
1



2



3



4



S Max和S Lock

- **S Max: As Draw**检索时有效
 - As Draw时，所有的原子不允许有取代
 - 标记上，S Max，等同于在As Draw时将这个位点全部开放
- **S Lock: As Substructure**检索时有效
 - As Substructure时，所有没有画出来的H，以及没有延展出来的H都可以随意取代
 - 标记上，S Lock，等同于该位点上只能是H，起到锁定作用

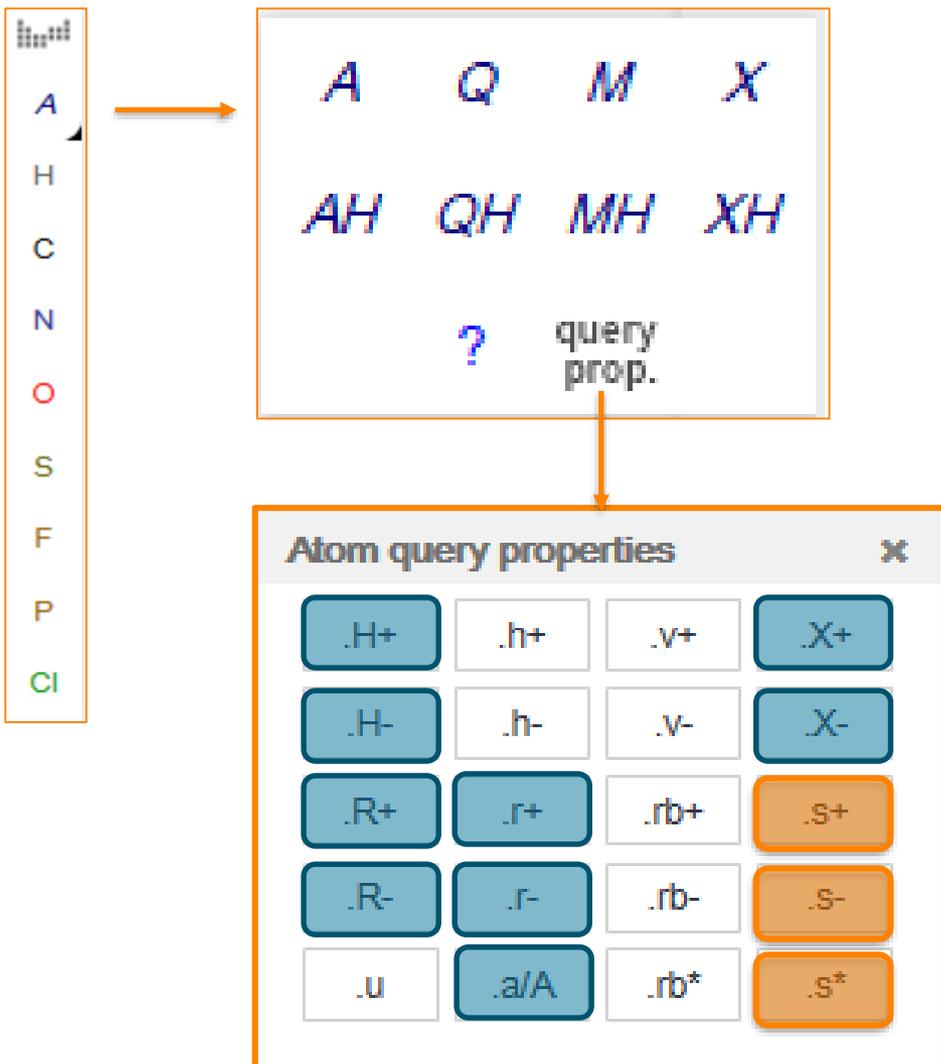


As Draw



As Substructure

原子属性列表



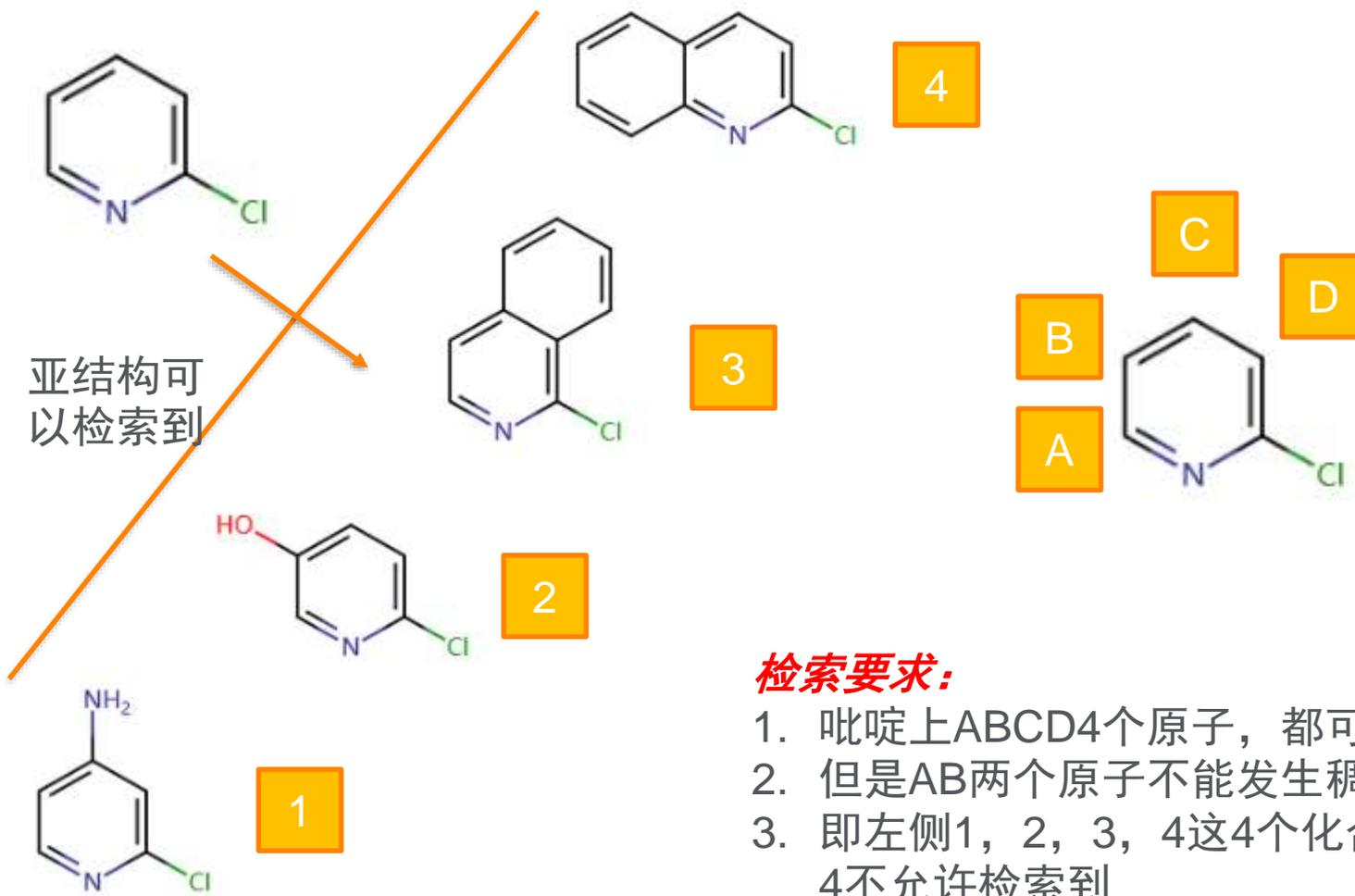
Tips:

- A: 任意非H原子
- Q: 任意非C, H原子
- M: 任意金属
- X: 卤素
- AH: 任意原子 (含H)
- QH: 任意非C原子 (含H)
- MH: 任意金属和H
- XH: 任意卤素和H
- Query prop: 原子属性列表

Tips:

- 蓝色标记的目前无功能
- S*等同于S Lock
- S+/S-大多数情况下用的是S6, 即S Max

一个很有意思的需求



检索要求:

- 吡啶上ABCD4个原子，都可以发生取代
- 但是AB两个原子不能发生稠环
- 即左侧1, 2, 3, 4这4个化合物，化合物4不允许检索到
- 俗称，**锁半环**

如果需要所有原子都不可以成环（即可以取代，但不能成环）

- 去除Additional Ring Closure

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

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

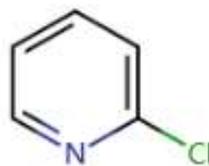
+ More options Feedback

Clear Cancel Transfer to query

去掉后，结构面板中所有的原子都不能成环

锁半环的解决方案

- 思考：是否允许成环
- 原子的标记，
- **rb***的定义，表示，在进行亚结构检索时，被标记的原子不能在成环



Reaxys

Quick search Query builder Results Synthesis planner History

Sam Yu

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

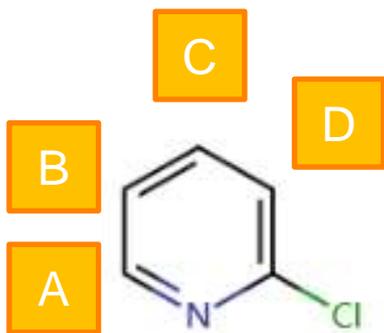
Atom query properties

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

Additional ring closures

案例的衍生....

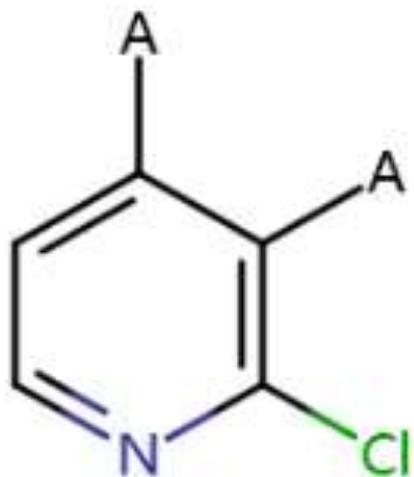
- 当前情况，AB不能成环，CD可以成环，也可以不成环



- 如果要求CD原子一定成环

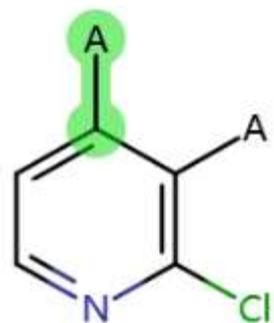
一定成环的定义

- 一定成环的条件
 - CD原子上一定会在连接一个非H原子
 - 且该非H原子一定与CD相接的一定是一个环键
- 所以.....



