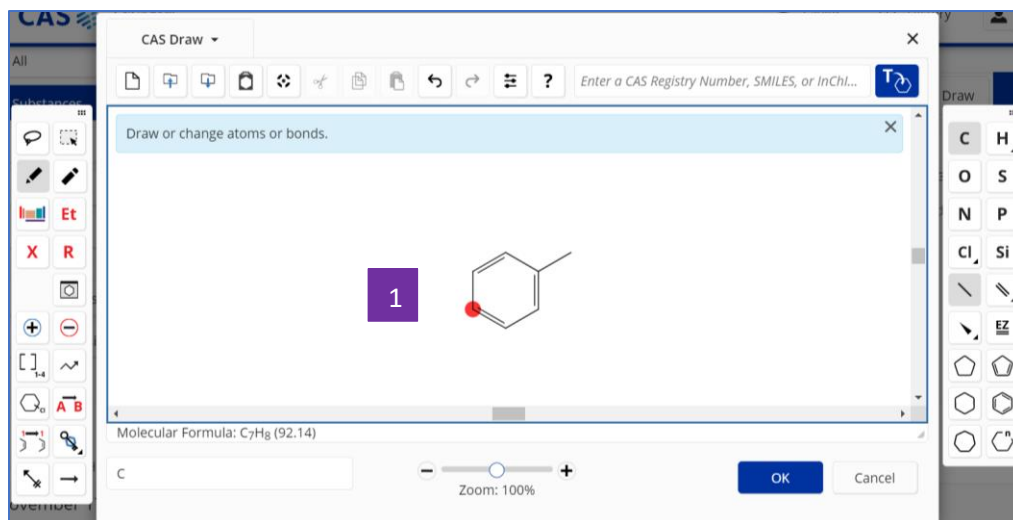
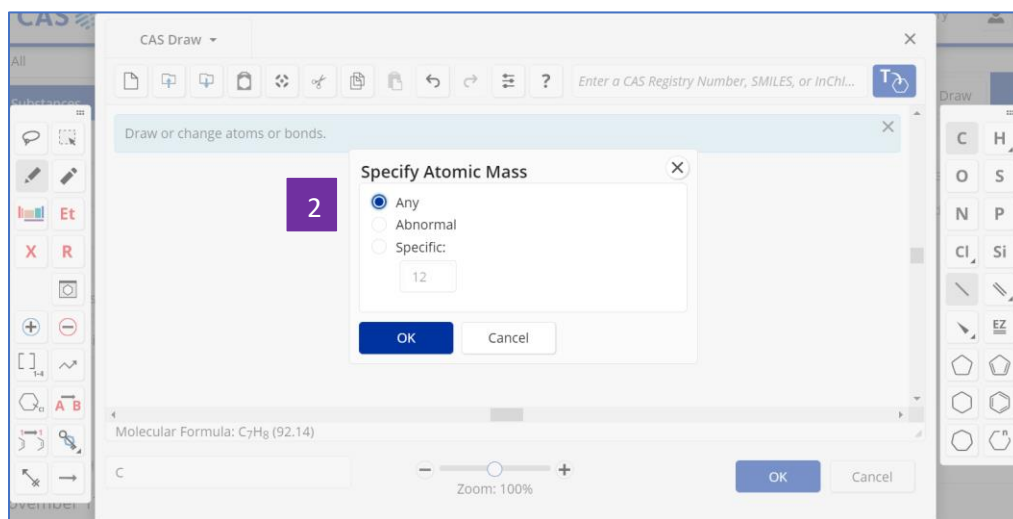


## CAS SciFinder<sup>®</sup> 使用技巧 | 绘制结构式时，如何绘制同位素

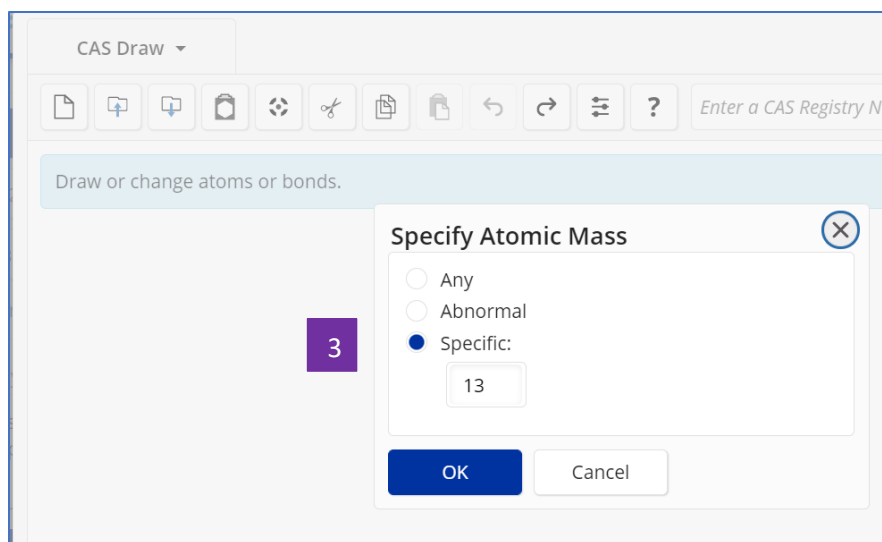
绘制结构时，可绘制特定原子的同位素，以获取其同位素标记的物质、同位素标记的物质参与的反应、研究同位素标记的物质的文献等信息。



