



## 生物科技實驗

# 分子入塢 — (I) 準備小分子

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實驗室：第一教學大樓 N1025室

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*YTLab Presents*

# Wet Lab vs Dry Lab

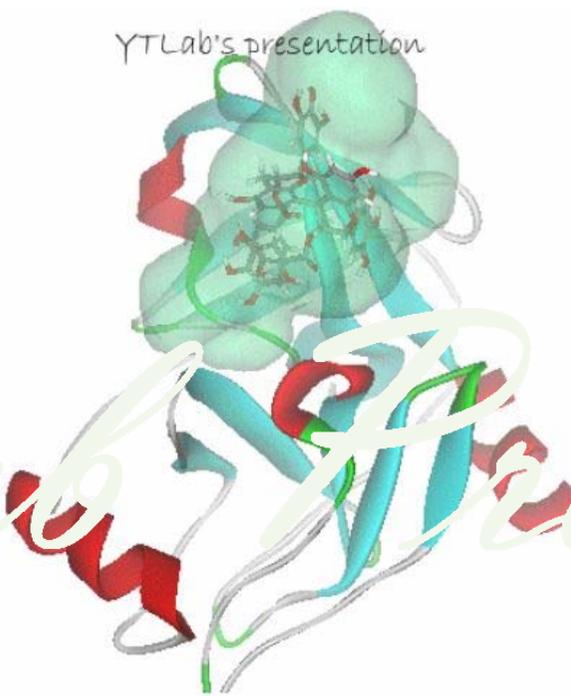
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# Molecular Docking

Molecular Docking

分子入場

YTLab's presentation



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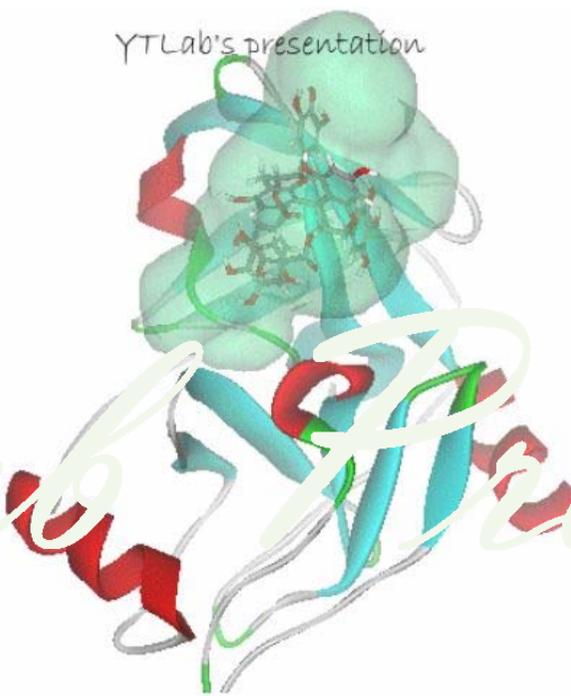
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# Handle Small Molecule

Molecular Docking

分子入場

YTLab's presentation



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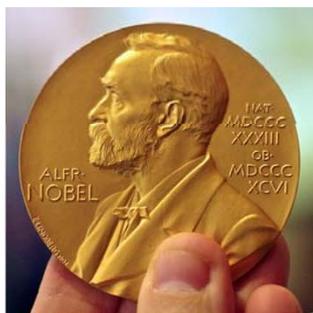
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西元2000年在”未來大趨勢”這本書中預測十年內，可以用筆記型電腦做藥物設計及開發！

Q1: 為何你還不能使用apple、acer、asus筆電做藥物開發？

- Ans:
1. 不會灌軟體
  2. 沒有錢買軟體
  3. 不知道有哪些軟體可以使用
  4. 覺得電腦模擬沒有用不可信
  5. 未選修電腦在生物醫學上的應用
  6. 未選修電腦輔助藥物開發
  7. 未選修生物資訊
  8. 沒有旋轉到 (rotation) yt實驗室

# Bringing the experiment to cyberspace



- Drs. Martin Karplus, Michael Levitt, and Arieh Warshel have been awarded the Nobel Prize in chemistry for developing computer models used to predict and understand chemical processes. The Royal Swedish Academy of Sciences announced the decision Wednesday morning at a press conference in Stockholm, Sweden. The three chemists will share a monetary prize of 8 million Swedish krona (\$1.2 million), to be awarded at a ceremony in December. (2013)

合抱之木，生於毫末；  
九層之台，起於累土；  
千里之行，始於足下。

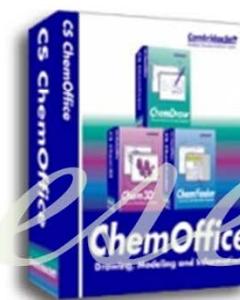
**Let's start experiment in cyberspace**

第一步：如何表達真實無誤的小分子在電腦裡？

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ChemOffice是化學和生物學家及一般研究人所推崇世界上最專業的生物化學結構繪圖辦公室軟體。是為了生物技術、製藥廠、化學公司和科學研究單位專門研究開發和行銷生命科學企業的解決方案。

第一步學會安裝軟體!!!



YTLab網址：<http://ytlab.kmu.edu.tw/>

YTLab's Home

YTLab

Ying-Ting Lin | Contact

ytLab

**ytLectures:**

- Computer Aided Biological Design
- Biotechnology Laboratory
- Computers In BioScience
- Bioinformatics
- BioPhysicalChemistry
- Structural Genomics
- Modern Technology
- Genomics
- more ...

*ytLectures: Ying-Ting Lin's Lectures.*

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- Duke
- Harvard
- Yale
- Carnegie Mellon

*MOOCs: Massive Open Online Courses.*

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# Molecular Docking



## Molecular Docking

### Experimental Protocols:

Handle Small Molecule:	<a href="#">MolecularDocking_SmallMolecule</a>
Handle Big Molecule:	<a href="#">MolecularDocking_BigMolecule</a>
Handle Binding Pocket:	<a href="#">MolecularDocking_BindingPocket</a>
Calculation of Molecular Docking:	<a href="#">MolecularDocking_Calculation</a>

### Computing Programs Installation:

Molecular Editor: [ChemBioOffice \(from SciStore\)](#)

A red arrow pointing downwards and to the left, highlighting the underlined text 'SciStore' in the link above.

### Other Installation:

Protein Viewer:	<a href="#">Chimera (from UCSF Chimera)</a>
Quantum Chemistry:	<a href="#">MOPAC2012, libiomp5md.dll (from OpenMOPAC)</a>

### Report:

[Hand in Your Report](#)

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ChemOffice® Professional 15.1 is very helpful in documenting chemical processes and drug substances for regulatory and patent filings. This innovative suite makes drawing correct and chemically intelligent structures and synthetic schemes intuitively easy.

ChemOffice® Professional 15.1 combines ChemDraw Professional, Chem3D,

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**Account Information**

**Required Information**

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<input type="text"/>	<input type="text"/>	<input type="text"/>
Type Email address again*	Organization*	Phone*
<input type="text"/>	<input type="text"/>	<input type="text"/>
Country*	Address Line 1 (no PO Boxes)*	Address Line 2 (Optional)
--Please choose one-- <span>▼</span>	<input type="text"/>	<input type="text"/>
City	State/Province/Region*	Zip*
<input type="text"/>	--Please choose one-- <span>▼</span>	<input type="text"/>
Primary Role*	Sub Role*	Industry*
--Please choose one-- <span>▼</span>	Please select a Primary Role fi <span>▼</span>	Please select a Sub Role first <span>▼</span>

填妥資料後送出!!!

3-5 mins即可收到信件

## 第二封信件含有個人的serial number 及下載網址

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If you have any questions or require assistance in getting the software installed and set up, you can contact Support by visiting the Support web site at :

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For a description of the Support Service, please see the following document:

[Global\\_Support.pdf](#)



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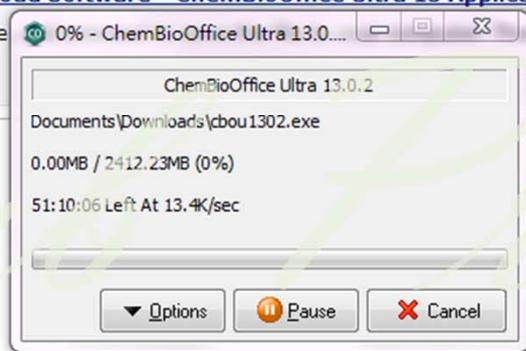
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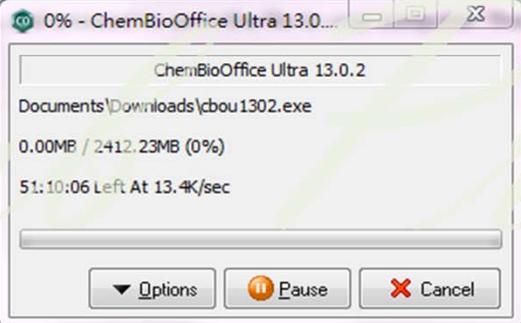
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(Click on the link above to see Installation Instructions.)

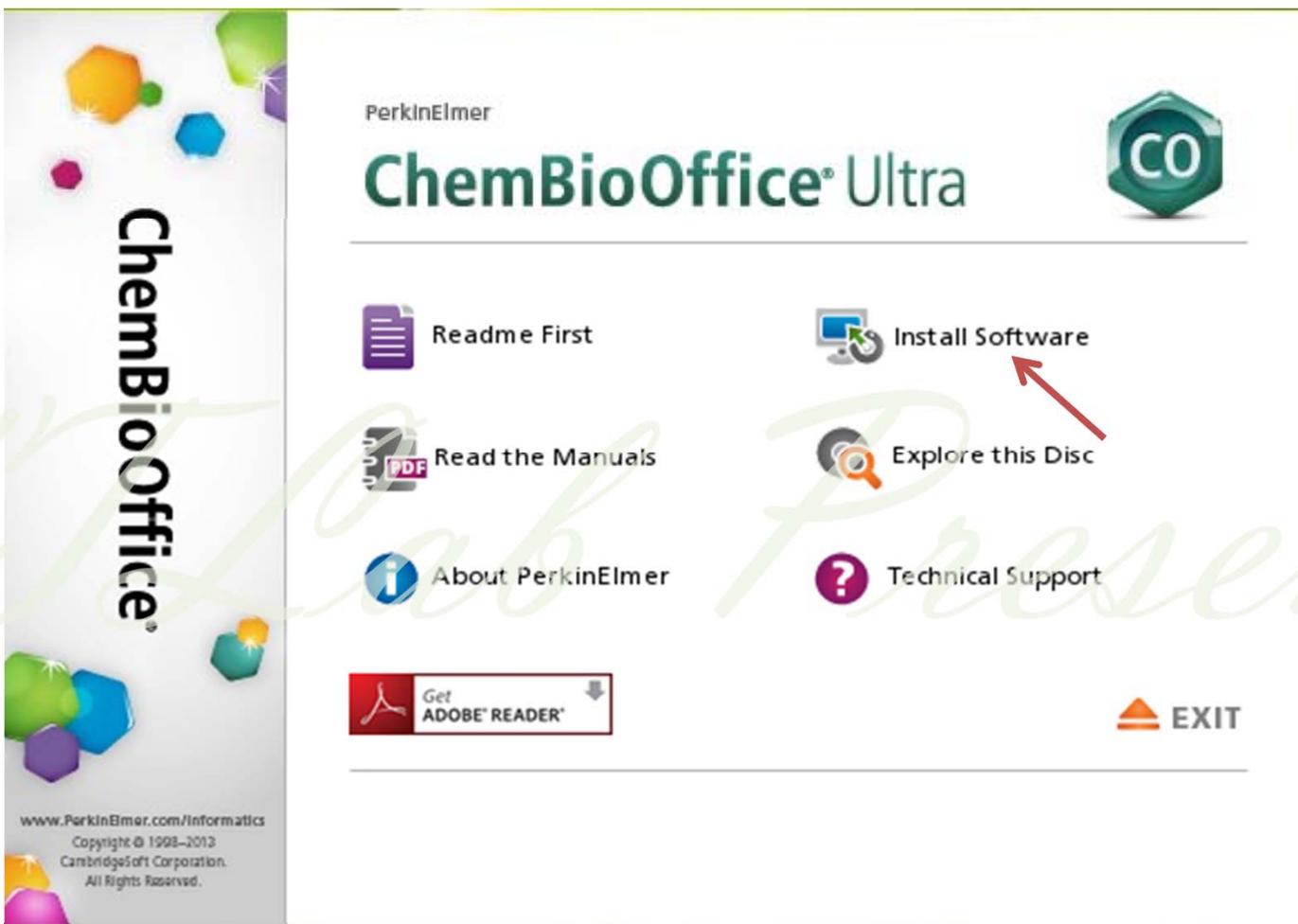


0% - ChemBioOffice Ultra 13.0.2  
Documents\Downloads\cbou1302.exe  
0.00MB / 2412.23MB (0%)  
51:10:06 Left At 13.4K/sec