键属性的定义

- 定义步骤
 - 右键点击需要定义的键，选择Bond Properties
 - 在Topology中选择in ring即可

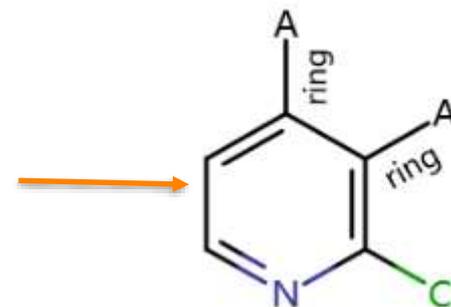


Attached Data...
Bond properties
Absolute stereo (chiral)
R-logic
Paste (Ctrl+V)

Bond properties

Type	single
Topology	undefined
Reacting center	undefined
Stereo search	in ring
	in chain

OK

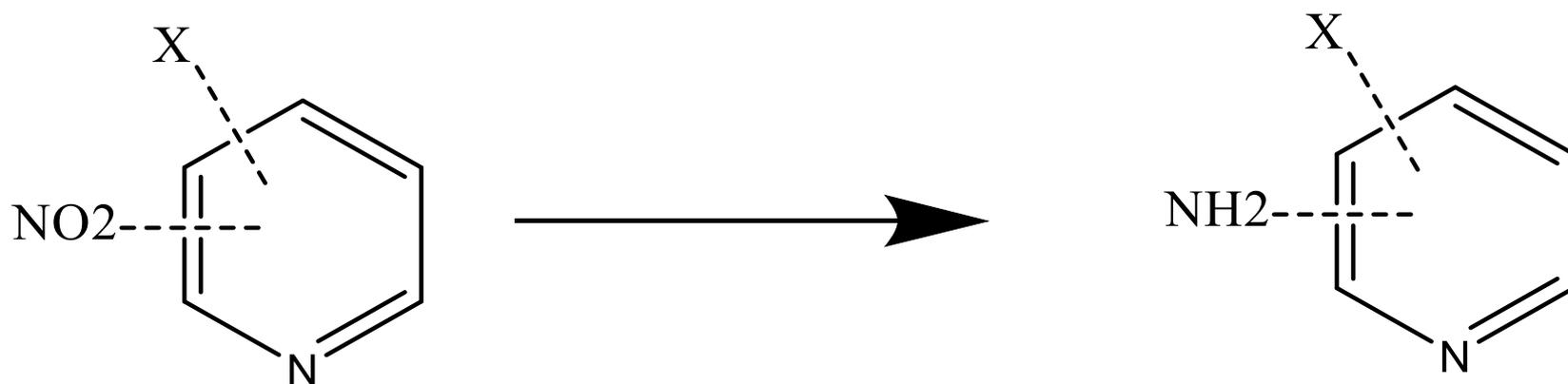


提纲

- Reaxys的基本介绍和数据索引
- Reaxys最新更新（近期即将）
- Reaxys中的检索
 - Reaxys中结构面板高级应用
 - Reaxys中的高级反应检索
 - Reaxys中的合成计划设计
- Reaxys检索小结

Case Study 1

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



Reaxys中的结构定义

The screenshot shows the Reaxys Structure editor interface. The main workspace displays a chemical reaction between two pyridine derivatives. The reactant on the left has a nitro group (NO₂) and a substituent (X) attached to different carbon atoms. The product on the right has an amino group (H₂N) and the same substituent (X) attached to different carbon atoms. The interface includes a toolbar on the left, a search panel on the right, and a 'Transfer to query' button at the bottom.

结构定义：

1: 使用两次不定位取代，将NO₂和X定义在吡啶环上

2: 使用原子映射功能，将反应前后的原子标记出来

3: As Draw检索

不定位取代的定义

1: 选择需要链接基团的原子，用不定位取代键和不同的基团相连

2: 吡啶环上的5个C原子需要使用两次不定位取代，一次链接X，一次链接NO₂

检索到的结果

29 Filters and Analysis

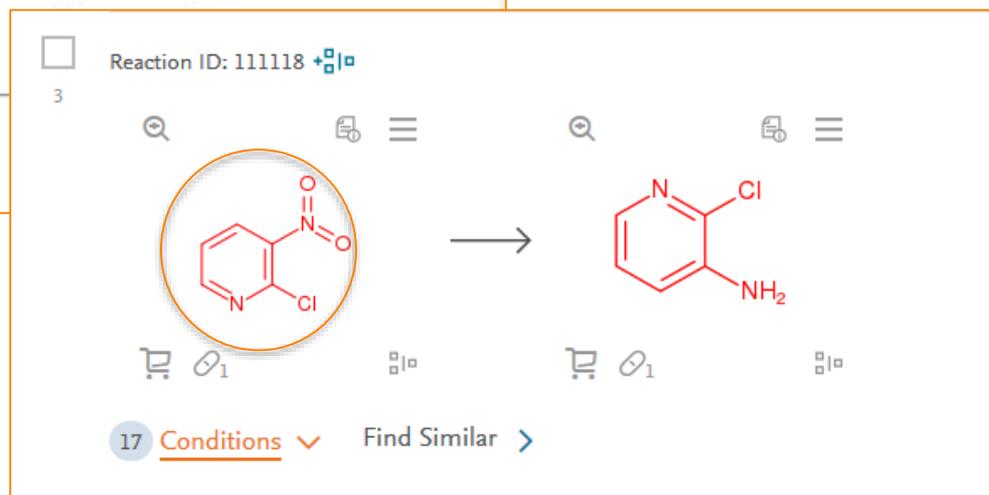
29 Reactions: 96 Documents 43 Substances, 18 Targets

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

Reaction ID: 91265

Reaction ID: 92348

检索到的反应，存在NO₂和X在邻位的，也存在对位的反应



如何对反应进行筛选

- 想要的一定属于这个结果集的子集，可以直接使用过滤工具

The screenshot displays the Reaxys web interface. On the left, the 'Filters and Analysis' sidebar is visible, with the 'By Structure' filter category highlighted by an orange box. Below this, a 'Create Structure Drawing' button is also highlighted. The main area shows search results for two reactions. Reaction 2 (ID: 92348) shows the reduction of 5-bromo-2-nitropyridine to 5-bromo-2-aminopyridine. Reaction 3 (ID: 111118) shows the reduction of 2-chloro-5-nitropyridine to 2-chloro-5-aminopyridine. Each reaction entry includes a search icon, a list icon, a zoom icon, and a 'Find Similar' link. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The user's name 'Sam Yu' and notification icons are also present.

输入限定的结构

The image shows the Reaxys software interface. The main window is the 'Structure editor' with a chemical structure of a 6-membered ring. The structure has an O_2N group and an X group attached to the ring. Four atoms in the ring are labeled with '[C, N]'. An orange box highlights the 'List' button in the 'Search this structure as:' panel. An orange arrow points from the periodic table to the structure editor. The periodic table shows the elements Carbon (C) and Nitrogen (N) highlighted in orange.

