

# Reaxys结构面板详解

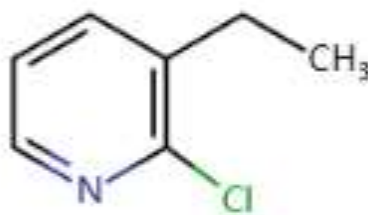
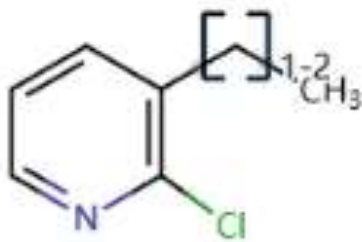
Presented By  
Date

## 提纲

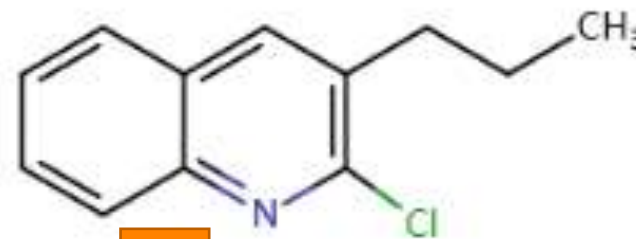
- Reaxys结构检索模式介绍
- Reaxys结构面板详解
  - 面板中简单功能介绍
  - Part A, 选择, 橡皮, 键, 链工具
  - Part B, 常见原子, 元素周期表中功能
  - Part C, 重复基团, R基团, 原子匹配
  - Part D, 常见环, 官能团, **Generic Group**
  - Part E, 通用官能团, 原子属性定义
  - Part F, 右键的应用

## Reaxys结构检索模式介绍

- As Draw
  - 检索到的结构完全和所绘制结构一样
- As Substructure
  - 对结构中没有绘制出来或者延展出来的H进行任意取代，但是核心结构必须和所绘制的一样



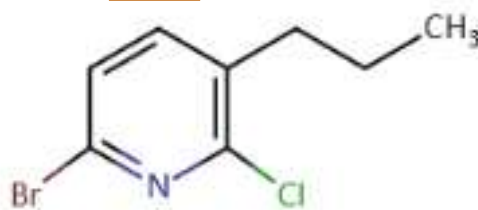
1



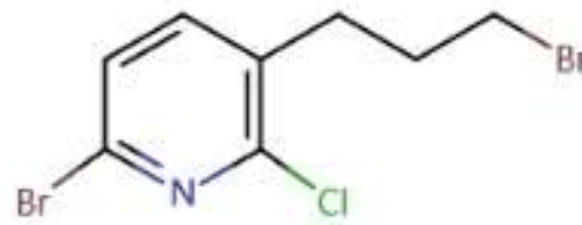
2

**思考:**

用两种方式检索上述结构，可以获得的结果有？



3



4

## 提纲

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- Reaxys结构面板详解
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  - Part C, 重复基团, R基团, 原子匹配
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## 面板中简单功能介绍

### Tips

1. 打开，保存结构
2. 复制，剪切，黏贴结构
3. 放大，缩小结构
4. Chemdraw中，复制结构的方式Ctrl+Alt+C

### Tips:

通过化学品名转化结构

The screenshot shows the Marvin JS Structure Editor interface. The top toolbar contains icons for file operations (open, save, copy, paste, zoom) and a button labeled "Create structure template from name". The main workspace displays the Marvin JS logo. On the right, there is a search and include options panel with checkboxes for "As drawn", "As substructure", "Similar", and various "Include" options like "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", and "Radicals".

# Reaxys的结构面板概览

The screenshot shows the Reaxys Structure editor interface. The main workspace is labeled "Structure editor" and contains a search bar "Create structure template from name". Below the search bar is a toolbar with various icons for editing and drawing. The interface is divided into several sections:

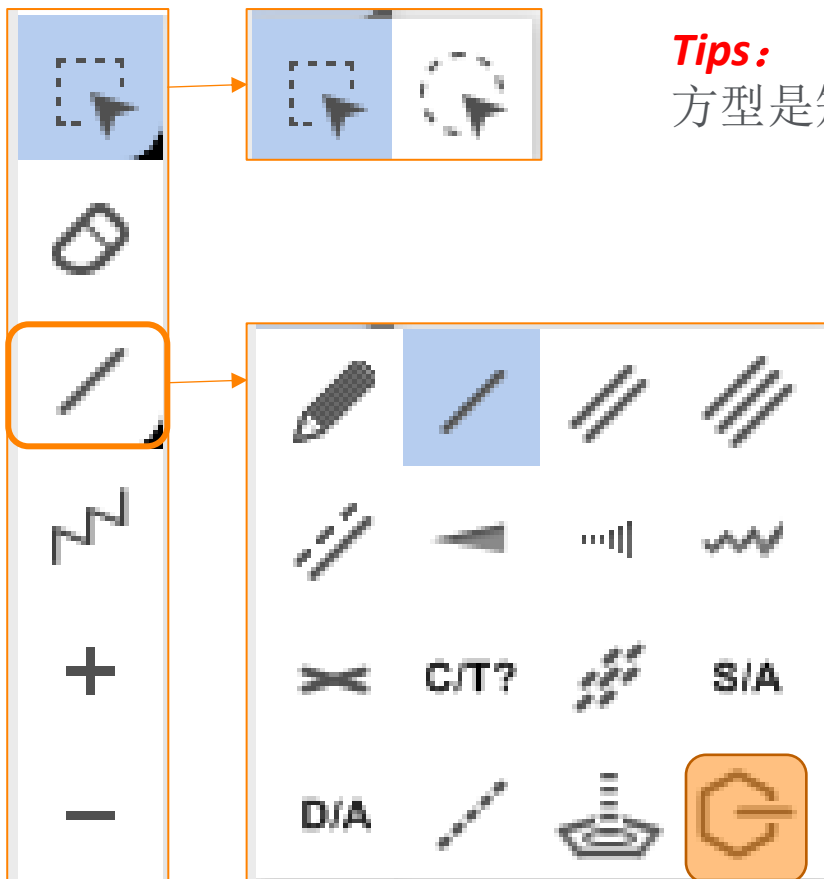
- Part A:** A vertical toolbar on the left side, containing icons for selection, erasing, drawing bonds, and adding/removing atoms.
- Part B:** A vertical toolbar on the right side, containing a list of elements (H, C, N, O, S, F, P, Cl, Br, I) and a search icon.
- Part C:** A vertical toolbar on the left side, containing icons for defining repeating groups (R), defining reactions, and matching atoms.
- Part D:** A horizontal toolbar at the bottom, containing icons for defining common rings and functional groups.
- Part E:** A vertical toolbar on the right side, containing a list of functional groups and a search icon.

On the right side of the interface, there is a search panel titled "Search this structure as:" with options: "As drawn" (selected), "As substructure", and "Similar". Below this is an "Include" section with checkboxes for: "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", and "Radicals". At the bottom of the search panel is a "+ More options" button.

## Part D:

常见的环，官能团，Reaxys的Generic Group定义

## Part A: 选择, 橡皮, 键, 链, 电子



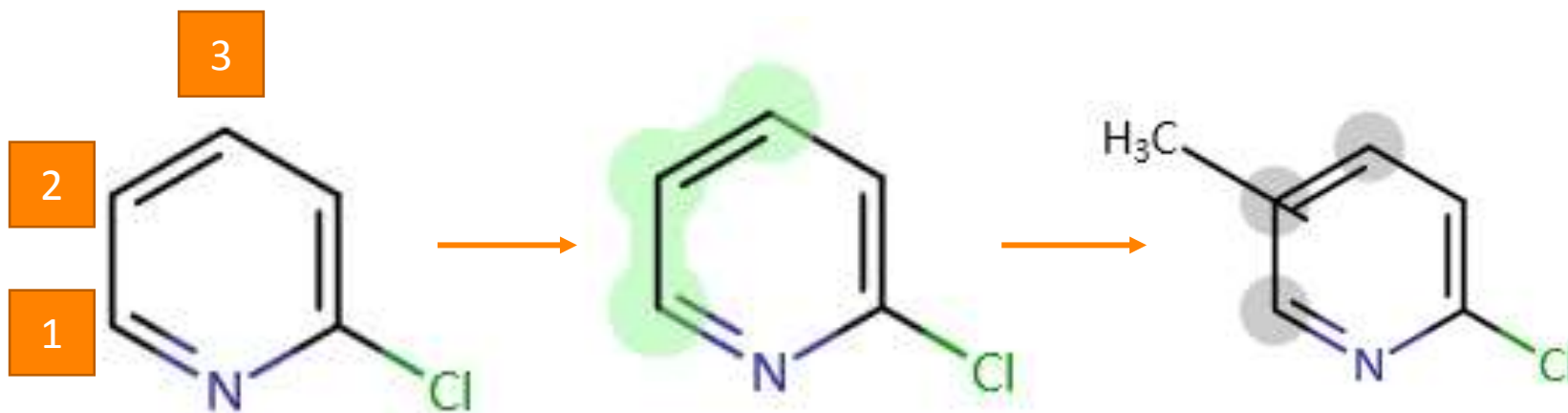
**Tips:**

方型是矩形选择, 圆形是自由选择工具

铅笔	单键	双键	三键
芳香键	单键上	单键下	单键上 或下
双键顺 或反	顺反或 未定义	单键或 双键	单键或 芳香键
双键或 芳香键	不确定 键	配位键	不定位 取代