1. 绘制结构，选中需要标记同位素的原子，点击鼠标右键。

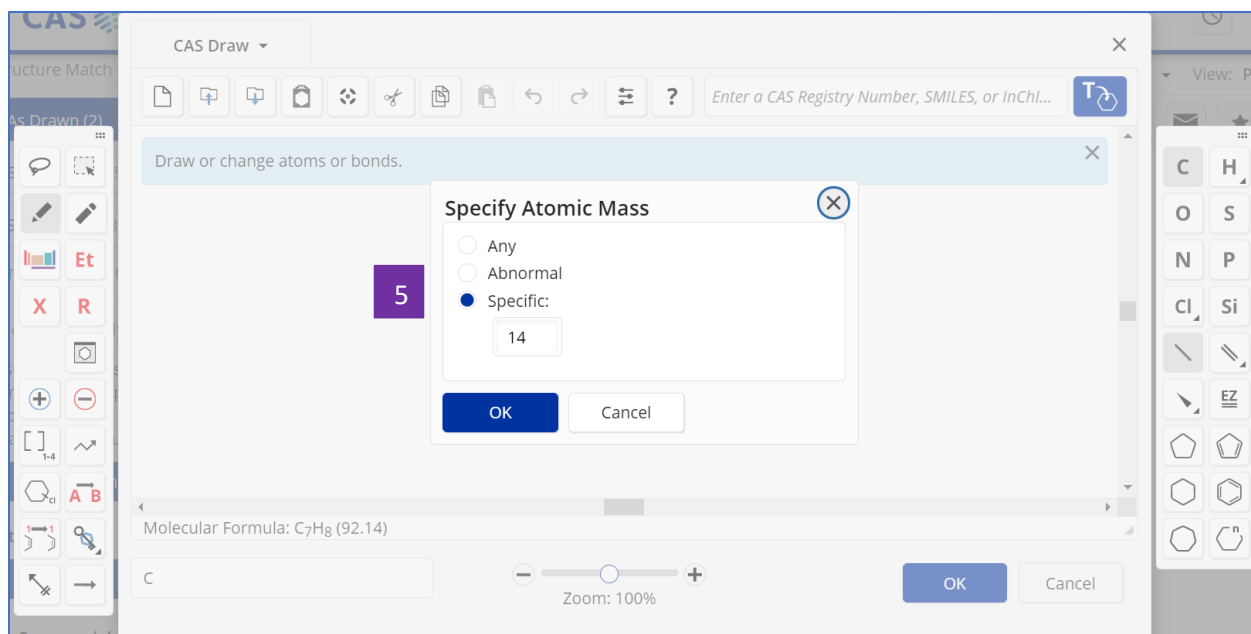


2. 在弹出窗口中，选择原子量为 Any（默认值，任意元素）、Abnormal（任意同位素）或 Specific（特定同位素）。



3. 选择 Specific，并输入数值 13，表面此处的碳原子为  $^{13}\text{C}$ 。

4. 所得结果均为满足设定需要：甲基对位的碳为  $^{13}\text{C}$ 。



5. 若希望甲基对位的碳原子为  $^{14}\text{C}$ ，则输入值 14

CAS SciFinder

Substances Enter a query...

