

# New Reaxys 使用介绍

Reaxys 解决方案咨询师  
俞靓

Presented By  
Date

## 提纲

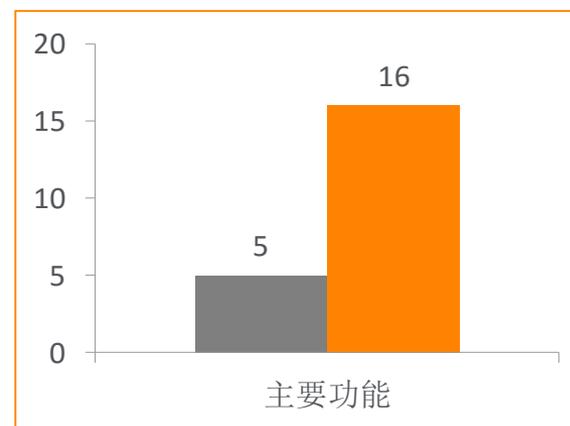
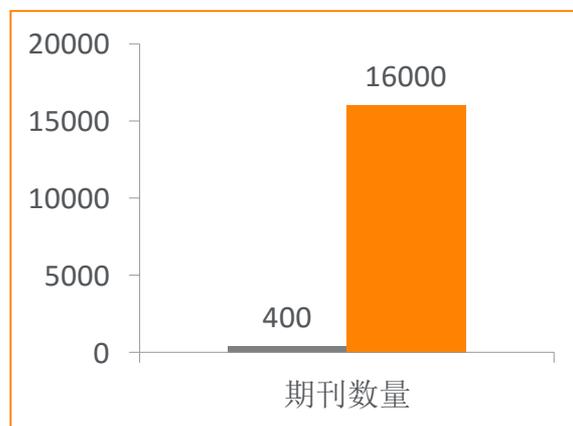
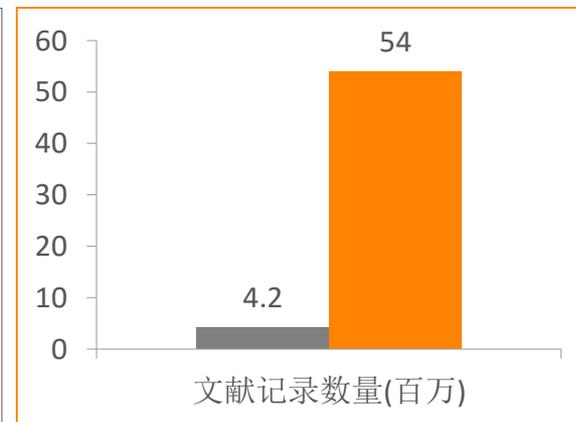
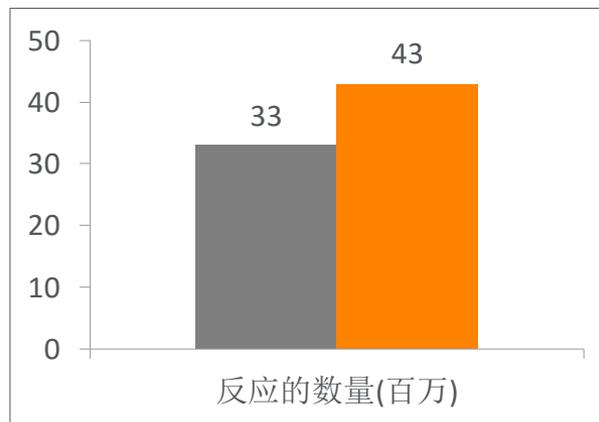
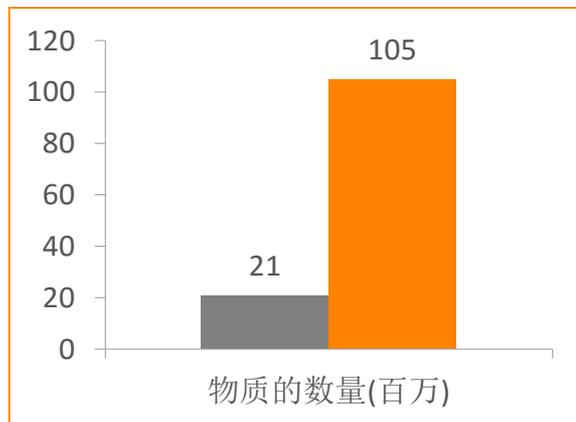
- Reaxys中的内容和数据索引介绍
- Reaxys中的检索案例
  - 如何利用Reaxys做物质分析研究
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行反应设计和反应筛选
  - 如何利用Reaxys进行合成计划制作
- Reaxys检索小结

# Reaxys的数据量在过去5年得到极大的提升...

2012 → 2017

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

■ REAXYS 2012 ■ REAXYS 2017



# New Reaxys中拥有更广泛的专利覆盖

- New Reaxys收录更多的亚太区域的专利



	World	US	Europe	Japan	S. Korea	China	Taiwan
≤2014	✓	✓	✓				
2015	✓	✓	✓	✓	✓		
2016	✓	✓	✓	✓	✓	✓	✓
2017	✓	✓	✓	✓	✓	✓	✓

July 2016

September 2016

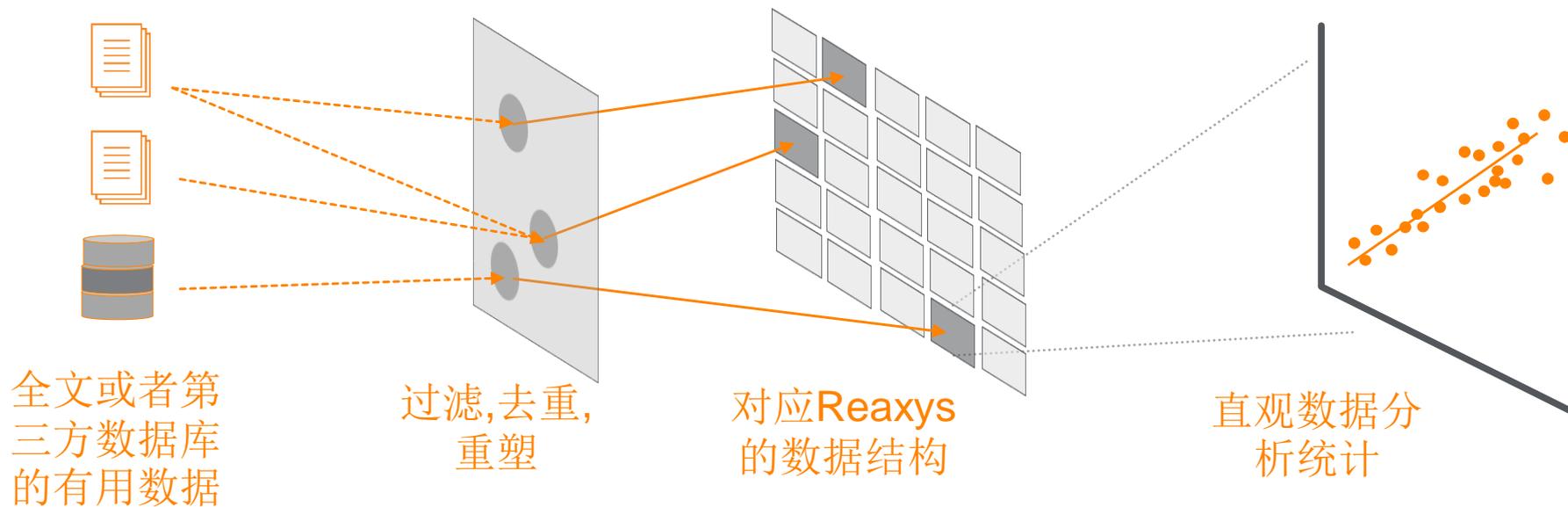
December 2016

2017



更多的源自亚洲专利中的物质将陆续添加到New Reaxys中

# Reaxys旨在弹指之间传递关键信息



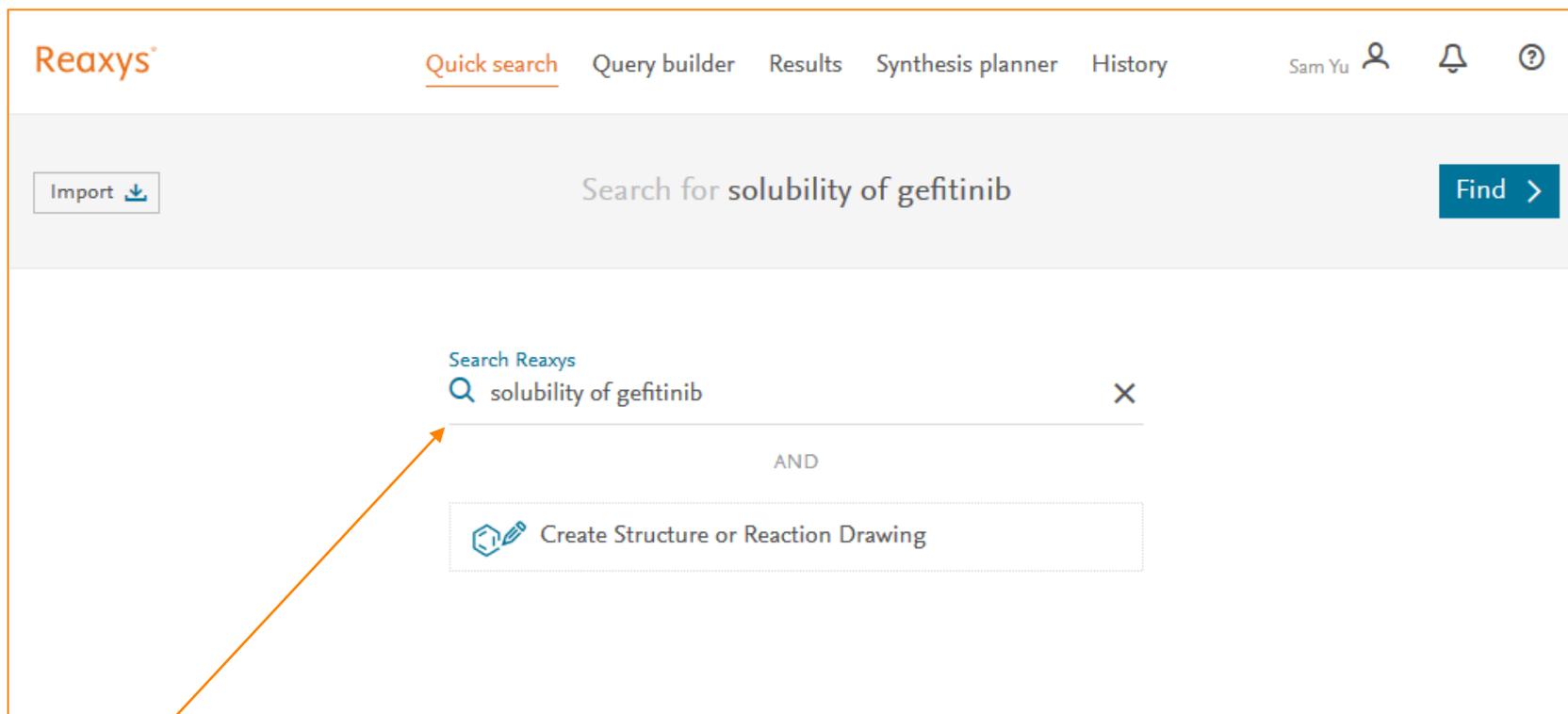
重在索引文献中的有用信息

## 提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索案例
  - 如何利用Reaxys做物质分析研究
  - 如何利用Reaxys结构面板实现复杂结构定义
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- Reaxys检索小结

## 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' and notification icons. 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 text to the search box.