## 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NH<sub>2</sub>

### 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CH<sub>3</sub>
3. 将CH<sub>3</sub>换成NH<sub>2</sub>



## Part B: 常见原子, 元素周期表定义



H

C

N

O

S

F

P

Cl

Br

Periodic table X

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	Ff	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

### Tips:

1. Atom List: 绘制允许取代的原子列表
2. Not List: 绘制不允许发生取代的原子列表

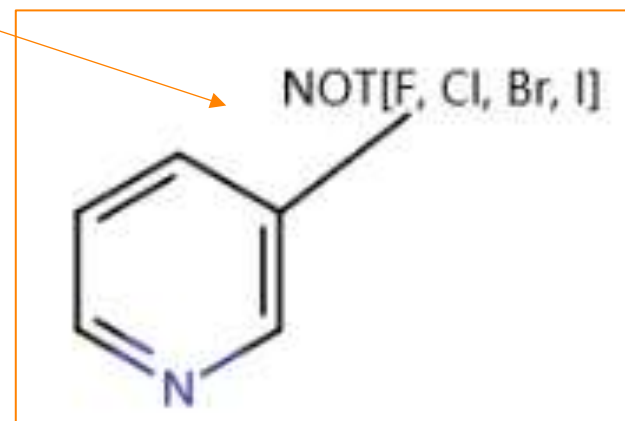
# Atom List/Not List画法

- Atom List/Not List的应用
  - Atom List: 定义允许取代的原子
  - Not List: 定义不允许发生取代的原子

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

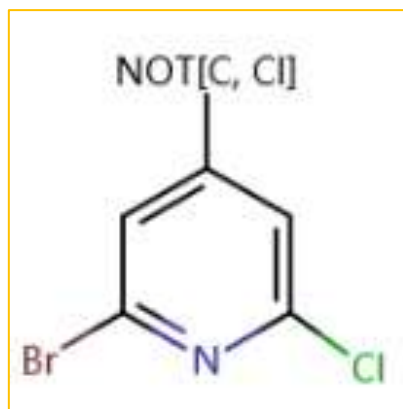
Ok



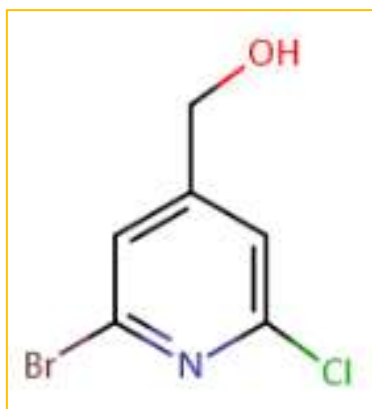
## Not List/Atom List定义Tips

- Atom List和Not List定义的是原子列表
  - 使用As Draw, 只接1个原子, 且该原子会处于Block状态
  - 使用As Substructure, 相当于基团的允许/不允许, 该原子默认开放
- Not List默认表示该位点是有取代的
  - Not List默认表示该位点是有取代的, 即Not Cl 和Not Cl H等效

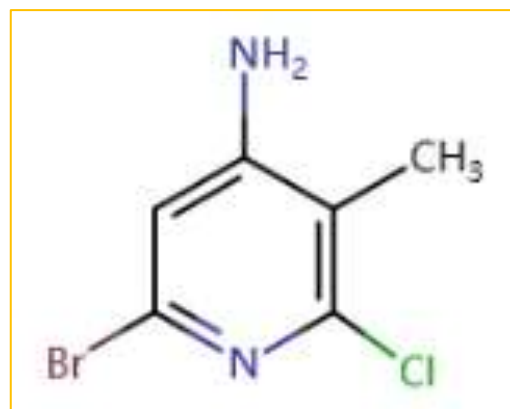
## 随堂小练习



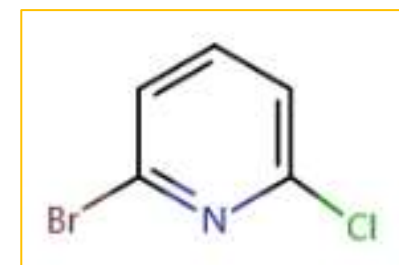
A



1



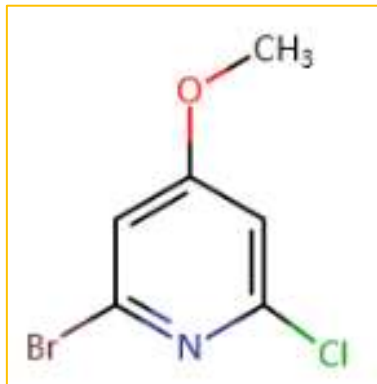
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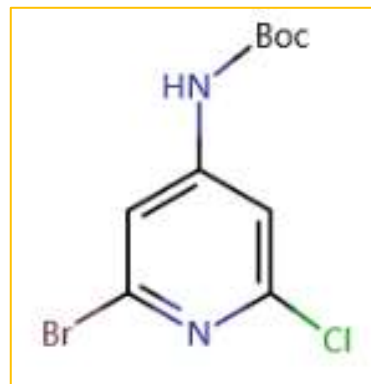
3



4



5



6

**思考:**

分别用As Draw和As Substructure检索结构A, 哪些结构可以被检索出来

## Part C: 重复基团, R基团定义工具, 原子匹配工具



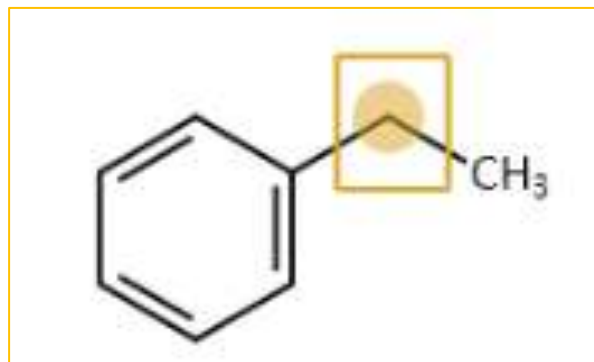
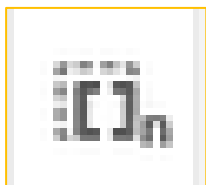
重复基团定义工具, 允许用在环和链上

R基团定义工具

R基团末端定义工具, 和R基团定义工具一起用

反应箭头, 原子匹配工具

## 重复基团定义工具的使用

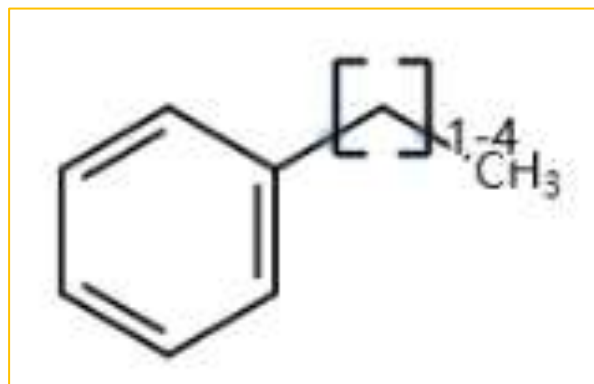


Repeating group ✕

[ ] (nt)