Options Pause Cancel



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# ChemBioOffice® Ultra



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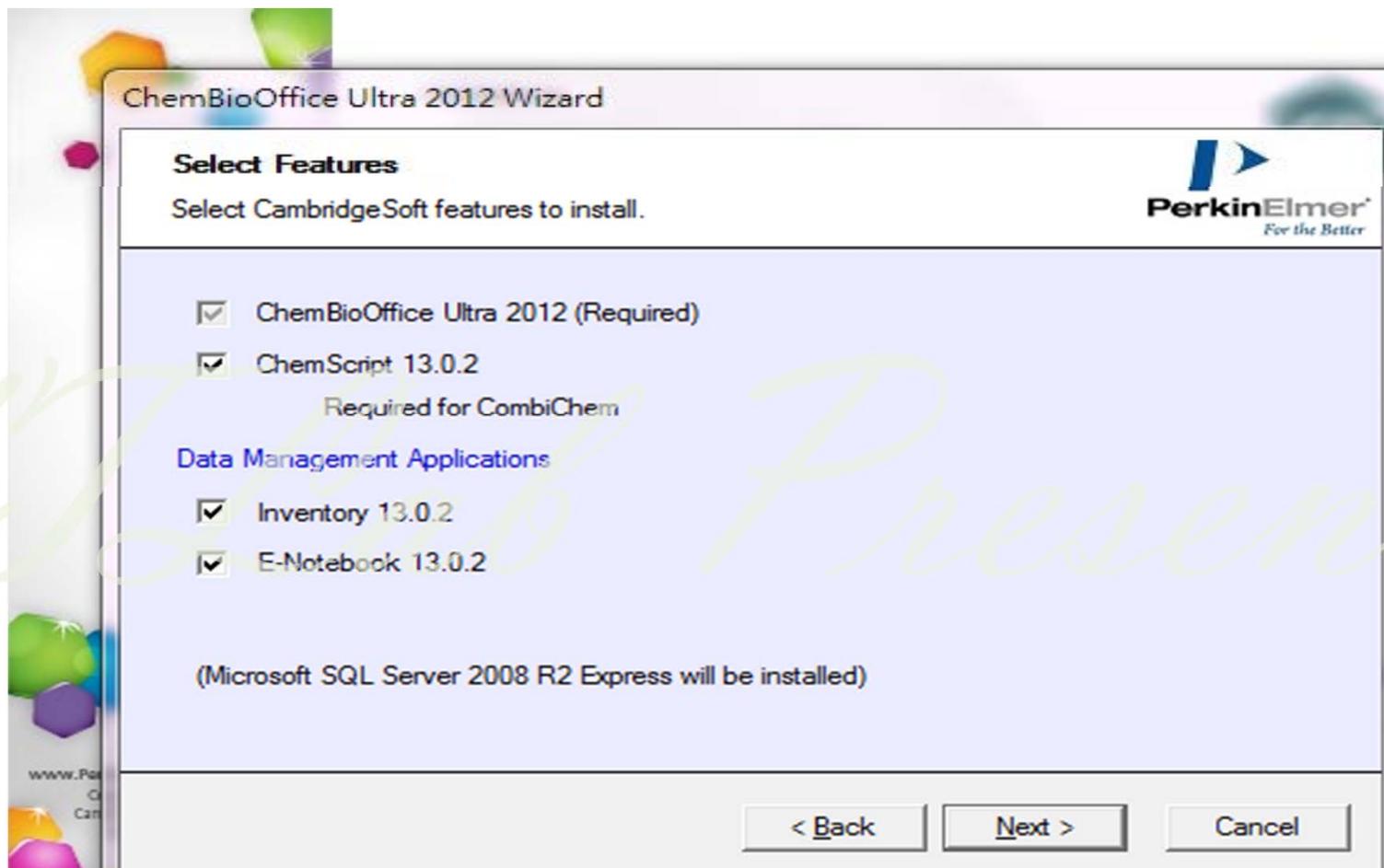
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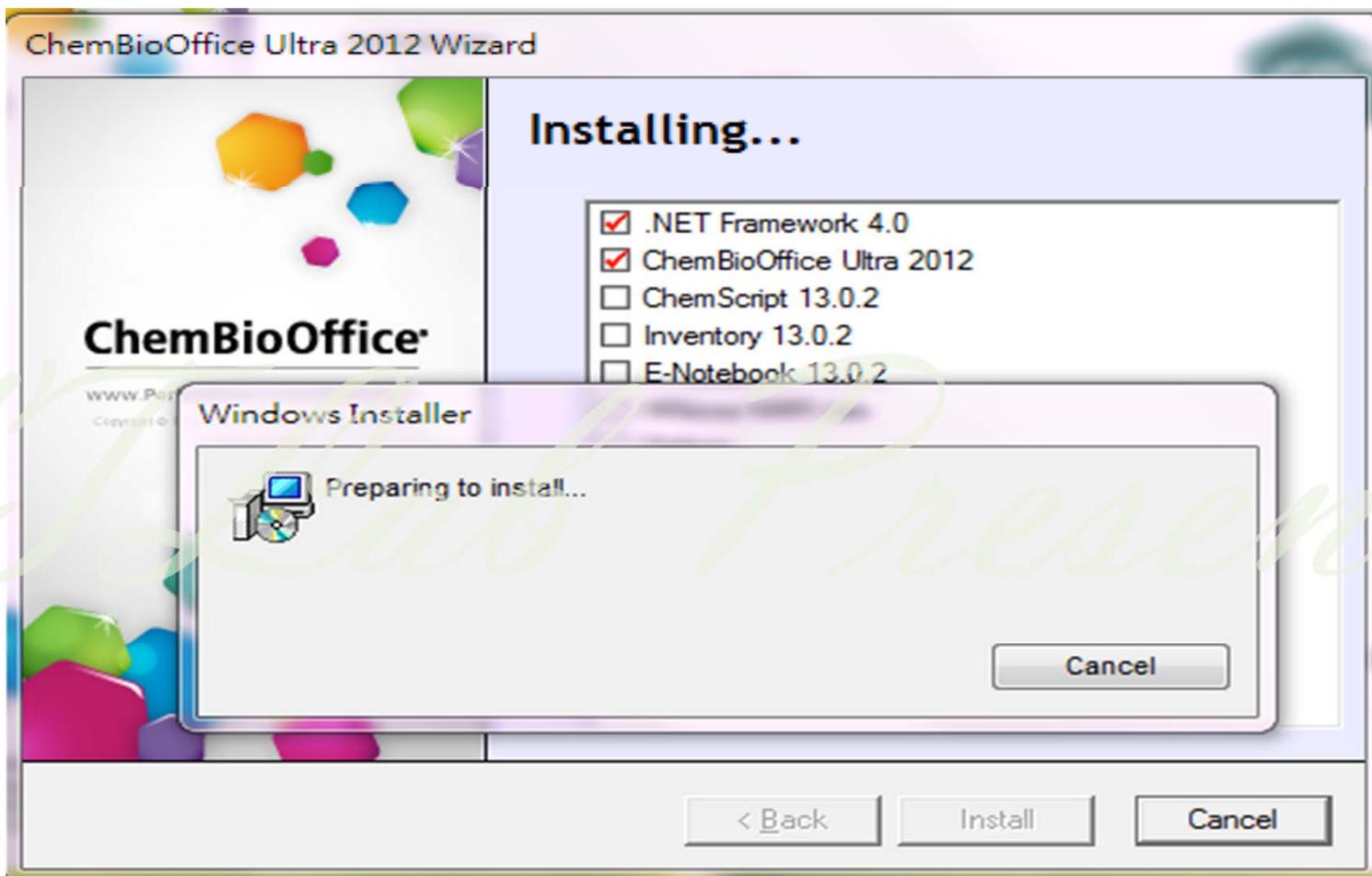
## Installing...

- .NET Framework 4.0
- ChemBioOffice Ultra 2012
- ChemScript 13.0.2
- Inventory 13.0.2
- E-Notebook 13.0.2
- MNova NMR Lite
- Python
- Microsoft SQL Server 2008 R2 Express

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Installation Complete

- .NET Framework 4.0
- ChemBioOffice Ultra 2012
- ChemScript 13.0.2
- inventory 13.0.2
- E-Notebook 13.0.2
- MNova NMR Lite
- Python
- Microsoft SQL Server 2008 R2 Express

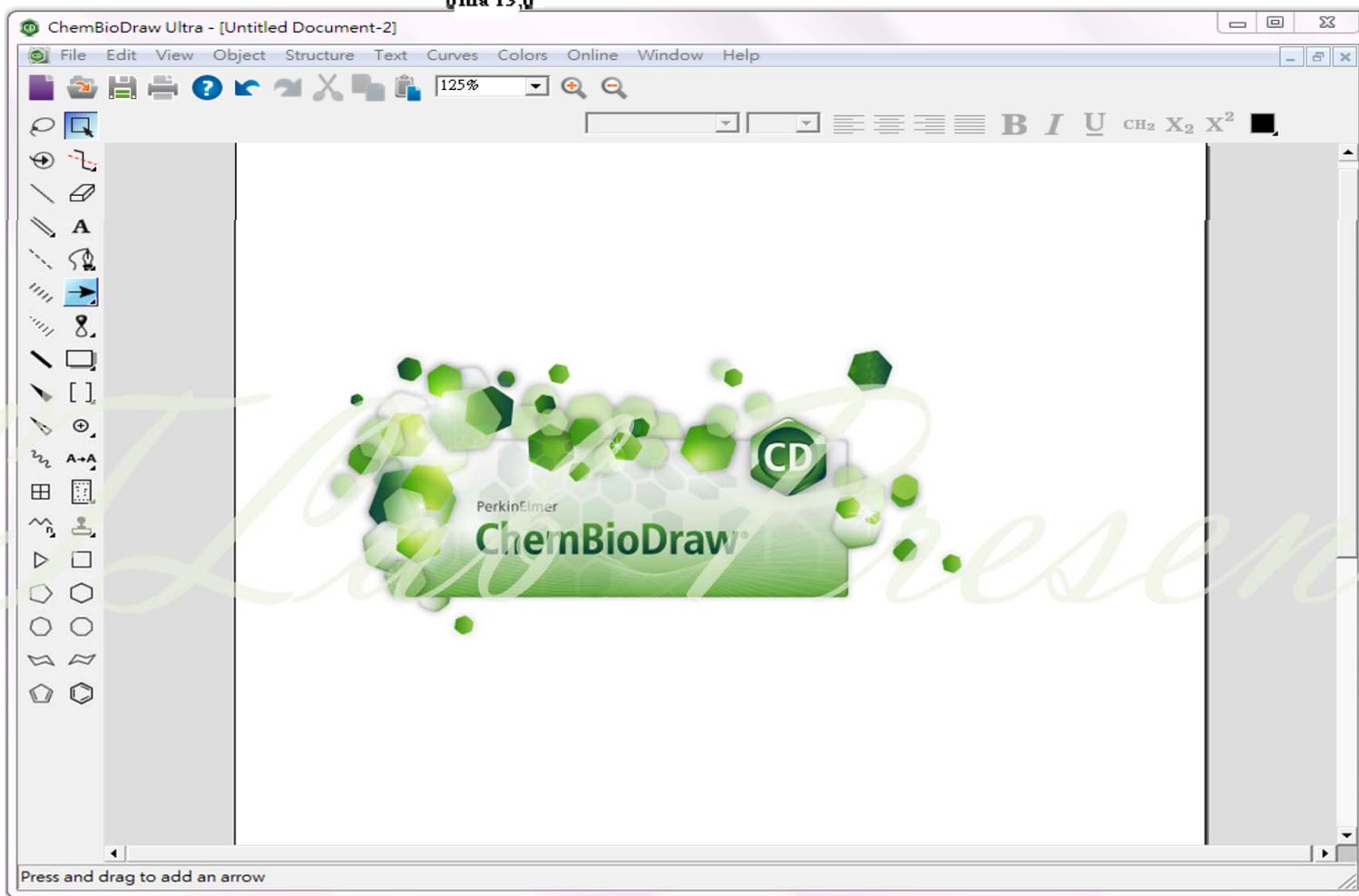
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Install

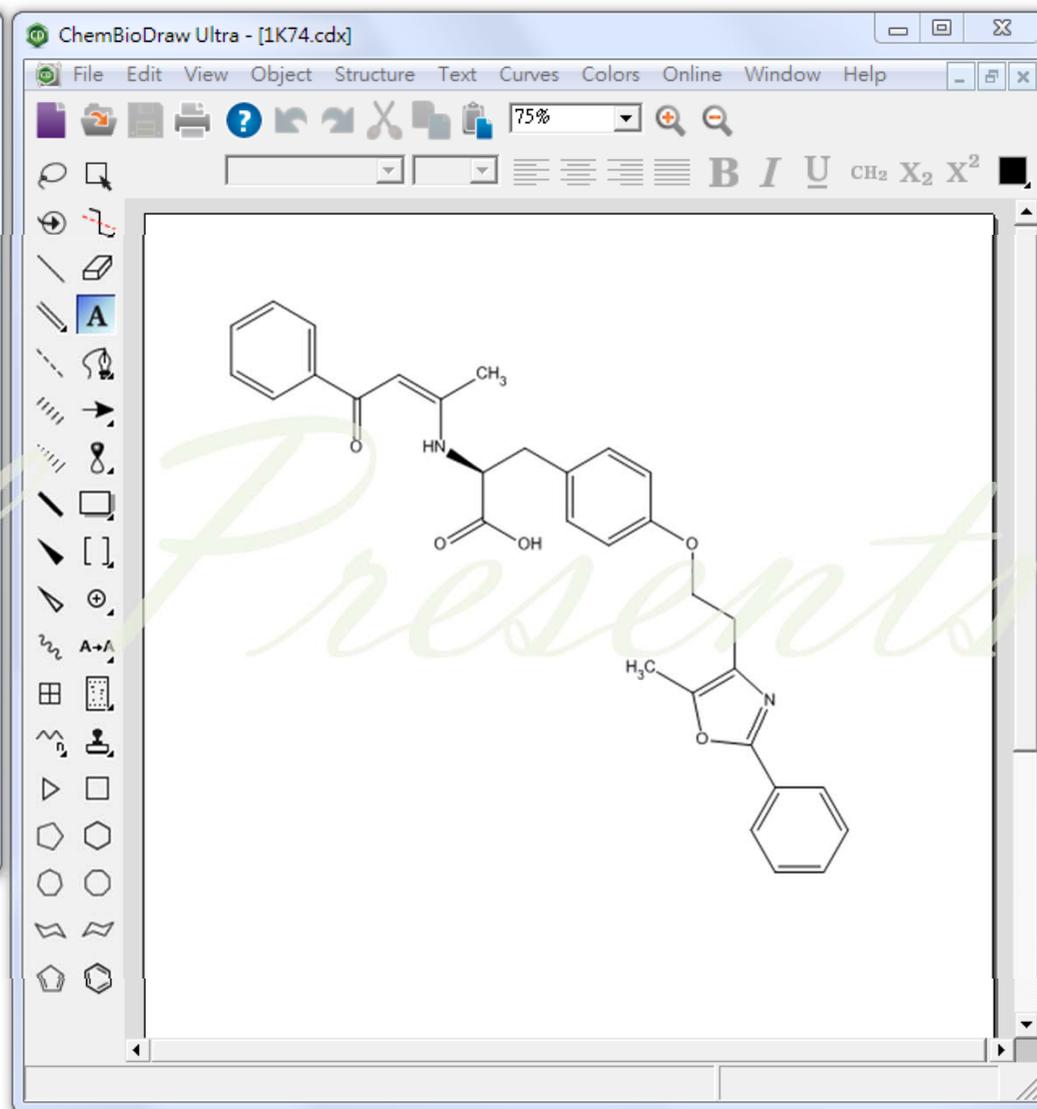
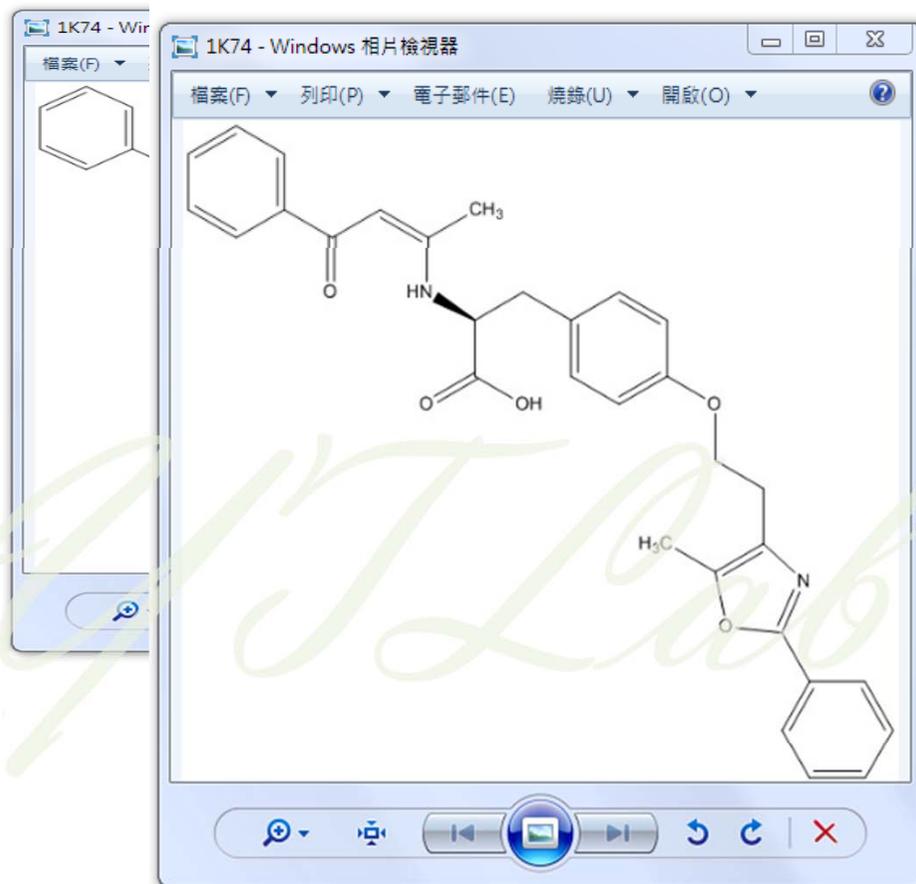
Finish

