

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

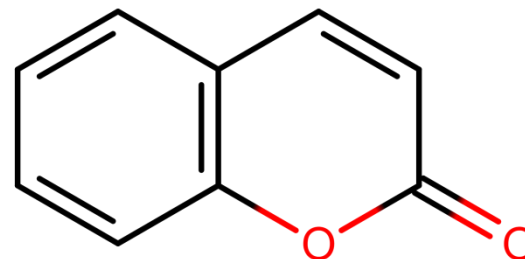
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由化合物名稱產生結構

Reaxys 結構搜尋 – 匯入與匯出 – 2

化合物名稱
Coumarin



Create structure template from name >

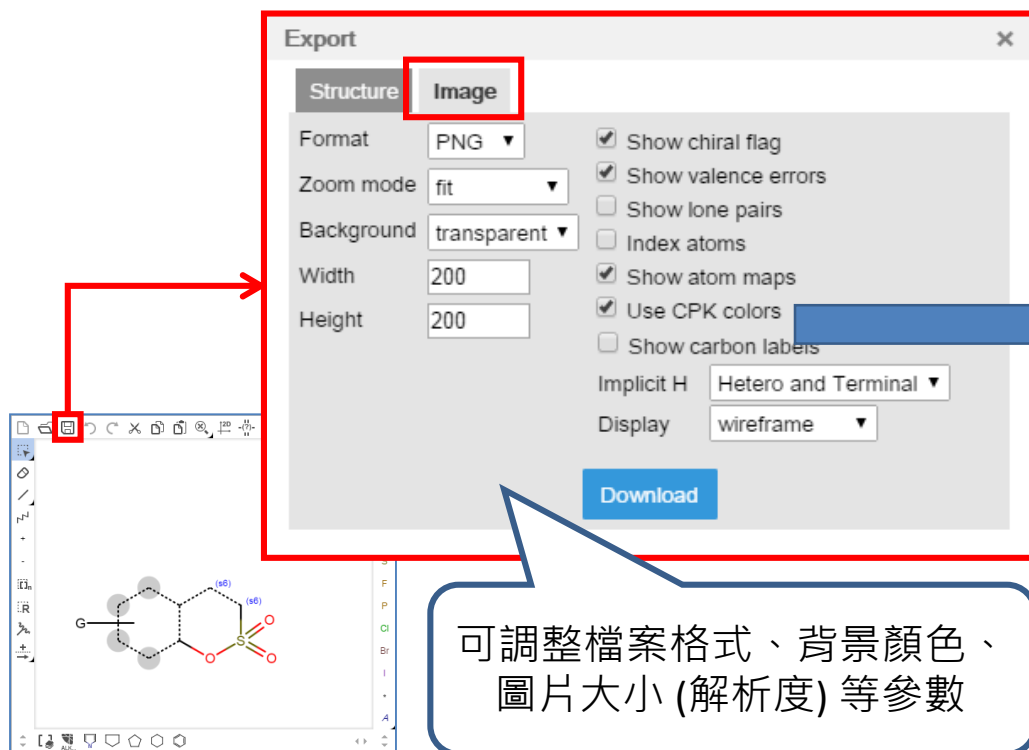
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<https://youtu.be/Y2sBPpaQpt4o>

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



Export

Structure **Image**

Format PNG

Zoom mode fit

Background transparent

Width 200

Height 200

Show chiral flag

Show valence errors

Show lone pairs

Index atoms

Show atom maps

Use CPK colors

Show carbon labels

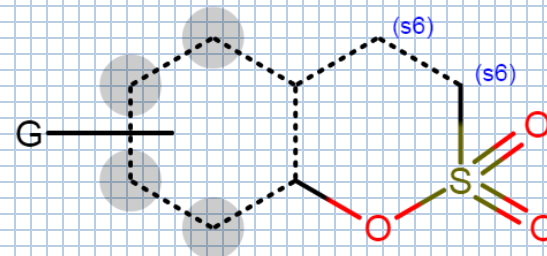
Implicit H Hetero and Terminal

Display wireframe

Download

可調整檔案格式、背景顏色、
圖片大小 (解析度) 等參數

背景透明的結構圖檔
可在 ppt 或海報使用



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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