1, 打开元素周期表, 选择Atom List定义C, N
 2: 在6元环上, 将其余4个C全部换成List

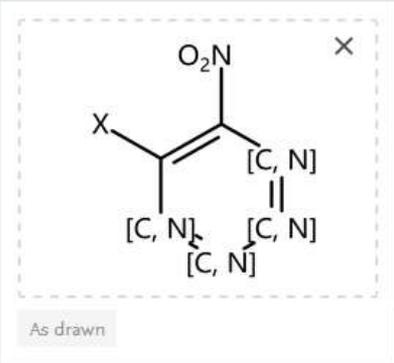
添加结构后的界面

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

29 Filters and Analysis

Limit to > Exclude >

By Structure 



As drawn

Yield 

Reagent/Catalyst 

Solvent 

Catalyst Classes 

Solvent Classes 

Product Availability 

29 Reactions out of 96 Documents containing 43 Substances, 18 Targets

0       Reaxys Ranking 

Reaction ID: 91265   

1      



36 Conditions  Find Similar >

Reaction ID: 92348   

2      



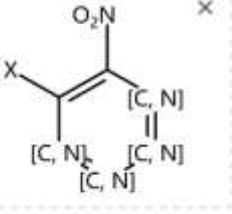
Feedback 

最后的结果

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

Filters and Analysis

By Structure



As drawn

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

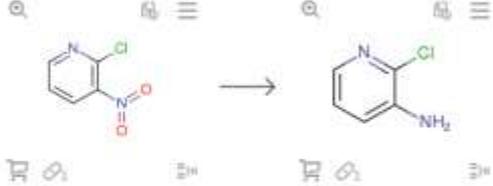
Solvent Classes

Product Availability

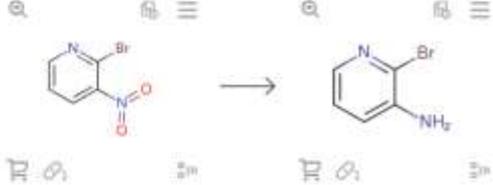
Reactant Availability

12 Reactions out of 29 Documents containing 18 Substances, 14 Targets

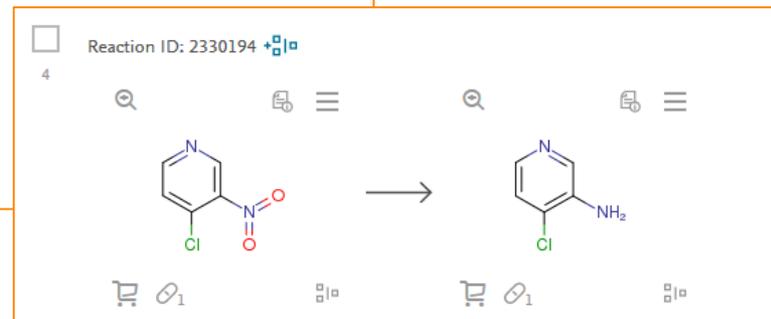
Reaction ID: 111118



Reaction ID: 111161

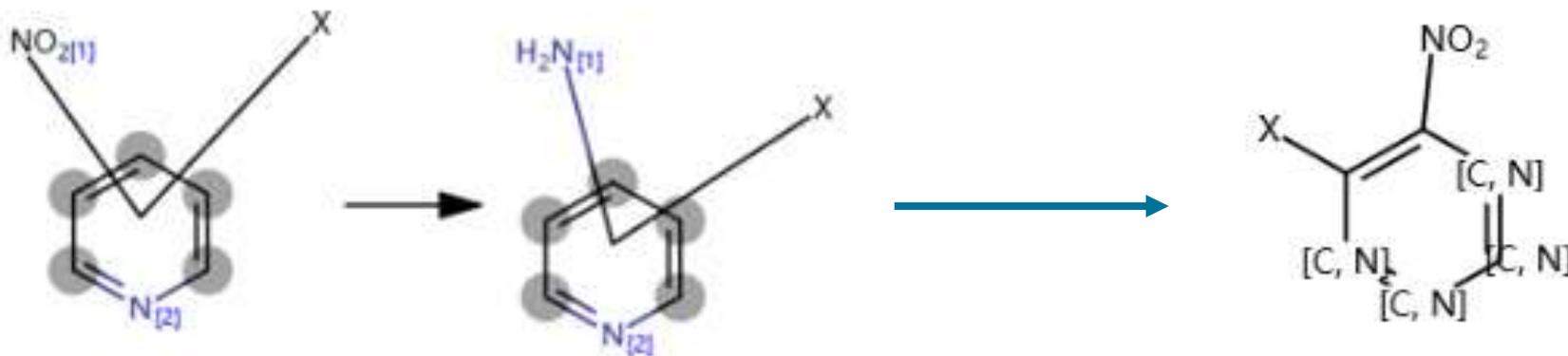


这种检索，出来的NO₂和X都处于邻位



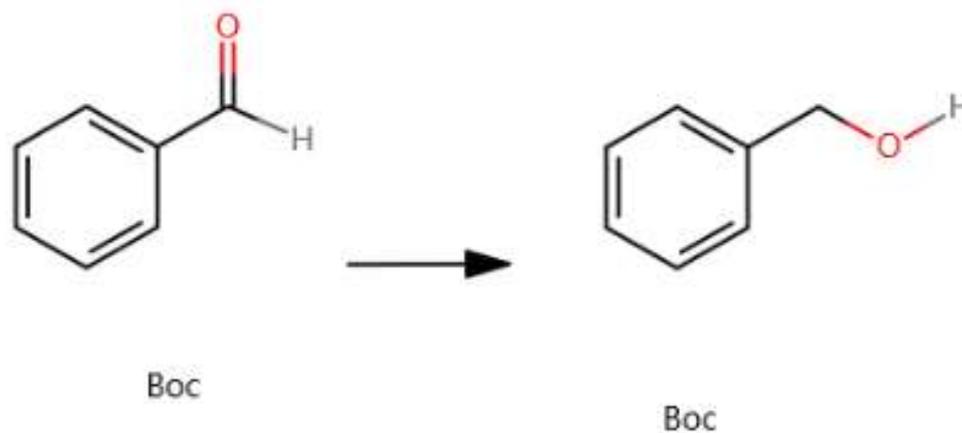
案例小结

- 当结构中存在一些特定要求，无法一次定义完全的时候，可以采用分次定义的方式
- 两次定义的结构，并不存在包容关系，这和通常意义上的限定不太一样
- 采用这种限定拿到的结果，是单独检索这两个结构的交集
- 采用这种限定策略，限定结构时必须将原有结构删除



Case Study 2

- 复杂结构中的常见问题
 - 反应中心，只是一个简单的化学变化
 - 反应物/产物，结构复杂或者新颖
 - 需要选择性的氧化，还原，脱保护等
- 检索符合以下条件的反应
 - 结构中不存在Boc和苯甲醛
 - 反应后苯甲醛变成苯甲醇



Reaxys中的定义

The screenshot displays the Reaxys Structure editor. The main workspace shows the chemical structure of benzaldehyde (O=Cc1ccccc1) on the left and benzyl alcohol (OCCc1ccccc1) on the right, connected by a reaction arrow. Below each structure is the label "Boc". The interface includes a top navigation bar with "Quick search", "Query builder", "Results", "Synthesis planner", and "History". A "Structure editor" toolbar is on the left, and a search options panel is on the right. The search options panel is titled "Search this structure as:" and includes several checkboxes. The "Additional ring closures" checkbox is highlighted with a red box. At the bottom of the editor, there are buttons for "Clear", "Cancel", and "Transfer to query".

1: 亚结构检索

2: 添加环的保护, Additional Ring closures.

3: S*, Atom Mapping

Reaxys中的结果

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

196 Filters and Analysis

By Structure ▾

Yield ▾

Reagent/Catalyst ▾

Solvent ▾

Catalyst Classes ▾

Solvent Classes ▾

Product Availability ▾

Reactant Availability ▾

Reaction Classes ▾

Document Type ▾

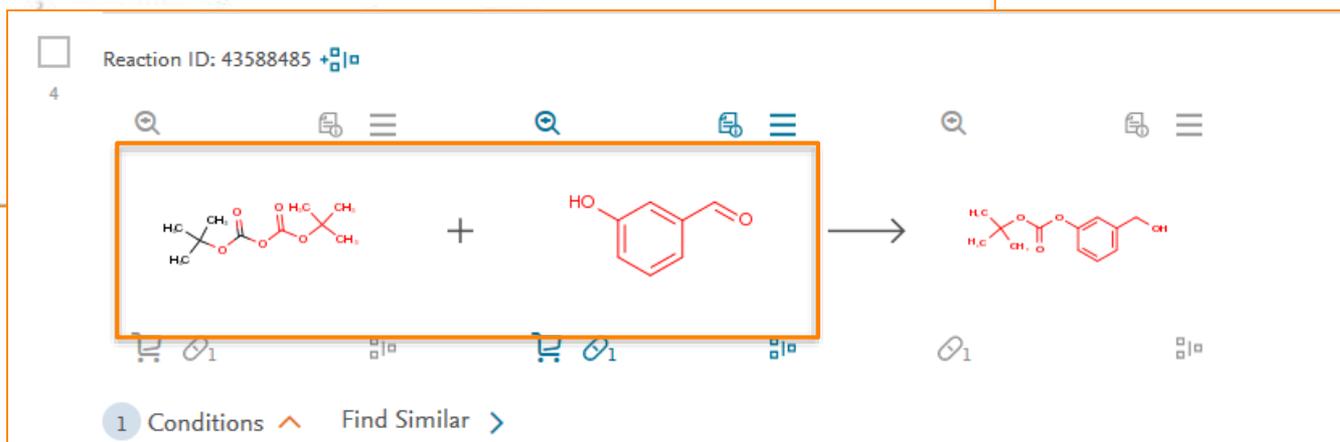
Publication Year ▾

Single step reactions only

196 Reactions out of 160 Documents containing 368 Substances, 46 Targets

Reaction ID: 46355509

Reaction ID: 9213594



在不做任何设置的情况下，会获得两个片段在不同结构中的反应

Reaxys在结构定义时直接定义碎片为一个整体

The screenshot displays the Reaxys Structure editor interface. The main workspace shows a chemical structure of benzaldehyde (left) and benzyl alcohol (right), with an arrow indicating the transformation. The search panel on the right is active, showing options for searching the structure: 'As drawn', 'As substructure' (selected), and 'Similar'. Under 'As substructure', there are radio buttons for 'On all atoms' (selected), 'On heteroatoms', and 'Similar'. A pop-up menu is overlaid on the search panel, showing options for 'Ignore Atom Mappings' (unchecked) and 'Keep fragments' (checked). Under 'Keep fragments', there are radio buttons for 'Separate' and 'Together' (selected). The 'More options' button is also visible.

New Reaxys定义的时候，可以直接选择Fragments是否在一个片段中

最后的结果

The screenshot displays the Reaxys search results interface. On the left, a sidebar titled "Filters and Analysis" lists various search criteria such as "By Structure", "Yield", "Reagent/Catalyst", "Solvent", "Catalyst Classes", "Solvent Classes", "Product Availability", "Reactant Availability", "Reaction Classes", "Document Type", and "Publication Year". The main area shows search results for "188 Reactions, 156 Documents, 350 Substances, 2 Targets". Three reaction entries are visible:

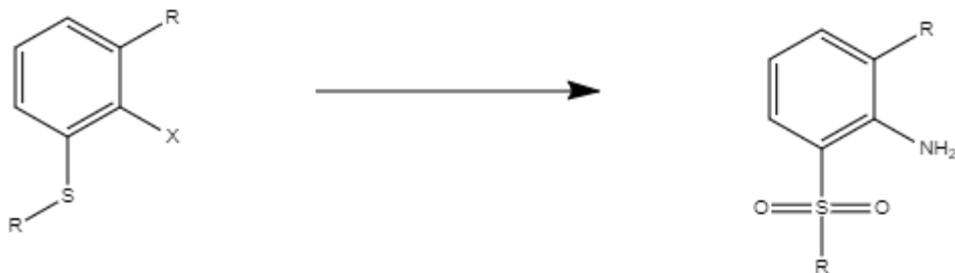
- Reaction ID: 46555509
- Reaction ID: 9213594
- Reaction ID: 29688187 (highlighted in a callout box)

Each reaction entry includes a chemical structure diagram showing the reactant and product, along with interactive icons for search, zoom, and conditions. The callout box for Reaction ID: 29688187 shows a reaction where a reactant with a chiral auxiliary and an aldehyde group is converted to a product with a chiral auxiliary and a primary alcohol group.

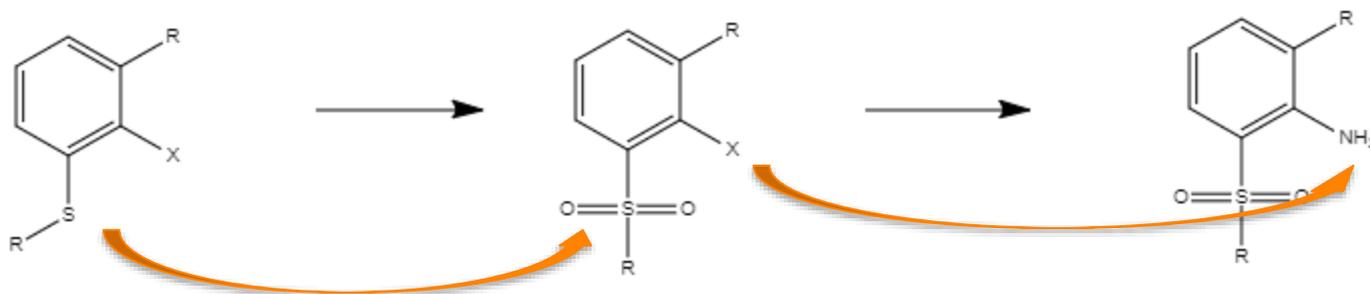
从结构上看，所有的结构中都包含2个片段

Case Study 3

- 检索以下的反应



- 常规做法如下



实际上的情况

- 实际的情况
 - 由于空间位阻的问题，无法取代NH₂
 - 由于砜也是一个离去基团，砜基团在第二步反应时脱落
- 修改的思路
 - 先变成亚砜，取代NH₂后，在变成砜



常规的检索

Reaxys® Quick search Query builder ^{new} Results Synthesis planner History Register > Sign in ?