直接用自然语言在输入，solubility of gefitinib，检索

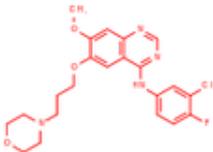
# Reaxys直接给出结果

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. The main heading is 'Results for solubility of gefitinib'. The results are listed in three rows:

Count	Category	Search Criteria	Preview Results	View Results
1	Substances	Structure :  as drawn AND Property : solubility	Preview Results ▾	<a href="#">View Results &gt;</a>
96	Documents	Titles, Abstract, Keywords : solubility, gefitinib	Preview Results ▾	<a href="#">View Results &gt;</a>
277,479	Documents	Titles, Abstract, Keywords : solubility	Preview Results ▾	<a href="#">View Results &gt;</a>

The 'View Results >' button for the first result (Substances) 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

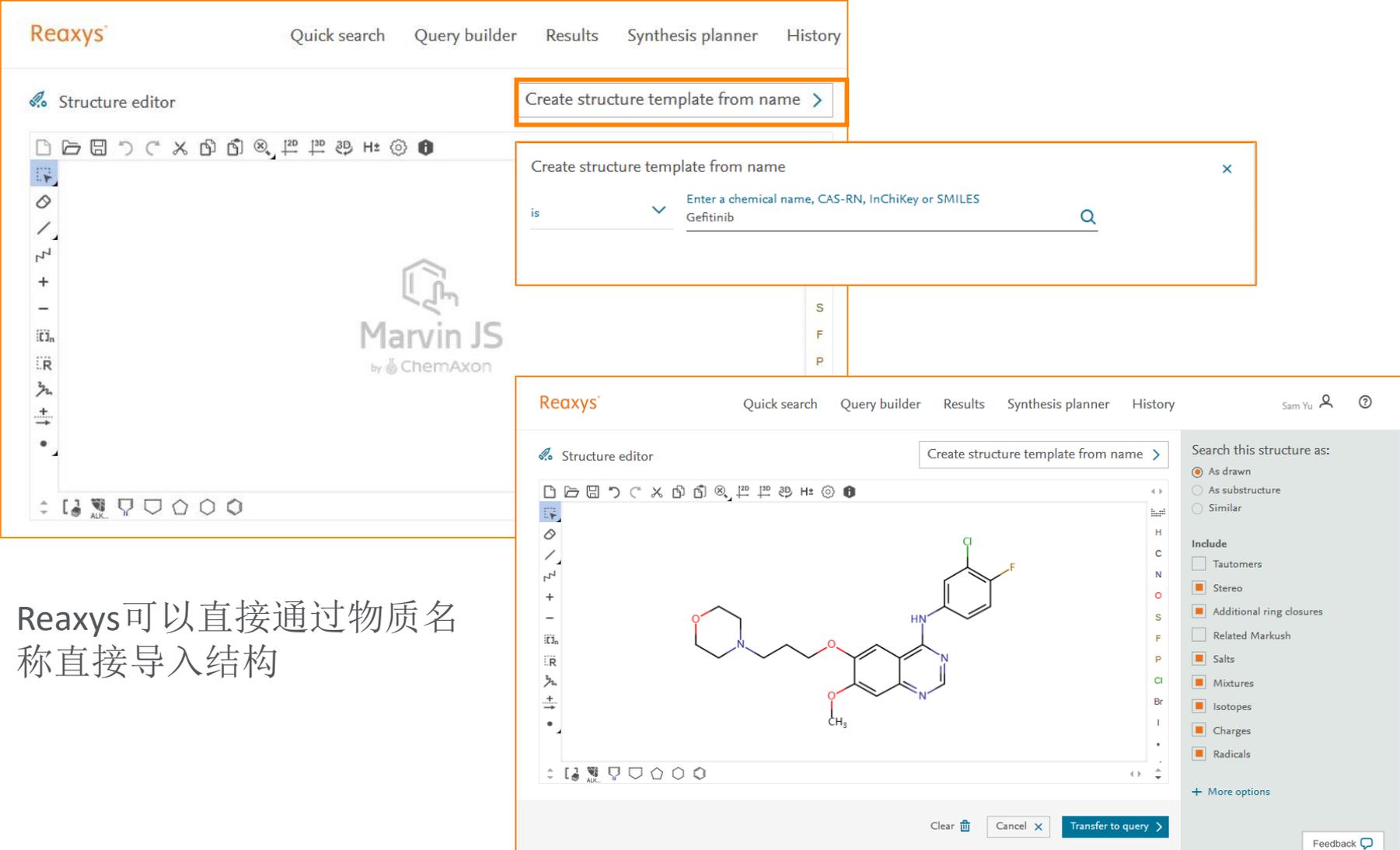
v Solubility (MCS) - 1 hits out of 1

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

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

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—获得药物的全部理化性质和分析方法



Reaxys

Quick search Query builder Results Synthesis planner History

Structure editor

Create structure template from name >

Create structure template from name

is Enter a chemical name, CAS-RN, InChiKey or SMILES

Gefitinib

Marvin JS  
by ChemAxon

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
- Similar

Include

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

+ More options

Clear Cancel Transfer to query

Feedback

Chemical structure of Gefitinib is shown in the main editor area.

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 ▾	<b>View Results &gt;</b>
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 interface.

# New Reaxys中的结果集

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sam Yu

222 Filters and Analysis

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

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes

0 Limit To Exclude Export No of References ↓ Heatmap

1

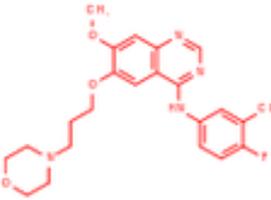
**gefitinib**  
C<sub>22</sub>H<sub>24</sub>ClFN<sub>4</sub>O<sub>3</sub> 446.909 8949523 184475-35-2

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**

C<sub>22</sub>H<sub>24</sub>ClFN<sub>4</sub>O<sub>3</sub> 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 >

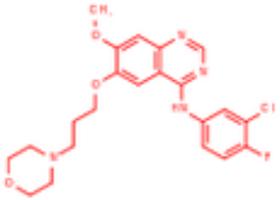
^ Physical Data - 52

- ∨ 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; <a href="#">+5 others</a> - CN105218476, 2016, A <a href="#">Full Text</a> ↗ <a href="#">Show details</a> >
white	Paragraph 0038	Southwest University of Science and Technology; WANG, CHUANFANG; <a href="#">+2 others</a> - CN105399688, 2016, A <a href="#">Full Text</a> ↗ <a href="#">Show details</a> >
white	Paragraph 0037	CSPC Zhongqi Pharmaceutical Technology(Shijiazhuang)Corporated; CSPC Ouyi Pharmaceutical Co., Ltd; Zhang, Yanqiao; <a href="#">+4 others</a> - CN103319422, 2016, B <a href="#">Full Text</a> ↗ <a href="#">Show details</a> >

# New Reaxys中的谱图



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

Identification  
 Druglikeness  
 Bioactivity (All)

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

^ Spectra - 43

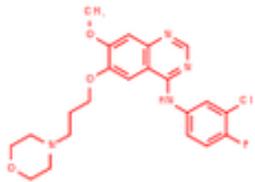
- ∨ NMR Spectroscopy - 27
- ∨ IR Spectroscopy - 4
- ∨ Mass Spectrometry - 7
- ∨ UV/VIS Spectroscopy - 4
- ∨ Raman Spectroscopy - 1

## Tips:

Reaxys直接摘录原文中的NMR谱图描述，并提供原文中的位置

<p><sup>1</sup>H NMR (400 MHz, d<sub>6</sub>-DMSO) 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>	<p>Paragraph 0035</p>	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1  <a href="#">Full Text ↗</a> <a href="#">Show details &gt;</a></p>
<p><sup>13</sup>C NMR (100 MHz, d<sub>6</sub>-DMSO) 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>	<p>Paragraph 0035</p>	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1  <a href="#">Full Text ↗</a> <a href="#">Show details &gt;</a></p>

# Reaxys中的分析文献的获取



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

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

**Tips:**

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

Reaxys<sup>®</sup>
Quick search   Query builder   Results   Synthesis planner   History
Sam Yu   

2,861

222

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

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

0 Limit To Exclude Export
Relevance v Heatmap 

- Oxindole derivatives  
<sup>1</sup> Zeneca Limited - US6265411, 2001, B1  
 Patent Family Members: GB9707800 D0; ZA9703844 B; WO1997/42187 A1; AU2647597 A; EP912557 A1; ...  
[Abstract](#) [Front Page Info](#) [Substances](#) 279 [Reactions](#) 182 [Targets](#) [Full Text](#) ↗
- Oxindolylquinazoline derivatives as angiogenesis inhibitors  
<sup>2</sup> Zeneca Limited - US6294532, 2001, B1  
 Patent Family Members: WO1999/10349 A1; AU8816298 A; EP1005470 A1; JP2001/514182 A; US6294532 B1; ...  
[Abstract](#) [Front Page Info](#) [Substances](#) 135 [Reactions](#) 81 [Full Text](#) ↗
- Use of tyrosine kinase inhibitors for the treatment of inflammatory processes  
<sup>3</sup> Boehringer Ingelheim Pharma GmbH and Co. KG - US2003/149062, 2003, A1  
 Patent Family Members: DE10204462 A1; US2003/149062 A1; CA2472293 A1; WO2003/66060 A2; ...

# Index Term Reaxys Tree的应用

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

Index Terms (List) ∨

Index Terms (ReaxysTree) ∧

- physico chemical properties 1,065
- chemical transformations 1,042
- physico chemical analysis methods 350
- quantum chemical calculation methods 165

+ More

Index Terms (ReaxysTree) 3 ×

- Index Terms (ReaxysTree) 2,861
  - physico chemical properties 1,065
  - chemical transformations 1,042
  - physico chemical analysis methods 350
    - spectroscopical analysis 165
      - luminescence spectroscopy 58
      - fluorescence spectroscopy 49
      - mass spectrometry 34
      - NMR spectroscopy 20
        - NMR spectroscopy type 15
          - 13C-NMR spectroscopy 3
          - 15N NMR spectroscopy 1

Selected search items:

13C-NMR s... troscopy ×

Clear selected × Limit To > Exclude >

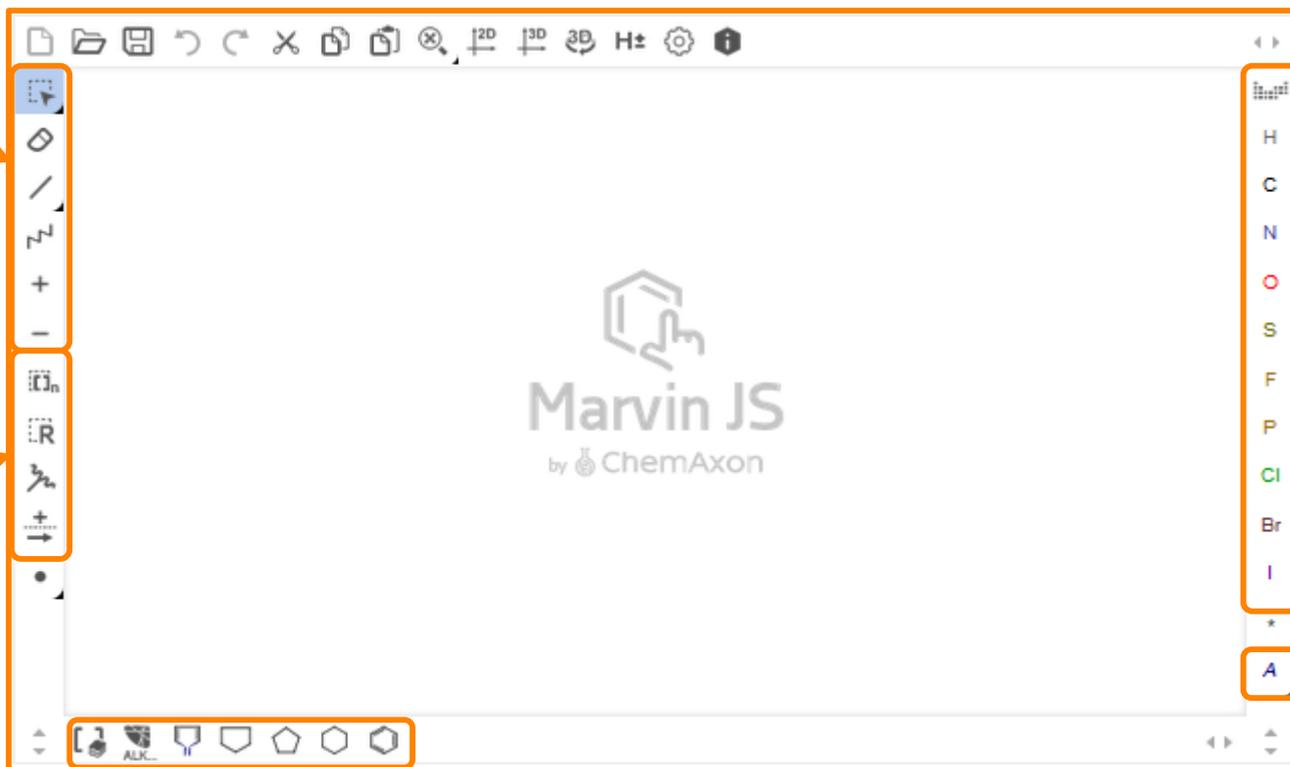
## 提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索案例
  - 如何利用Reaxys做物质分析研究
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# 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