1-4

Ok

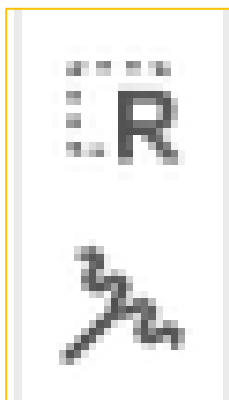


### **Tips:**

1. 使用重复基团工具
2. 选择需要重复的结构
3. 输入范围，确定
4. 重复的阈值，可以写成：2，4-6

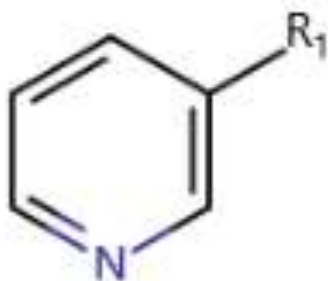
## R基团定义及R基团末端定义工具

- R基团定义和R基团末端定义是一组功能

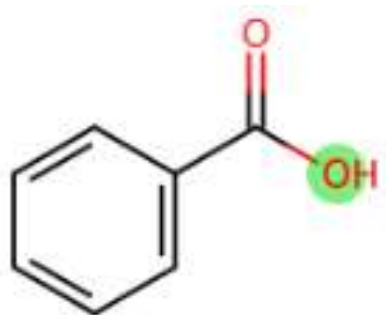


### 定义要求:

1. 定义一个结构A
2. 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

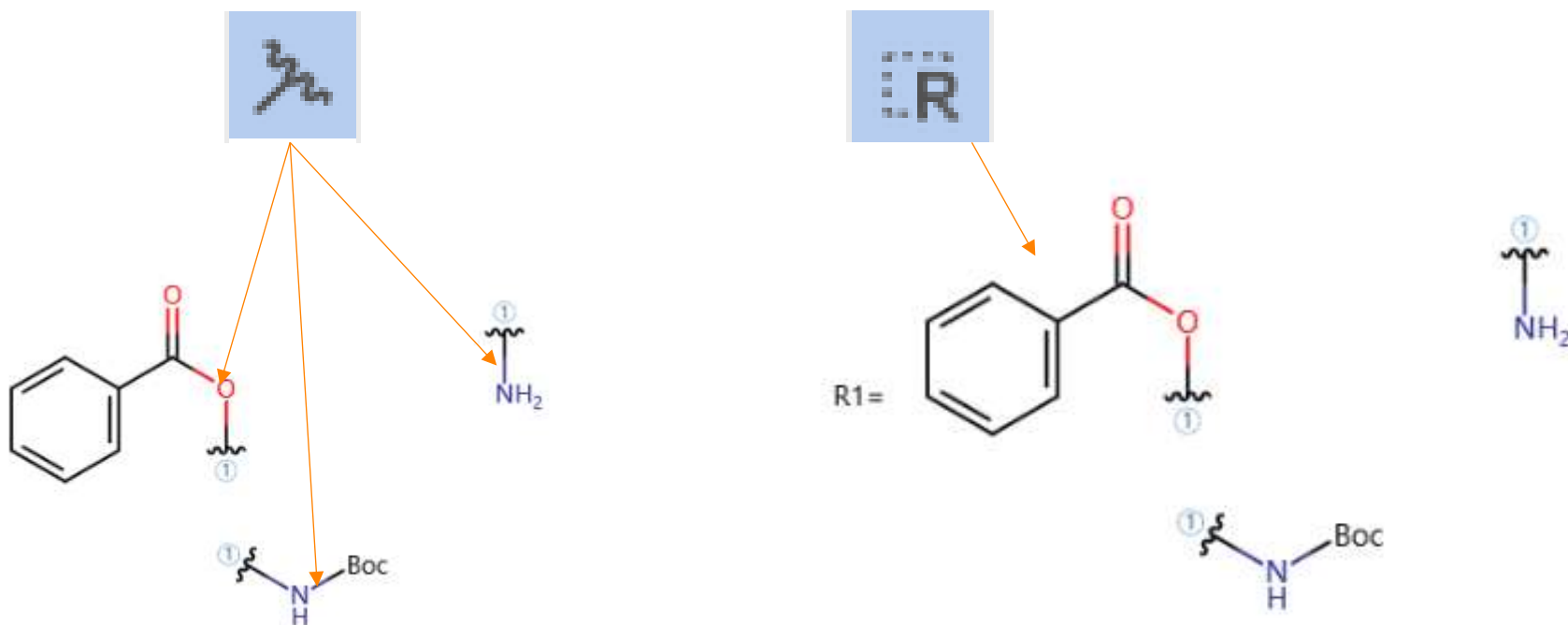


A



## 绘制方法

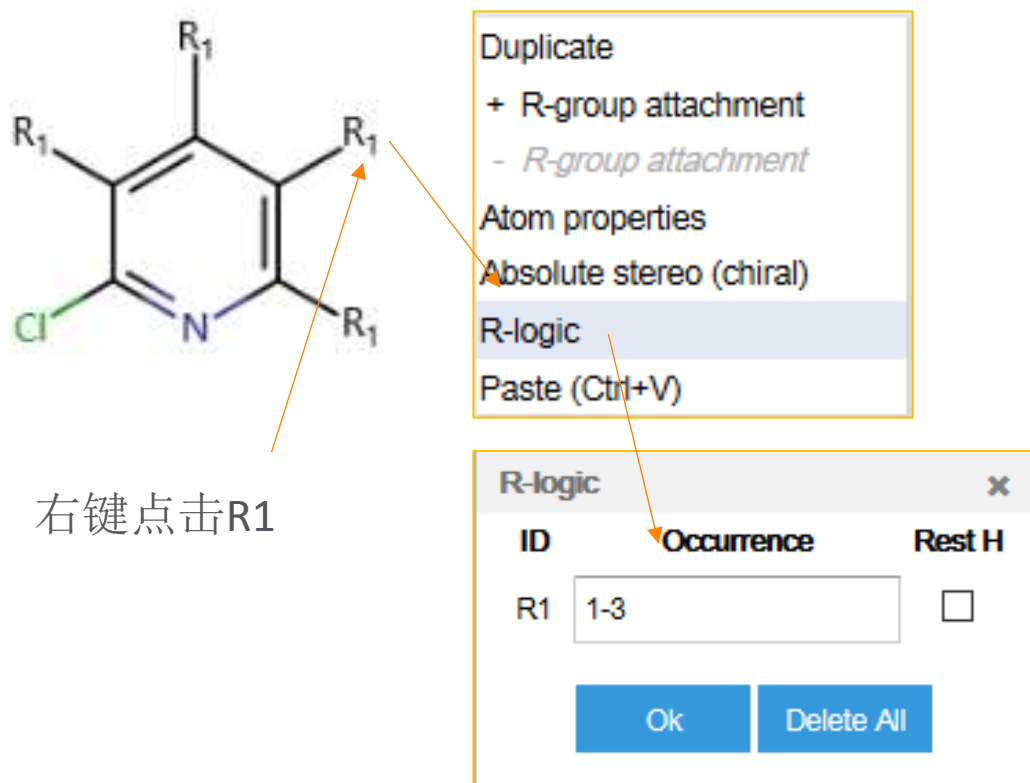
- 定义步骤：
  - 使用R基团末端定义工具定义绿色原子
  - 使用R基团定义工具，选择全部片段，即可完成R1的定义





## R基团定义的延展

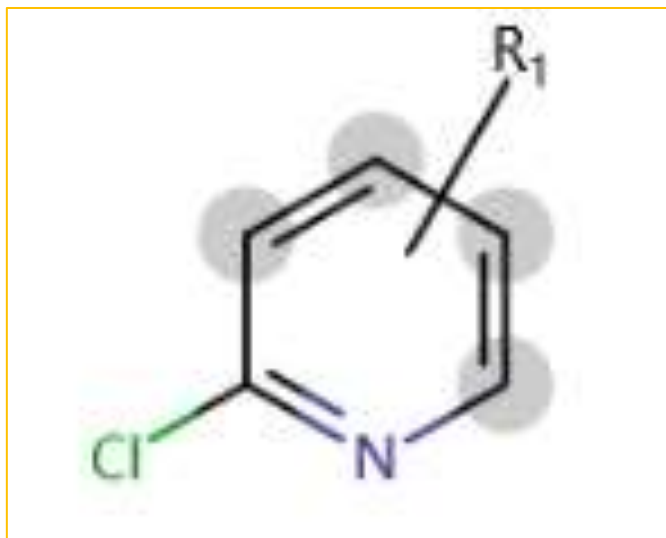
- 如下结构
  - R1可以出现在4个不同的位点，
  - 但是，需要R1基团只能出现1-3次



### Tips:

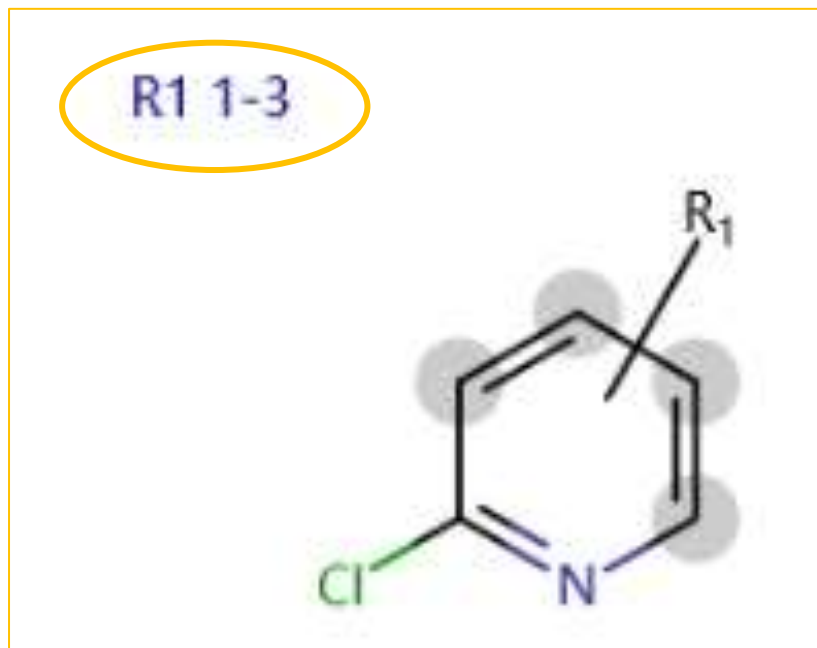
1. 当R基团有多个位点，且R的个数可变的时候，需要用R-Logic定义R的阈值
2. 右键R，打开R-Logic
3. 输入R的阈值

