由 ChemDraw 複製結構到 MarvinJS

Reaxys 結構搜尋 – 匯入與匯出 – 1

Edit → Copy as → SMILES

Ctrl + V 貼上

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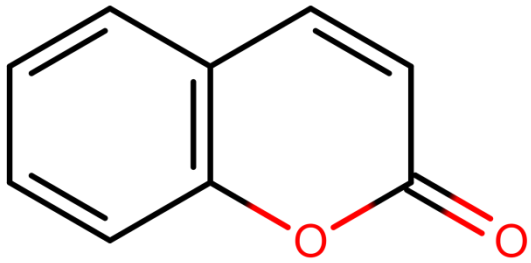
由化合物名稱產生結構

Reaxys 結構搜尋 – 匯入與匯出 – 2

化合物名稱
Coumarin

Create structure template from name >



https://youtu.be/Y2sBPaQpt4o

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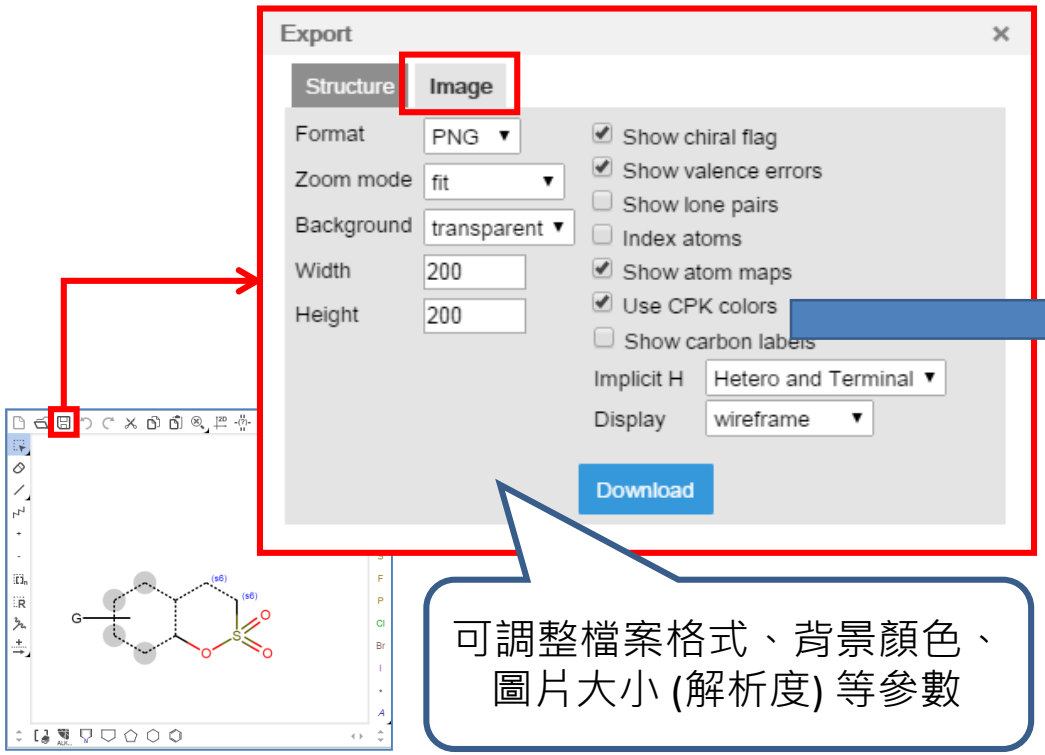
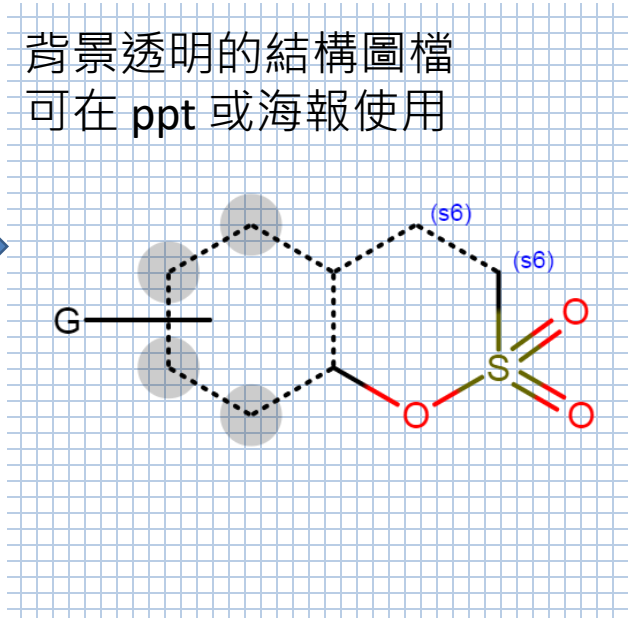
將化學結構存成透明背景的圖檔