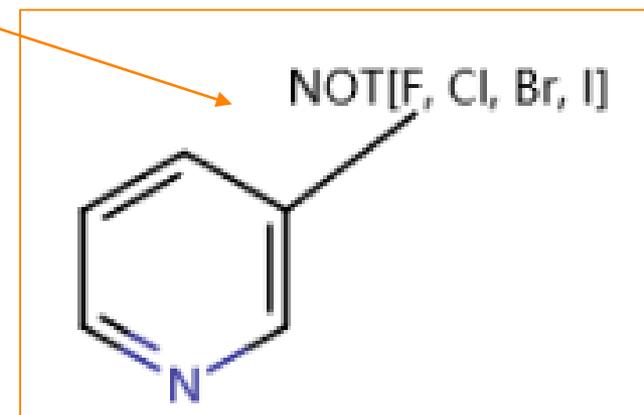
## 结构定义案例1—Not List的应用

- 案例:
  - 定义某位点上不能发生F, Cl, Br, I取代

Periodic table

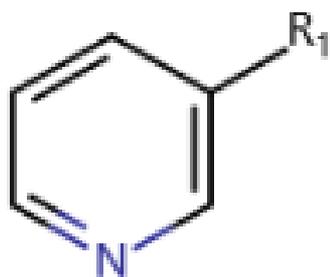
1	H	2																18	He
2	Li	Be											B	C	N	O	F	Ne	
3	Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	#	Rf	Db	Sg	Bh	Hs	Mt	Ds	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

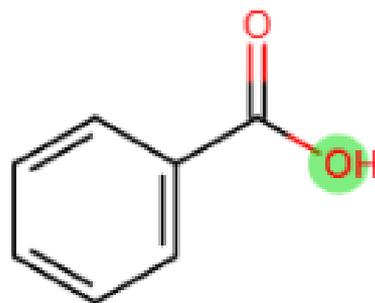


## 自定义R基团

- 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

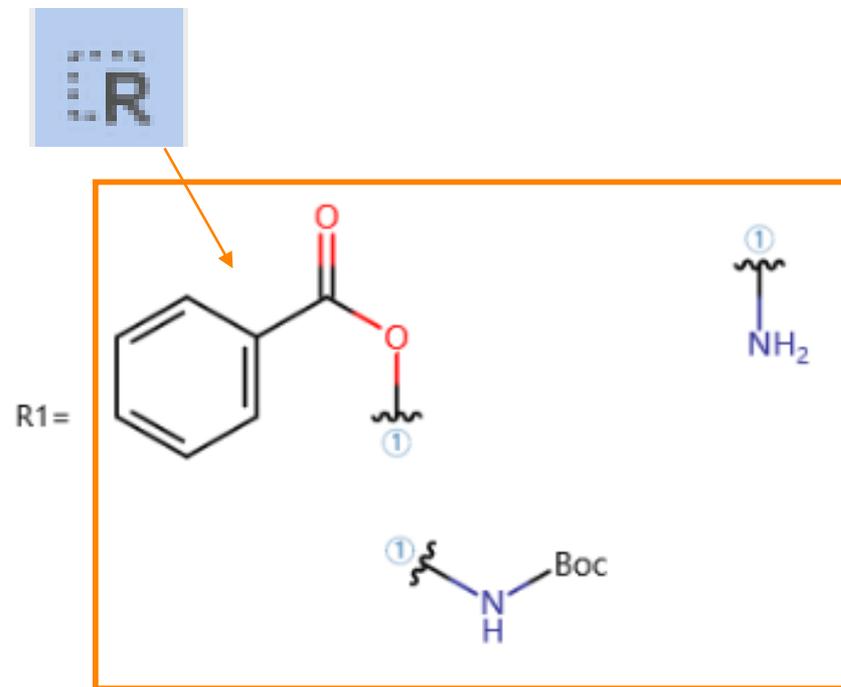
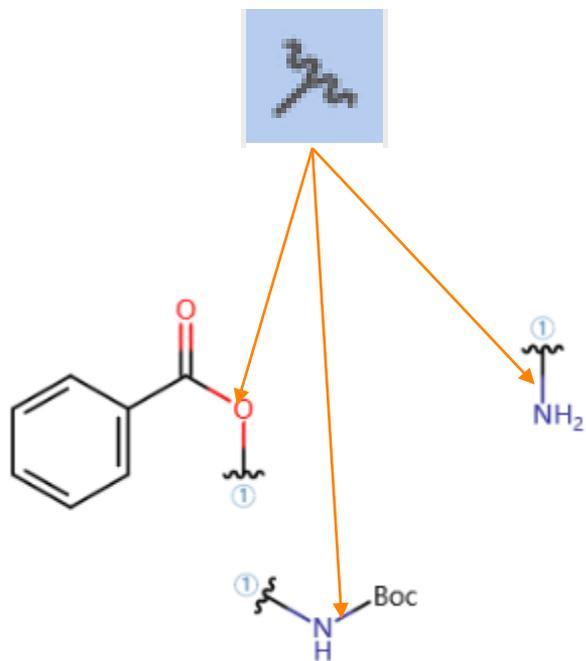


A



## 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



## 提纲

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  - 如何利用Reaxys做物质分析研究
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行反应设计和反应筛选
  - 如何利用Reaxys进行合成计划制作
- Reaxys检索小结



ELSEVIER

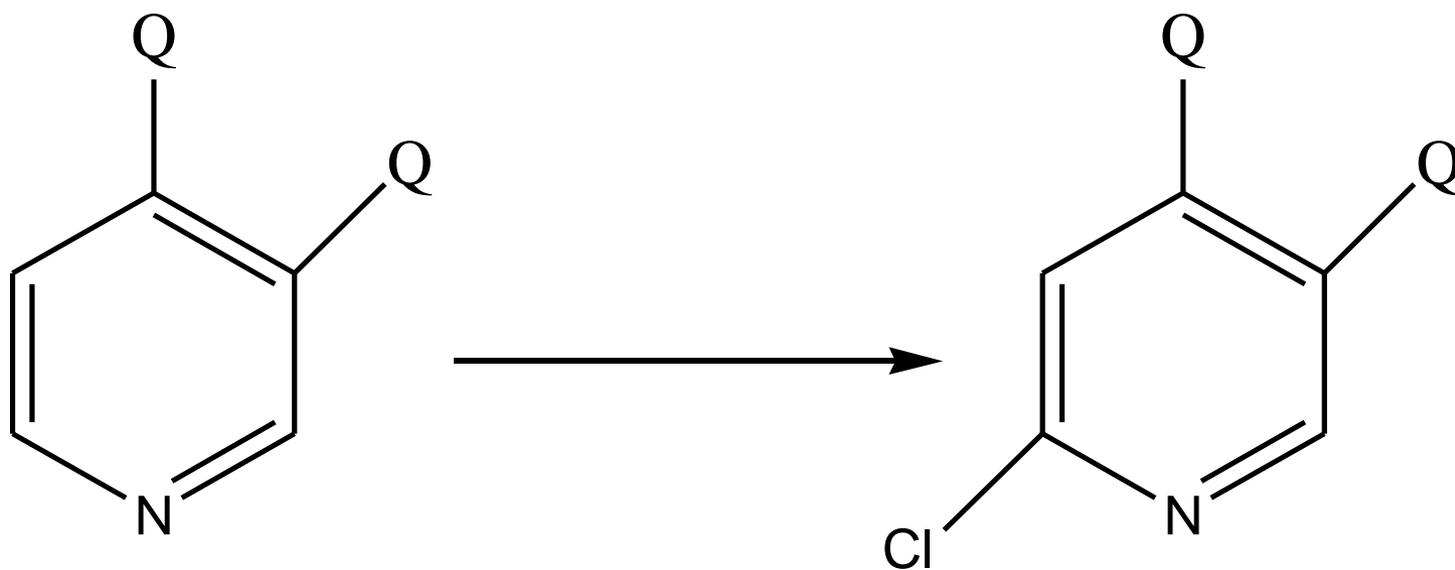
# Reaxys合成案例1—Reaxys中的筛选策略

Presented By

Date

## Reaxys中的反应筛选策略

- 寻找包含以下反应中心的反应
  - 吡啶环的3,4位存在任意的非C,H原子或基团
  - 检索在6位引入Cl的反应



# Reaxys中的结构定义

The screenshot displays the Reaxys interface with the following elements:

- Header:** Reaxys logo, navigation links (Quick search, Query builder, Results, Synthesis planner, History), and user profile (Sam Yu).
- Structure editor:** A central workspace showing a chemical structure transformation. On the left is a pyridine ring with two 'Q' substituents. An arrow points to the right, where the same pyridine ring is shown with a 'Cl' substituent at the 4-position. A vertical element list on the right side of the editor includes H, C, N, O, S, F, P, Cl (highlighted), Br, and I.
- Search options (highlighted in orange):**
  - Search this structure as:
    - As drawn
    - As substructure
      - On all atoms
      - On heteroatoms
    - Similar
  - Include:
    - Tautomers
    - Stereo
    - Additional ring closures
    - Related Markush
    - Salts
    - Mixtures
    - Isotopes
    - Charges
    - Radicals
  - [+ More options](#)
  - [Feedback](#)
- Footer:** Clear, Cancel, and Transfer to query buttons.