## R基团定义和不定位与R联用时

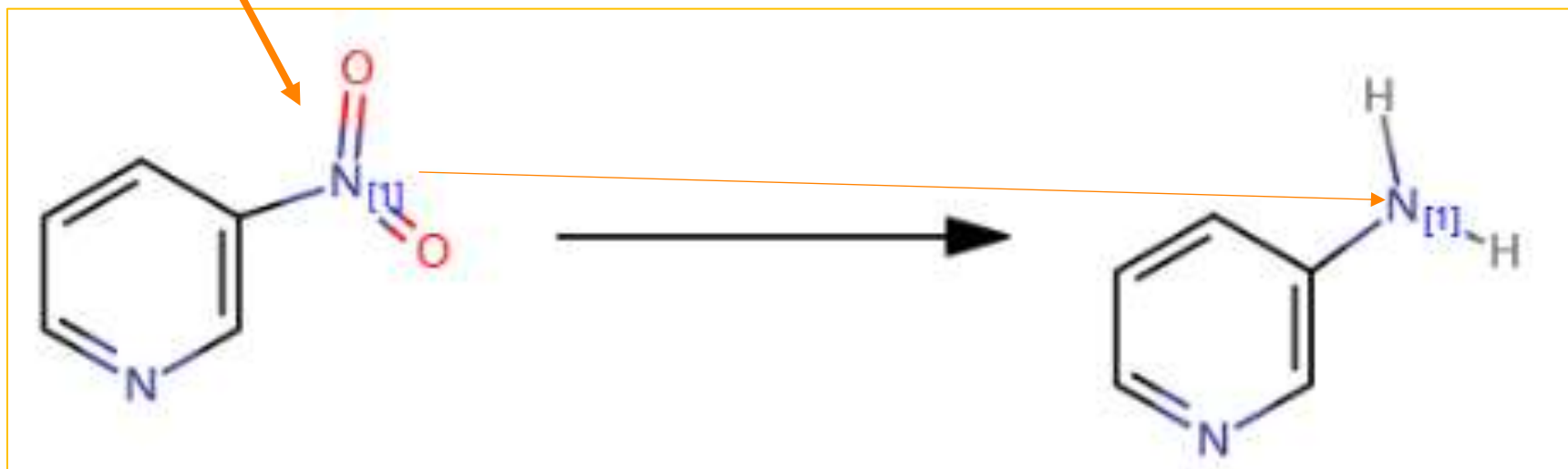
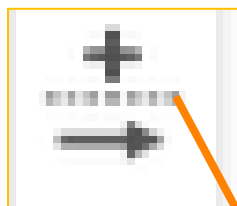


### **Tips:**

1. 当不定位工具和R基团联用时，默认是R接在所有原子上，即左图是必须接有4个R
2. 需要用到R-Logic去定义R的个数



## 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

## Part D: 常见环, 官能团, Reaxys的Generic Group定义



**Abbreviated groups** [X]

BOC  Expand

**Boc** **Ok**

**Reaxys Group Generics** [X]

**Acyclic** **Cyclic**

ACY ACH

Carb: ABC ABH

Hetero: AHC AHH

Alkynyl: AYL AYH

Alkoxy: AOX AOH

Alkyl: ALK ALH

Alkenyl: AEL AEH

G GH G\* GH\* Pol

### 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

Reaxys Group Generics

Acyclic Cyclic

ACY ACH

Carb Hetero

ABC ABH AHC AHH

Alkynyl Alkoxy

AYL AYH AOX AOH

Alkyl

ALK ALH

Alkenyl

AEL AEH

G GH G\* GH\* Pol

## 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' window with the 'Cyclic' tab selected. The interface is organized into several categories, each with a sub-category and two options (e.g., 'H' and 'H\*'). The 'Cyclic' tab is active, and several groups are highlighted with orange boxes:

- CYC** (Cyclic)
- CYH** (Cyclic with H)
- Carb** (Carbon-containing rings):
  - CBC** (Cyclic Carbon)
  - CBH** (Cyclic Carbon with H)
- Aryl** (Aromatic rings):
  - ARY** (Aromatic)
  - ARH** (Aromatic with H)
- Cycloalkyl** (Saturated carbon rings):
  - CAL** (Cycloalkyl)
  - CAH** (Cycloalkyl with H)
- Cycloalkenyl** (Unsaturated carbon rings):
  - CEL** (Cycloalkenyl)
  - CEH** (Cycloalkenyl with H)
- Hetero** (Heterocyclic rings):
  - CHC** (Cyclic Hetero)
  - CHH** (Cyclic Hetero with H)
- Heteroaryl** (Aromatic heterocyclic rings):
  - HAR** (Heteroaryl)
  - HAH** (Heteroaryl with H)
- No carbon** (Non-carbon rings):
  - CXX** (No carbon)
  - CXH** (No carbon with H)

At the bottom of the window, there are five buttons: **G**, **GH**, **G\***, **GH\***, and **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/G\*

G

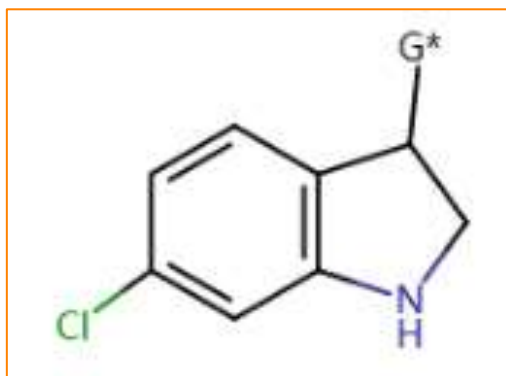
GH

G\*

GH\*

### Tips:

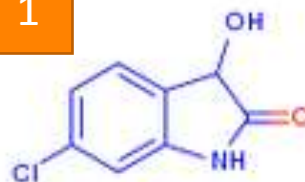
1. G代表的是任意基团，GH表示的是任意基团或H
2. G\*和G的区别是，G\*所连接的基团允许和母体成环，G不允许成环



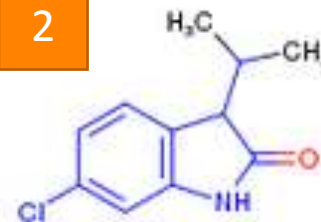
### 思考:

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



## Part E: 通用官能团, 原子属性定义

A

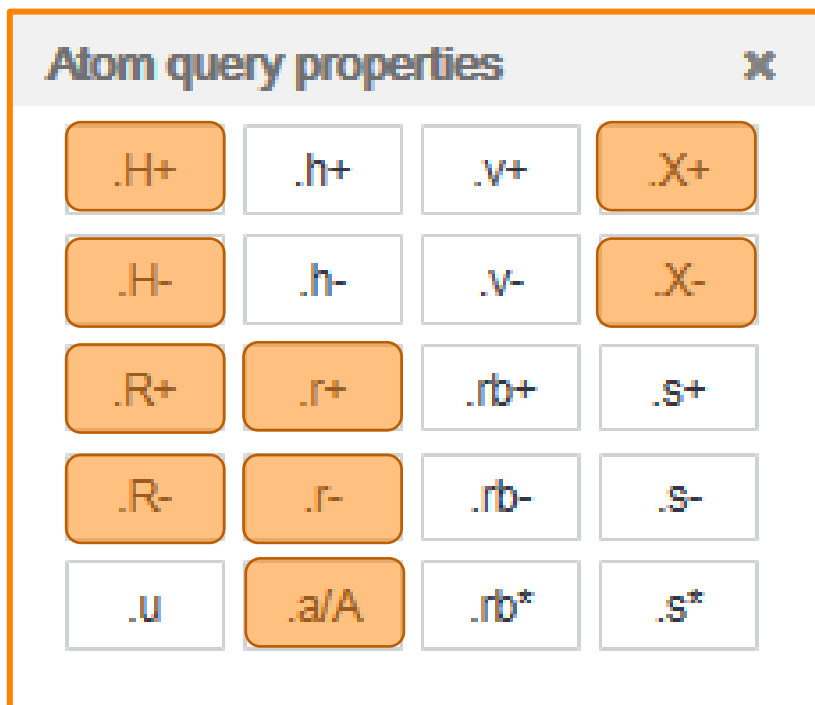
<i>A</i>	<i>Q</i>	<i>M</i>	<i>X</i>
<i>AH</i>	<i>QH</i>	<i>MH</i>	<i>XH</i>
	<i>?</i>	query prop.	