Structure editor ¹ Create structure template from name >

Search this structure as:

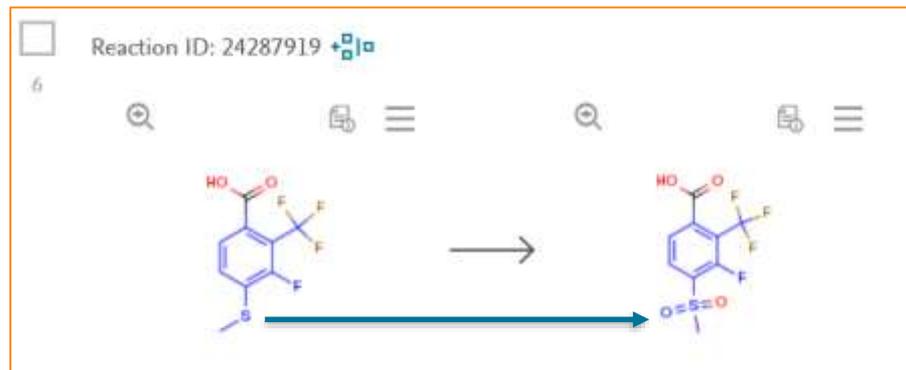
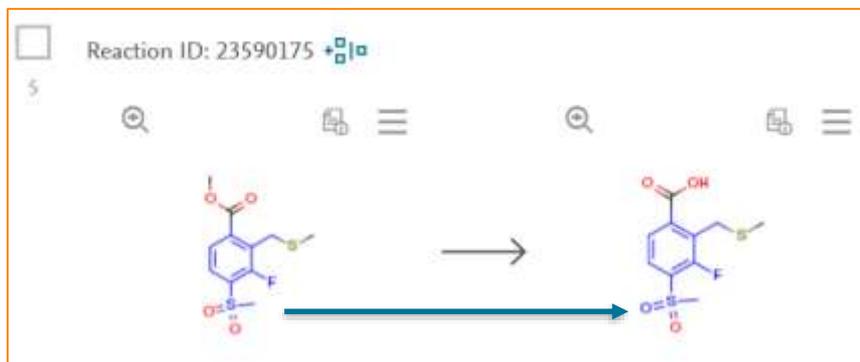
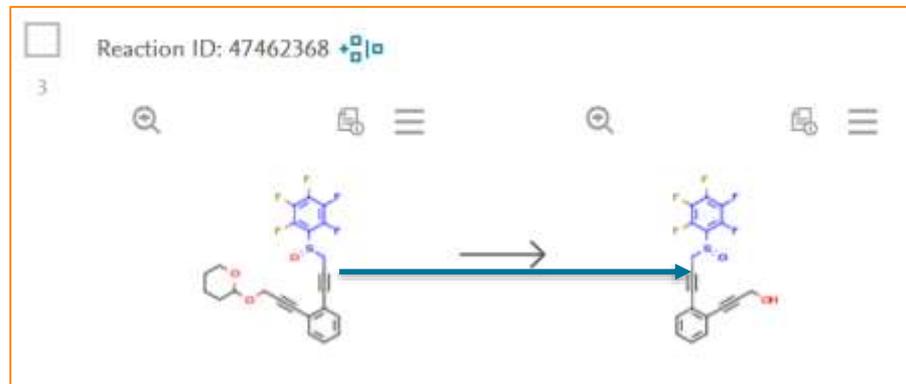
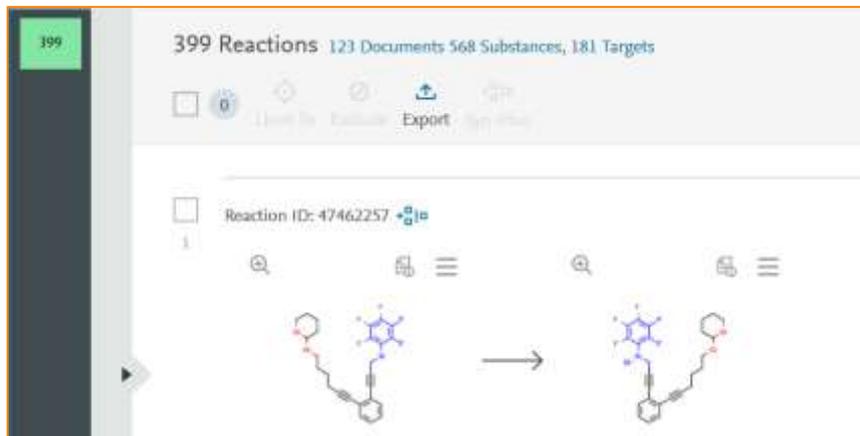
- As drawn
- As substructure
 - On all atoms
 - On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear Cancel Transfer to query >

Feedback

检索到的结果



常见的不符合要求的反应：

1. 亚砷变成亚砷的
2. 砷变成砷的
3. 硫醚变成砷的

问题解决出发点

- 不符合要求的反应
 - 亚砷变成亚砷的
 - 砷变成砷的
 - 硫醚变成砷的
- 原因分析
 - S原子在进行检索时，价态的变化而导致
- 如何解决
 - Solution 1:
 - Solution 2:

Solution 1: S*的应用

The screenshot displays the Reaxys software interface. At the top, there are navigation options: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". On the right, there are buttons for "Register" and "Sign in". The main area is the "Structure editor", which contains a chemical reaction scheme. The reactant is a benzene ring with substituents G and X, and a methyl group (H₃C) attached to a sulfur atom (S). The product is the same benzene ring with G and X, but the sulfur atom is now double-bonded to an oxygen atom (S=O). Two orange arrows originate from the sulfur atom in the reactant and point to the sulfur atom in the product, indicating that the sulfur atom is locked (S Lock) during the reaction. The right sidebar shows search options: "Search this structure as:" with radio buttons for "As drawn", "As substructure", "On all atoms", and "On heteroatoms"; "Similar" with a radio button; and checkboxes for "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", and "Radicals". At the bottom of the editor, there are buttons for "Clear", "Cancel", and "Transfer to query".

利用S Lock将反应物，产物中的S锁定即可

Solution 2: v+/v-的应用

The screenshot shows the Reaxys Structure editor interface. The main workspace displays a chemical reaction where a methyl-substituted benzene ring with substituents G and X reacts to form a corresponding sulfonamide derivative. The sulfur atom in the product is highlighted with a blue box and labeled with a query property. On the right side, the 'Search this structure as:' panel is open, showing various search options. A red box highlights the 'Similar' section, specifically the 'A' (Atom) query type. Below this, a table of query properties is shown, with a red box highlighting the 'v+' and 'v-' options. A red arrow points from the 'v+' option in the table to the sulfur atom in the product structure. Another red arrow points from the 'v+' option in the table to the 'v+' option in the 'Atom query properties' dialog box. The 'Atom query properties' dialog box is also open, showing a grid of query properties including .H+, .h+, .v+, .X+, .H-, .h-, .v-, .X-, .R+, .r+, .rb+, .s+, .R-, .r-, .rb-, .s-, .u, .a/A, .rb*, and .s*.

Tips:

1. V+/V-的定义，表示被标记的原子的价位
2. 类似的情况还有，氮氧化合物

最后的结果

Reaxys® Quick search Query builder ^{new} Results Synthesis planner History Register > Sign in ?

77 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

77 Reactions out of 38 Documents containing 129 Substances, 8 Targets

0 Limit To Exclude Export Syn-Plan Product Availability ↓ ▾

1 Reaction ID: 36121047

1 Conditions ▾ Find Similar >

2 Reaction ID: 36121123

1 Conditions ▾ Find Similar >

Case Study 4

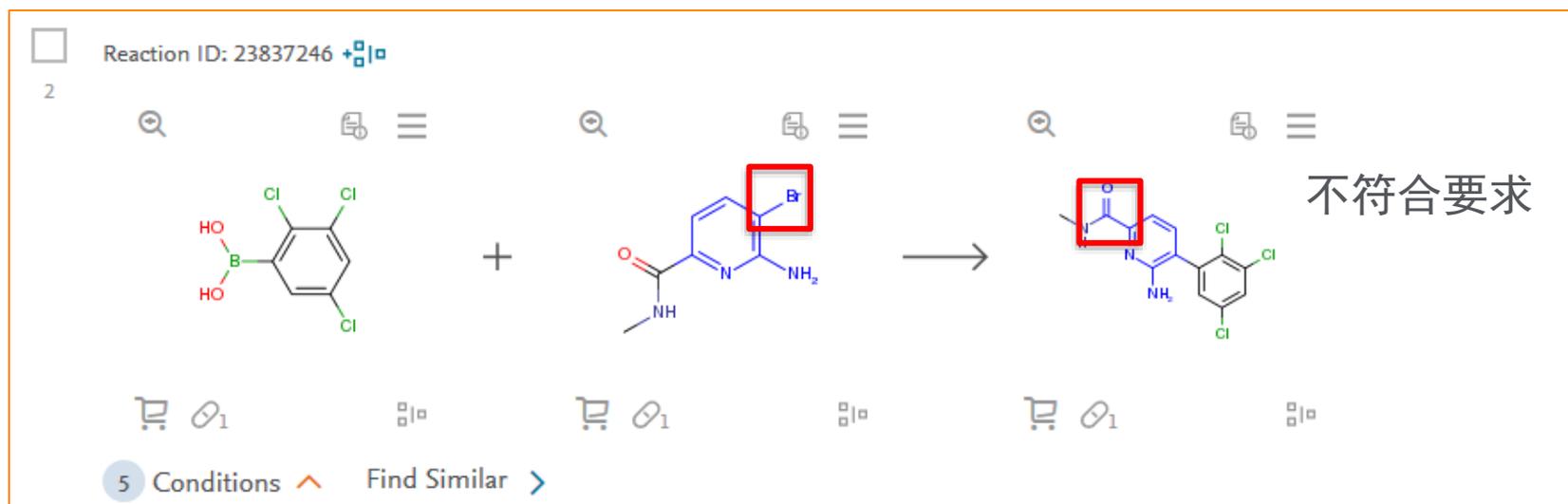
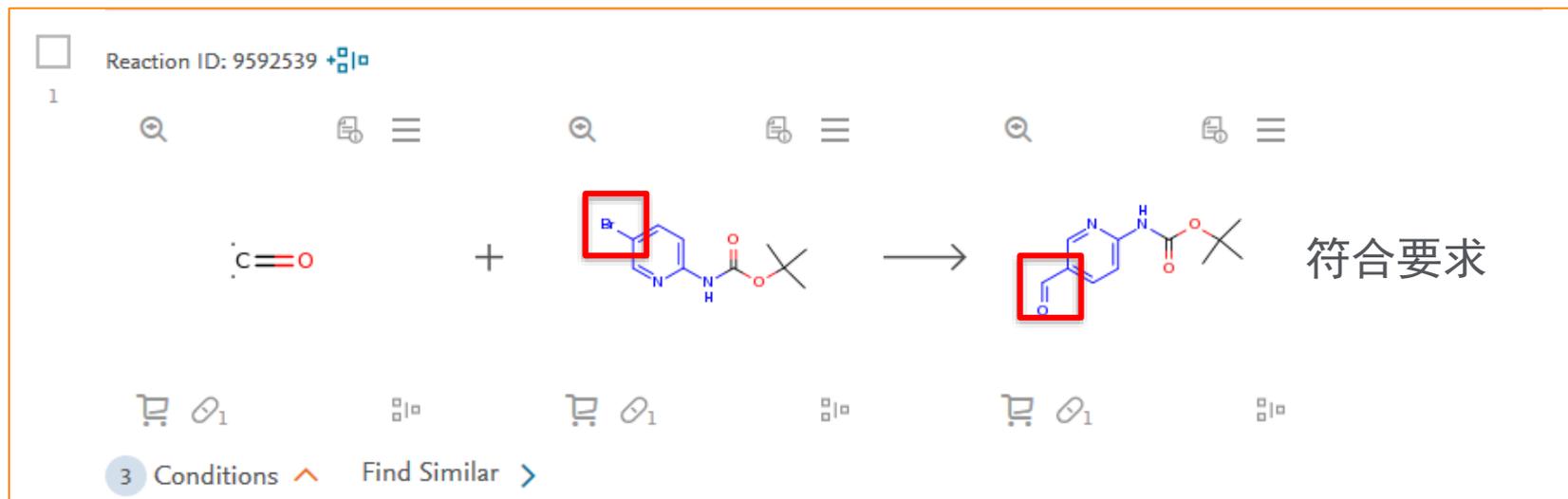
- 检索以下反应，将Br变成羰基