亚结构检索，并开放所有原子

# Reaxys中的结果

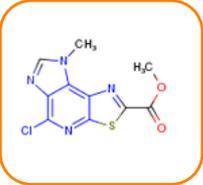
Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sam Yu  

3,686 [Back to Results Preview](#)

3,686 Reactions out of 564 Documents containing 2,878 Substances

0 selected: [Limit To](#) [Exclude](#) [Export](#) [Reaxys Ranking](#) [↑](#) [↓](#)

1    

HO-CH<sub>3</sub> +  + C=O → 

Show All Details [Find Similar Reactions](#)

Yield	Conditions	Reference
91%	With bis-triphenylphosphine-palladium(II) chloride; triethylamine In acetonitrile at 60°C under 5171.62 Torr for 24h; Inert atmosphere	Kempson, James; Spergel, Steven H.; Guo, Junqing; +27 others - Journal of Medicinal Chemistry, 2009, vol. 52, # 7, p. 1994 - 2005 <a href="#">Full Text</a> <a href="#">Cited 21 times</a> <a href="#">Show details</a>

[Feedback](#)

虽然找到了3600+反应，但是大致扫一眼，发现存在结构的环发生的稠环变化，如何保证环系不发生破坏

# Reaxys中的环保护工具

The screenshot displays the Reaxys Structure editor interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Synthesis planner, and History. The main workspace shows a chemical structure transformation: a pyridine ring with two 'Q' substituents on the left, which is converted to a pyridine ring with two 'Q' substituents and a 'Cl' substituent on the right. A toolbar on the left contains various editing tools. On the right, a search options panel is visible, titled 'Search this structure as:'. It includes radio buttons for 'As drawn', 'As substructure' (selected), and 'Similar'. Under 'As substructure', there are radio buttons for 'On all atoms' (selected), 'On heteroatoms', and 'Similar'. Below this, there is an 'Include' section with checkboxes for 'Tautomers', 'Stereo', 'Additional ring closures' (highlighted with an orange box and an arrow), 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom of the interface, there are buttons for 'Clear', 'Cancel', and 'Transfer to query', along with a 'Feedback' button.

在亚结构检索时，一键保护所有的环系

# Reaxys中的结果

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sam Yu  

1,600

[← Back to Results Preview](#)

**1,600 Reactions** out of 426 Documents containing 1,505 Substances

0 selected: [Limit To](#)  [Exclude](#)  [Export](#)  [Reaxys Ranking](#)   

1

  
O=[N+]([O-])c1cc(F)c(Cl)cc1[N+](=O)[O-]>>Nc1cc(F)c(Cl)cn1

[Show All Details](#)  [Find Similar Reactions](#) 

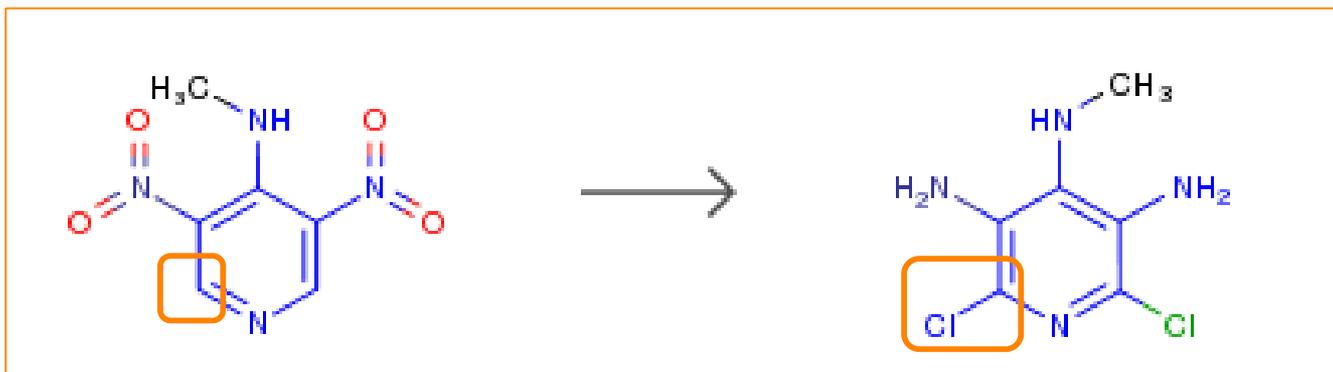
Yield	Conditions	Reference
-------	------------	-----------

所有反应中都没有稠环的出现

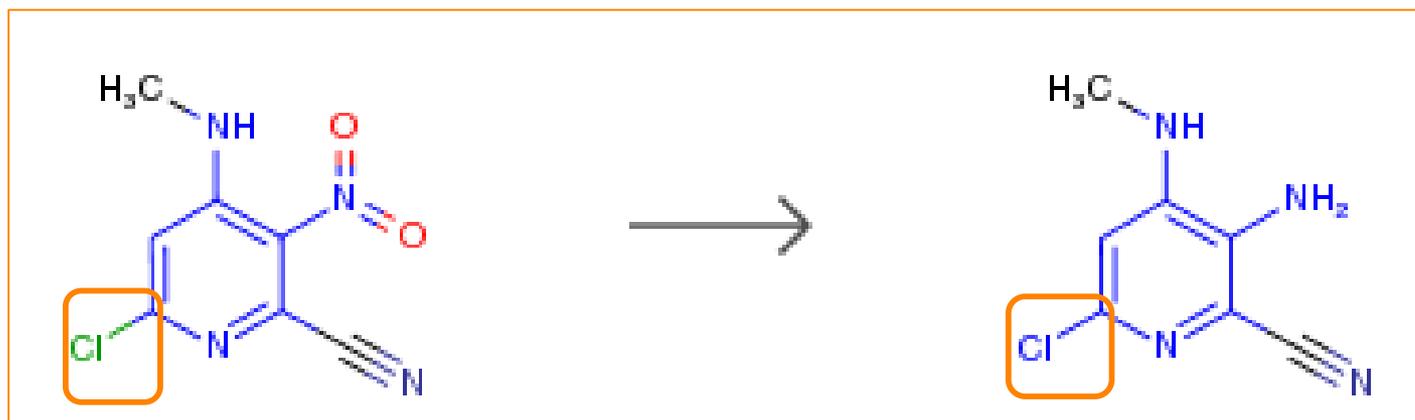
## 简单的看一下这些反应



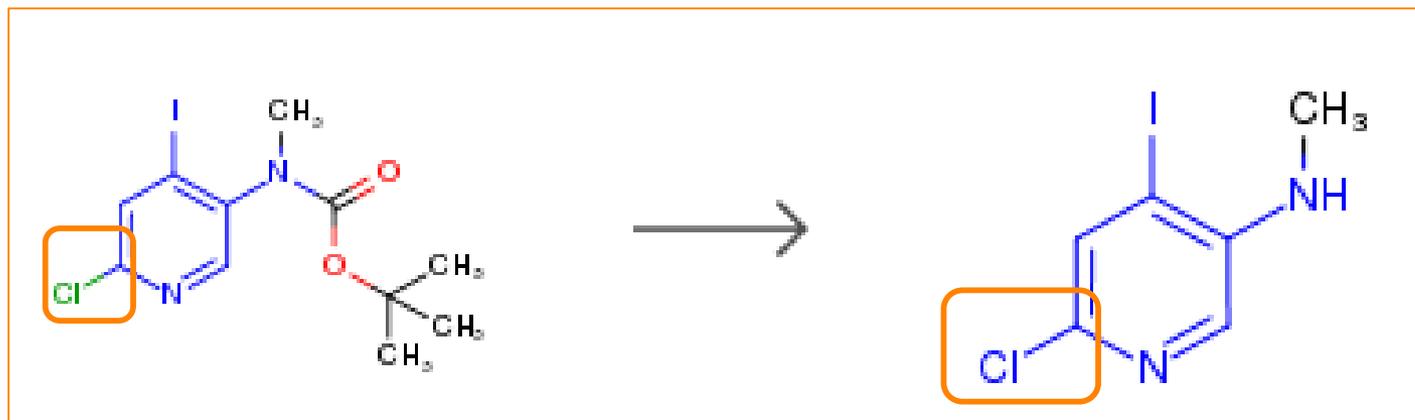
这些都是符合要求的反应，底物的6位都是H，反应过后变成了Cl



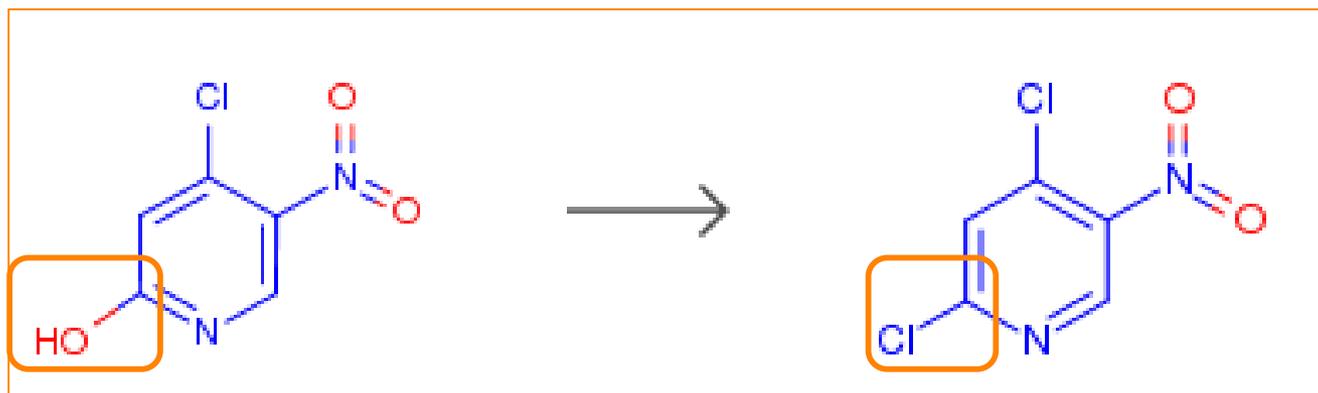
## 继续浏览



这些都不符合我们的要求，产物6位是Cl是底物直接带过来的



## 继续浏览



这些底物6位非  
H, 非Cl的反应,  
或许符合我们的要  
求



## 思考：什么样的反应是我们想要的

- 第一条反应：6位H变成6位C1—肯定是我们想要的
- 第二条反应：6位C1变成6位C1—肯定不是我们想要的
- 第三条反应：6位非H非C1变成6位C1—有可能是我们想要的

不同的人在这里的选择不一样，我们先假设只想获得第一类的反应。

## 直接对底物6位上的C原子进行属性设定

The screenshot displays the Reaxys interface for editing a chemical structure. The main window shows a pyridine ring with two 'Q' substituents and a chlorine atom at the 6-position. A blue arrow points to the carbon atom at the 6-position, which is labeled with a blue 's' in parentheses. The right panel shows the 'Atom query properties' dialog box, which is used to define the atom's properties. The 'A' property is selected, and the 's\*' property is highlighted in the list of options.