### **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



# Atom Properties全图



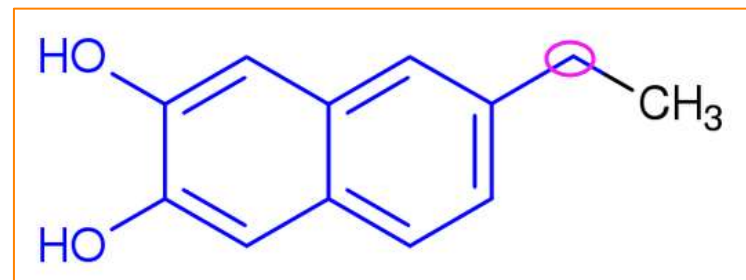
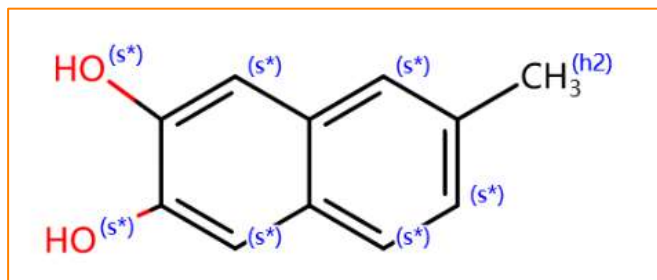
## Tips:

1. 有颜色标记的键目前RX中不起任何作用
2. h+/h-: 定义确定H的个数
3. v+/v-: 定义原子价位
4. rb+/rb-: 定义原子上环键个数
5. s+/s-: 定义原子上取代基个数
6. u: 定义原子取代基类型
7. rb\*: 封环
8. s\*: 封原子

所有功能使用时，需要配合As Draw，As Substructure。

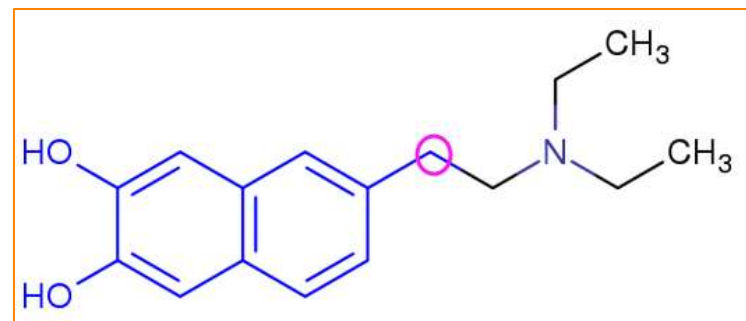
## h+/h-功能

- 定义：确定的H的取代个数
- 亚结构检索下面的结构



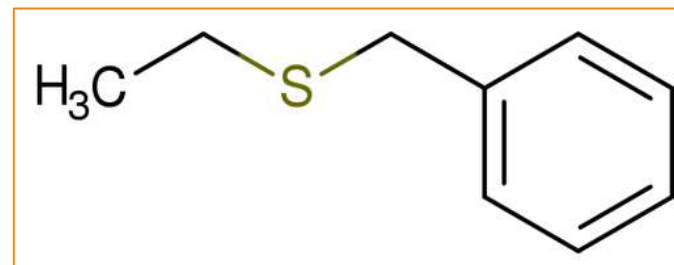
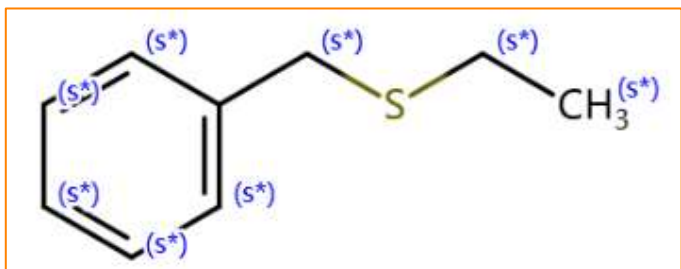
### Tips:

1. 一定要亚结构才有效用
2. 标记h<sub>2</sub>的C，通过亚结构检索后的结果中，该C上一定存在2个H，



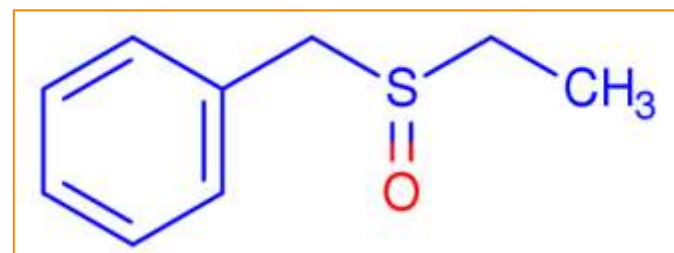
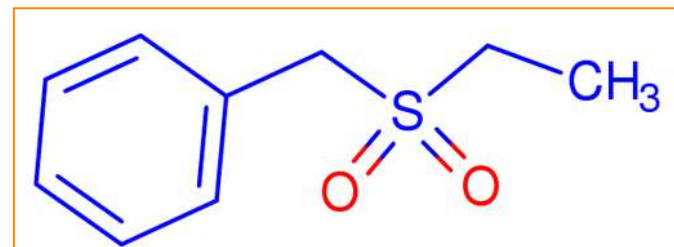
## v+/v-功能

- 定义：键的个数，通常来说指的是原子效价
- 亚结构检索带有S，N的物质中会经常遇到，如

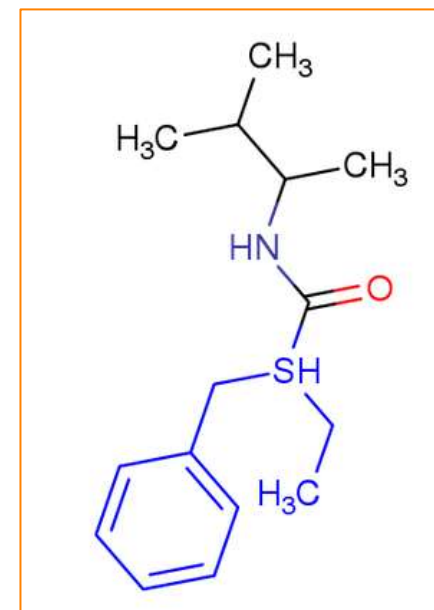
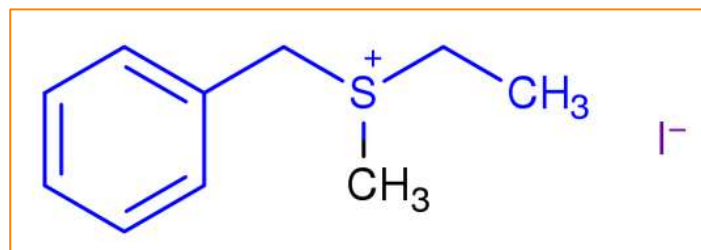
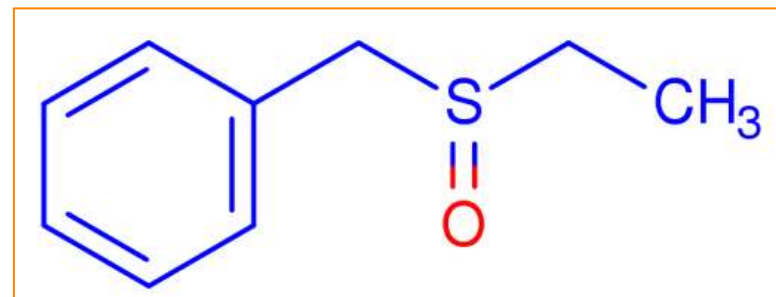
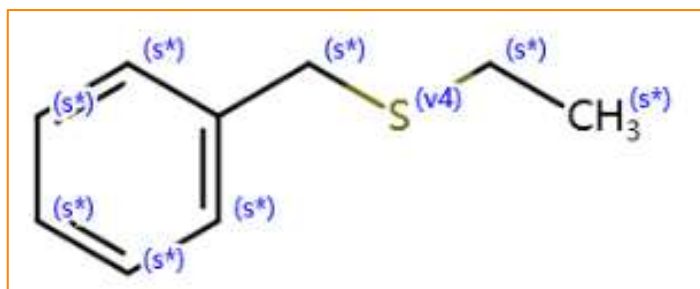


### Tips:

1. 一定在亚结构检索有效
2. 不使用v+/v-，可以拿到上述结构中S的所有效价的化合物，如右图
3. 如果标记v.....



## v+/v-功能---续

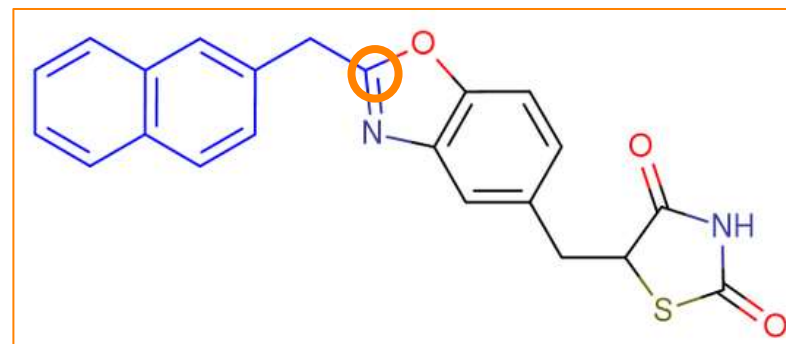
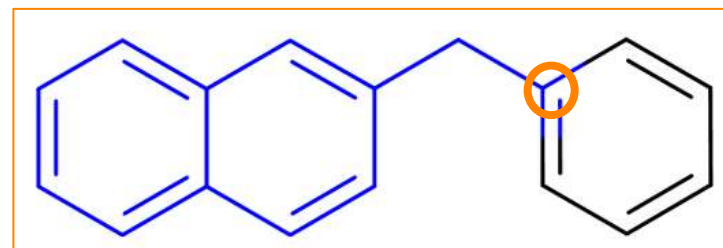
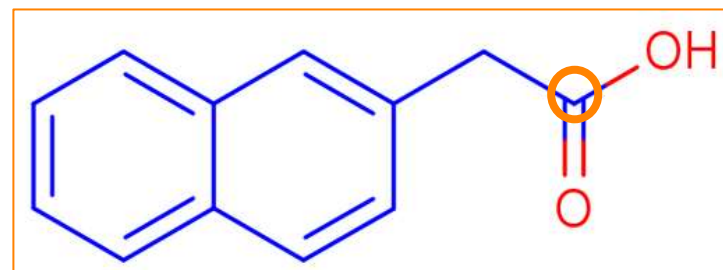
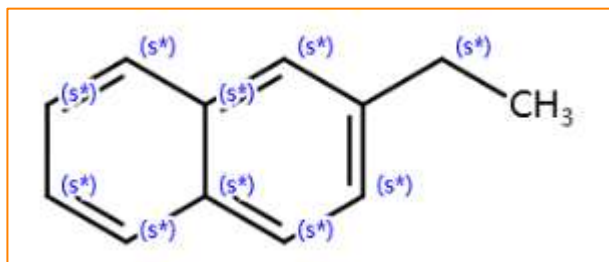