Reaxys 結構搜尋 – 匯入與匯出 – 3



可調整檔案格式、背景顏色、圖片大小 (解析度) 等參數



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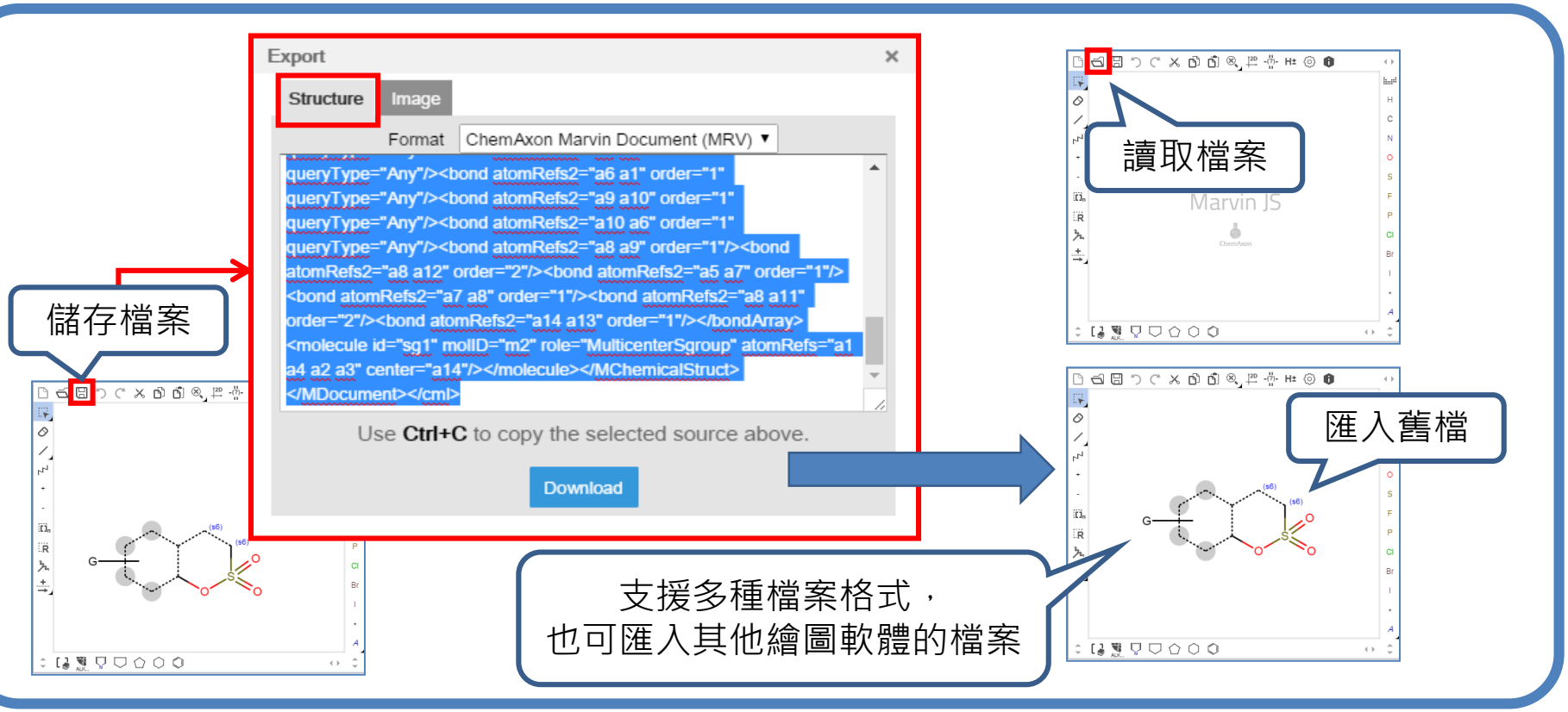
儲存可編輯的結構檔 .mrv