安裝完畢!

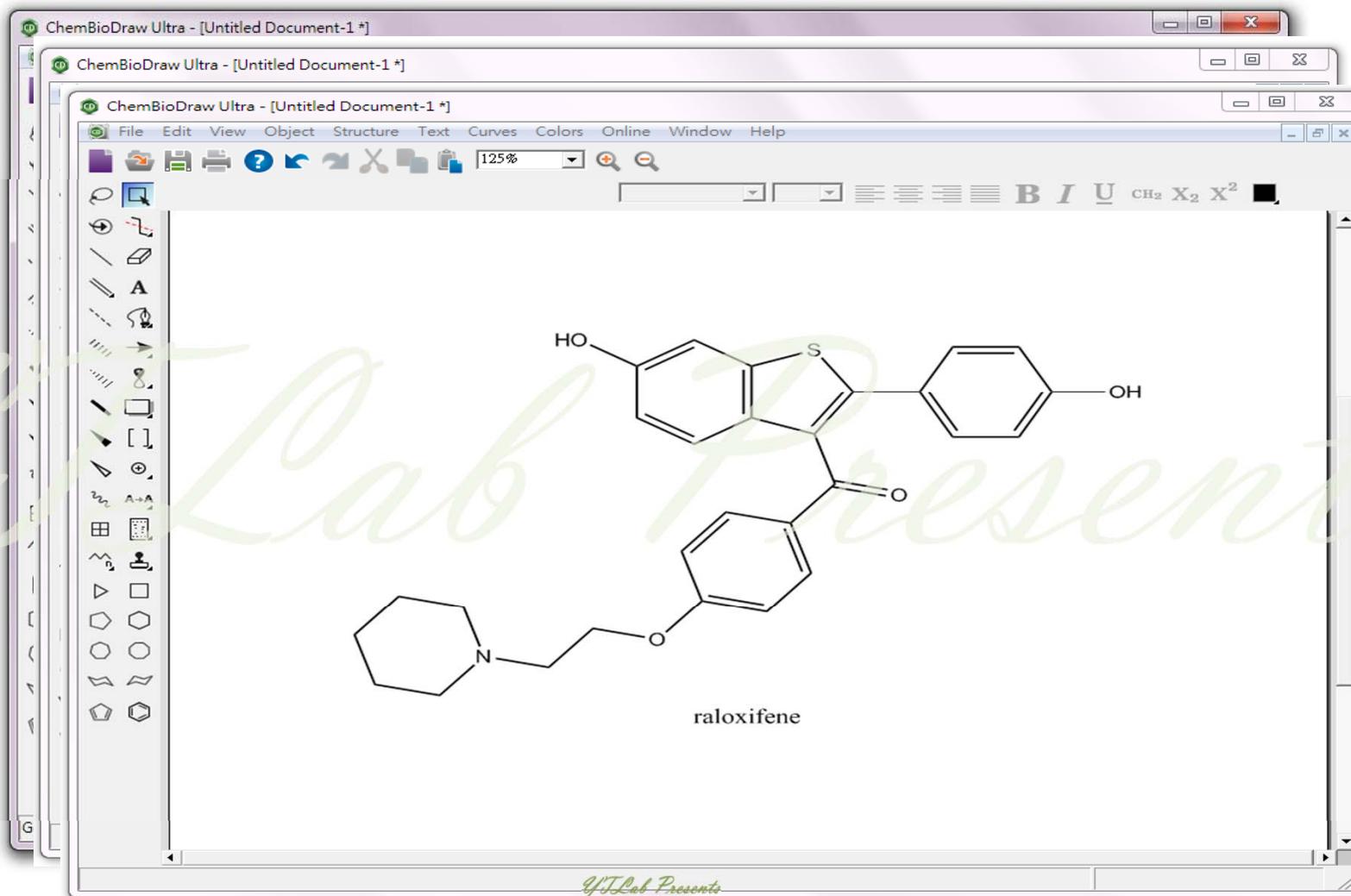
# 開啟ChemBio2D



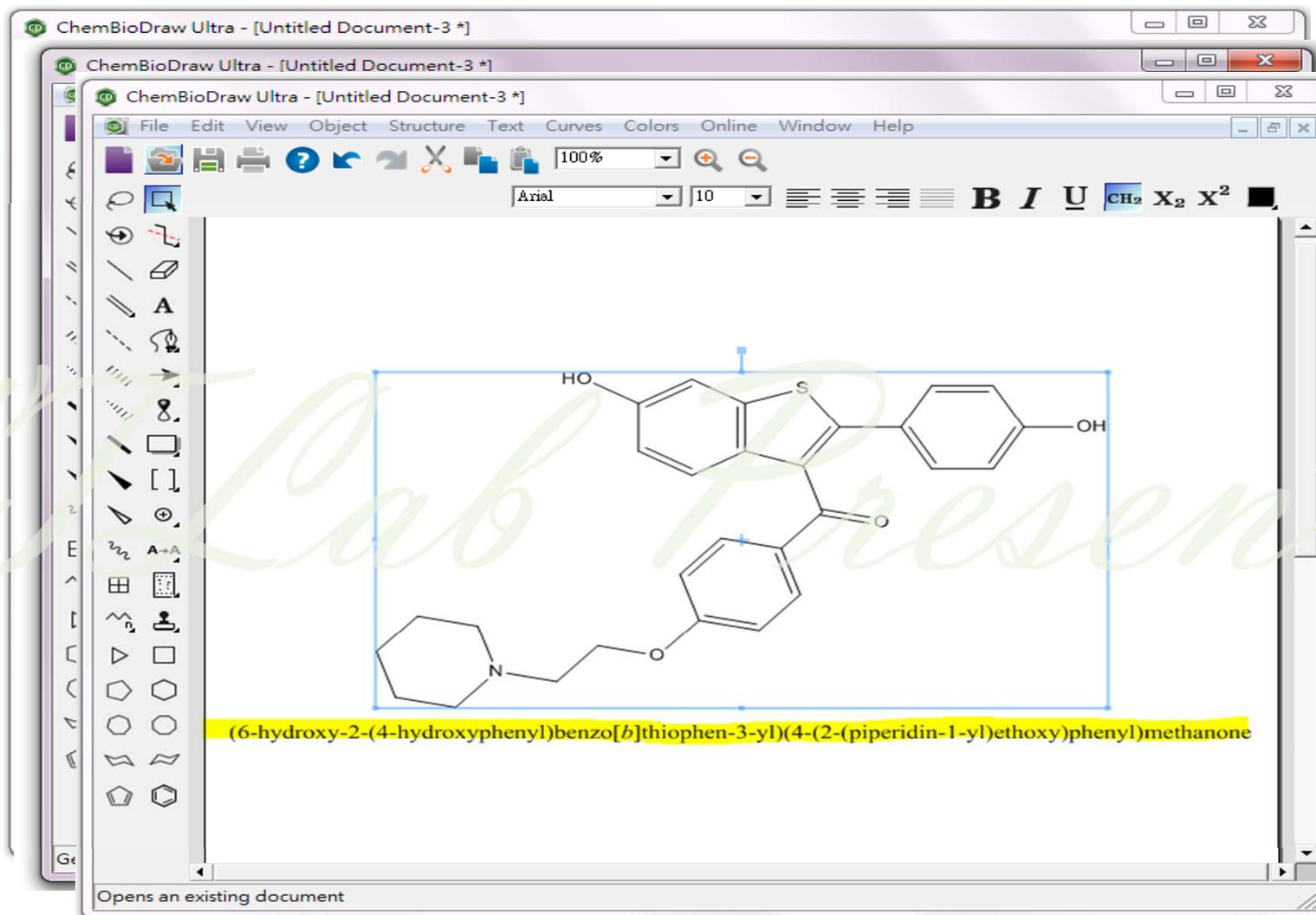
# 依樣畫葫蘆



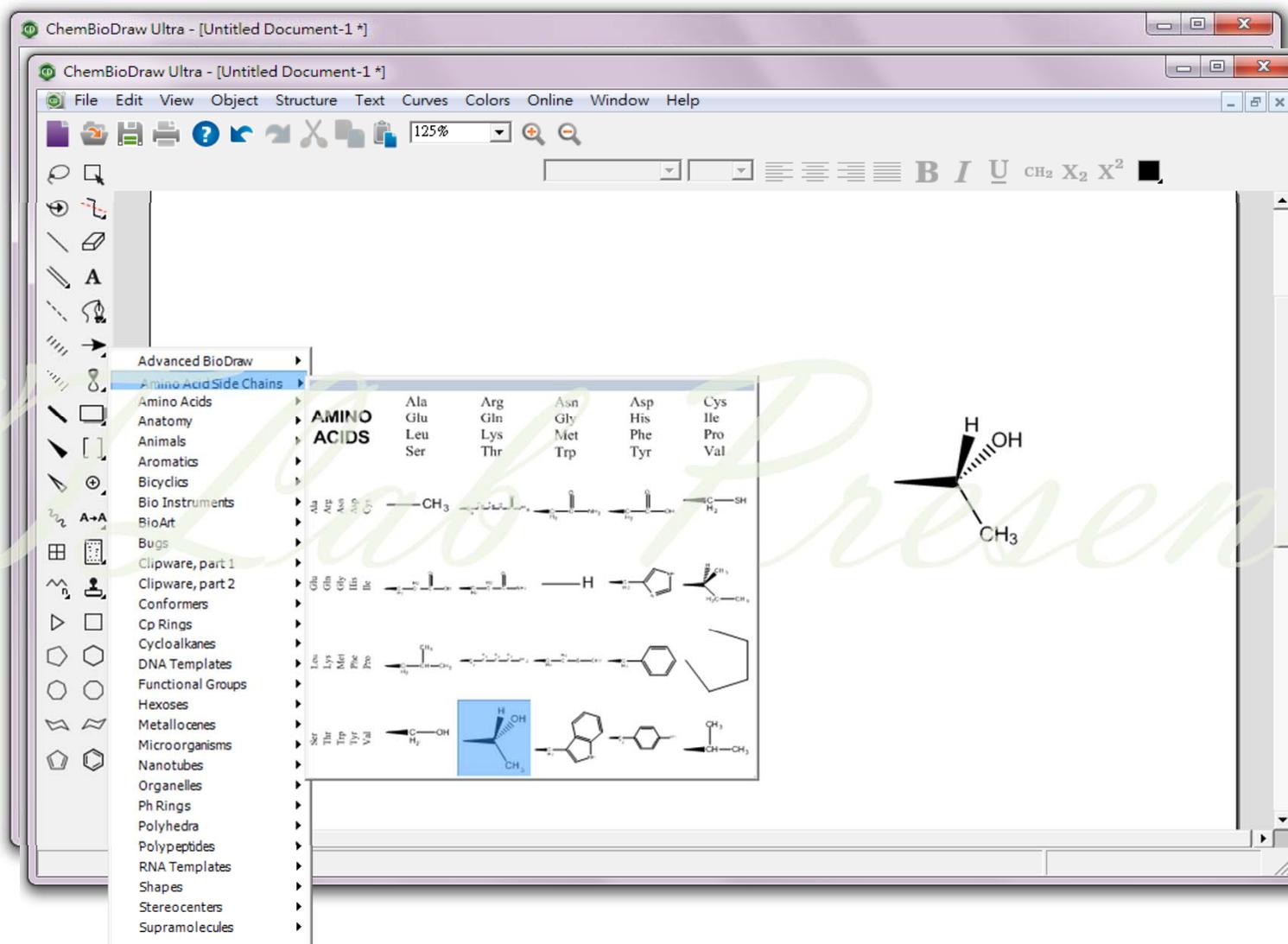
Structure → name to structure



Structure → structure to name

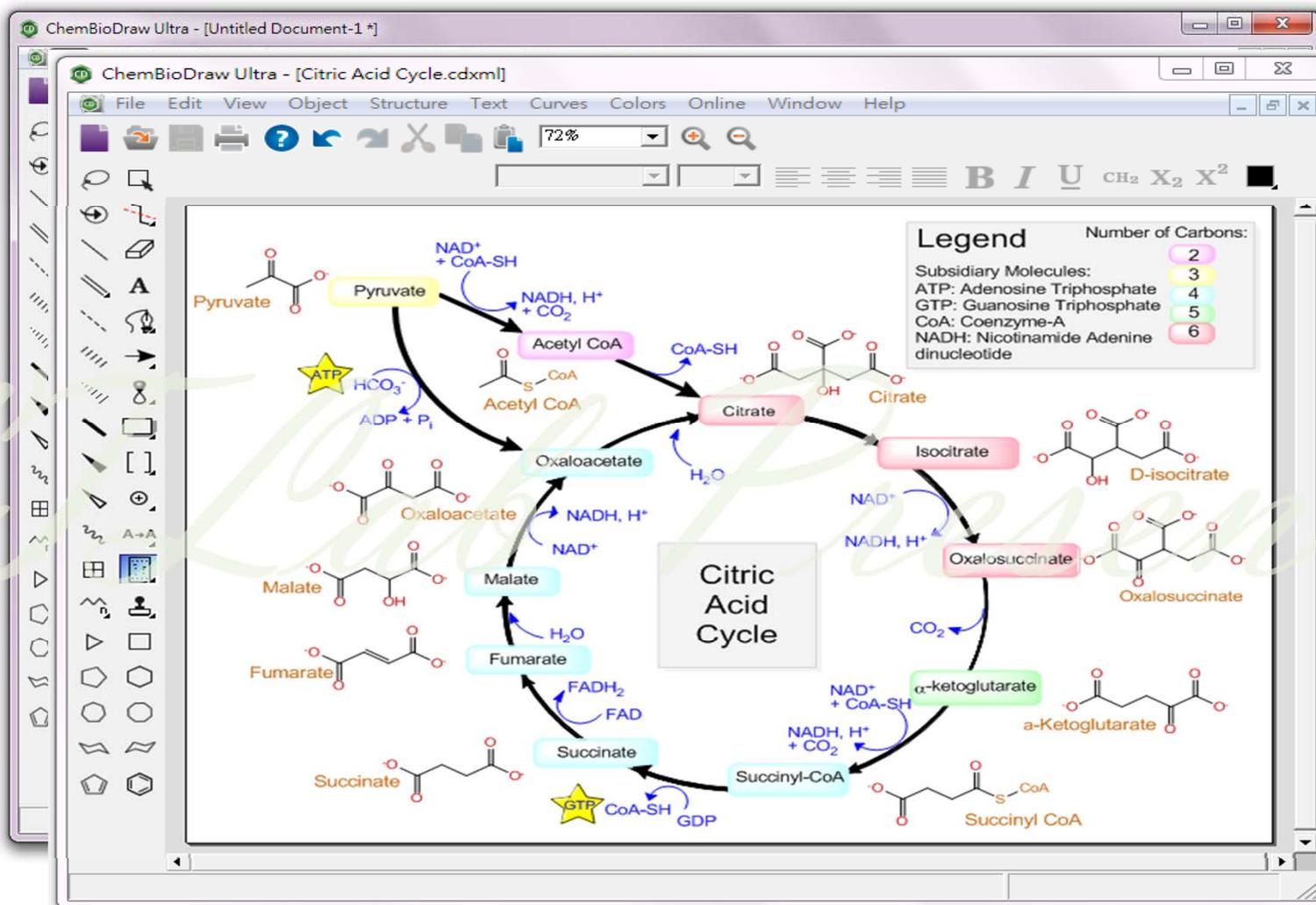


# Templates

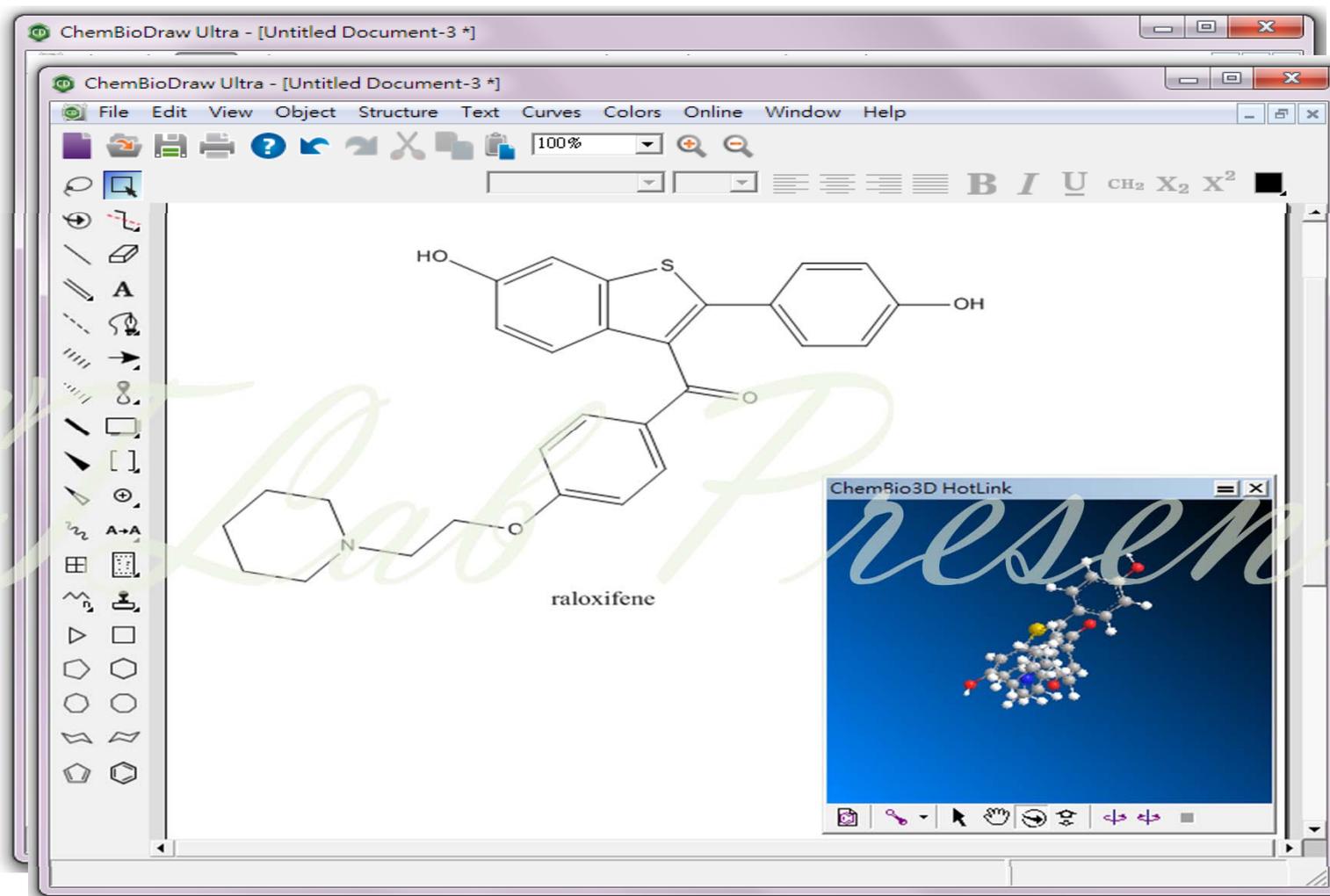


sample

舉手加分:請試著說明citric acid cycle



# Chem3D Preview



Structure → clean up structure

ChemBioDraw Ultra - [Untitled Document-4 \*]

File Edit View Object Structure Text Curves Colors Online Window Help

Anal [100%]