The screenshot displays the Reaxys Structure editor interface. At the top, there are navigation links: Quick search, Query builder, Results, Synthesis planner, and History. On the right, there are buttons for Register and Sign in. The main workspace shows a chemical reaction: 2-amino-5-bromopyridine (left) reacts to form 2-amino-5-formylpyridine (right). The interface includes a search sidebar on the right with the following options:

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

At the bottom of the editor, there are buttons for Clear, Cancel, and Transfer to query. A Feedback button is located in the bottom right corner.

检索到的结果

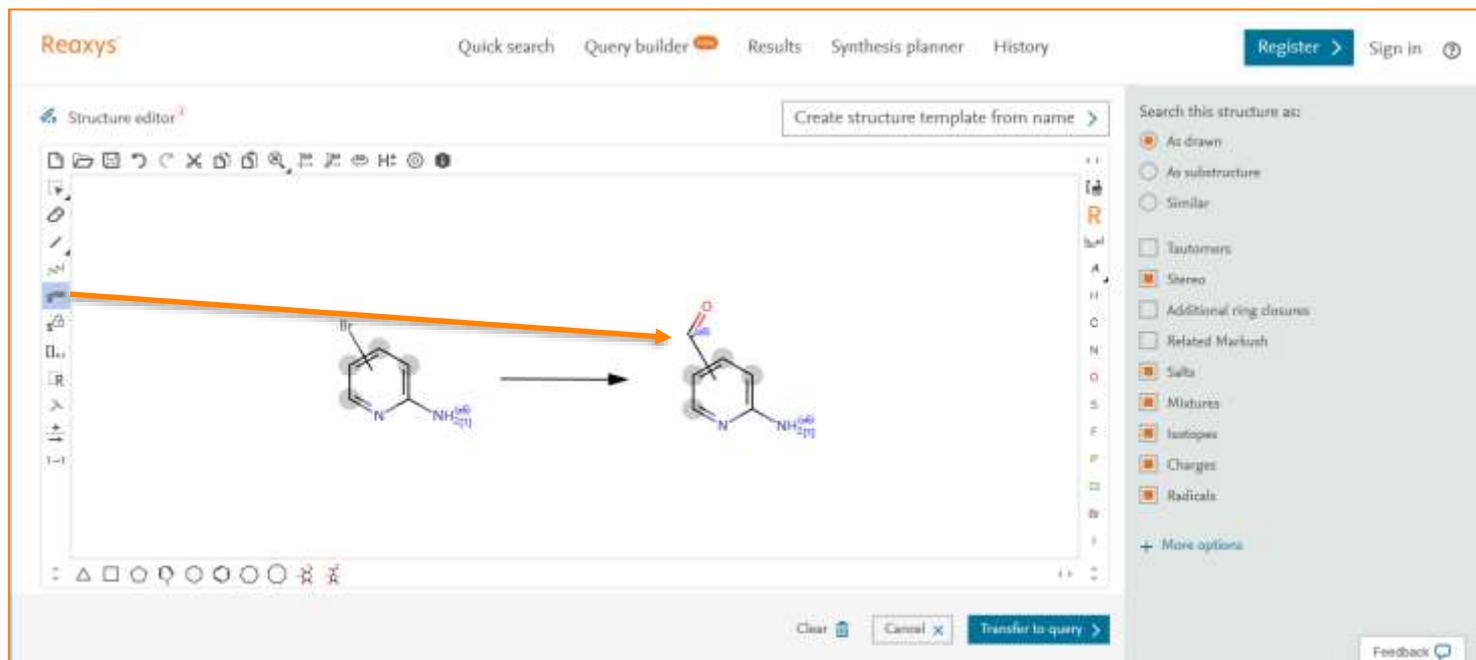


如何解决

- 不符合要求的反应
 - C=O在原来反应物中带过来
 - 不是在Br的地方换成C=O
- 原因分析
 - 不定位取代的时候没有办法做原子映射
- 如何解决
 - Solution 1:
 - Solution 2:

Solution 1: 换一个检索模式

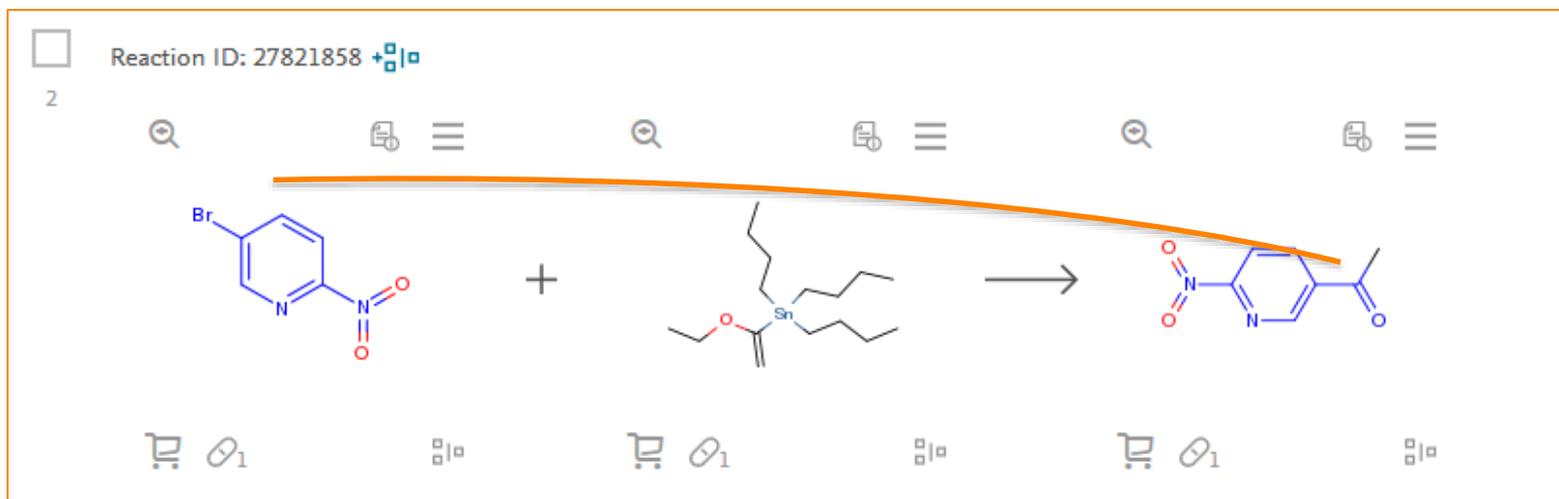
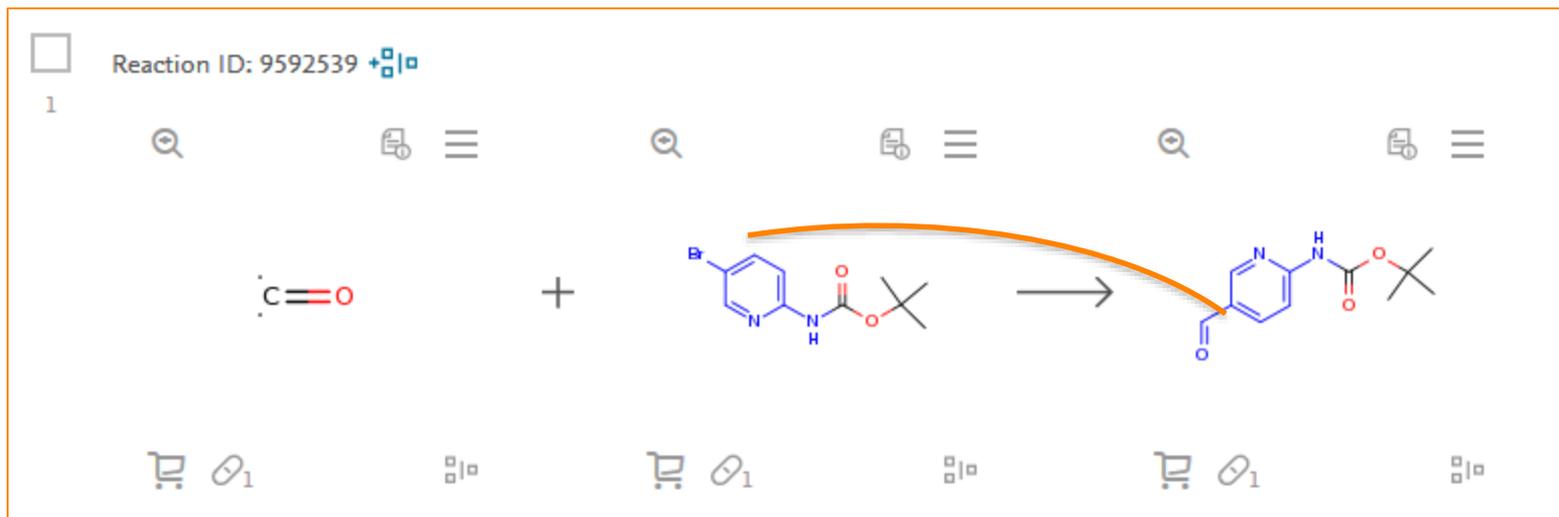
- As Draw检索同样结构