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner His

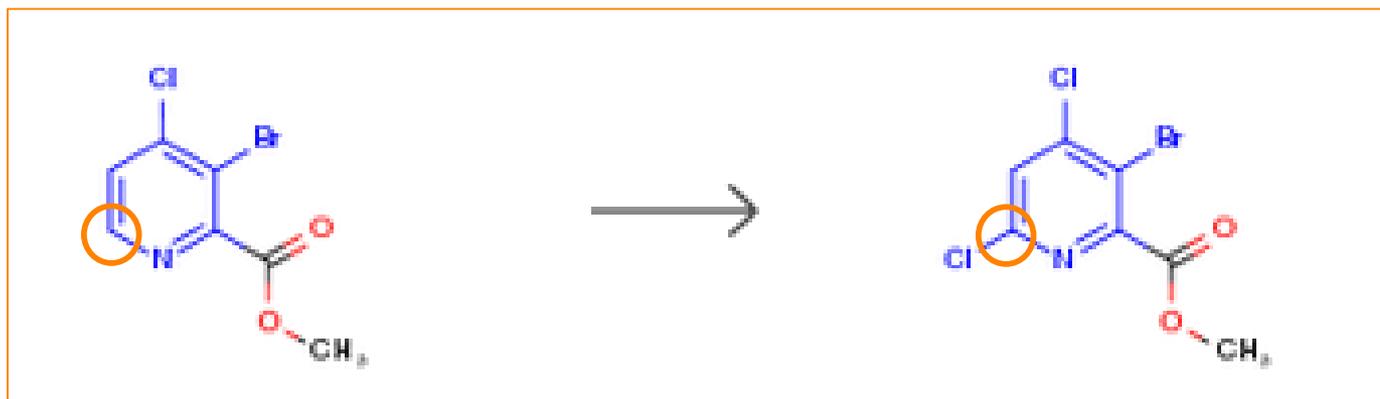
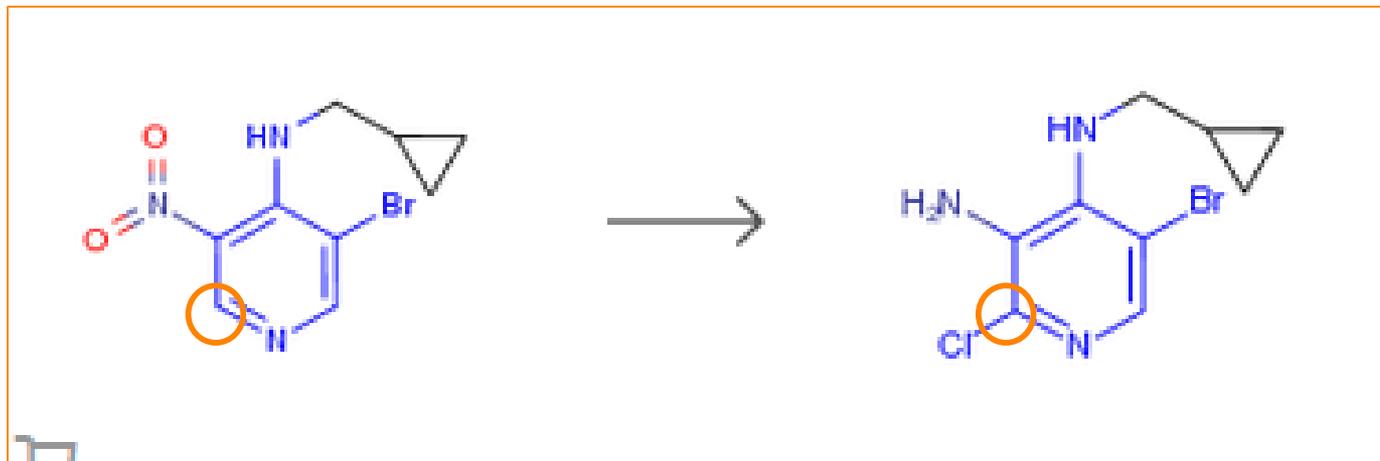
Structure editor Create structure template from name >

Atom query properties

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

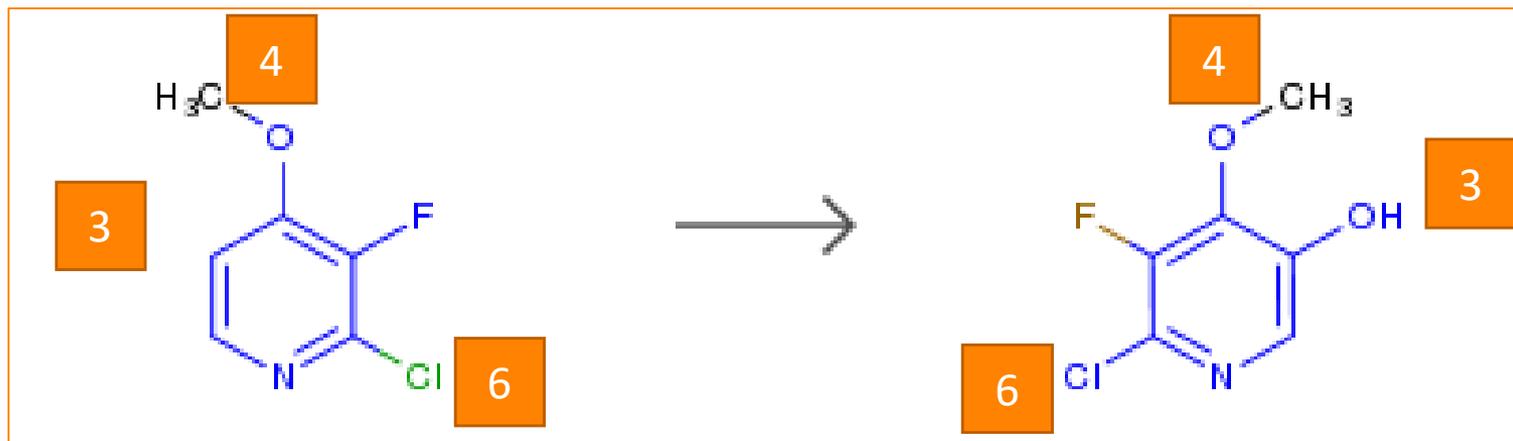
- 1: 打开原子属性工具
- 2: 选择原子属性
- 3: 使用s\*将底物6位上的C标记，这可以保证在亚结构检索时，这个C原子不允许有取代。

## 检索的结果

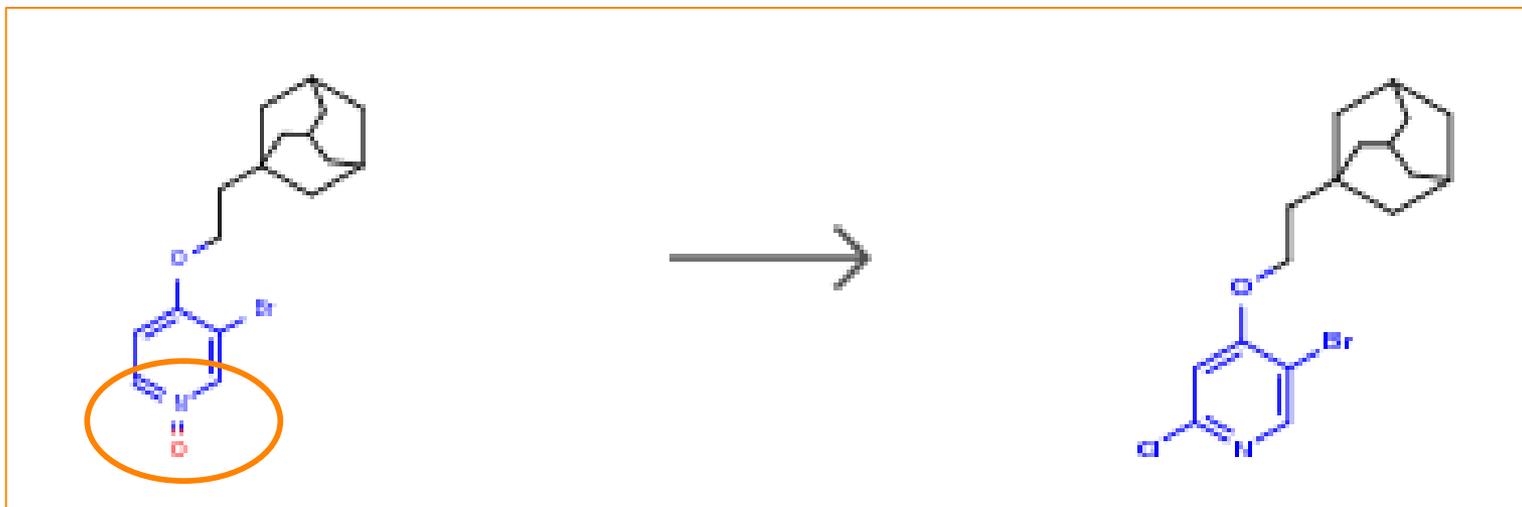


检索到结果中就能发现更多的我们感兴趣的反应

但是，当细看的时候，我们还发现……



反应前后  
原子不匹  
配的问题



极少量的  
反应中存  
在吡啶的N  
上存在双  
键O

# 原子匹配的定义

The screenshot displays the Reaxys Structure editor interface. At the top, there are navigation options: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". The "Structure editor" section is active, showing a "Create structure template from name" button. The main workspace contains two chemical structures: a pyridine ring with two 'Q' substituents on the left, and a chlorinated pyridine ring with two 'Q' substituents on the right. An orange arrow points from the nitrogen atom in the first structure to the nitrogen atom in the second structure, indicating atom mapping. A blue box highlights the "Add" (+) button in the left-hand toolbar. On the right side, there is a search configuration panel with the following options:

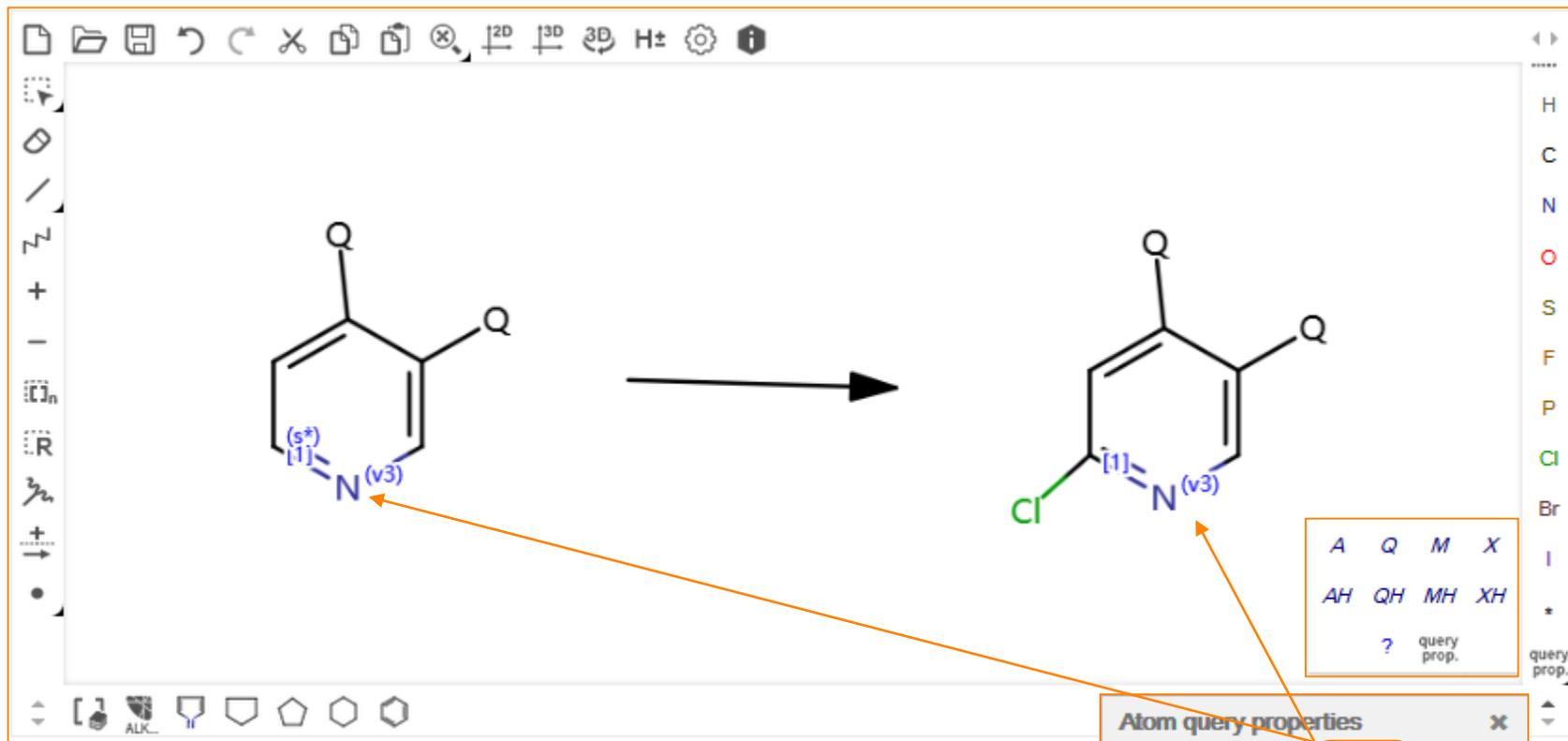
- Search this structure as:
  - As drawn
  - As substructure
    - On all atoms
    - On heteroatoms
  - Similar
- Include:
  - Tautomers
  - Stereo
  - Additional ring closures
  - Related Markush
  - Salts
  - Mixtures
  - Isotopes
  - Charges
  - Radicals
- [+ More options](#)

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

## Tips:

使用原子匹配，帮助匹配反应前后相同的原子，避免一些相似结构的干扰。

## 如何处理N上双键氧的问题



### Tips:

1. 使用v+/v-, 标记N的价位, 常用的还能用在亚砷, 砷相关结构

# 如果要求6位为非H, 非Cl, 如何定义

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History

Structure editor Create structure template from name >

The screenshot shows the Reaxys interface with a structure editor. A pyridine ring is shown with a 'NOT[H, Cl]' label at the 6-position. An arrow points from this label to the 'NOT list' in the periodic table window.