**B I U** CH<sub>2</sub> X<sub>2</sub> X<sup>2</sup>

(6-hydroxy-2-(4-hydroxyphenyl)benzo[*b*]thiophen-3-yl)(4-(2-(piperidin-1-yl)ethoxy)phenyl)methanone

Before clean

Prints the document

Analyze Stoichiometry  
Predict <sup>1</sup>H-NMR Shifts  
Predict <sup>13</sup>C-NMR Shifts  
Make Spectrum-Structure  
Define Nickname...  
Convert Name to Structure  
Convert Structure to Name

Reposition the selected atom(s)

Window Help

**B I U** CH<sub>2</sub> X<sub>2</sub> X<sup>2</sup>

Shift+Ctrl+K  
Shift+Ctrl+X

ChemBioDraw Ultra - [Untitled Document-4 \*]

File Edit View Object Structure Text Curves Colors Online Window Help

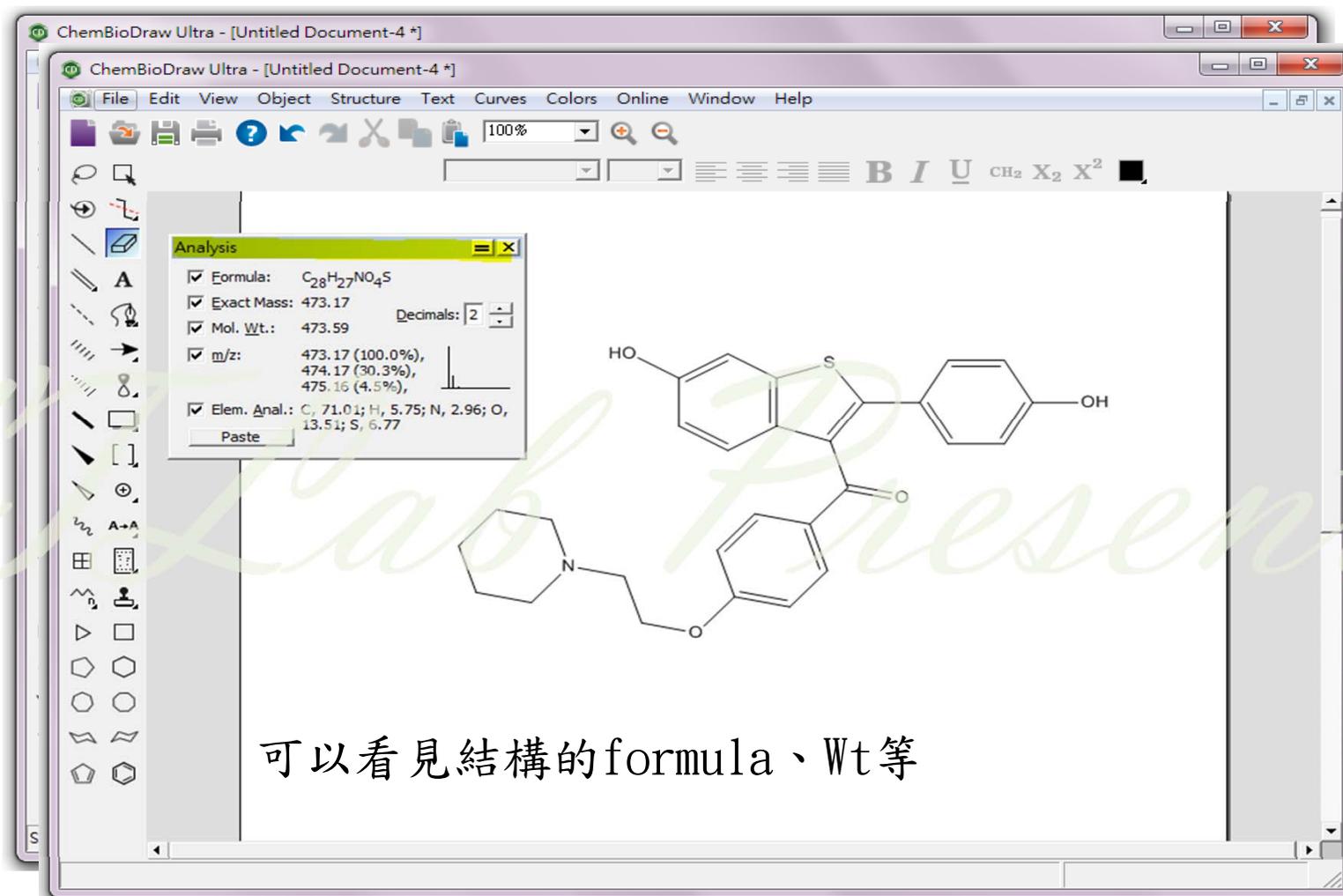
Anal [100%]