Tips:

1. 使用As Draw，可以使得Br变成C=O，但也封闭了C=O，NH₂上的取代可能性
2. 可以使用S Max标记C=O，NH₂，在进行As Draw检索时，实现原子的开放
3. 该检索结果，吡啶上只能有一个取代基

检索结果



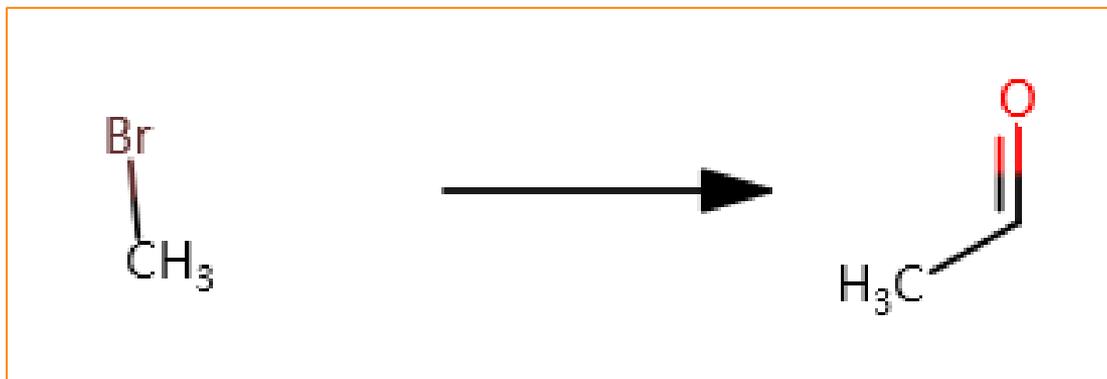
Solution 2: 对于As Substructure结果的筛选

- 利用结构进行筛选

The screenshot displays the Reaxys web interface. On the left, a sidebar titled "Filters and Analysis" is visible, with the "By Structure" filter selected. A "Create Structure Drawing" button is highlighted. The main area shows a list of reactions. The first reaction, with ID 9592539, shows the reaction of a carbonyl compound with a substituted pyridine derivative to form a product. The second reaction, with ID 23837246, shows the reaction of a chlorinated benzene derivative with a substituted pyridine derivative to form a product. The interface includes navigation options like "Quick search", "Query builder", "Results", "Synthesis planner", and "History", along with "Register" and "Sign in" buttons.

筛选的出发点

- 问题的结症
 - Br和C=O接在吡啶上的位置不确定，无法保证对应
- 反应的共性
 - 但是Br，C=O都是接在C上，且该C原子一定在一个芳环，或者一定要有一个不饱和键
- 筛选的结构
 - 基本上反应中心如下

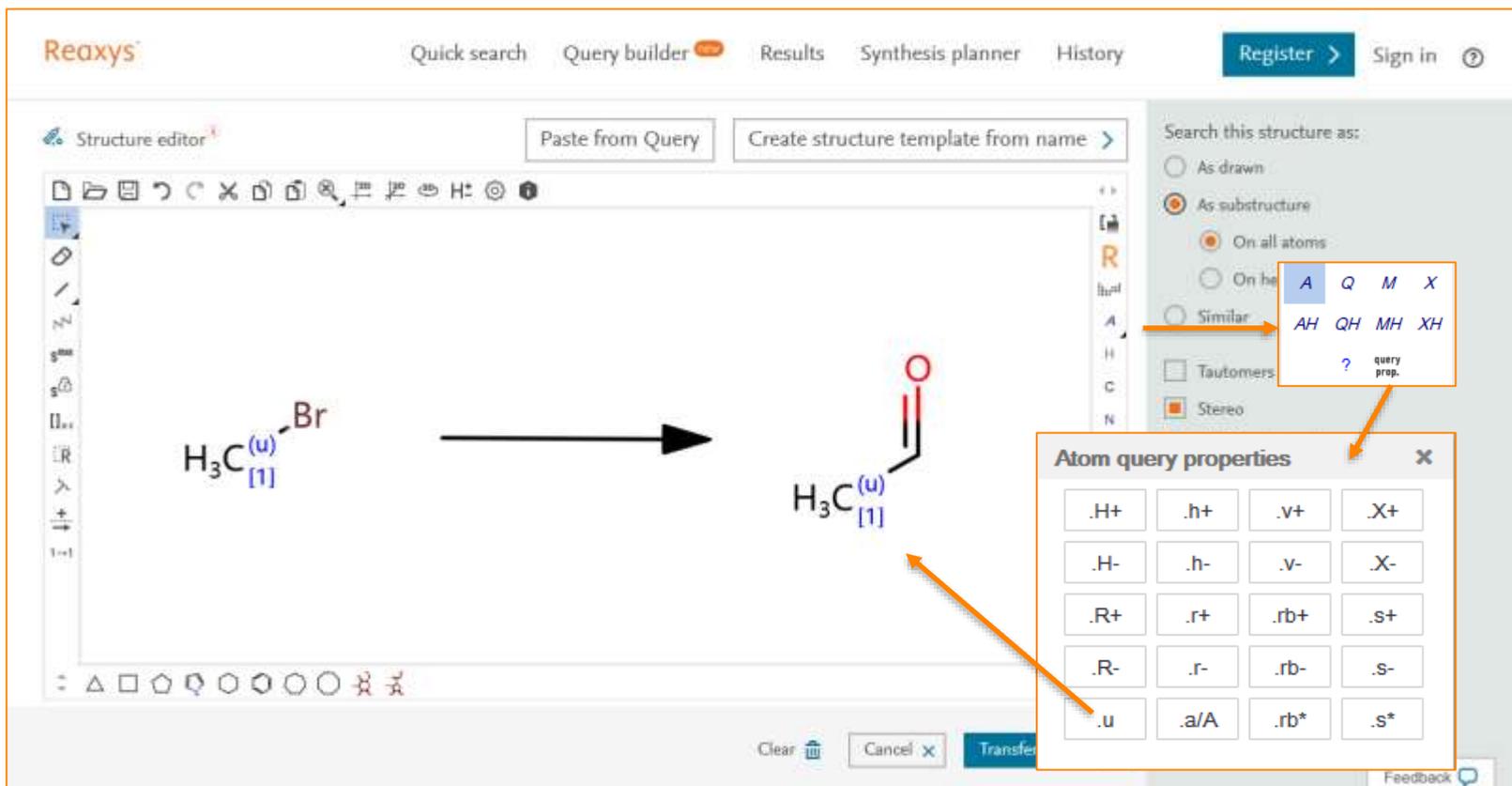


如何绘制



Tips:

1. 如果对于C原子有要求，可以带上U的定义，
2. 如果没要求，也可以不画



The screenshot shows the Reaxys Structure editor interface. On the left, a structure of methyl bromide ($\text{H}_3\text{C}-\text{Br}$) is shown with the carbon atom labeled $\text{H}_3\text{C}(\text{u})$ and a [1] in brackets below it. An arrow points to the right, where the resulting structure is shown: a methyl group (H_3C) with the carbon atom labeled $\text{H}_3\text{C}(\text{u})$ and a [1] in brackets below it, and a carbonyl group ($\text{C}=\text{O}$) attached to the right. The interface includes a toolbar with various drawing tools, a search bar, and a 'Structure editor' panel. On the right side, there is a 'Search this structure as:' panel with options like 'As drawn', 'As substructure', 'On all atoms', 'On he', and 'Similar'. The 'Similar' option is selected, and a dropdown menu shows 'A Q M X' and 'AH QH MH XH'. Below this, there is a 'Atom query properties' panel with a grid of query properties: .H+, .h+, .v+, .X+, .H-, .h-, .v-, .X-, .R+, .r+, .rb+, .s+, .R-, .r-, .rb-, .s-, .u, .a/A, .rb*, .s*.

添加筛选后的界面

Reaxys

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

558 Filters and Analysis

Limit to > Exclude >

By Structure

On all atoms

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

558 Reactions out of 220 Documents containing 888 Substances, 103 Targets

Reaction ID: 9592539

100%

With N,N,N,N-tetramethylethylenediamine; hydrogen; cat-
axonium A; palladium diacetate in tetrahydrofuran at 100°C;
under 3750.38 Torr, for 16h;

Experimental Procedure

References

SANOPI; BOEHM, Claudius; KLEIN, Susanne; NAPIERSKI, Bernd;
SOMMER, Christian - WO2012/62730, 2012, A1
Location in patent: Page/Page column 22
Full Text > Details > Abstract >