Reaxys 結構搜尋 – 匯入與匯出 – 4



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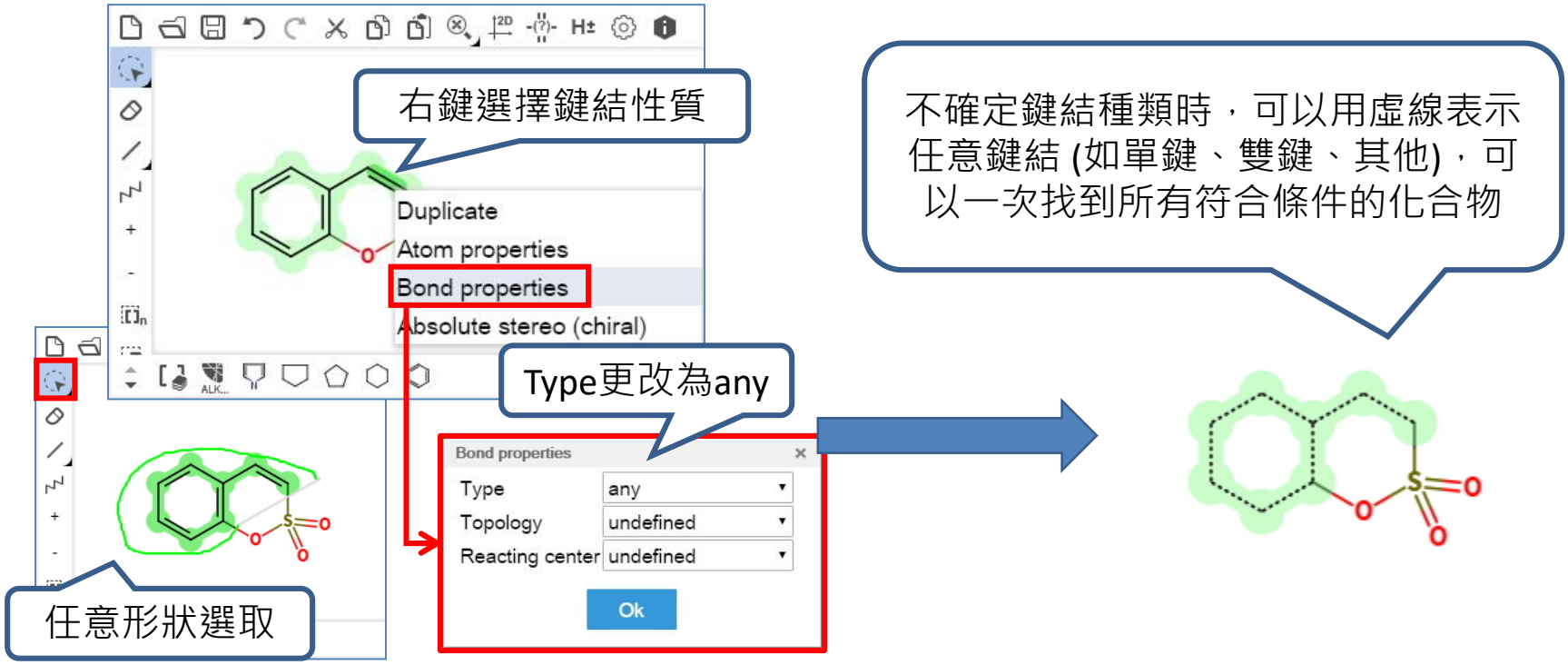
不確定鍵結種類，該如何搜尋?