**B I U** CH<sub>2</sub> X<sub>2</sub> X<sup>2</sup>

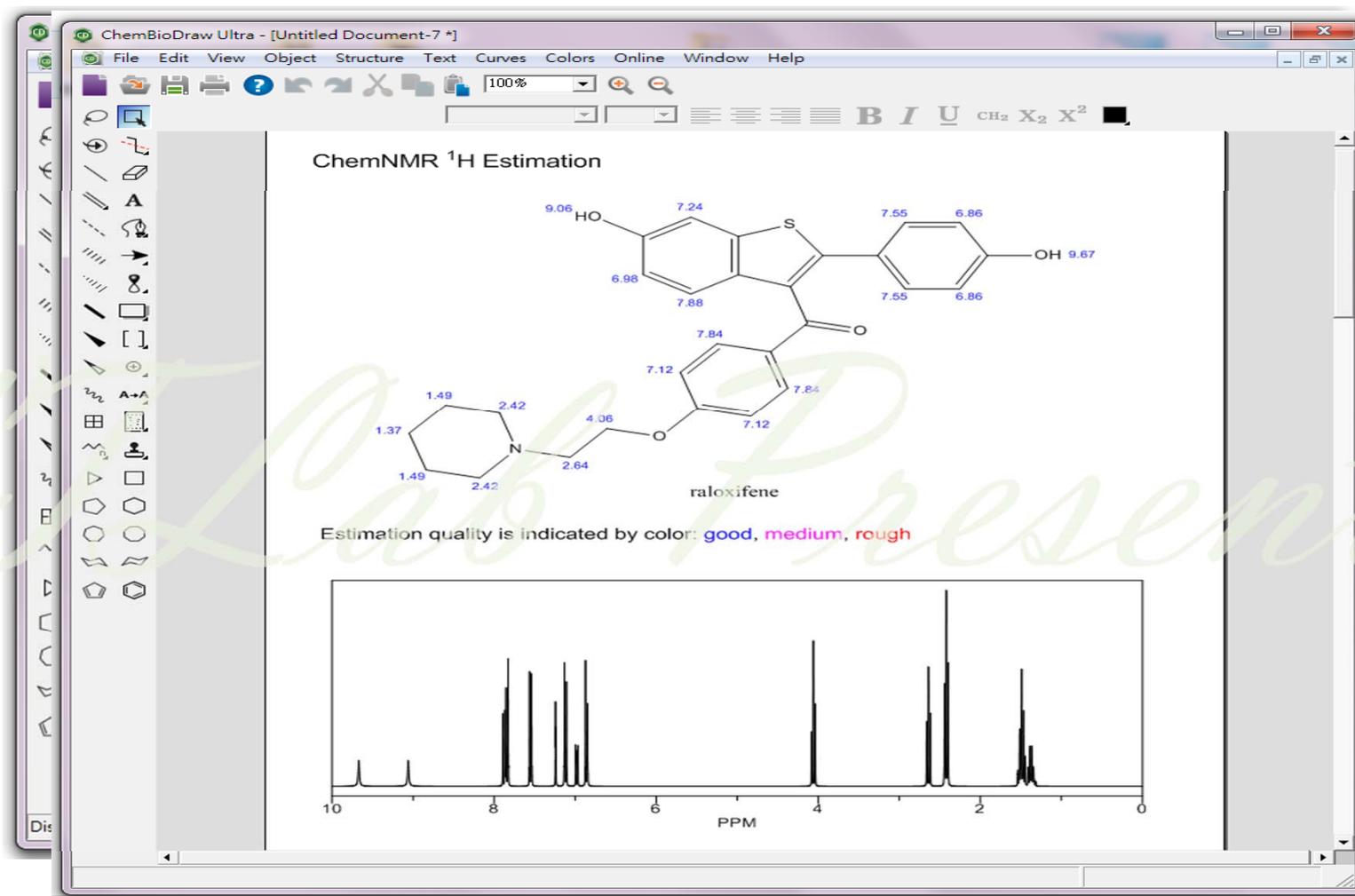
(6-hydroxy-2-(4-hydroxyphenyl)benzo[*b*]thiophen-3-yl)(4-(2-(piperidin-1-yl)ethoxy)phenyl)methanone

After clean

## Analysis window

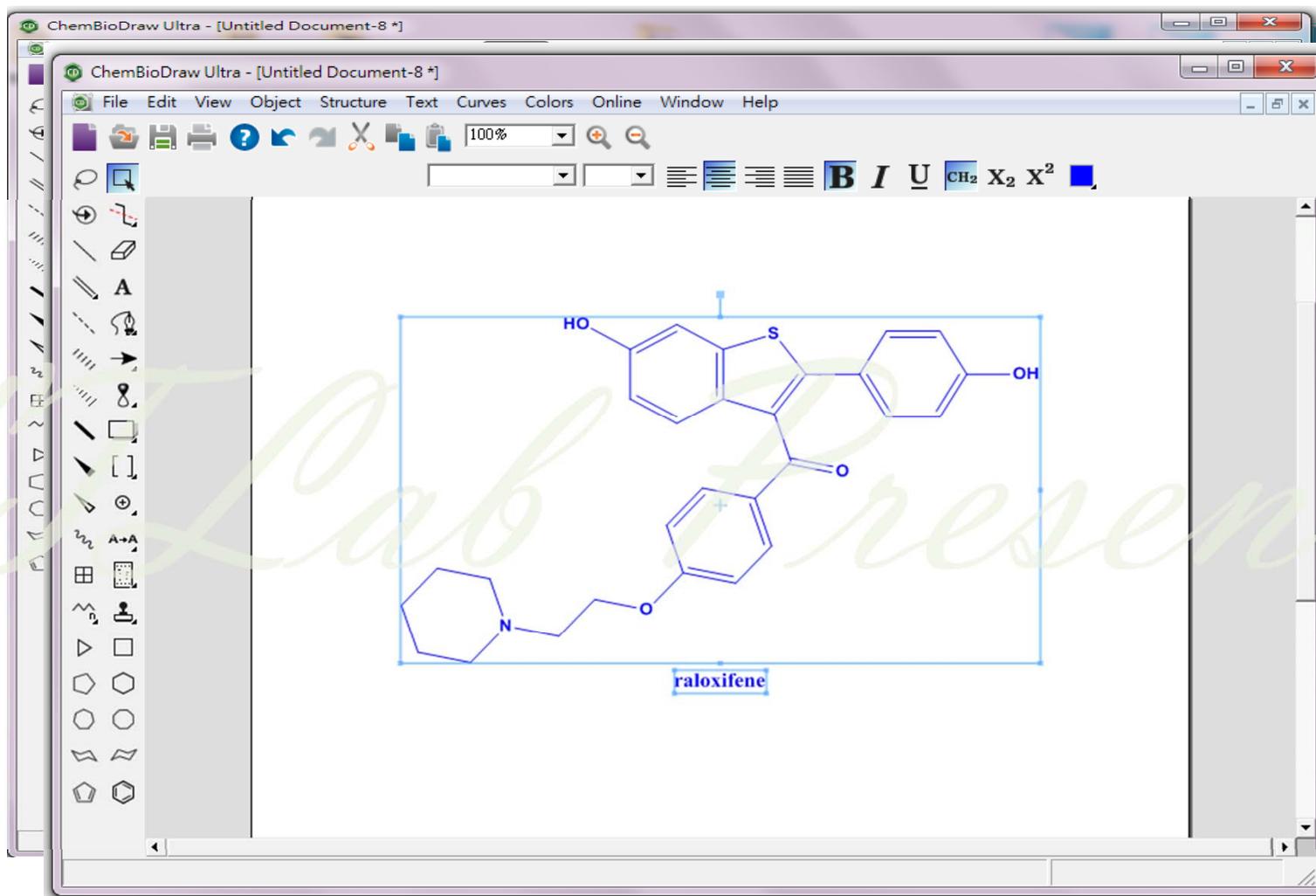


Structure → predict H-NMR Shifts

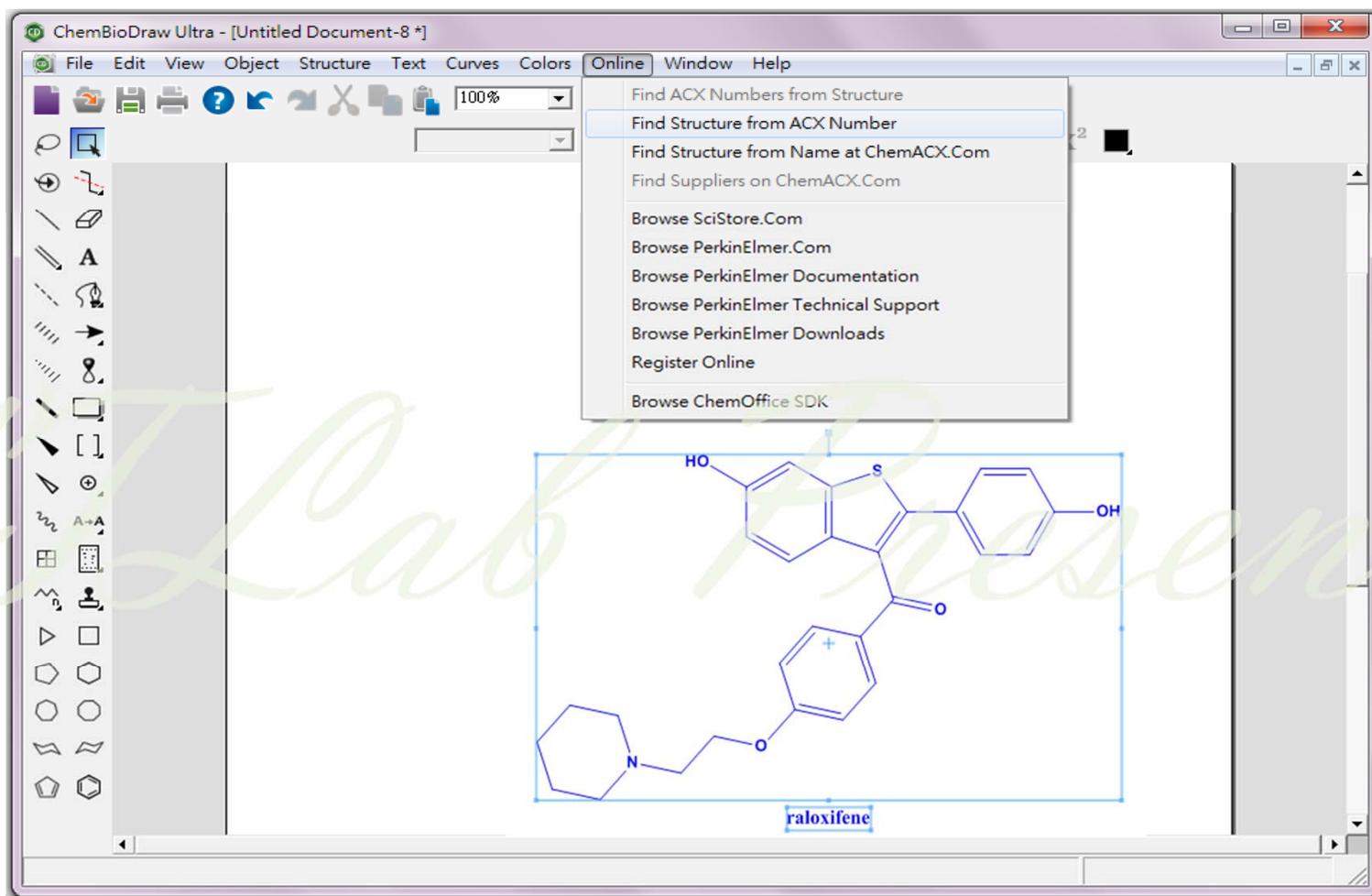


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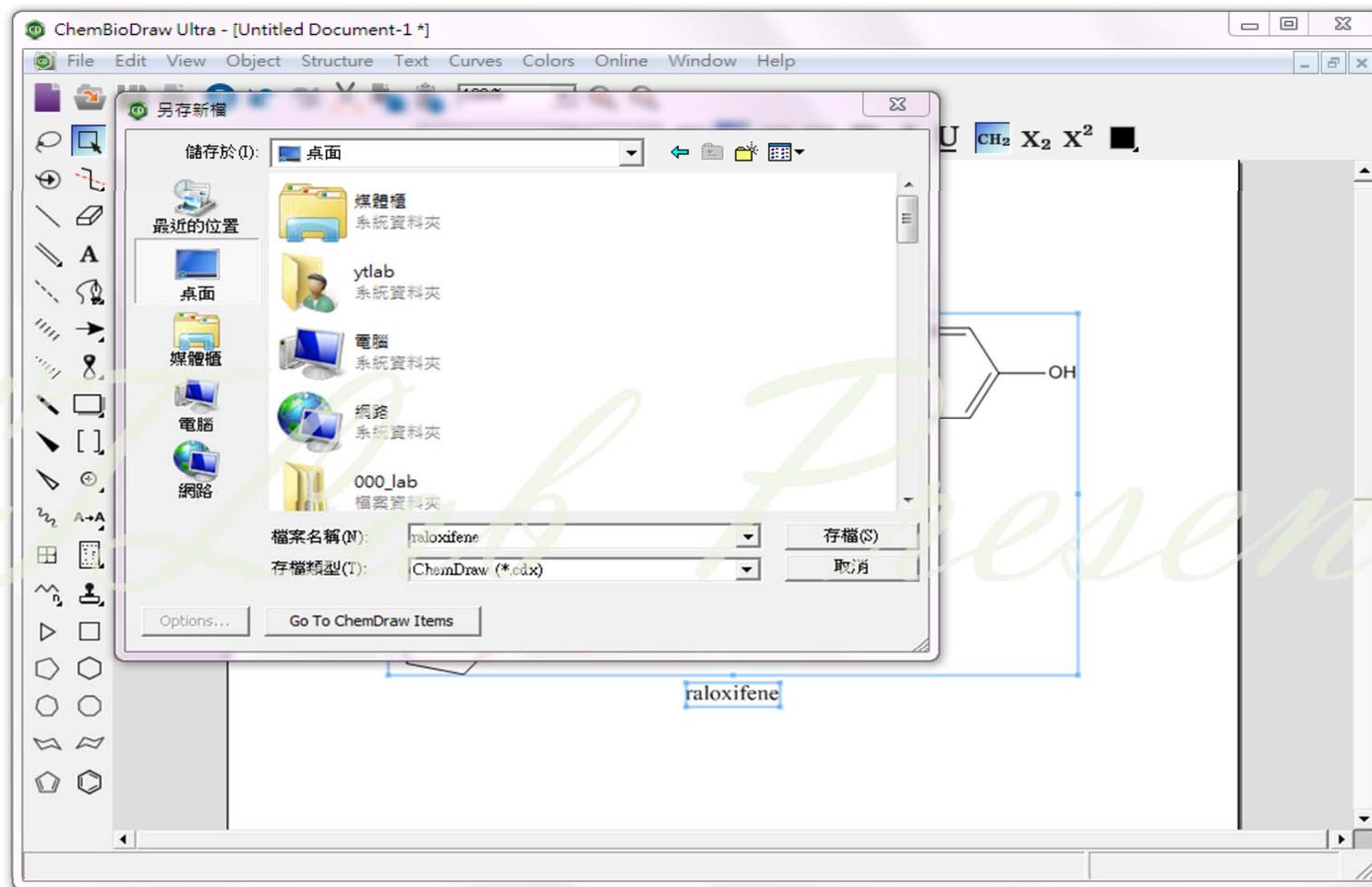
# Colors



