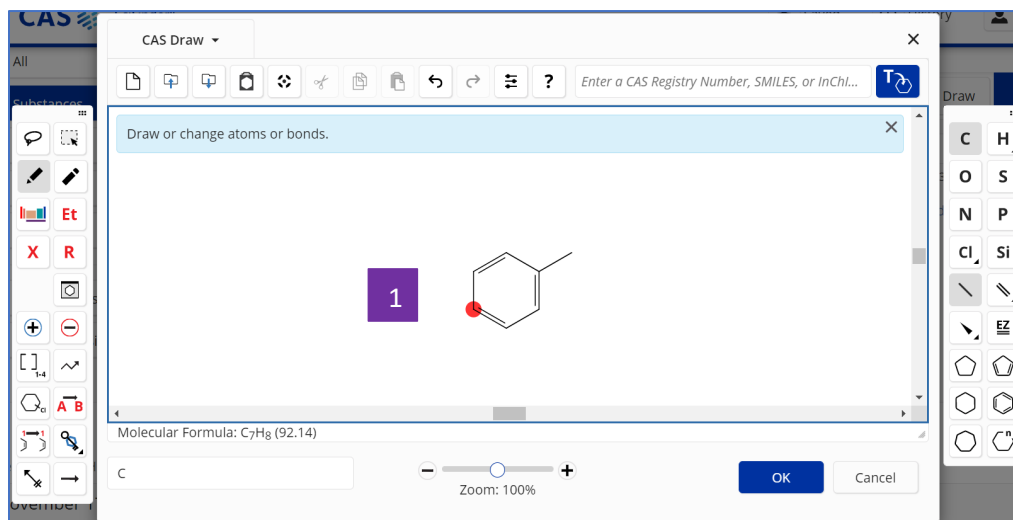
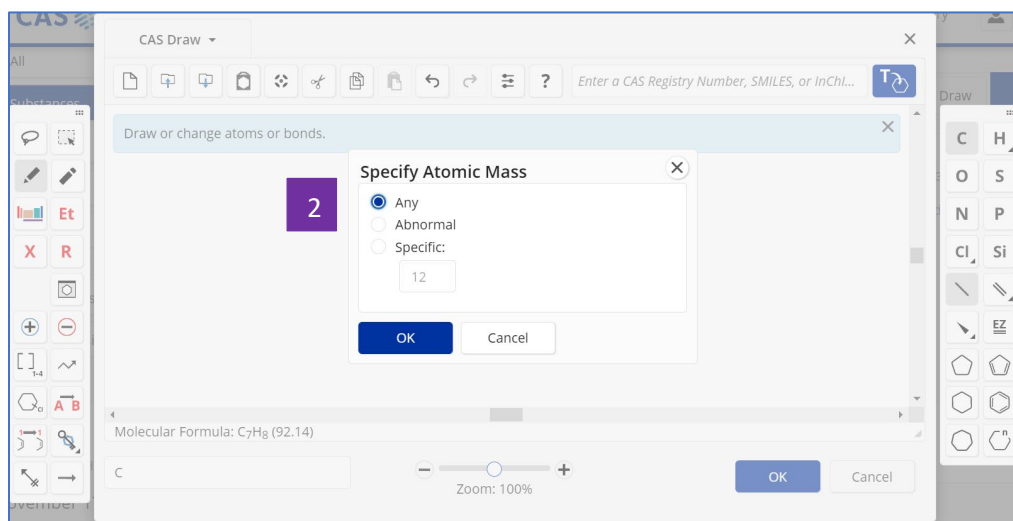