- 1: 打开原子周期表
- 2: 选择Not list, 选择H, Cl,
- 3: 在底物6位上直接定义 NOT Cl

Periodic table

1	H	2																18	
1	H	2																	He
2	Li	Be																	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	
			*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			#	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Atom list

NOT list

Ok

## 最后的检索结果

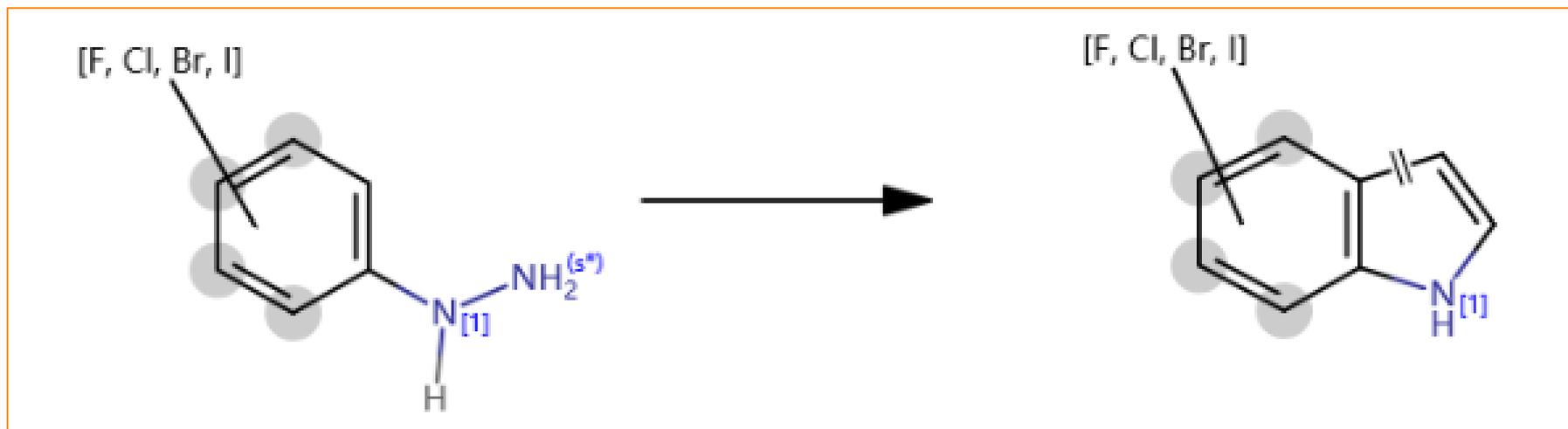


最终的结果都是从非H，非Cl变成Cl的反应

## Reaxys中的反应筛选策略

- 并不是所有的科研工作者，一开始就能准确的定义反应结构。
- 建议先大致浏览下反应结果集，然后去思考如何去除我们不想要的反应。
- 使用**Reaxys**中的结构定义工具，或其他的检索策略，去除不想要的反应。

## 一个随堂小练习



请列举至少3个这条反应中应用到的功能：

功能1: \_\_\_\_\_

功能2: \_\_\_\_\_

功能3: \_\_\_\_\_



ELSEVIER

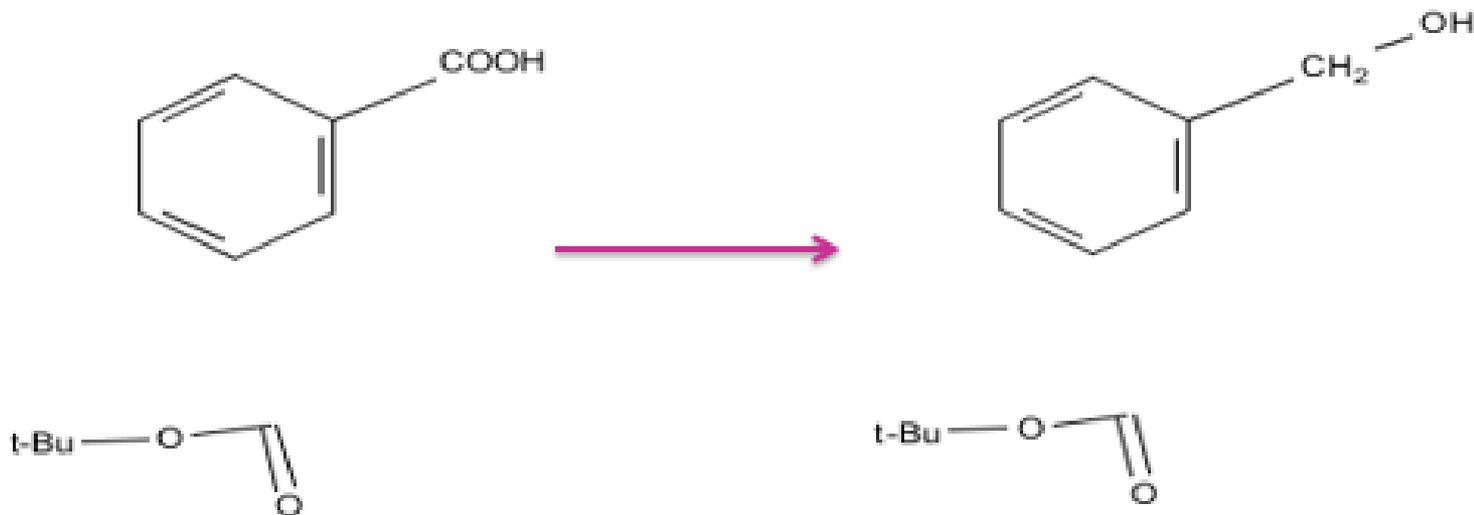
# 合成案例2—Reaxys中的碎片反应检索及衍生

Presented By

Date

## Reaxys中的碎片反应检索

- 检索符合以下条件的反应
  - 结构中存在Boc和苯甲酸
  - 反应后苯甲酸变成苯甲醇



# Reaxys中的定义

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 a help icon are visible in the top right. The main area is the "Structure editor", which contains a toolbar with various drawing tools and a central workspace. In the workspace, a chemical structure of benzoic acid is shown on the left, with an arrow pointing to a structure of benzamide on the right. Both structures are labeled "Boc". To the right of the workspace is a search configuration panel titled "Search this structure as:". It includes radio buttons for "As drawn", "As substructure", and "Similar". Under "As substructure", there are options for "On all atoms", "On heteroatoms", and "Similar". Below this is an "Include" section with checkboxes for "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", "Radicals", and "Ignore Atom Mappings". The "Additional ring closures" checkbox is highlighted with a red box. At the bottom of the interface, 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.

# Reaxys中的结果

[← Back to Results Preview](#)

**882 Reactions** out of 744 Documents containing 1,694 Substances

0 selected: [Limit To](#) [Exclude](#) [Export](#) [Reaxys Ranking](#) [↑](#) [↓](#)

1

[Show All Details](#) [Find Similar Reactions](#)

Yield | Conditions

[Show All Details](#) [Find Similar Reactions](#)

Yield | Conditions | Reference

检索结果:

两个片段可以出现在一个结构中,也可以出现在2个结构中。

## 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 transformation: a benzene ring with a carboxylic acid group (C(=O)OH) on the left, which is converted to a benzene ring with a hydroxymethyl group (CH<sub>2</sub>OH) on the right. Both structures are labeled "Boc". The interface includes a top navigation bar with "Quick search", "Query builder", "Results", "Synthesis planner", and "History". A "Structure editor" header is present, along with a "Create structure template from name" button. A toolbar with various editing tools is visible above the workspace. On the right side, a settings panel titled "Search this structure as:" is open, showing options for "As drawn", "As substructure" (selected), and "Similar". Under "Include", "Stereo" and "Keep fragments" are checked. The "Keep fragments" section has "Together" selected over "Separate". A "+ More options" button is highlighted at the bottom of the settings panel. The bottom of the interface features "Clear", "Cancel", "Transfer to query", and "Feedback" buttons.

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

[← Back to Results Preview](#)

**289 Reactions** out of 193 Documents containing 561 Substances

0 selected: [Limit To](#) [Exclude](#) [Export](#) [Reaxys Ranking](#) [↑](#) [↓](#)

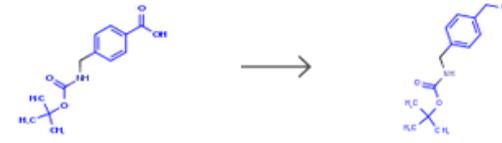
1



[Find Similar Reactions](#) >

Yield | Conditions

2



[Show All Details](#) [Find Similar Reactions](#) >

Yield | Conditions

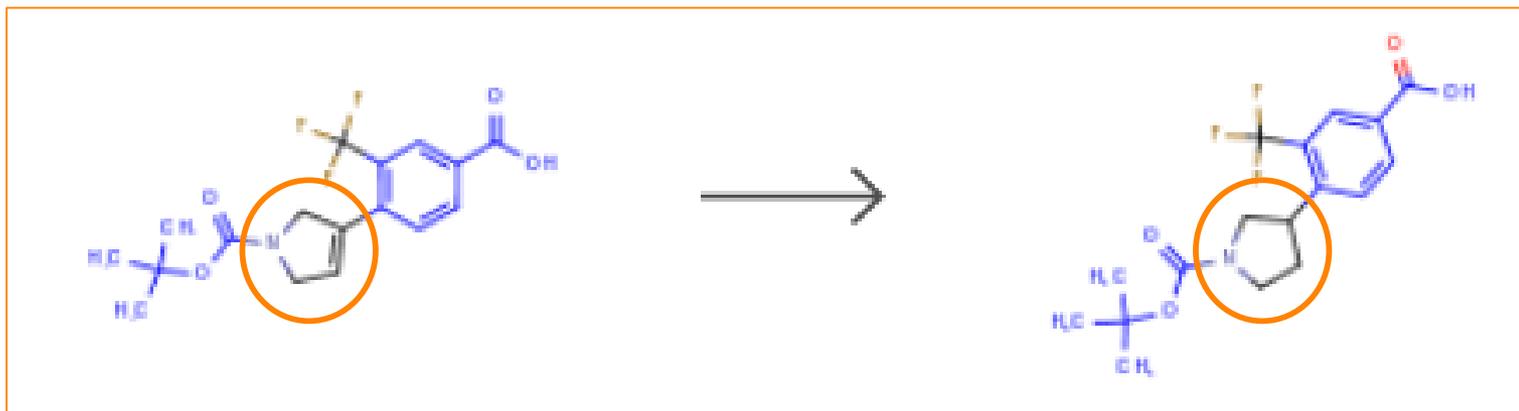
100% **With lithium aluminium tetrahydride** In tetrahydrofuran; 1,4-dioxane at 0 - 20°C for 16.25h;