Return to Home

Structure Match

As Drawn (2)

Substructure (585)

Similarity (6,335)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

**Substances (2)**

References Reactions Suppliers

1 859793-75-2

$\text{H}^{14}\text{C}$

C<sub>7</sub>H<sub>8</sub>  
Toluene-*p*-C<sup>14</sup>

1 Reference 0 Reactions 0 Suppliers

2 115760-59-3

$\text{H}^{14}\text{C}$   $^{14}\text{C}$   $^{14}\text{C}$   $^{14}\text{C}$   $^{14}\text{C}$   $^{14}\text{C}$

C<sub>7</sub>H<sub>8</sub>  
Benzene-<sup>14</sup>C<sub>6</sub>, methyl-

3 References 3 Reactions 3 Suppliers

6

Edit Drawing Remove

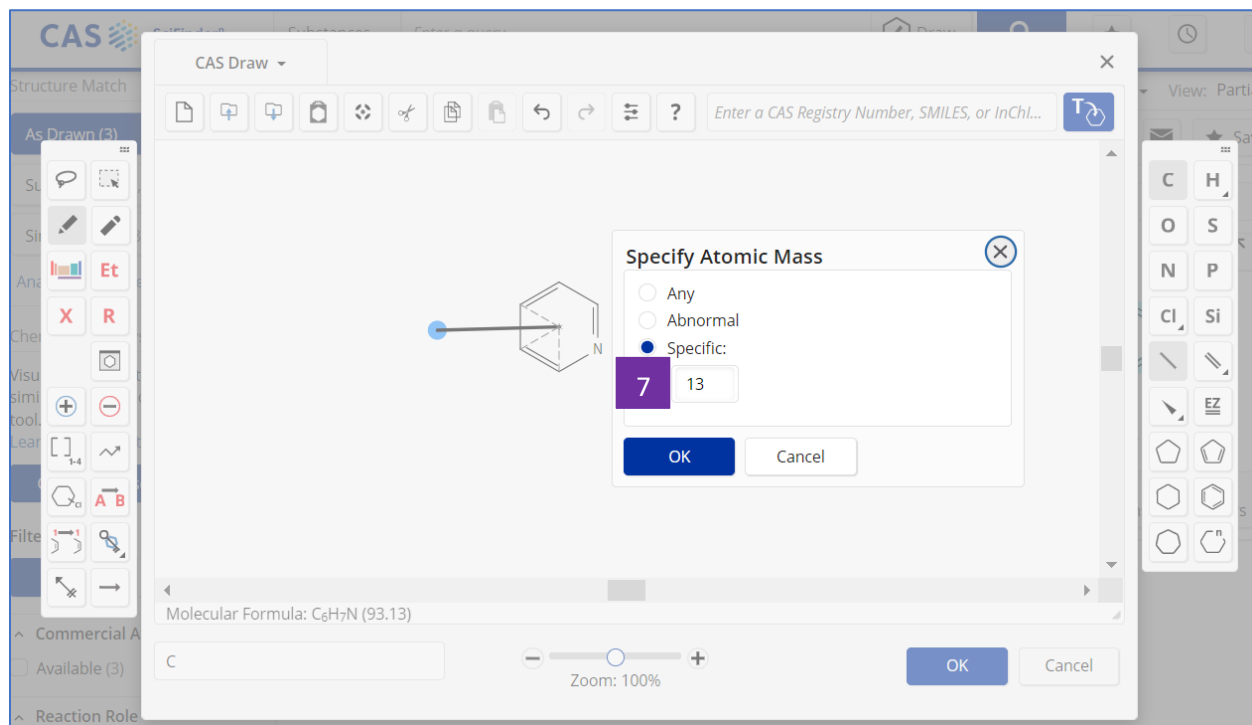
Search Patent Markush

6. 获得指定原子为  $^{14}\text{C}$  的物质。

## 案例

获取具如下结构特征的物质：

吡啶环中 N 原子的邻位、间位或者对位至少连接一个甲基，且甲基碳为  $^{13}\text{C}$ 。



7. 将甲基碳的原子量设置为 13

CAS SciFinder® Substances  Edit Search Star Clock User

Return to Home 8

## Substances (4)

References Reactions Suppliers

Descending View: Partial

As Drawn (4) Substructure (292) Similarity (3,128) Analyze Structure Precision

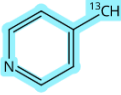
Chemscape Analysis Visually explore structure similarity with a powerful new tool. Learn more about Chemscape. Create Chemscape Analysis

Filter Behavior Filter by Exclude

Commercial Availability  Not Available (4) Reaction Role

1

**1630788-91-8**

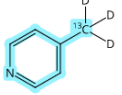


$C_6H_5N$   
4-Pyridinylmethylene- $^{13}C$

1 Reference 8 Reactions 0 Suppliers

2

**1529772-81-3**

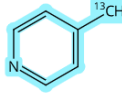


$C_6H_4D_3N$   
4-(Methyl- $^{13}C$ - $d_3$ )pyridine

1 Reference 1 Reaction 0 Suppliers

3

**1404120-05-3**

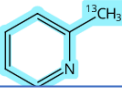


$C_6H_7N$   
4-(Methyl- $^{13}C$ )pyridine

3 References 4 Reactions 0 Suppliers

4

**813432-91-6**



8. 获得满足要求的物质。