儲存檔案

讀取檔案

匯入舊檔

支援多種檔案格式，
也可匯入其他繪圖軟體的檔案

```
queryType="Any"/><bond atomRefs2="a6 a1" order="1"
queryType="Any"/><bond atomRefs2="a9 a10" order="1"
queryType="Any"/><bond atomRefs2="a10 a6" order="1"
queryType="Any"/><bond atomRefs2="a8 a9" order="1"/><bond
atomRefs2="a8 a12" order="2"/><bond atomRefs2="a5 a7" order="1"/>
<bond atomRefs2="a7 a8" order="1"/><bond atomRefs2="a8 a11"
order="2"/><bond atomRefs2="a14 a13" order="1"/></bondArray>
<molecule id="sg1" molID="m2" role="MulticenterSgroup" atomRefs="a1
a4 a2 a3" center="a14"/></molecule></MChemicalStruct>
</MDocument></cm>
```

Use **Ctrl+C** to copy the selected source above.

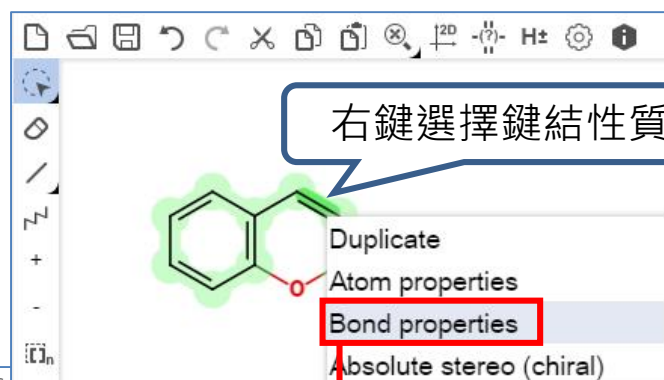
Download

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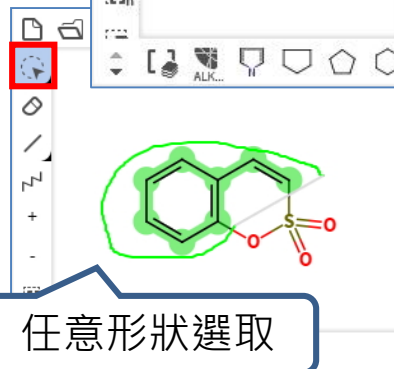
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不確定鍵結種類，該如何搜尋？

Reaxys 結構搜尋 – 衍生物搜尋 – bond property



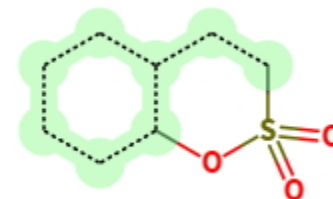
不確定鍵結種類時，可以用虛線表示任意鍵結 (如單鍵、雙鍵、其他)，可以一次找到所有符合條件的化合物



Type更改為any

Bond properties	
Type	any
Topology	undefined
Reacting center	undefined

Ok

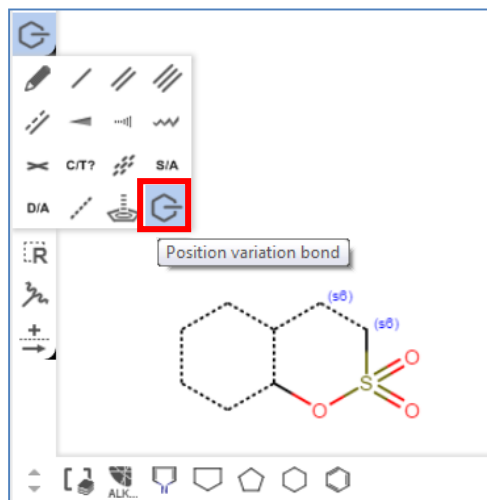


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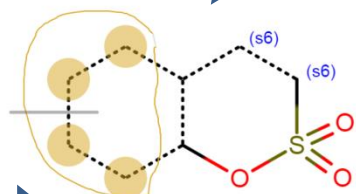
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不確定鍵結位置，該如何搜尋？