[Experimental Procedure](#) [Show Reference](#) >

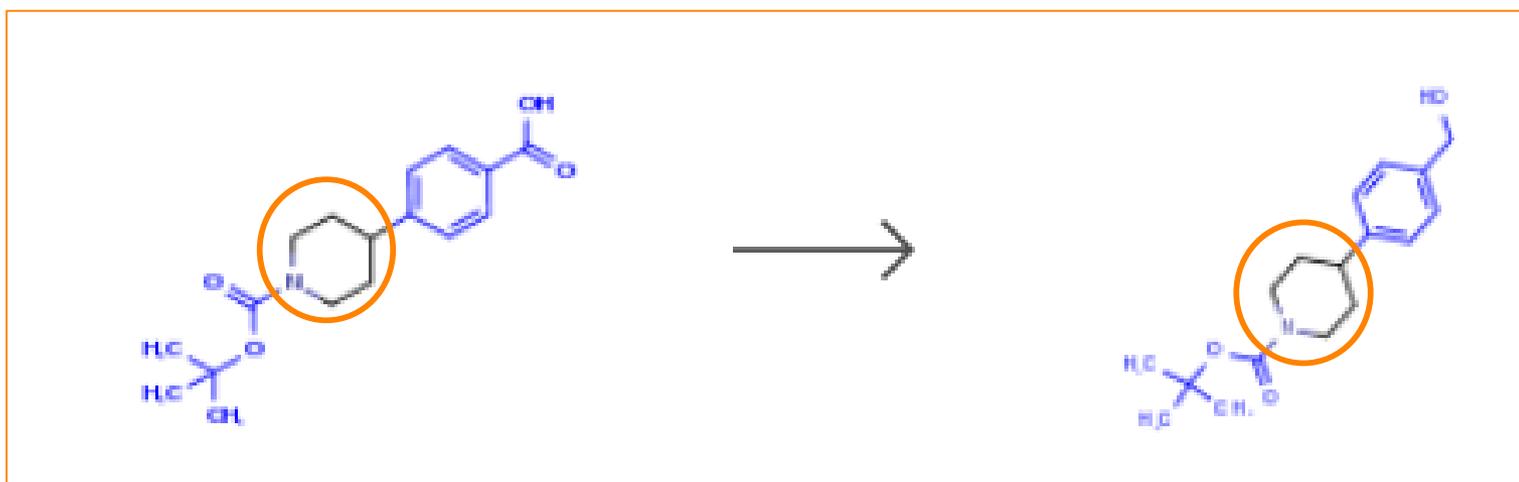
从结构上看，所有的结构中都包含2个片段

## 一些筛选的假设

- 假设，我们希望反应结果集中不能出现



假设我们不  
希望出现成  
环的叔胺



# 排除结构的绘制

The image illustrates the process of defining bond properties for a structure in Reaxys. The main window shows a chemical structure with a nitrogen atom highlighted in green. A context menu is open over the nitrogen atom, and a 'Bond properties' dialog box is also open, showing the 'in ring' option selected for the 'Reacting center' property.

**Bond properties**

- Absolute stereo (chiral)
- R-logic*
- Paste (Ctrl+V)

**Bond properties**

Type	single
Topology	undefined
Reacting center	undefined
	in ring
	in chain

Structure editor

Search this structure as:

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

Include

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

Clear

+ More options Feedback

右键点击N上的键，直接定义这两根键在环中。

## 绘制好的结构

Reaxys<sup>®</sup> 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

Include

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

+ More options Feedback

和前面谈到的排除策略一致，选择Exclude，

Reaxys<sup>®</sup> Quick search

82

289

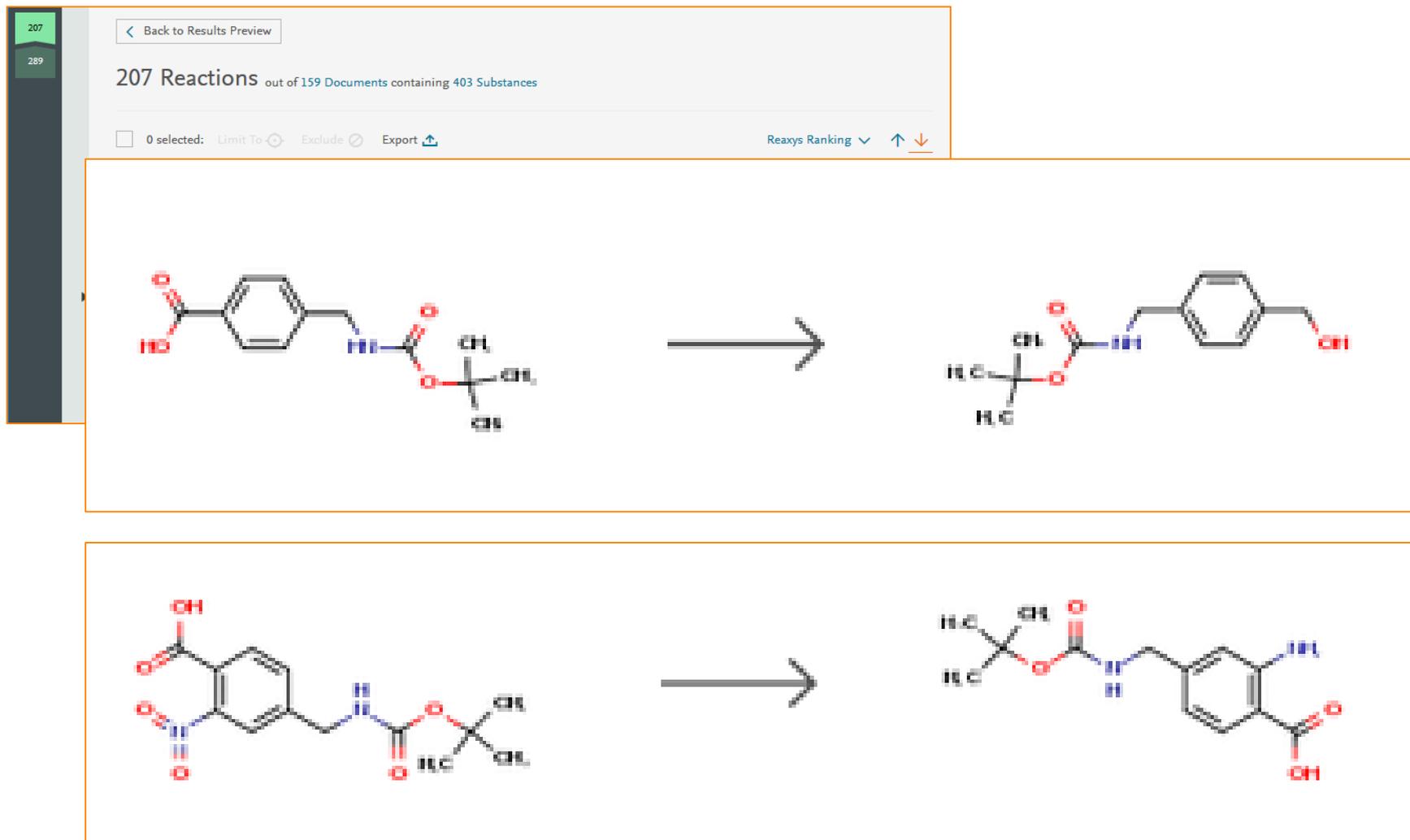
Filters and Analysis

Limit to > Exclude >

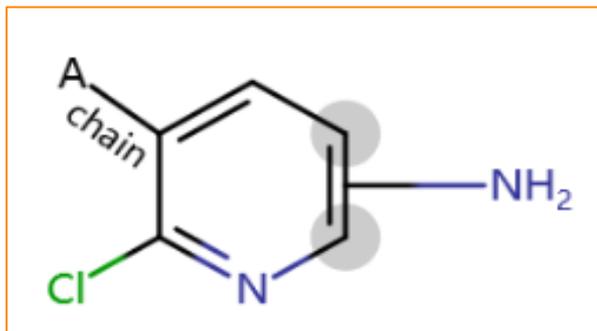
By Structure

On all atoms

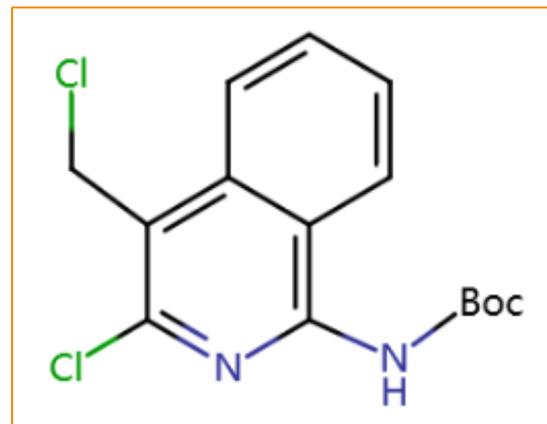
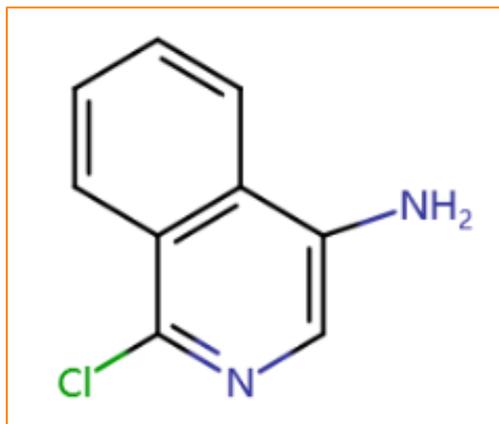
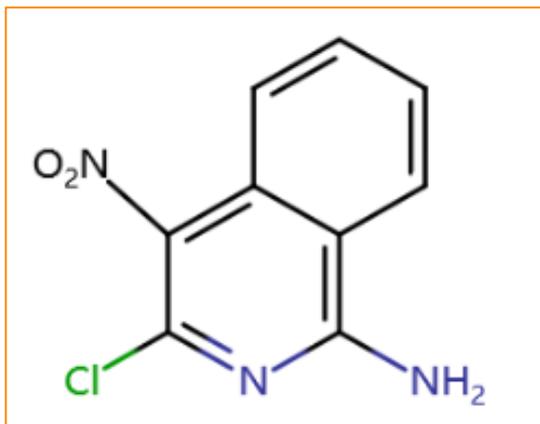
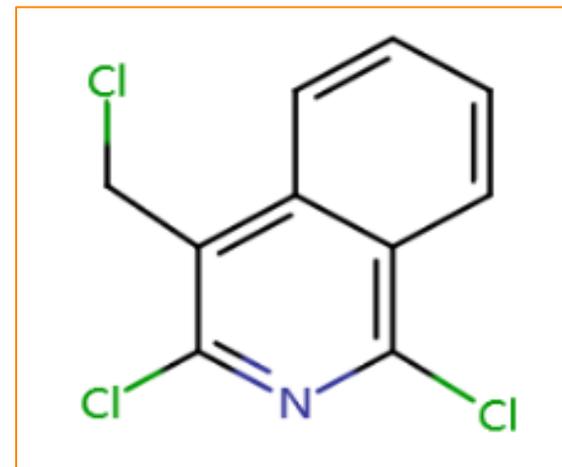
# 最后的结果