Reaxys 結構搜尋 – 衍生物搜尋 – bond property



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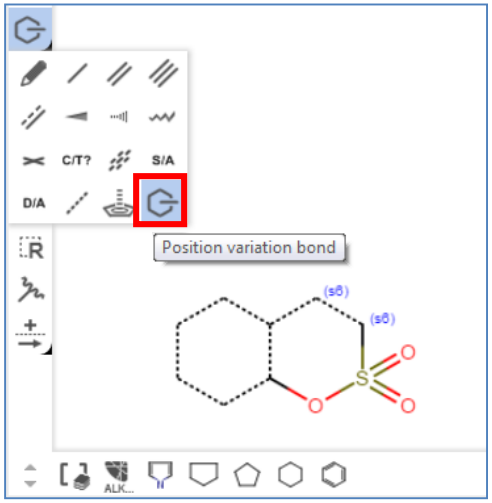
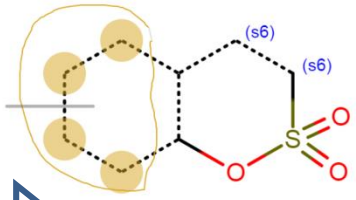
不確定鍵結位置，該如何搜尋?

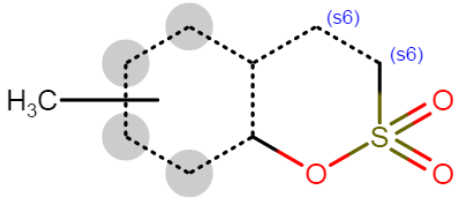
Reaxys 結構搜尋 – 衍生物搜尋 – position variation bond



圈選可能接上
取代基的原子



鍵結與官能基種類
可以再調整



4 個灰色標記的原子
任 1 個接上甲基
就會被搜尋到

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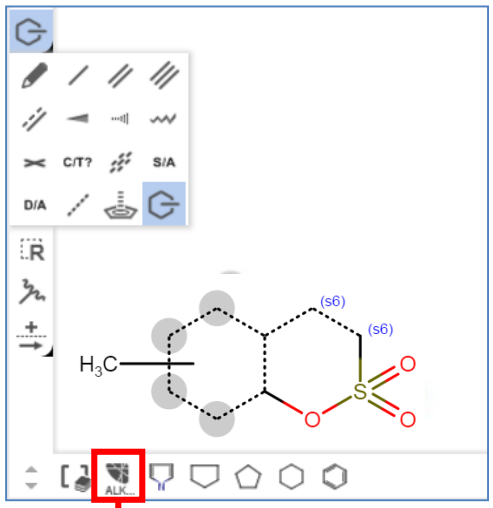
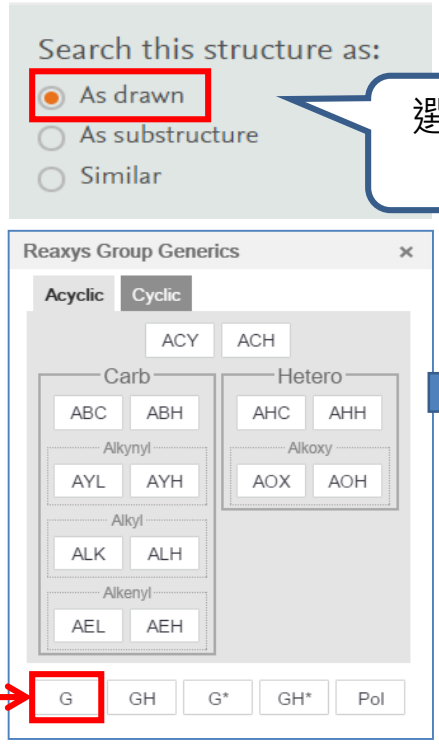
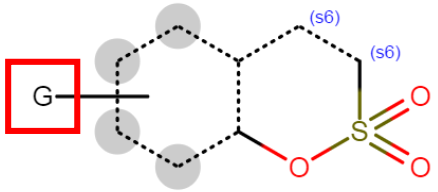
在指定位置，搜尋任意官能基