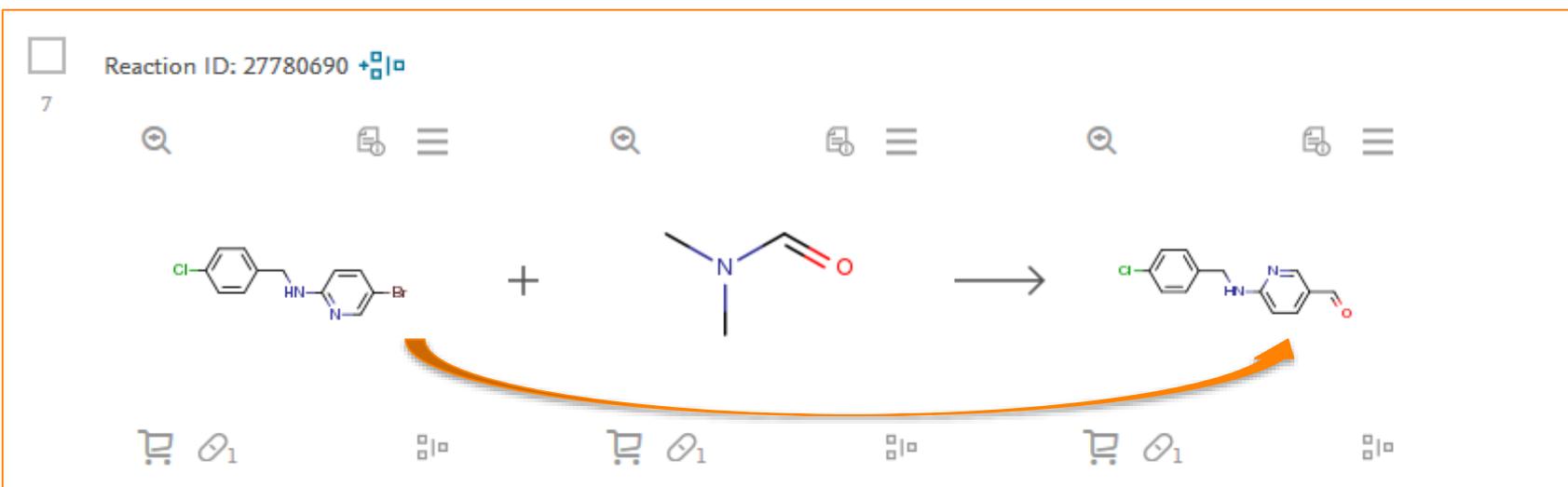
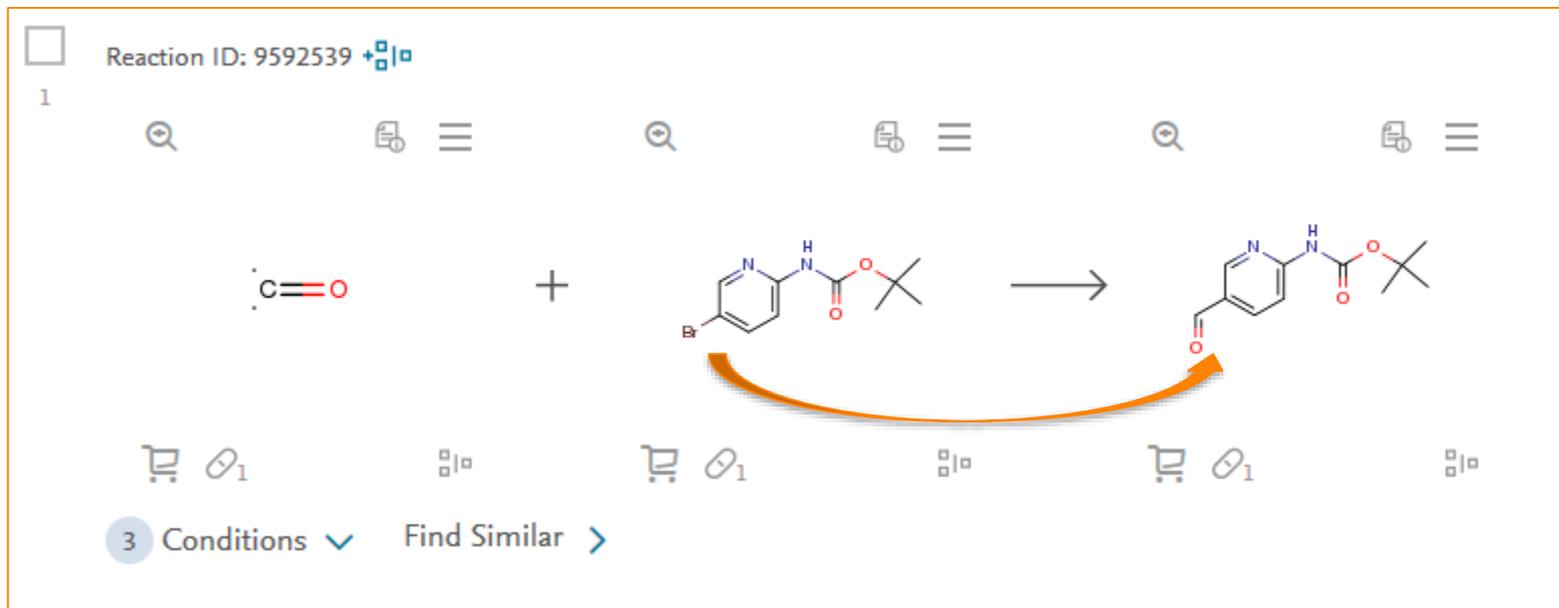
100%

With N,N,N,N-tetramethylethylenediamine;
ladium diacetate; cataxonium A in tetrahydrofuran at 100°C;
under 3750.38 Torr, for 16h;

Show Less

Feedback

最后的结果



提纲

- Reaxys的基本介绍和数据索引
- Reaxys最新更新（近期即将）
- Reaxys中的检索
 - Reaxys中结构面板高级应用
 - Reaxys中的高级反应检索
 - Reaxys中的合成计划设计
- Reaxys检索小结

Reaxys中的合成计划

- 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

gefitinib
C22H24ClFN4O3 446.909 8949523 184475-35-2

Identification Bioactivity (All) Spectra - 53 Preparations - 65 >
Druglikeness Physical Data - 67 Other Data - 2,552 Reactions - 101 >
Targets - 1,047 >
Documents - 3,884 >

Tips:

- 1: 通过前述的操作找到物质
- 2: 点击Synthesize图标
- 3: 打开Synthesis Plan, 这里选择手动

Synthesize X

> Manually

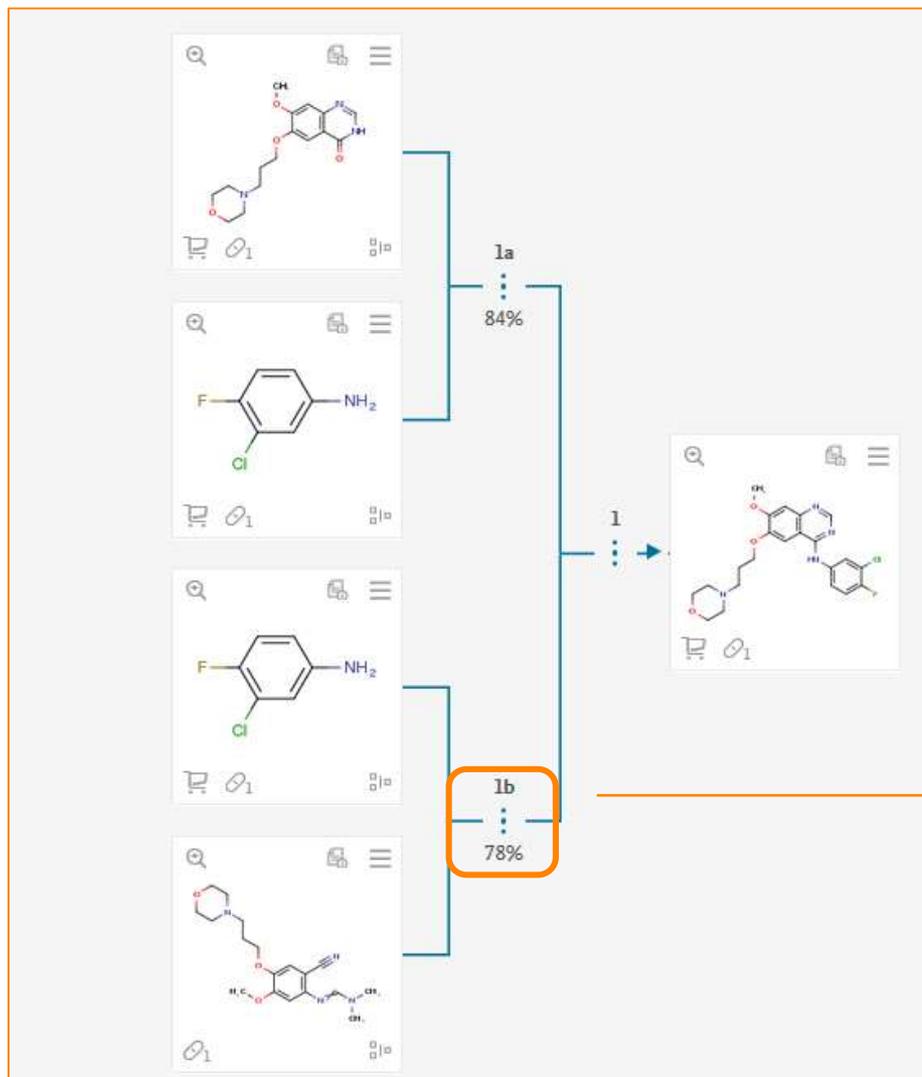
> Autoplan

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

The screenshot displays the Reaxys Synthesis Planner interface. On the left, a sidebar titled "Filters and Analysis" lists various search criteria such as "By Structure", "Yield", "Reagent/Catalyst", "Solvent", "Catalyst Classes", "Solvent Classes", "Product Availability", "Reactant Availability", "Reaction Classes", "Document Type", and "Publication Year". The main area shows a list of 64 reactions. Two reactions are highlighted with orange boxes and arrows pointing to the "+ Syn-Plan" button. The first reaction, with ID 11041177, shows a complex polycyclic aromatic hydrocarbon reacting with 4-chloroaniline. The second reaction, with ID 36604056, shows 4-chloroaniline reacting with a complex polycyclic aromatic hydrocarbon. The interface includes navigation tabs for "Quick search", "Query builder", "Results", "Synthesis planner", and "History". The top right corner shows the user name "Sam Yu" and notification icons. The bottom of the screen shows the "Conditions" and "Find Similar" options for each reaction.