# 一个随堂小练习



亚结构检索左侧结构，右侧及下面的4个结构哪些可以被检索出来



4

1

2

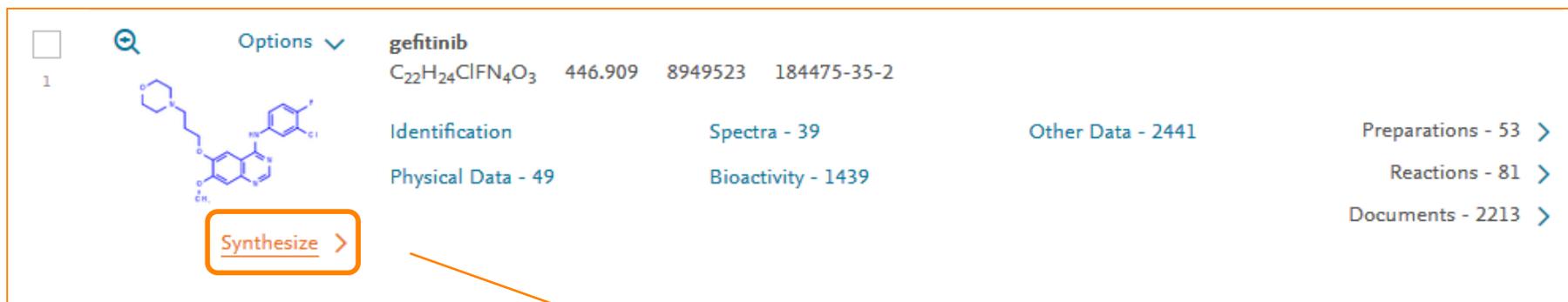
3

## 提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索案例
  - 如何利用Reaxys做物质分析研究
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行反应设计和反应筛选
  - 如何利用Reaxys进行合成计划制作
- Reaxys检索小结

# Reaxys的Synthesis Plan是全球最先进的合成路线设计工具

- 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 ▾

1

gefitinib  
C22H24ClFN4O3 446.909 8949523 184475-35-2

Identification Spectra - 39 Other Data - 2441 Preparations - 53 >

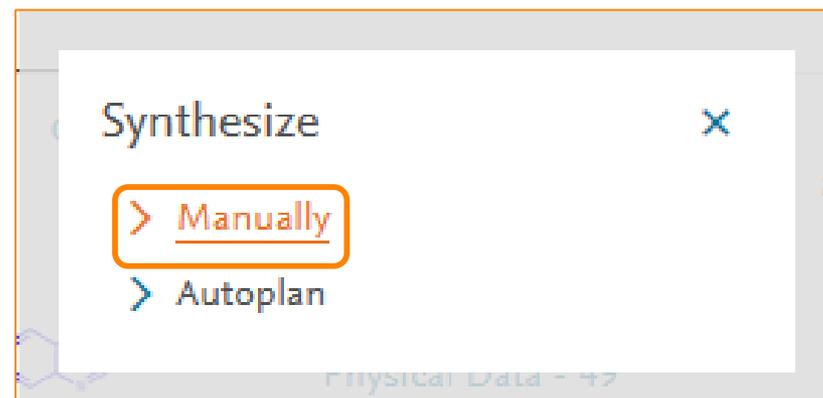
Physical Data - 49 Bioactivity - 1439 Reactions - 81 >

Documents - 2213 >

Synthesize >

## Tips:

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



Synthesize X

> Manually

> Autoplan

Physical Data - 49

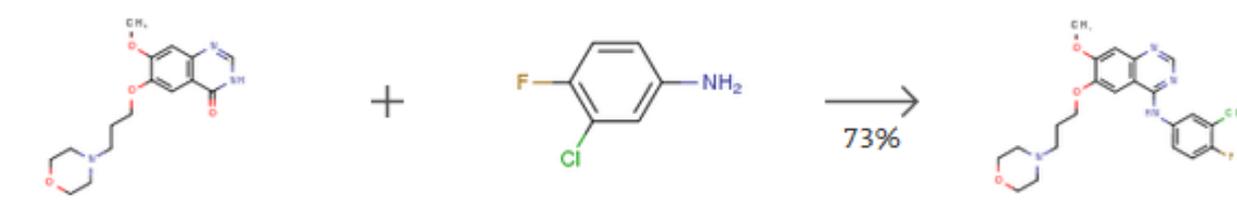
## Synthesis Plan—添加感兴趣的反应

- 可以添加多条反应在一个Plan中，用于比较

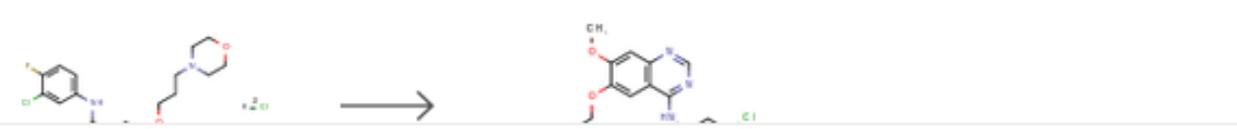
Add preparation - 52 ×

Preparation

1



2

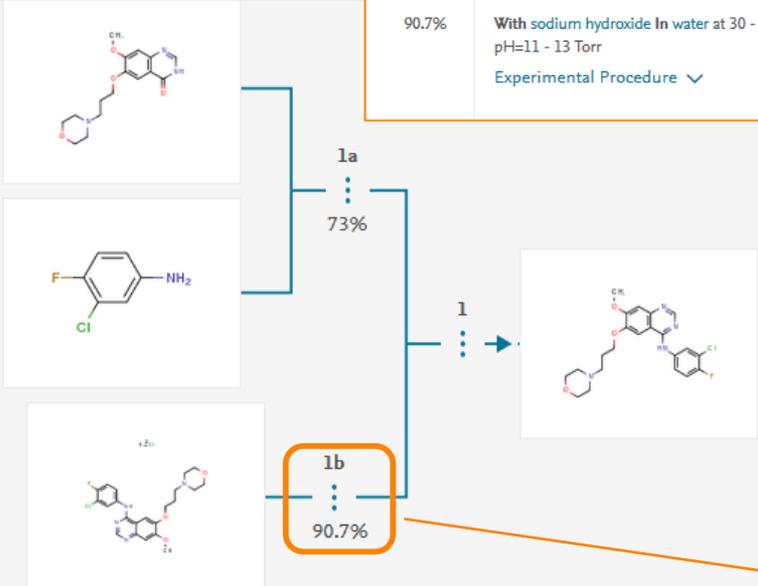


[+ Load more](#) [Cancel X](#) [Add 2 to plan >](#)

# 添加好的结果界面

Synthesis plan 3

Import  Save  Export 



Conditions

Preparation - 1b

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

 Show conditions 

 Hide preparation

 Remove preparation

## Tips:

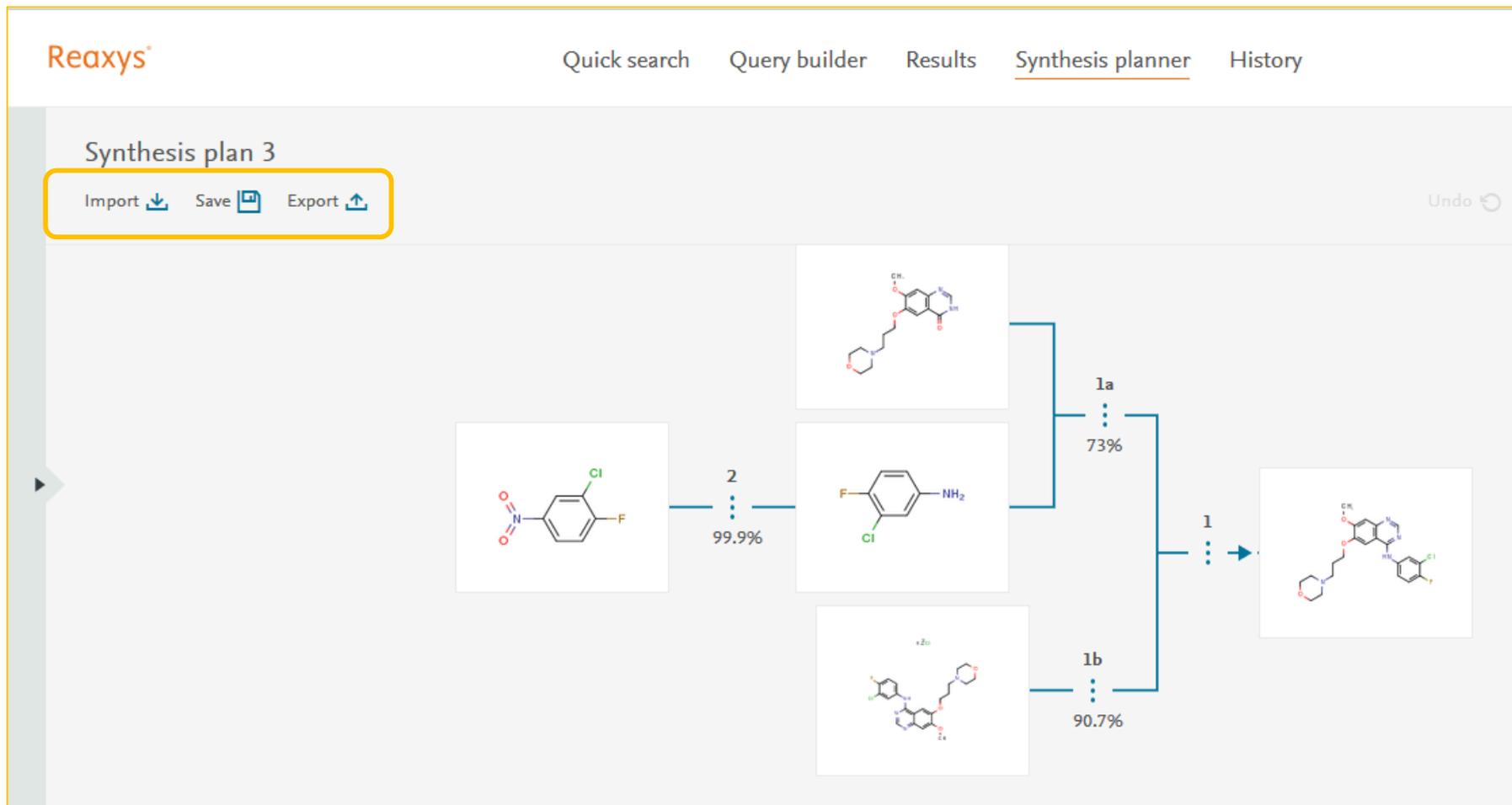
- 1: 通过添加多条反应，可以用来评估反应信息
- 2: 点击虚线的地方，可以查看条件，或者隐藏，移除反应

## 继续的扩充反应路线

The image displays a software interface for managing a synthesis plan. The main window, titled "Synthesis plan 3", shows a reaction network. A central node is a 2,4-dichloroaniline derivative. Two arrows branch out from it: one labeled "1a" with a yield of 73%, and another labeled "1b" with a yield of 90.7%. Both lead to a final product node. A "Synthesize" button is highlighted in a yellow box, with an arrow pointing to a "Synthesize" dialog box. This dialog box has two options: "Manually" (highlighted with a red box) and "Autoplan". Below the dialog box is a window titled "Add preparation - 4" which shows two chemical reactions. Reaction 1 shows the conversion of 2,4-dichloro-1-nitrobenzene to 2,4-dichloroaniline with a 99.9% yield. Reaction 2 shows the conversion of 2,4-dichloro-1-nitrobenzene to 2,4-dichloroaniline. At the bottom of this window are "Cancel" and "Add 1 to plan" buttons.

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

# 最后的结果



可以对Synthesis Plan进行导入，导出或者保存等操作。

## 提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索案例
  - 如何利用Reaxys做物质分析研究
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行反应设计和反应筛选
  - 如何利用Reaxys进行合成计划制作
- Reaxys检索小结

## New Reaxys检索小结

- **New Reaxys**从大量文献中摘取和物质性质相关的所有数据，帮助科研人员获得标准化，规范化，格式化的物性数据列表及参考文献
- **New Reaxys**中的**Query Builder**检索帮助科研人员通过简便的方式，获得精准，跨学科的精确定案
- **New Reaxys**中的结构面板，能实现科研人员绝大部分的结构绘制要求，帮助科研人员用最直接的方式获得相应的物质和反应



ELSEVIER

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