Reaxys 結構搜尋 – 衍生物搜尋 – G 代表 any functional group





選擇精準搜尋
As drawn



搜尋結果中 G 的位置
可能接上任意官能基

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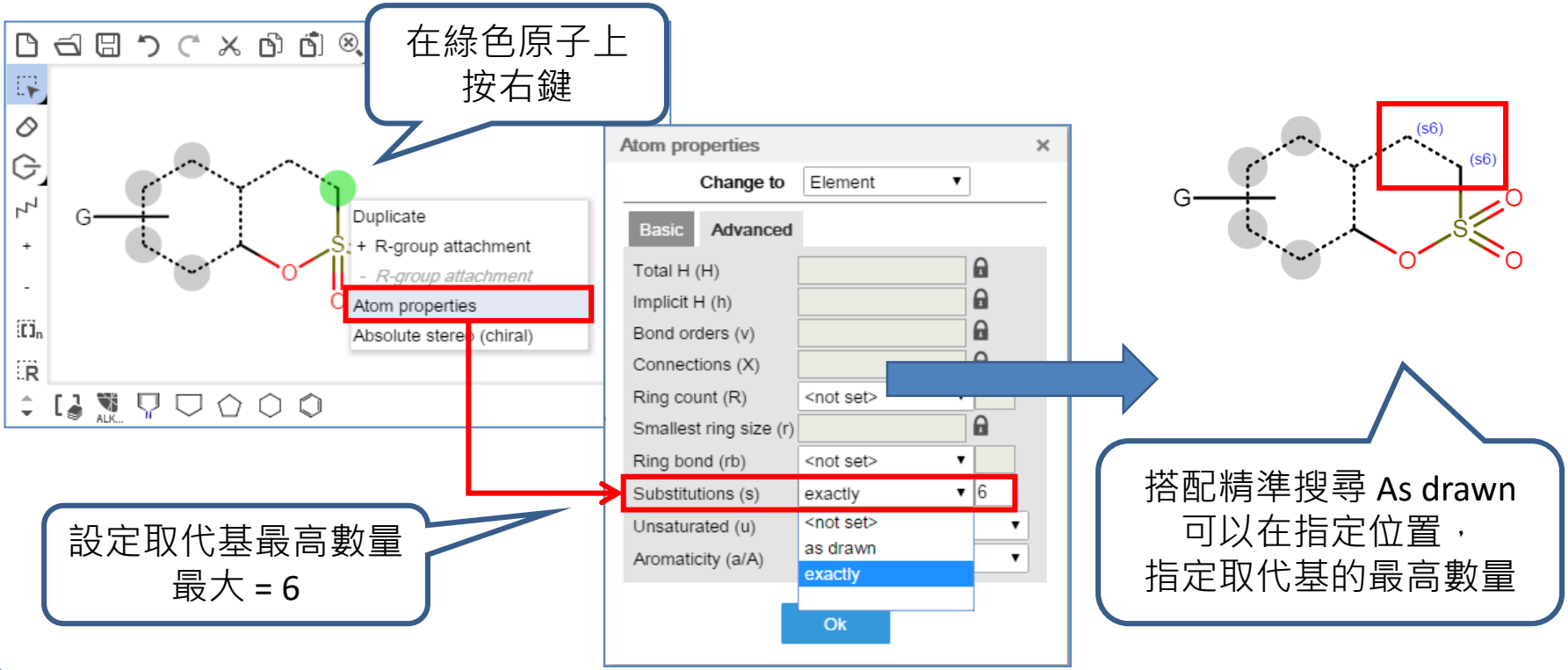
允許取代基

Reaxys 結構搜尋 – 衍生物搜尋 – Substitution 最高數量



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