添加好的结果界面



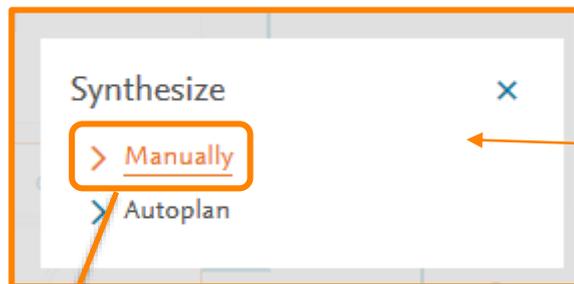
Preparation - 1b

Yield	Conditions	Reference
78%	With acetic acid at 130°C; for 3h; Temperature; Experimental Procedure \downarrow	Guangzhou Baiyunshan Pharmaceutical Group Co., Ltd. Baiyunshan Pharmaceutical Zong Factory; Chen Mao; Zhu Shaowen; Huang Xiaoguang - CN104072426, 2017, B Location in patent: Paragraph 0030, 0031, 0052, 0053, 0054, 0055 Full Text \uparrow Details \gt Abstract \gt
71.1%	With acetic acid in 5,5-dimethyl-1,3-cyclohexadiene at 135°C; Experimental Procedure \downarrow	Shanxi Normal University; Li, Baolin; Ren, Yufei; Wang, Liuchang; Jia, Yuwei; Qing, Siyi; Wang, Wei - CN101519702, 2016, B Location in patent: Paragraph 0094-0096 Full Text \uparrow Details \gt Abstract \gt
70%	With acetic acid at 125 - 130°C; for 3h;	- Organic Process Research and Development, 2007, vol. 11, # 5, p. 813 - 816 Full Text \uparrow Cited 51 times \uparrow Details \gt Abstract \gt

Context menu options:

- Show conditions
- Hide preparation
- Remove preparation

继续的扩充反应路线



Reaxys

Quick search Query builder Results Synthesis planner History

Filters and Analysis

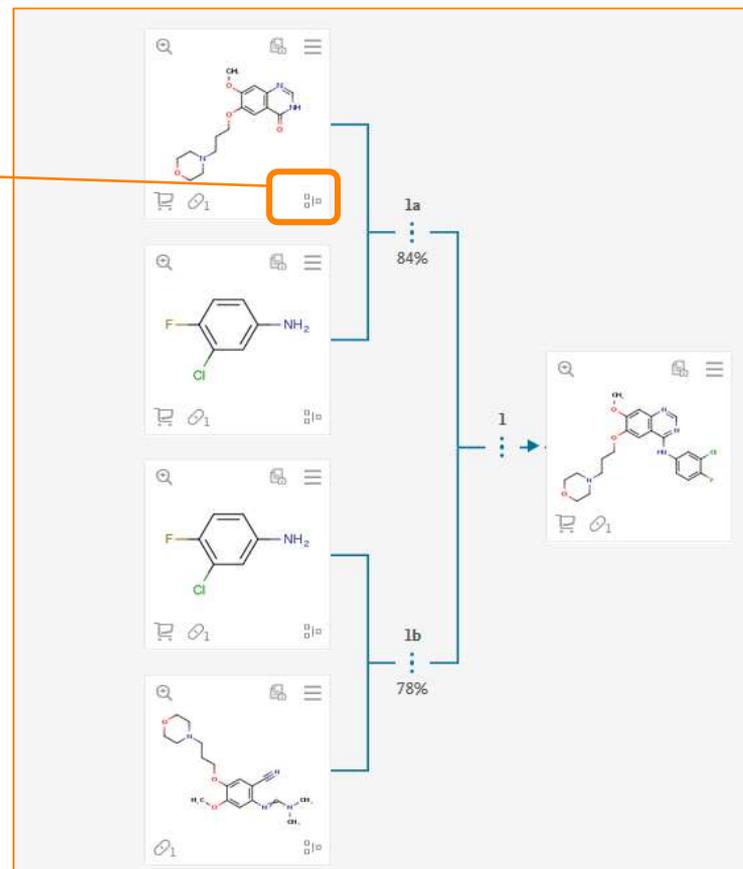
By Structure Yield Reagent/Catalyst Solvent Catalyst Class Solvent Class Product Availability Reagent Availability Reaction Class Document Type Publication Year

33 Reactions out of 28 documents containing 17 substances, 6 targets

Reaction ID: 2922877

Reaction ID: 4204370

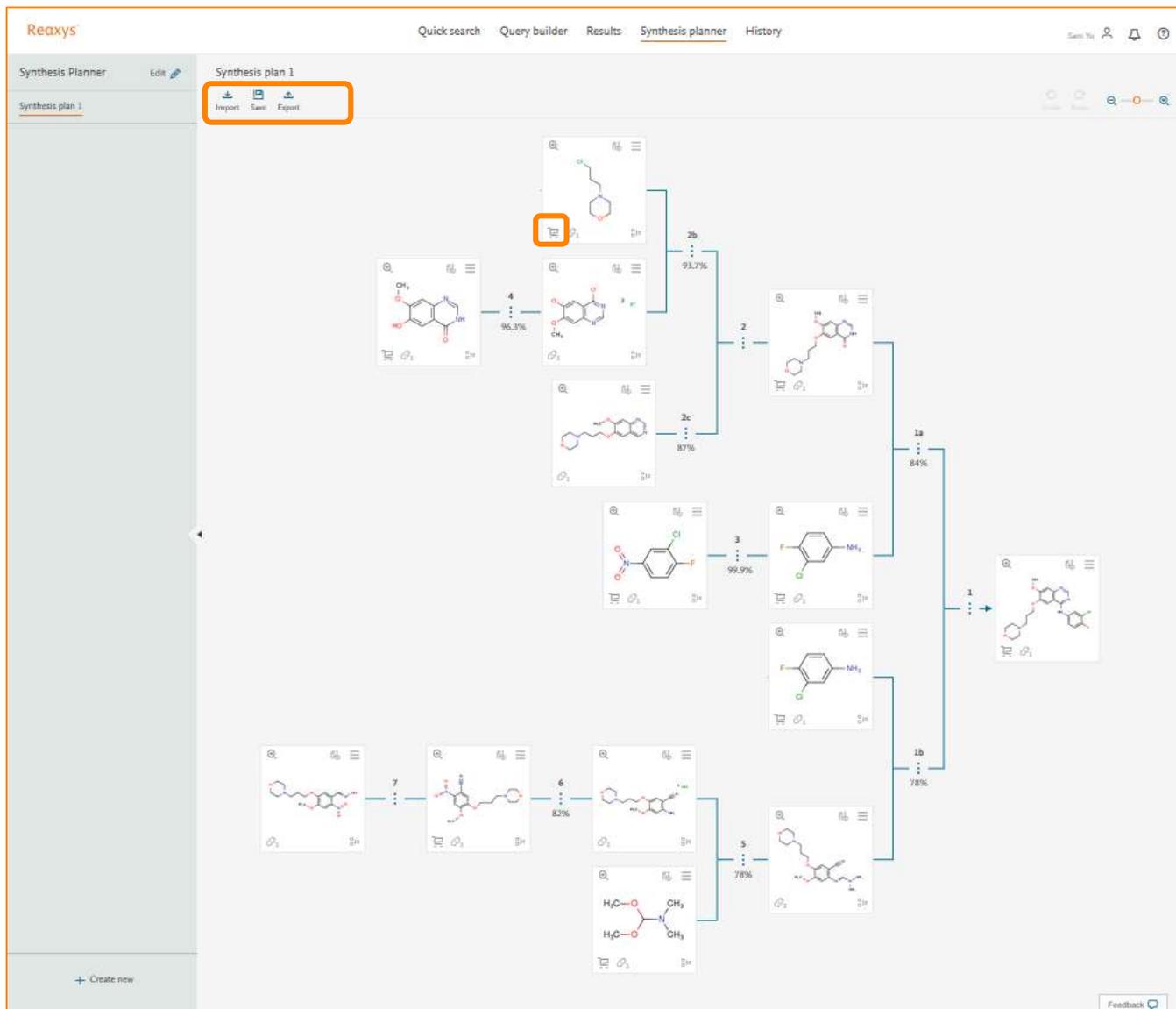
Reaction ID: 4204371



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
- CambridgeSoft ACX
- Labnetwork
- Sigma Aldrich

LabNetwork 药明康德 WuXi AppTec

4-(3-chloropropyl)morpholine

Chemical structure:

宽博网化合物ID: LN00004308
 CAS: 7367-67-7
 MDL: MFCD00039714
 分子式: C7H14ClNO
 分子量: 163.6464
 Log P: 暂无
 重原子个数: 10
 同位素原子数: 暂无

SMILES: ClCCCNC1CCOCC1
 InChi 编码: PIAZYBLGBSMNLX-UHFFFAO YSA-N
 InChi: InChi=1S/C7H14ClNO/c8-2-1-3-9-4-6-10-7-5-9/r1-7/H2
 氢键受体数: 2
 氢键给体数: 0
 旋转键数: 3

共显示 51 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
4-(3-Chloropropyl)morpholine(WX630132) 规格ID: WX630132	上海药明康德新药开发有限公司	★★★★★	¥875.00 (100g)	96%	询盘	- 展开
N-(3-Chloropropyl)morpholine 规格ID: Runsheng222	郑州润东化工有限公司	★★★★★	¥85.00 (10g)	暂无	50g - CN	- 展开
4-(3-Chloropropyl)morpholine 规格ID: 14-02393	Atlantic Research Chemicals	★★★★★	¥89.25 (1g)	97%	494.75g - UK	- 展开
4-(3-Chloro-propyl)morpholine 规格ID: 15-030-003	Advanced Chemical Intermediates (ACINTS)	★★★★★	¥81.00 (1g)	96%	9g - UK	- 展开
4-(3-chloropropyl)morpholine 规格ID: 48-61-0228201	Specs	★★★★★	¥208.00 (100mg)	暂无	询盘	- 展开
N-(3-Chloropropyl)morpholine 规格ID: AB10000002	萨奥化学技术(上海)有限公司	★★★★★	¥85.00 (5g)	96%	3225g - CN	- 展开
4-(3-Chloropropyl)morpholine 规格ID: C3602	绿希斯上海化成工业发展有限公司	★★★★★	¥390.00 (5g)	96%	5g - CN-SH 10g - CN-TJ	- 展开
4-(3-Chloropropyl)morpholine 规格ID: 1100388	北京飞达瑞商贸有限公司	★★★★★	¥2118 (5g)	96%	95g - CN	- 展开
4-(3-Chloropropyl)morpholine 规格ID: 104081	上海皓鸿生物医药科技有限公司(乐研品牌)	★★★★★	¥77.00 (25g)	96%	1000g - CN-SH	- 展开
4-(3-Chloropropyl)morpholine 规格ID: 127673	Toronto Research Chemicals	★★★★★	¥425.00 (100mg)	暂无	询盘	- 展开

提纲

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 - Reaxys中的高级反应检索
 - Reaxys中的合成计划设计
- Reaxys检索小结

Reaxys反应检索小结

- As Draw检索和As Substructure检索的区别
- 结构面板上的一些功能，必须配合不同的检索模式才能实现，如S Max, S Lock
- Reaxys的结构面板给予用户更多的自由度，可以实现原子，键的各类属性定义。
- Limit to和Exclude的处理，帮助用户用最简便的方式，去实现对需要，和不需要结果集的获取和排除
- 反应检索遇到困难时，多思考下共性，看如何用结构面板解决，更多的是可以反向思考，如何排除不需要的答案
- 有问题，欢迎随时交流。



**If you have questions feel
free to reach out**

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p.wu.1@Elsevier.com