Online=> Find Structure from ACX Number



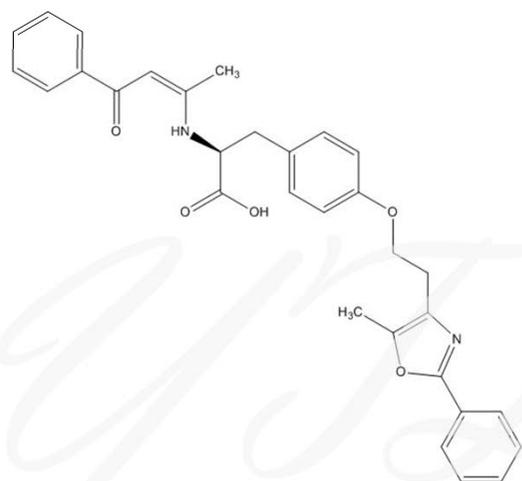
Save as → 選取.cdx檔



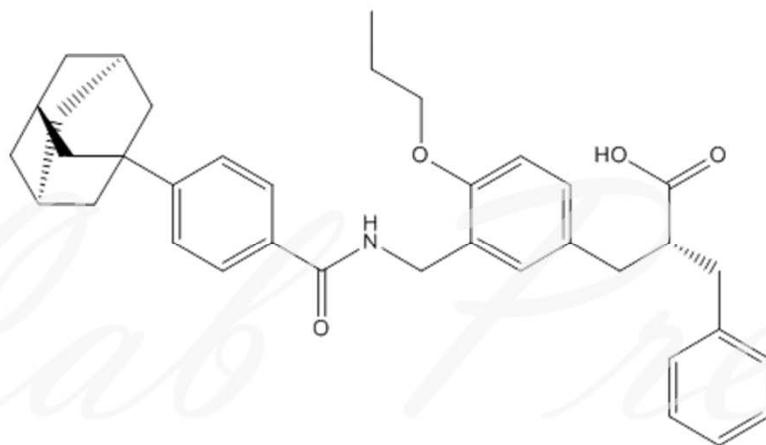
Experiment 1 :

以ChemDraw畫出下列三種Group(共九個)，  
並標記其化合物ID，存檔(.cdx)以備下星期上課使用。

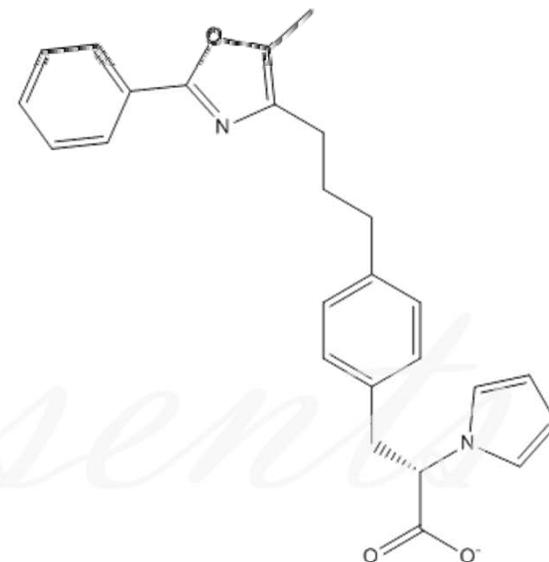
# Group 1 :



1K74\_L

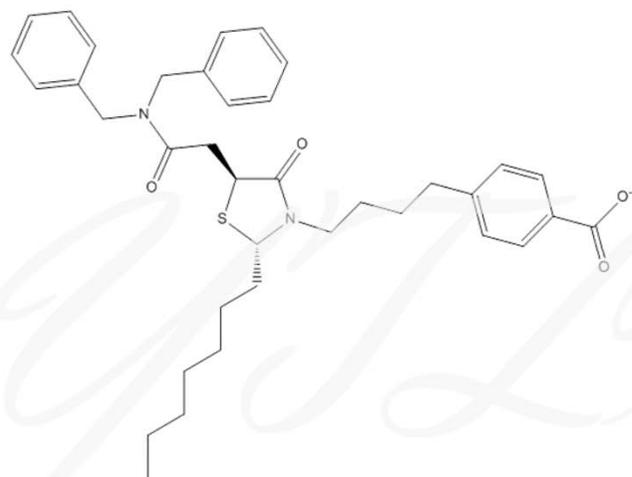


3AN4\_L

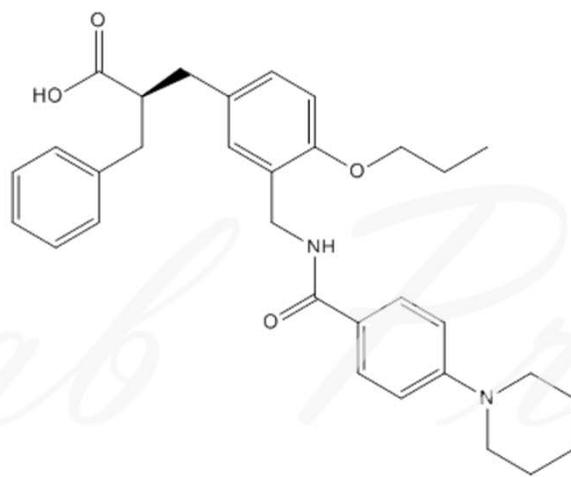


2Q8S\_L

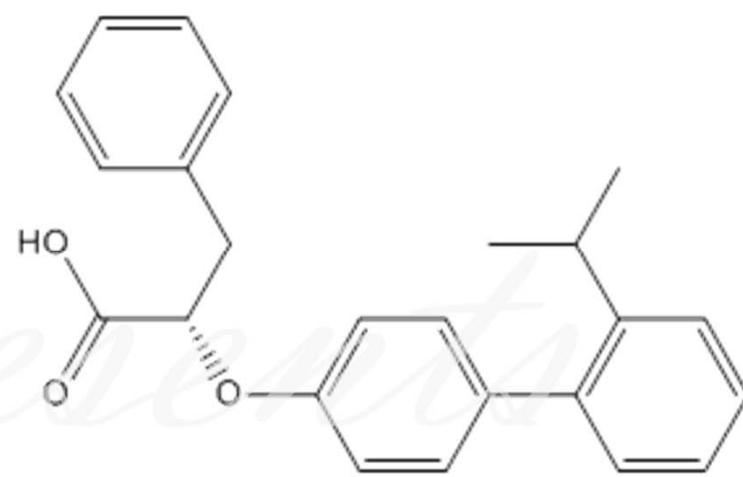
## Group 2 :



4PRG\_L

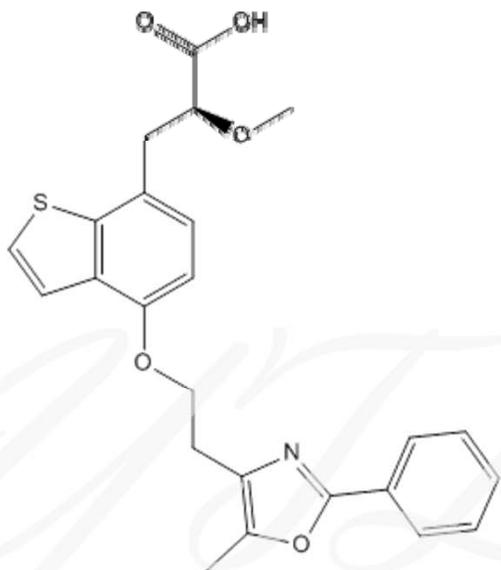


3VSP\_L

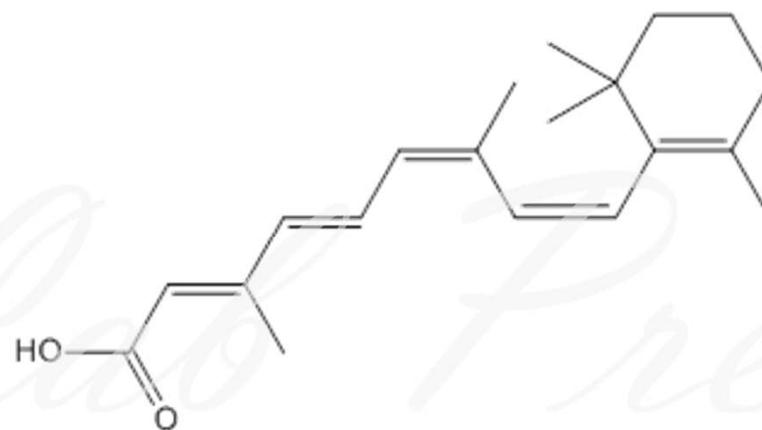


4E4K\_L

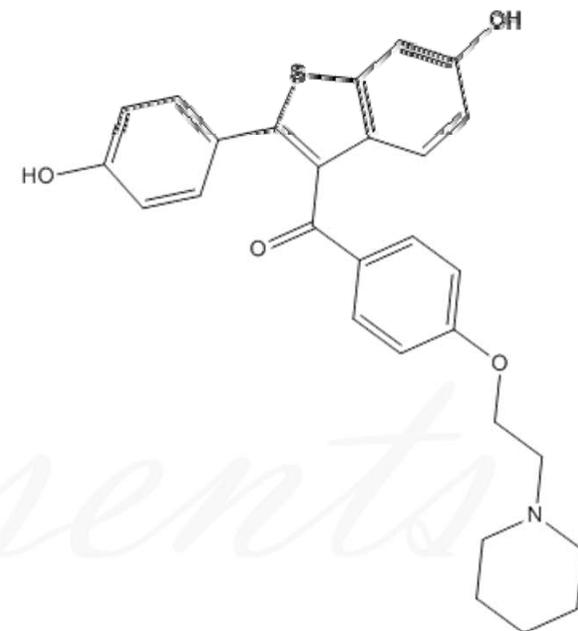
# Group 3 :



3G8I\_L



3DZU\_L



1QKN\_L

# 開一個目錄到桌面上

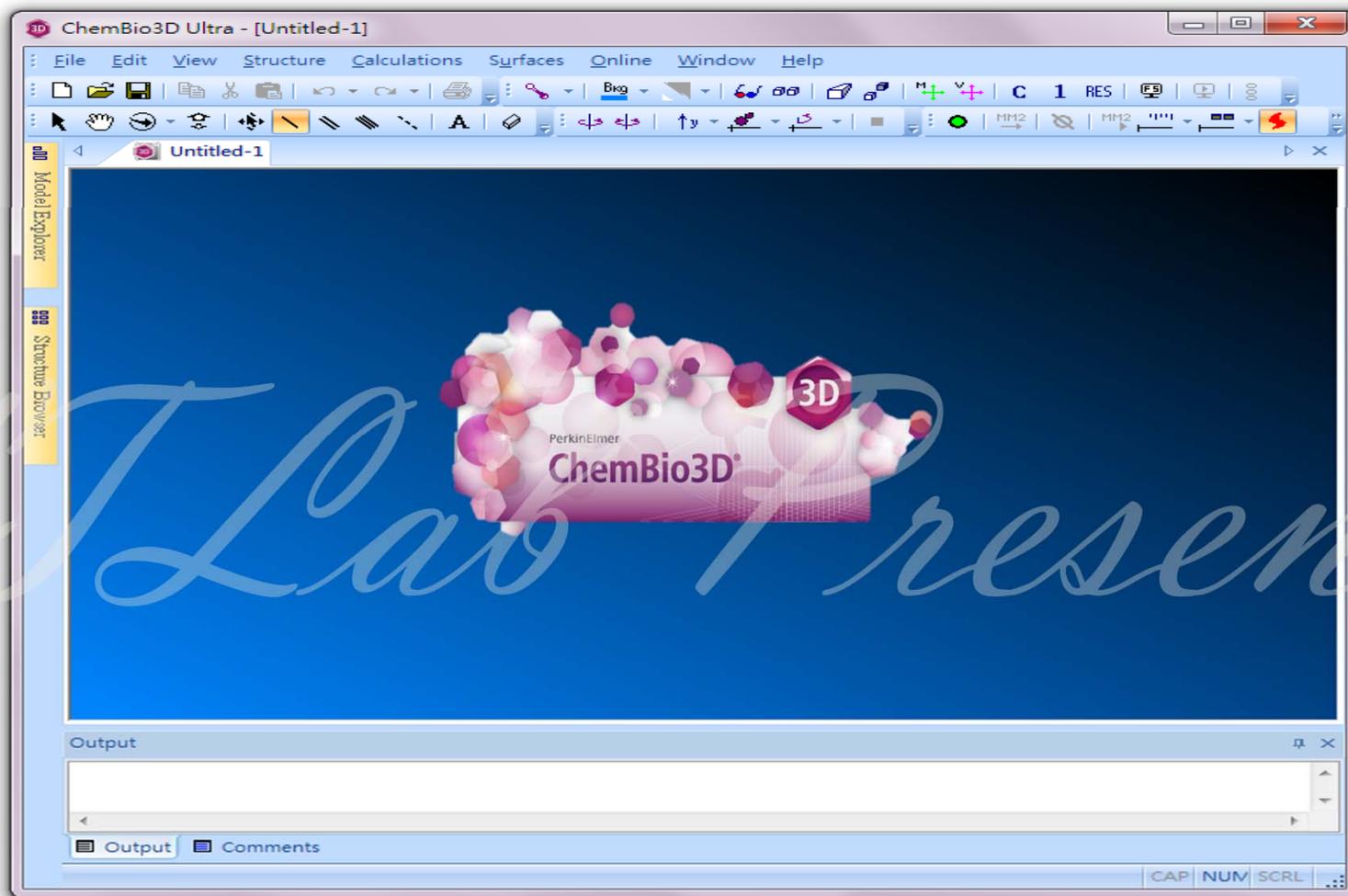
- 目錄名稱:

(例) 20171012\_MolecularDockingI\_1060220168\_林盈廷\_01



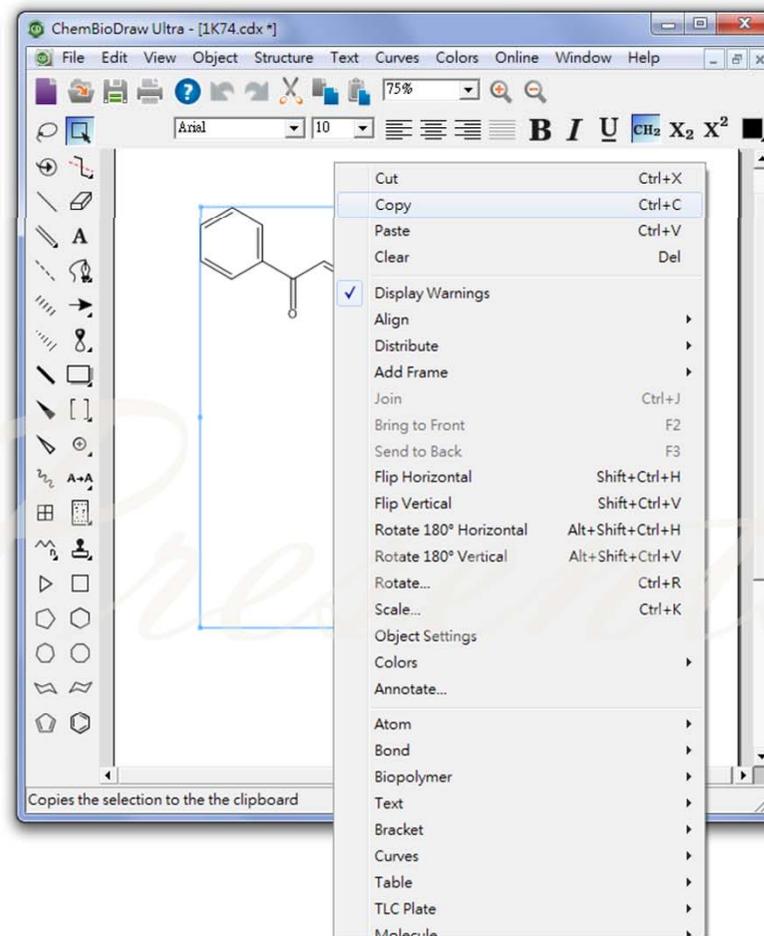
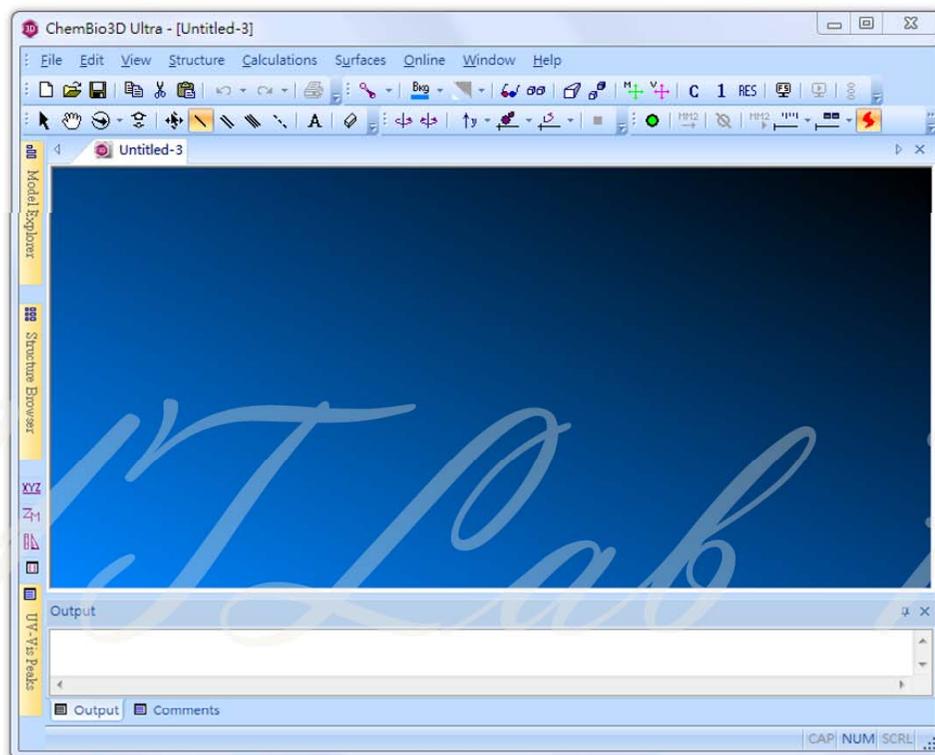
所有實驗用檔案 cdx, mol, word 放進去;  
用來交今日實驗報告

開啟Chem3D

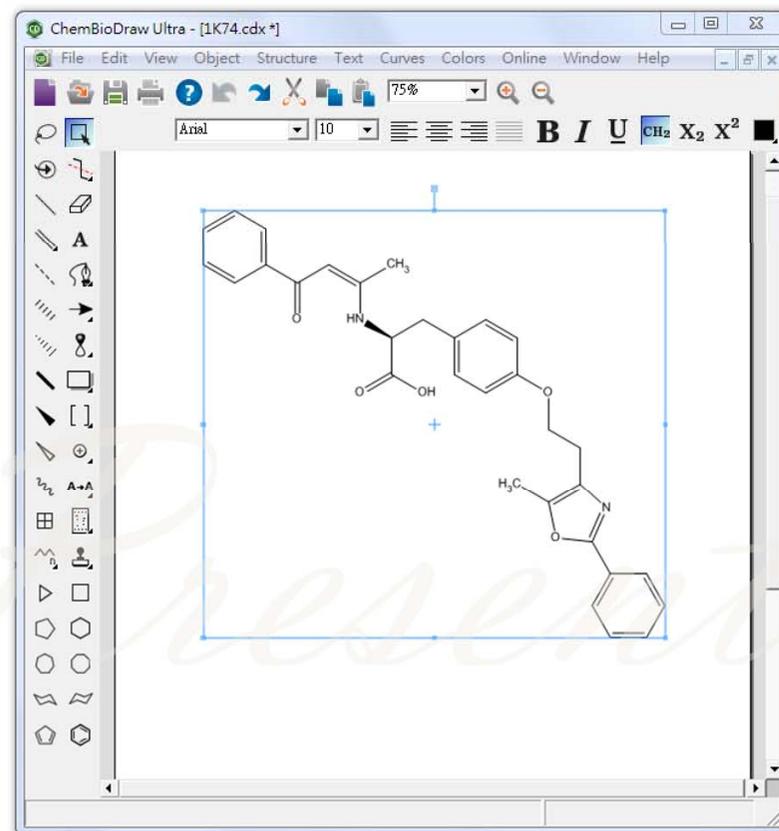
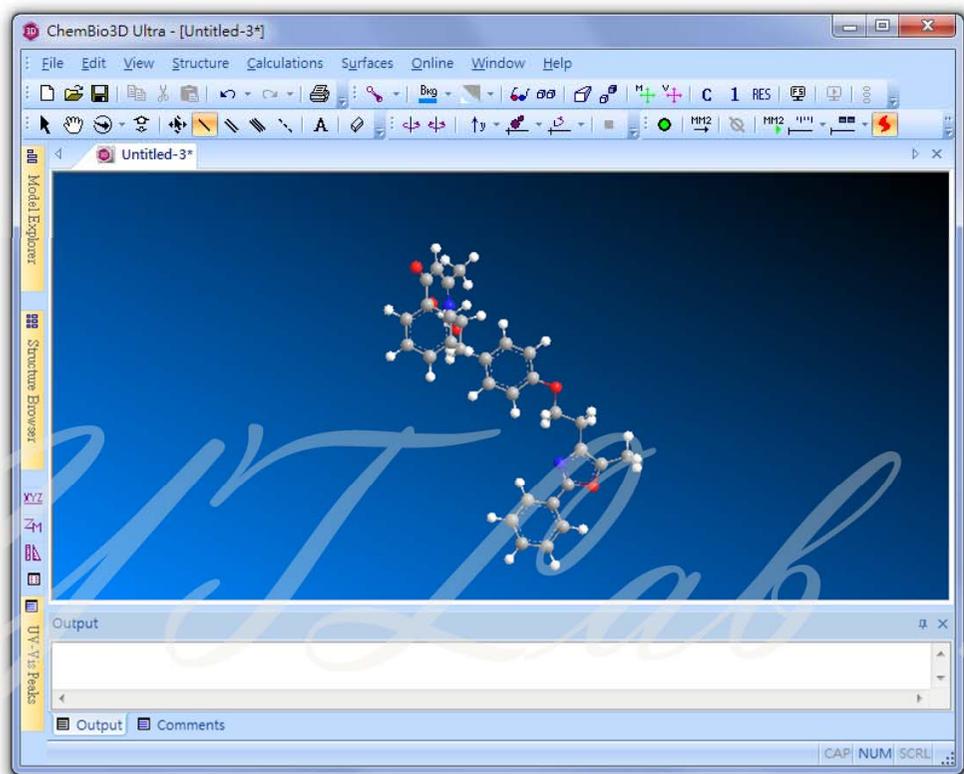


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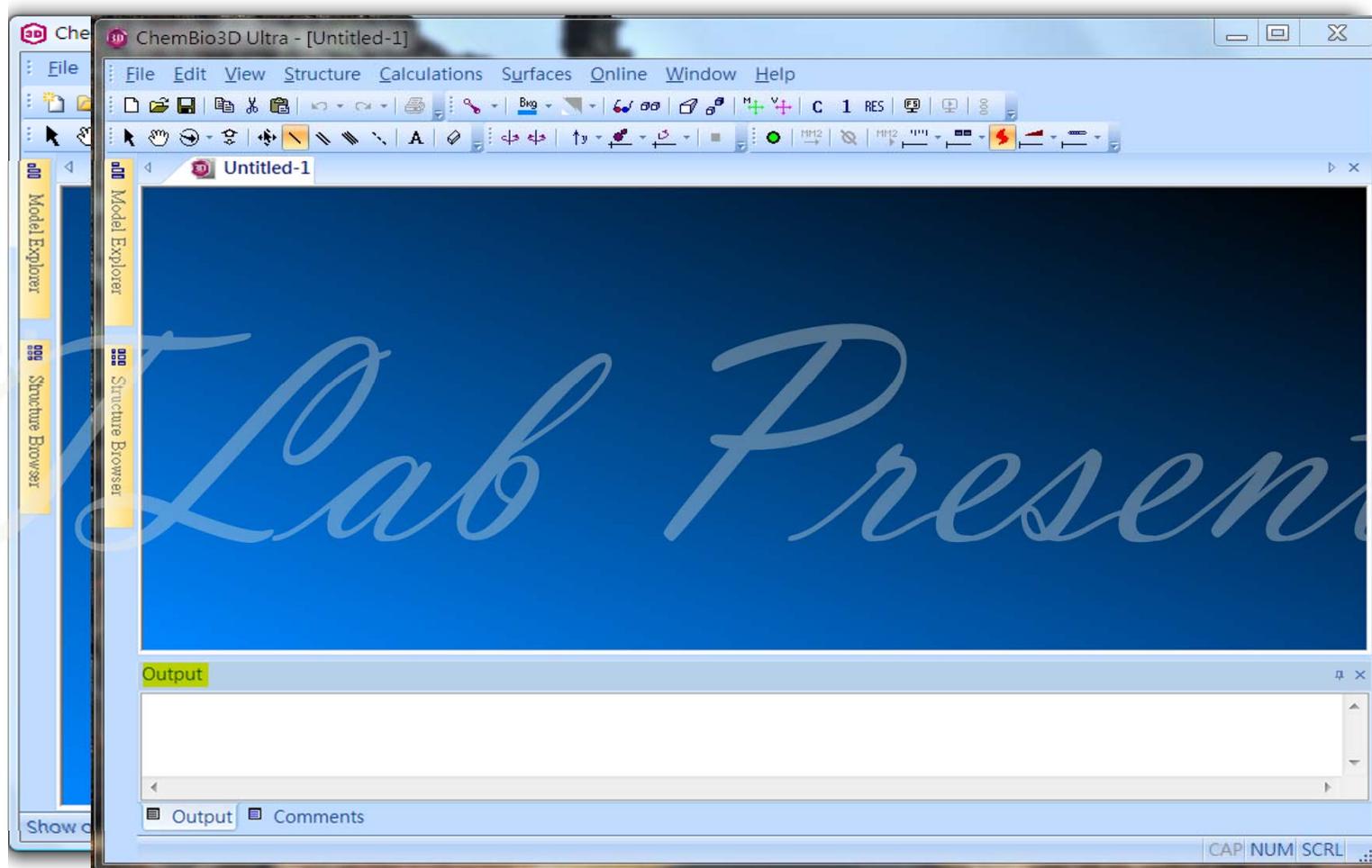
## 將化合物copy進Chem3D