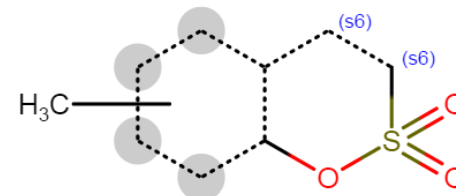
Reaxys 結構搜尋 – 衍生物搜尋 – position variation bond



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



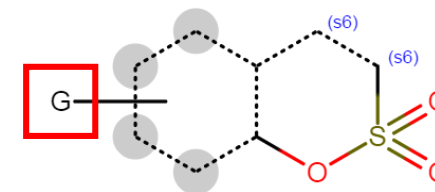
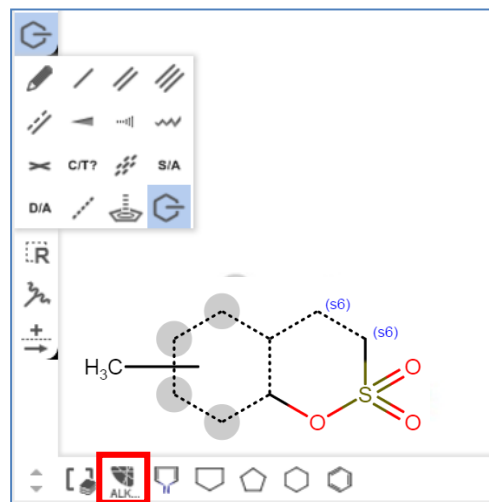
4 個灰色標記的原子
任 1 個接上甲基
就會被搜尋到

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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

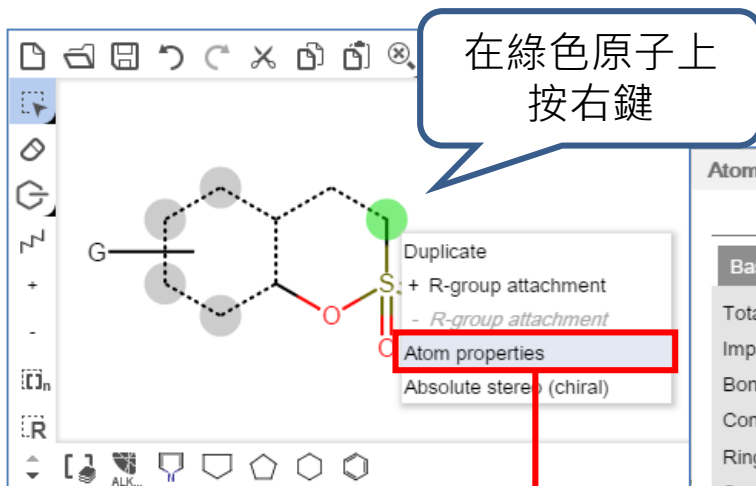


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允許取代基

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



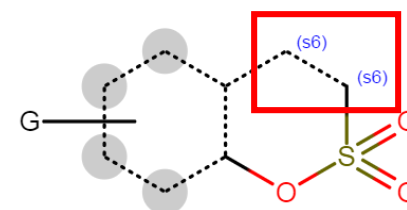
Atom properties

Change to: Element

Basic	Advanced
Total H (H)	
Implicit H (h)	
Bond orders (v)	
Connections (X)	
Ring count (R)	<not set>
Smallest ring size (r)	
Ring bond (rb)	<not set>
Substitutions (s)	exactly 6
Unsaturated (u)	<not set>
Aromaticity (a/A)	as drawn

Ok

設定取代基最高數量
最大 = 6



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