CAS SciFinder[®] 使用技巧 | 绘制结构式时，如何绘制同位素

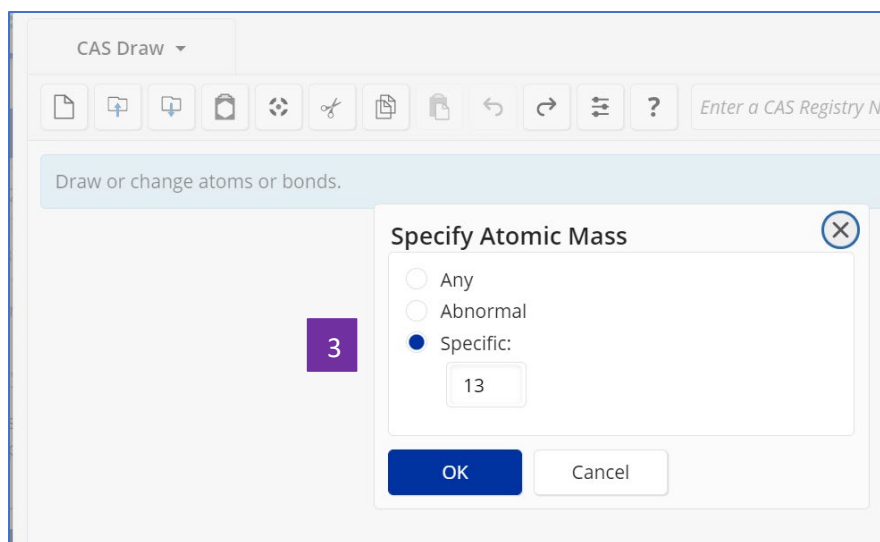
绘制结构时，可绘制特定原子的同位素，以获取其同位素标记的物质、同位素标记的物质参与的反应、研究同位素标记的物质的文献等信息。



1. 绘制结构，选中需要标记同位素的原子，点击鼠标右键。

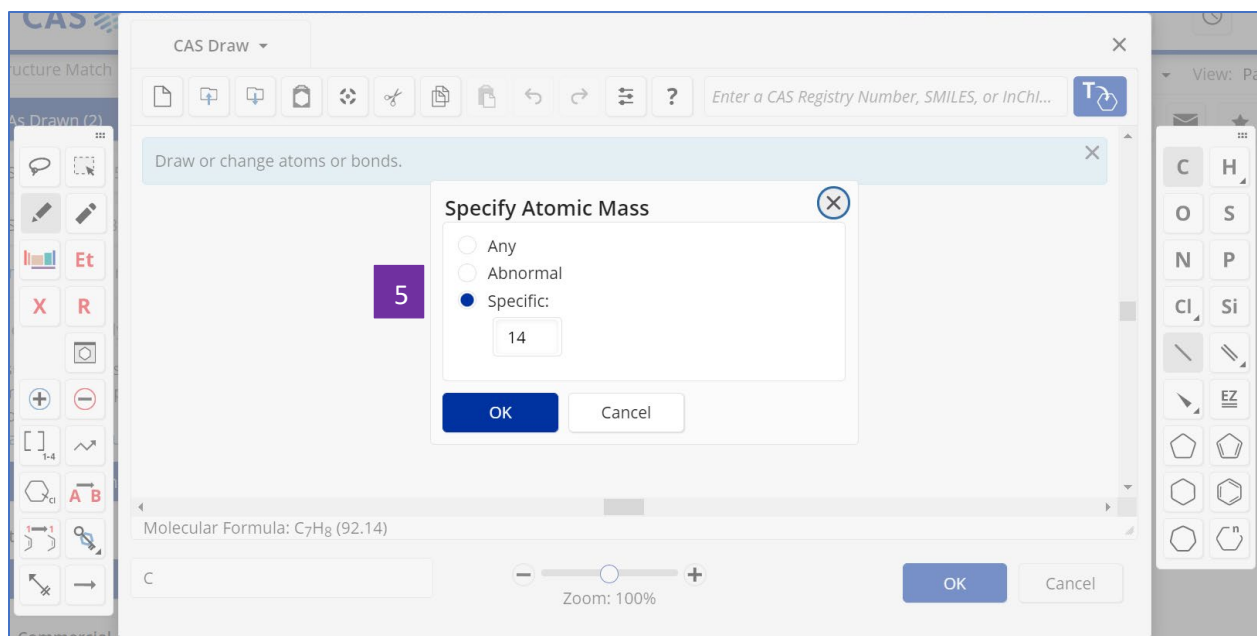


2. 在弹出窗口中，选择原子量为 Any（默认值，任意元素）、Abnormal（任意同位素）或 Specific（特定同位素）。



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

4. 所得结果均为满足设定需要：甲基对位的碳为 ^{13}C 。



5. 若希望甲基对位的碳原子为 ^{14}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

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Create Chemscape Analysis

Filter Behavior

Substances (2)

