

## SciFinder Academia Tips on Searching Similar Reaction

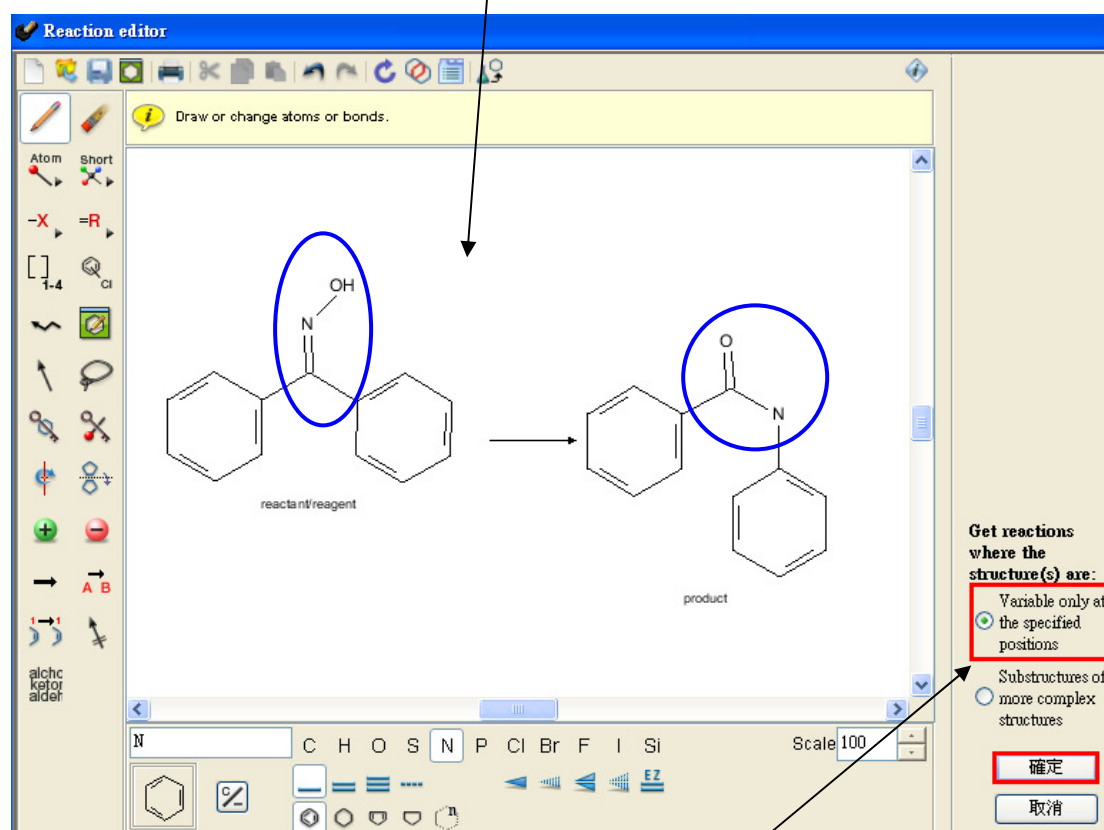
Quiz:

如何尋找相似反應機構方程式(例如  $R_1R_2-CN-OH \rightarrow R_1-CO-NH-R_2$ )

Ans:

當我們檢索一組化學反應時，我們要知道該反應方程式的相似反應，我們可以進入畫板

在畫板上畫出欲檢索的反應方程式，其中 C=N-OH 反應後變成 O=C-N-H 鍵

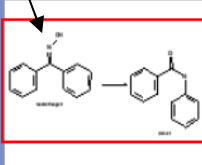


選擇 variable only at the specified position 並按下確定鍵

反應方程式會呈現出來

選擇 Allow variability only as specified，點選尋找

Reaction Structure



Click image to change structure or view detail

Search type:  Allow variability only as specified  
 Substructure

Search

選擇適當的反應條件，如：溶劑、催化劑、回收率...後，從確認的反應方程式中點選 Similar Reactions

1. Reaction Detail [Similar Reactions](#) NEW

$$\text{Ph}_2\text{C}=\text{N}-\text{OH} \xrightarrow{\text{R: C}_5\text{H}_5\text{N}, \text{R: HCl}, \text{S: H}_2\text{O}} \text{Ph}-\overset{\text{O}}{\parallel}{\text{C}}-\text{NHPh}$$

100%

NOTE: HCl/Pyridine, 1,2-Shift, Amide formation, Arylation, Dearomatization, Dehydroxylation, Deoxygenation, Hydroxylation, Isomerization, Migration, N-Arylation, N-Deoxygenation, Oxygenation, Rearrangement,  
Reactants: 1, Reagents: 2, Solvents: 1,  
Steps: 1, Stages: 1

依相似程度不同，勾選適合的相似反應，點選 Get Reactions

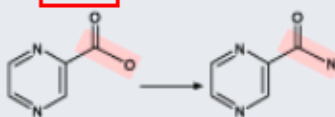
### Get Similar Reactions ⓘ

Retrieve similar reactions from:

- All reactions
- Current answer set

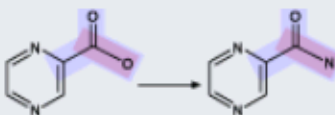
Include this level of similarity:

- Broad** - Reaction centers only (907)



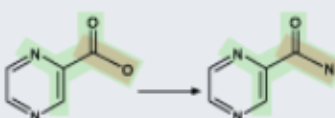
只有反應中心相同，相似度最低，有 907 筆

- Medium** - Reaction centers plus adjacent atoms and bonds (224)



除了反應中心，周圍原子相同，有 224 筆

- Narrow** - Reaction centers plus extended atoms and bonds (167)



反應中心往外延伸之原子都相同，相似度最高，有 167 筆

Get Reactions

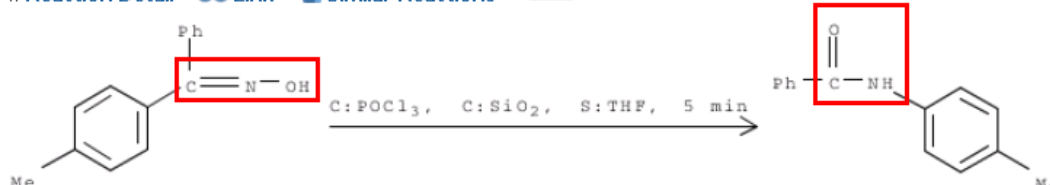
Cancel

如此即可獲得相似反應方程式，如：以下兩組反應式都是  $C=N-OH \rightarrow O=C-N-H$  的反應

2. Reaction Detail [Link](#) [Similar Reactions](#) NEW



4. Reaction Detail [Link](#) [Similar Reactions](#) NEW



需要知道更多....

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