### Tips:

1. S标记V4后,
2. 检索出来的结果, S都是4价的, 如亚砷
3. 同样如果标记V6, S都是6价的, 会出现砷的结构

## rb+/rb-功能

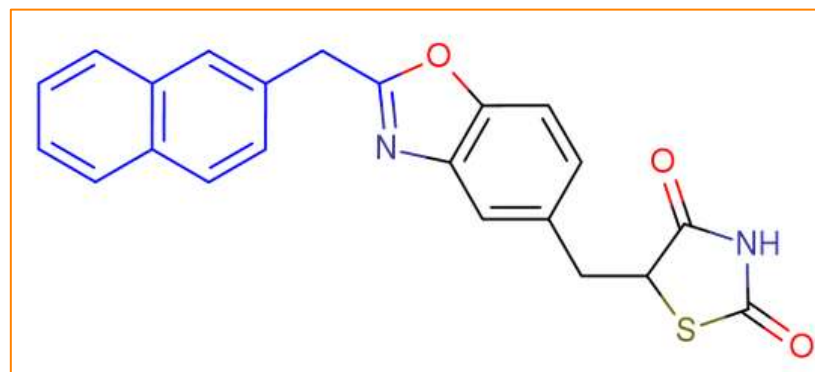
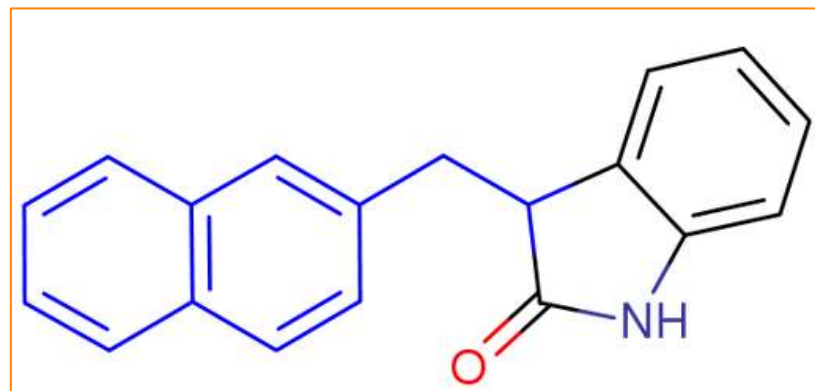
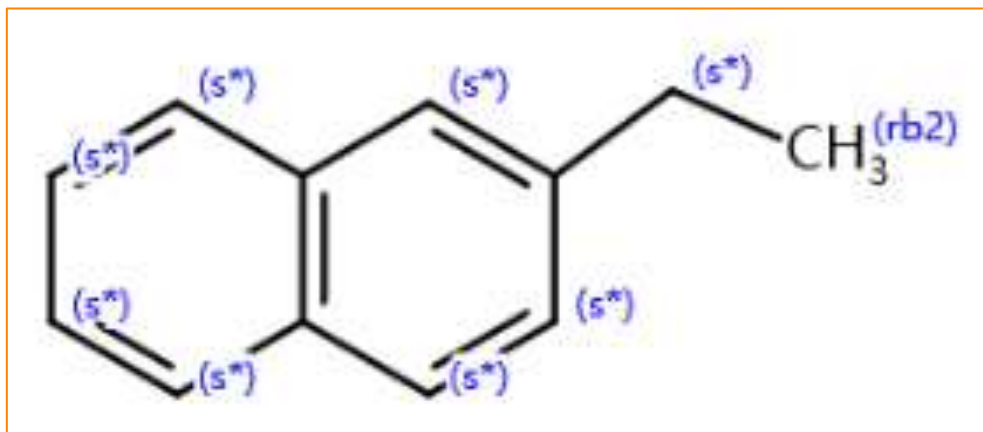
- 定义：原子上存在的，确定的，环键的个数
- 最主要的作用是控制原子是否在环上面



### Tips:

1. 一定要在亚结构中才有效用
2. 如上图，如果不用任何标记，亚结构检索可以获得右图，末端C可以在链中，也可以在环中
3. 如果添加rb+/rb-.....

## rb+/rb-功能—续

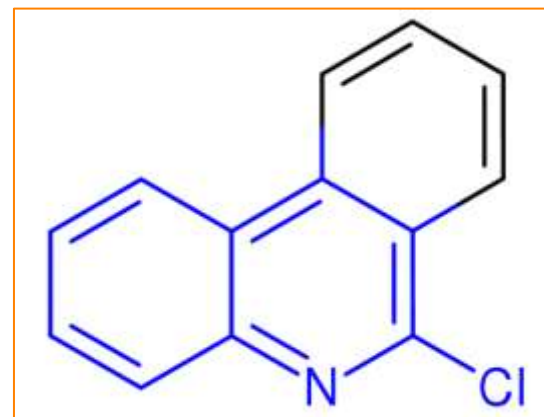
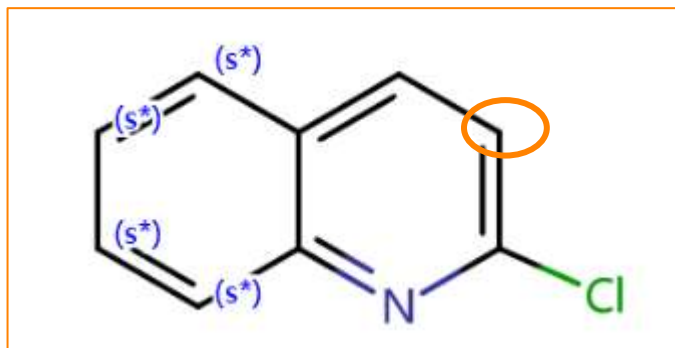


### Tips:

1. 末端C原子定义上rb后，末端C都是在C上的，如右图。
2. 一般来说，r0，r2，r3表示确切的个数，r4表示4跟环键或者更多环键。

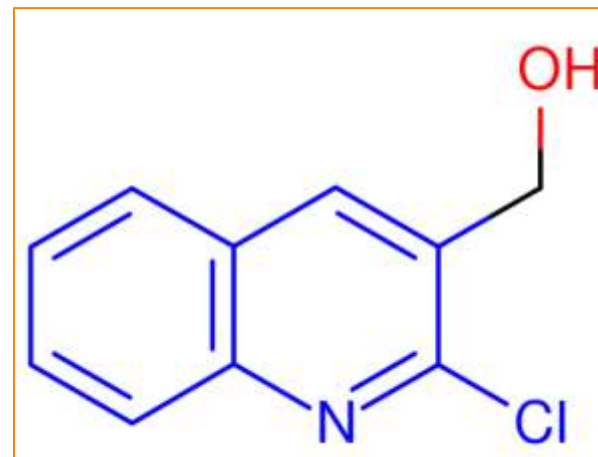
## rb\*功能

- 定义，在环上的原子，定义rb\*后，在进行亚结构检索时，只能是链取代，不能在发生环融合

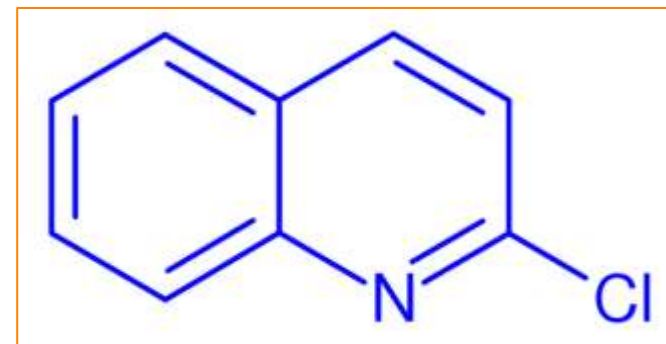
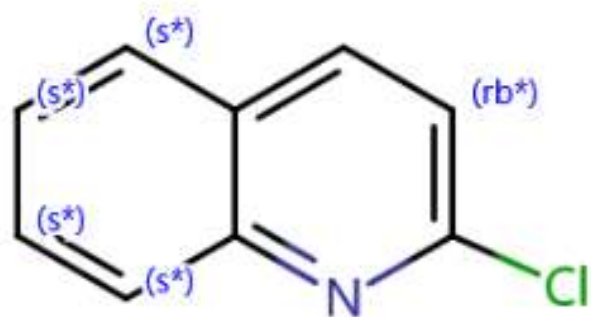