References Reactions Suppliers

1 859793-75-2

C₇H₈
Toluene-*p*-C¹⁴

1 Reference 0 Reactions 0 Suppliers

2 115760-59-3

C₇H₈
Benzene-¹⁴C₆, methyl-

3 References 3 Reactions 3 Suppliers

6

Edit Drawing Remove

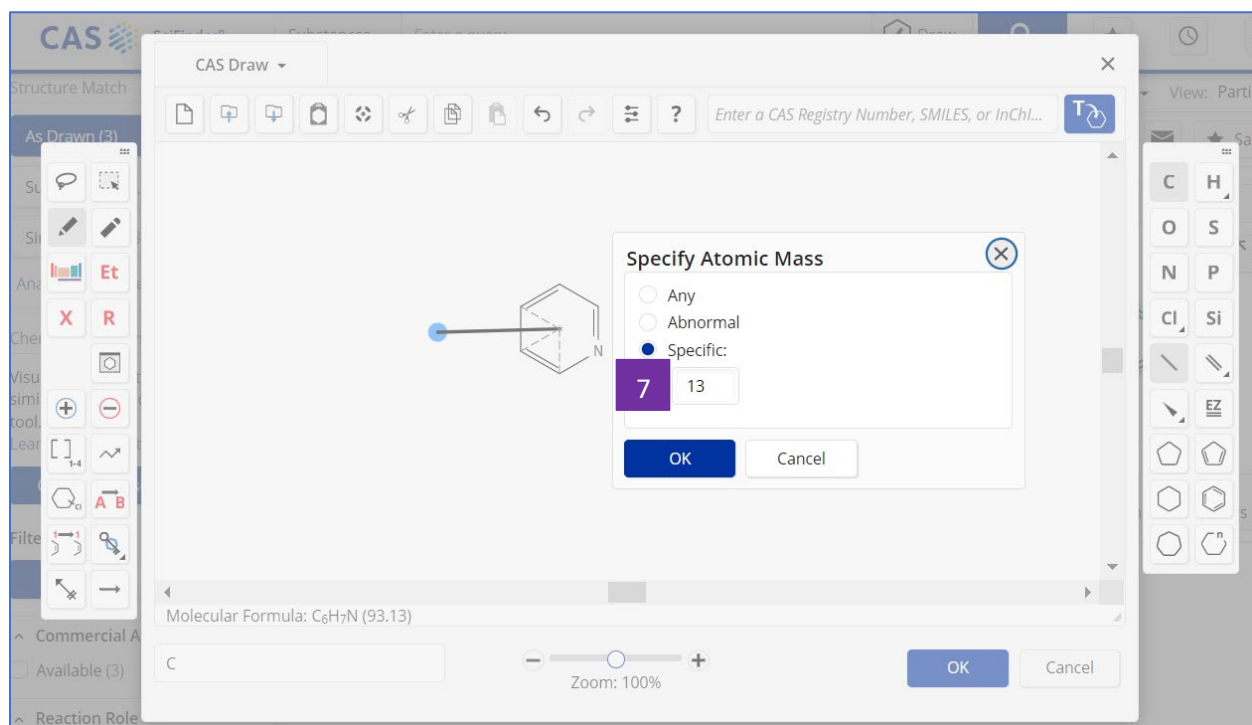
Search Patent Markush

6. 获得指定原子为 ^{14}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}C 。



7. 将甲基碳的原子量设置为 13

CAS SciFinder[®] Substances Enter a query...

8

Substances (4)

Structure Match

As Drawn (4)

Substructure (292)

Similarity (3,128)

Analyze Structure Precision

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Filter Behavior

Filter by Exclude

Commercial Availability

Not Available (4)

Reaction Role

References Reactions Suppliers

1 8 0

Reference Reactions Suppliers

1 1 0

Reference Reaction Suppliers

3 4 0

References Reactions Suppliers

4

1630788-91-8

Cc1cccnc1

C_6H_5N
4-Pyridinylmethylene- ^{13}C

1529772-81-3

Cc1cccnc1

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

1404120-05-3

Cc1cccnc1

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

813432-91-6

Cc1cccnc1

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

Edit Drawing Remove

Search Patent Markush

Descending View: Partial

Download Email Save

8. 获得满足要求的物质。