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。

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1. 绘制结构,选中需要标记同位素的原子,点击鼠标右键。

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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)。

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

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4. 所得结果均为满足设定需要: 甲基对位的碳为 ¹³C。

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5. 若希望甲基对位的碳原子为¹⁴C,则输入值 14

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Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.	C ₇ H ₈ Toluene- <i>p</i> -C ¹⁴		C7H8 Benzene− ¹⁴ C6,	methyl-		
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Filter Behavior						

6. 获得指定原子为 ¹⁴C 的物质。

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 ¹³C。



7. 将甲基碳的原子量设置为 13

案例



8. 获得满足要求的物质。