### Tips:

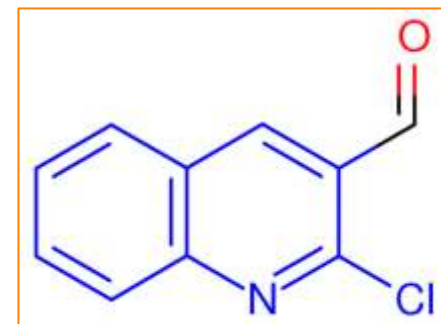
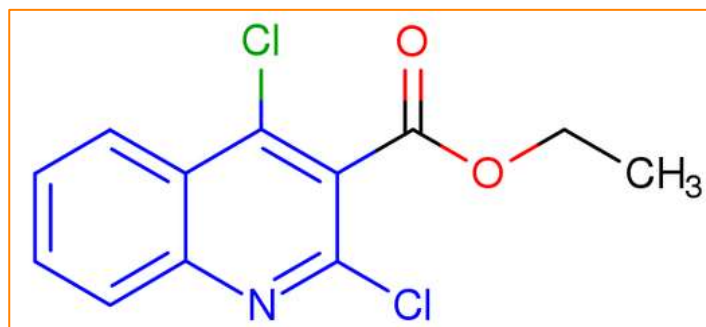
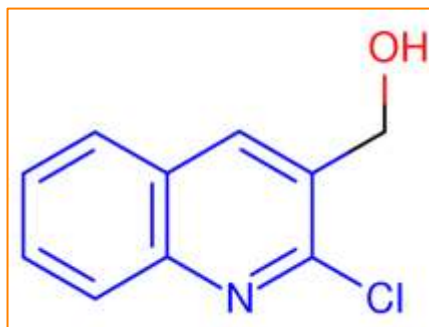
1. 只能使用在环原子上，亚结构检索有效，使用在链原子上无效
2. 如对上述结构进行亚结构检索，可以检索到右侧结构
3. 如果添加rb\*.....



## rb\*功能—续



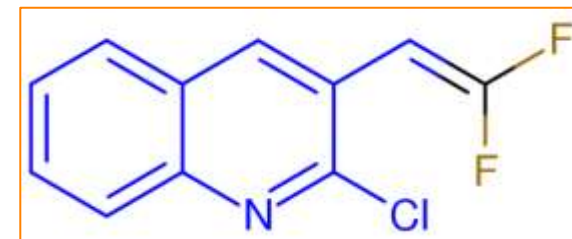
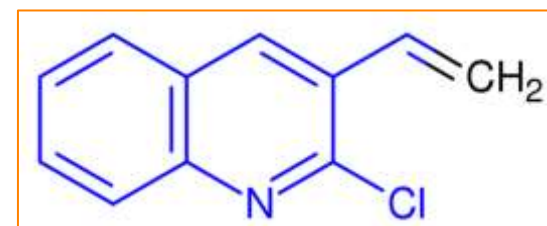
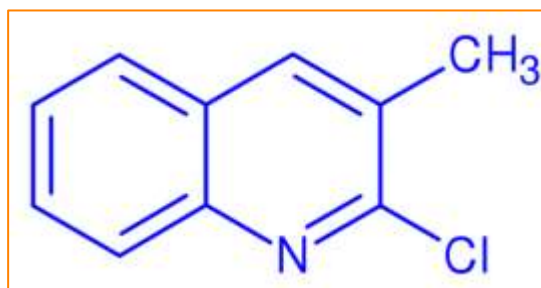
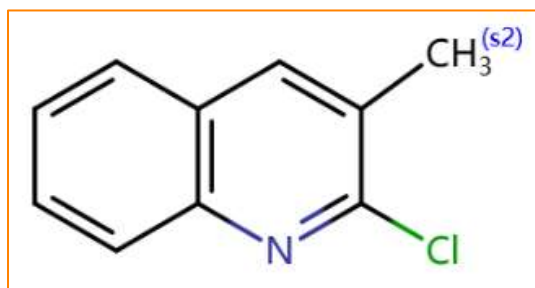
所有在标记位点上在融合成环结构全部去掉





## S+ / S- 功能

- 定义：原子上最大取代基数，S0-S5，最大取代基数，S6，开放所有取代。

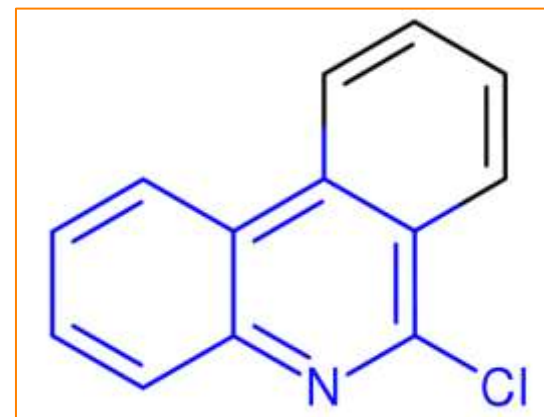
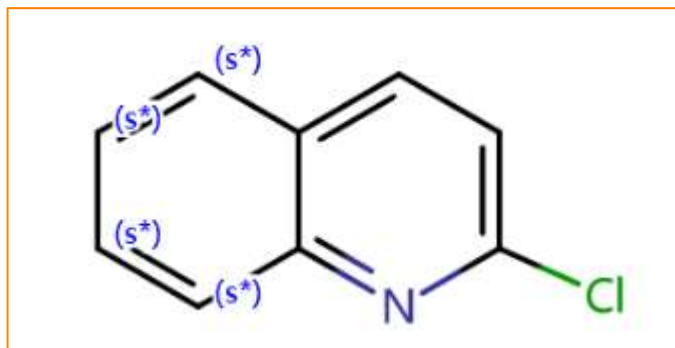


### Tips:

- As Draw中有效，亚结构无效
- 这是用As Draw做的检索，可以看到标记S2的原子在进行检索时都最多存在2个取代基（苯并吡啶算一个）

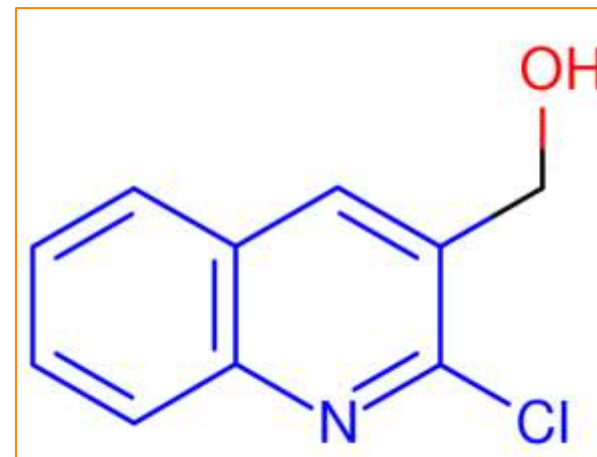
## S\*功能

- 定义：在进行亚结构检索的时候，被标记的原子处于封闭状态



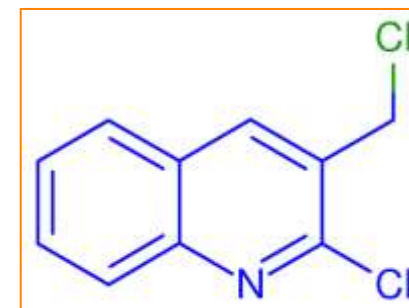
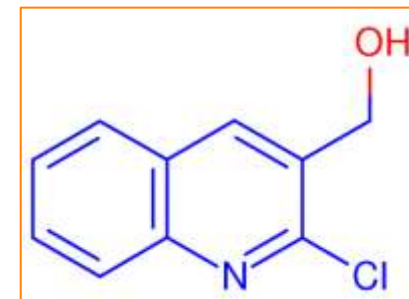
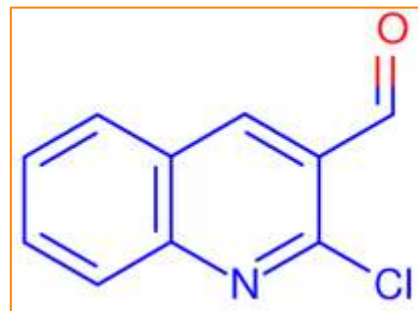
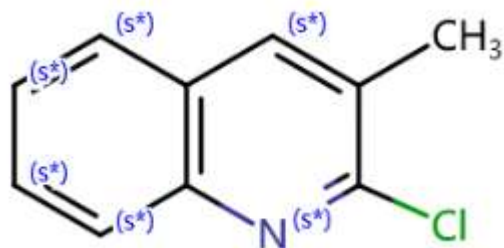
### Tips:

1. 亚结构中有效
2. 这是用Substructure做的检索，可以看到标记的4个C原子在进行检索时都没有取代发生



## U功能

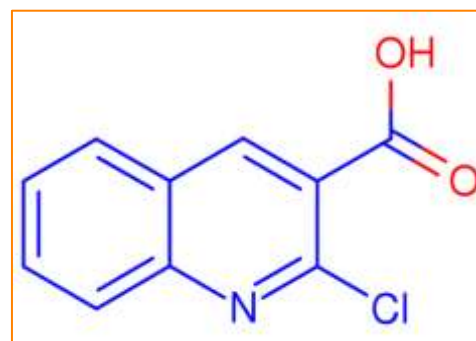
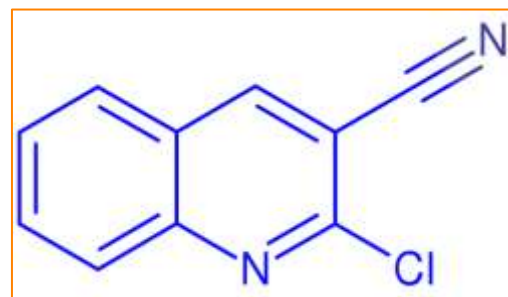
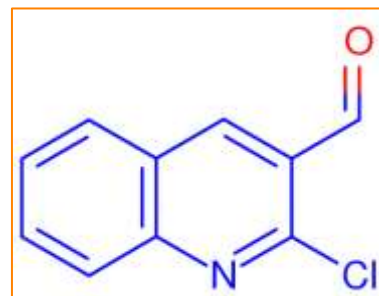
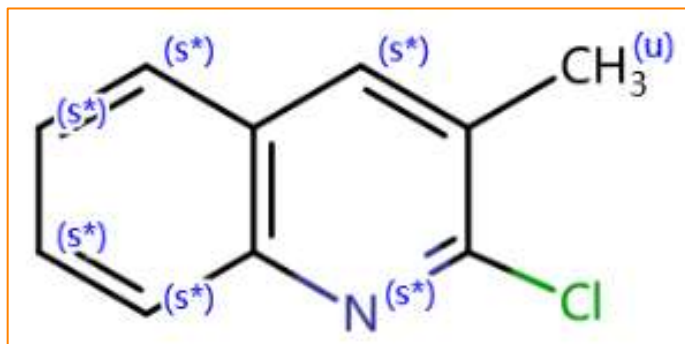
- 定义：在检索时，被标记的原子一定会存在双键，三键或者在芳环中



### Tips:

1. 亚结构中有效
2. 亚结构检索上述物质，可以发现C原子上可以接的键所有可能性都存在，饱和，不饱和
3. 使用U定义苯并吡啶的CH3

## U功能—续



### **Tips:**

1. 标记上U后，这个 $\text{CH}_3$ 上的取代，C上必须存在不饱和键

## Part F: 右键的使用—原子右键的重要功能

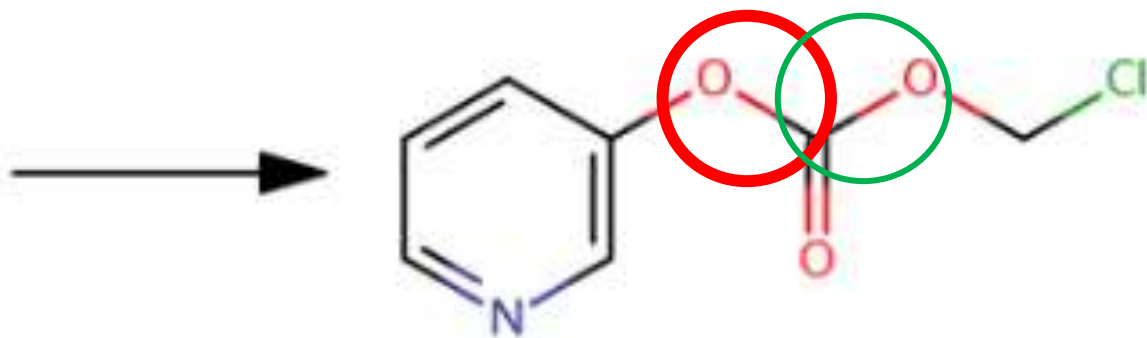
- 原子右键的使用，定义同位素

The diagram illustrates the process of defining an isotope for an atom in a chemical structure. It consists of several components:

- Top Left:** A benzene ring with a green circle highlighting one of its carbon atoms.
- Bottom Left:** A context menu with the following options: Duplicate, + R-group attachment, - R-group attachment, Atom properties (highlighted), Absolute stereo (chiral), R-logic, and Paste (Ctrl+V). An arrow points from the 'Atom properties' option to the 'Atom properties' dialog box.
- Center:** The 'Atom properties' dialog box. It has a title bar with a close button (x). Below the title bar is a 'Change to' dropdown menu set to 'Element'. The dialog is divided into 'Basic' and 'Advanced' tabs. The 'Basic' tab is active, showing fields for Atom (C), Alias (locked), Isotope (locked), Charge (0), Radical (none), Enhanced stereo (Off), and Map (locked). The 'Isotope' field is highlighted with an orange box. An arrow points from this field to a separate input field on the right.
- Top Right:** A separate input field labeled 'Isotope' with the value '13' and a lock icon.
- Bottom Right:** A benzene ring with the label  $^{13}\text{C}$  next to one of its carbon atoms, indicating the final result.

## Part F: 右键的使用—化学键右键的重要功能

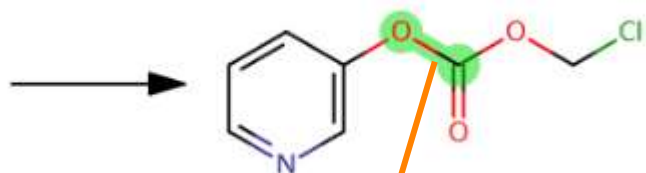
- 化学键右键的使用，定义反应中心



### **Tips:**

1. 对于这个化合物的合成，可以将结构拆成2个部分，理论上可以从红色和绿色两个部分进行拆分
2. 如果一定要是从红色部分拆分，如何定义

# 反应中心的定义



**Bond properties**

Absolute stereo (chiral)

*R-logic*

Paste (Ctrl+V)

**Bond properties** x

Type	single	▼
Topology	undefined	▼
Reacting center	undefined	▼

Ok

## Tips:

Center:

Make or Break:

Change:

Make and Change:

Not Center:

反应中心

生成或断裂

变化

生成和变化

不是反应中心

undefined

center - #

make or break - ||

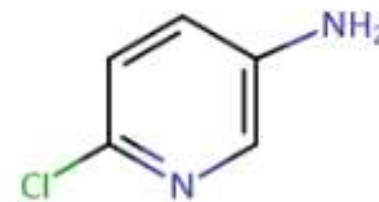
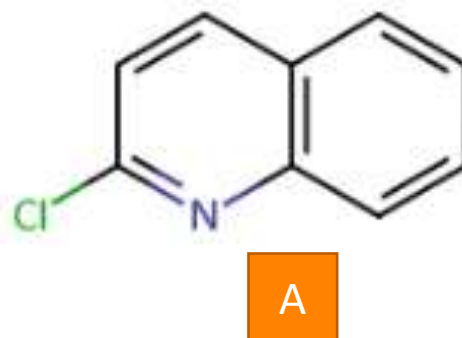
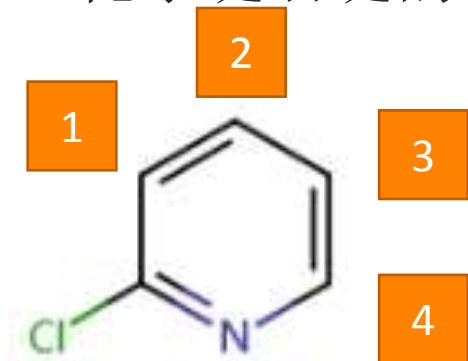
change - |

make and change - |||

not center - x

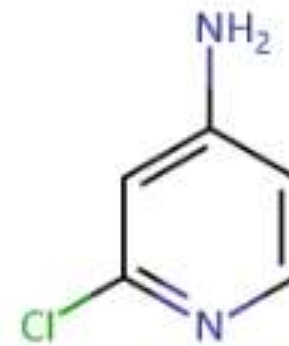
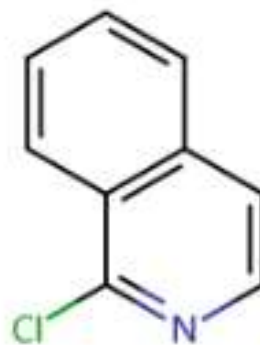
## Part F: 右键的使用—化学键右键的重要功能

- 化学键右键的使用，键的拓扑



### 思考:

- 使用As Substructure检索吡啶氯可以获得右侧所有结构
- 但是如何实现，3，4位点上不发生稠环的检索，即A结构不允许检索到，但其他3个结构可以





## 键的属性定义



Bond properties

Absolute stereo (chiral)

*R-logic*

Paste (Ctrl+V)

Bond properties

Type	single
Topology	undefined
Reacting center	undefined

Ok

Bond properties

Type	single
Topology	in chain
Reacting center	undefined

### Tips:

1. 用AH定义吡啶上的可能的取代原子
2. 右键绿色的键，
3. 利用Topology功能定义这根键在环上，还是在链上



Thank you!

刘佳

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