## 將化合物copy進Chem3D

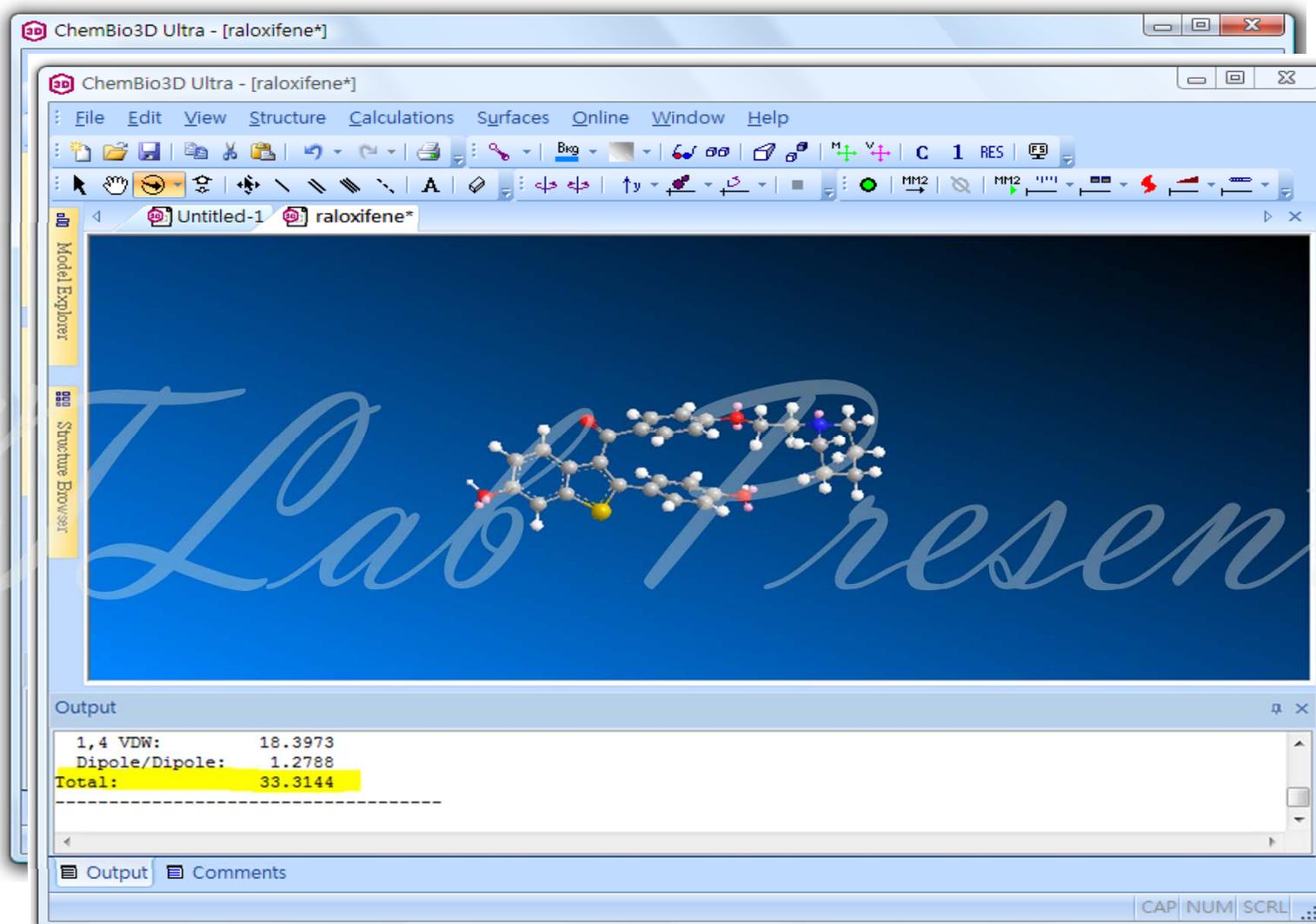


選取 View 中 Output Box

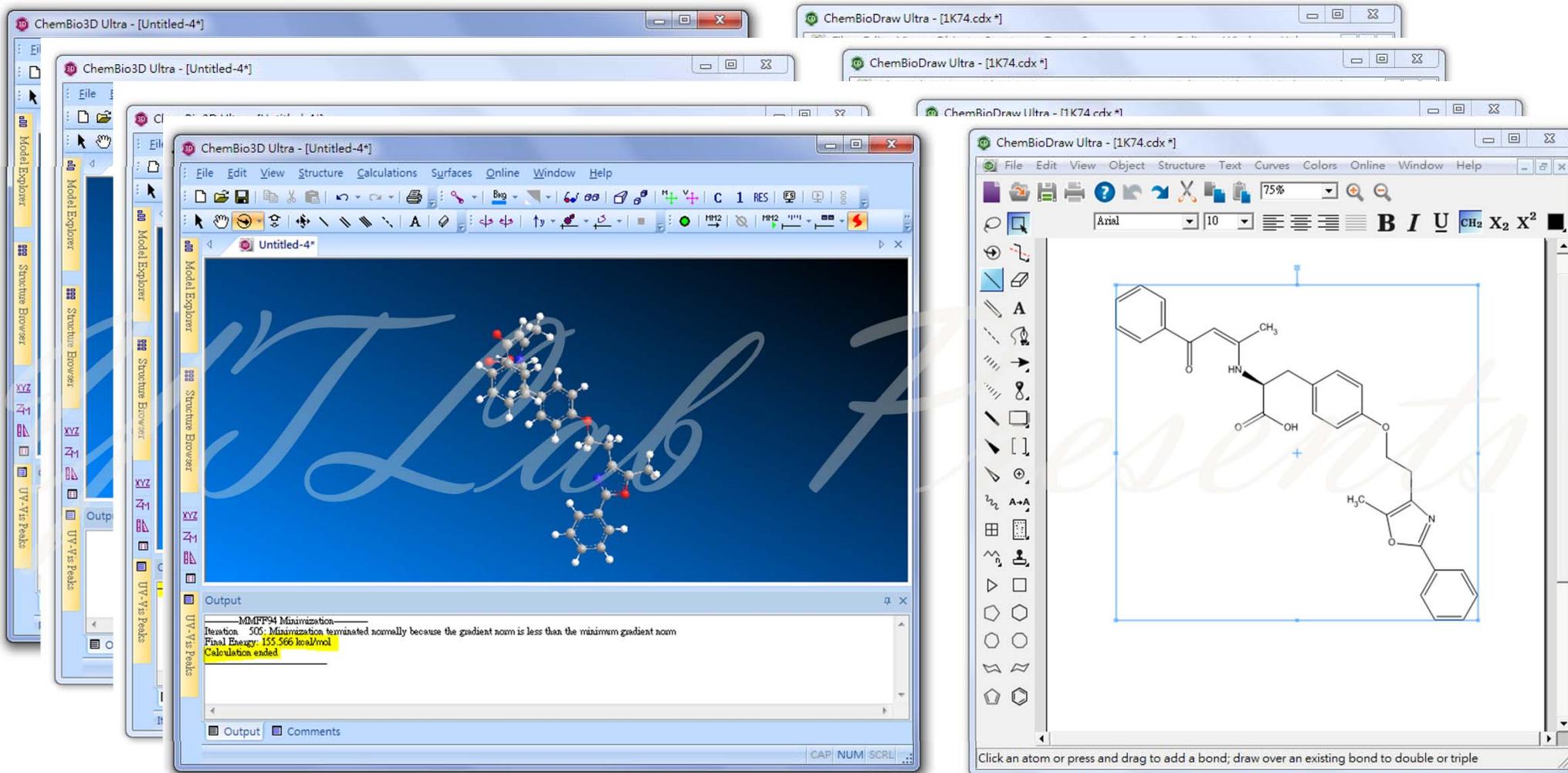


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## MM2 Minimize



# MMFF94 Minimize



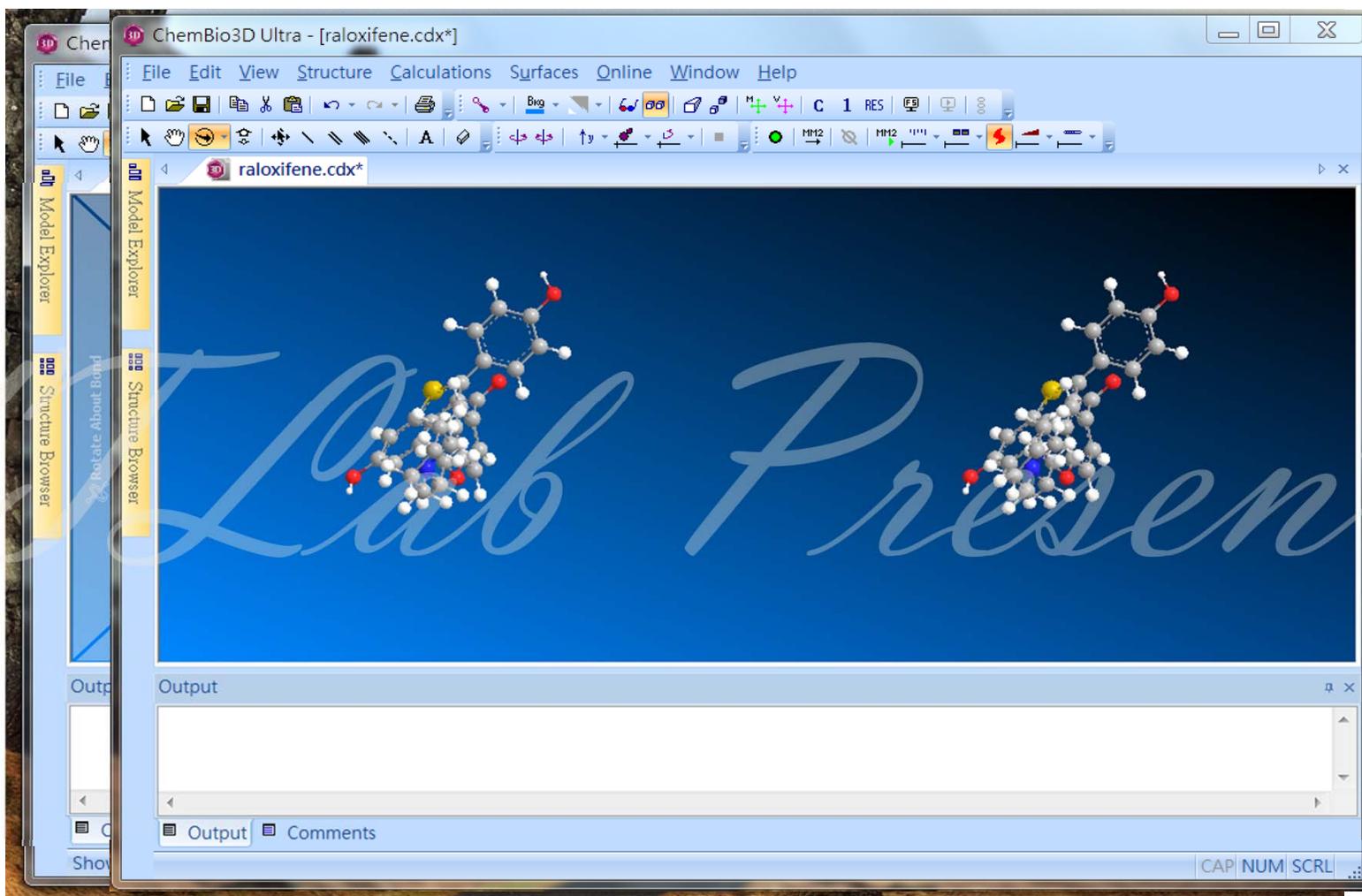
## **Molecular mechanics**

[http://en.wikipedia.org/wiki/Molecular\\_mechanics](http://en.wikipedia.org/wiki/Molecular_mechanics)

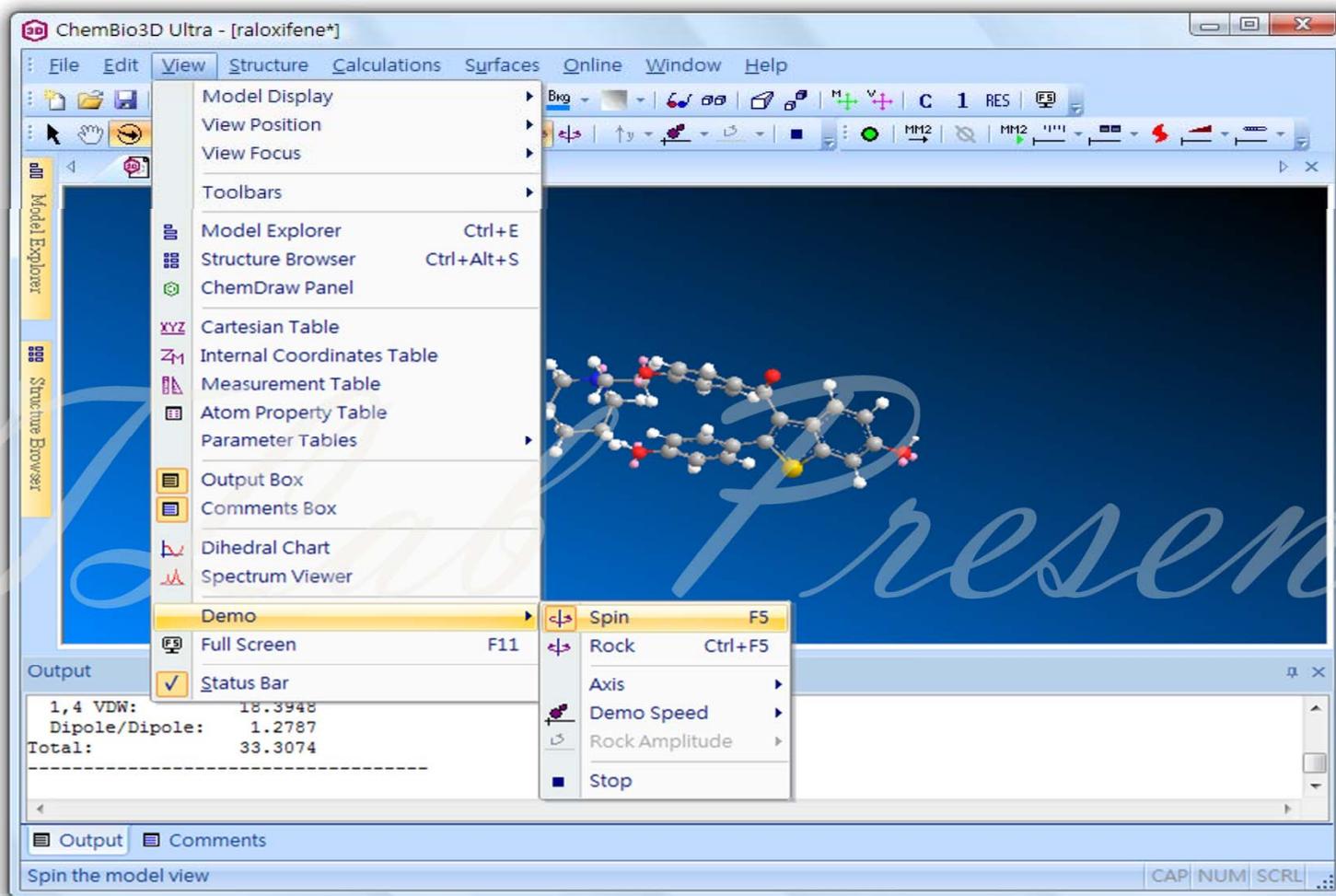
## **Molecular dynamics**

[http://en.wikipedia.org/wiki/Molecular\\_dynamics](http://en.wikipedia.org/wiki/Molecular_dynamics)

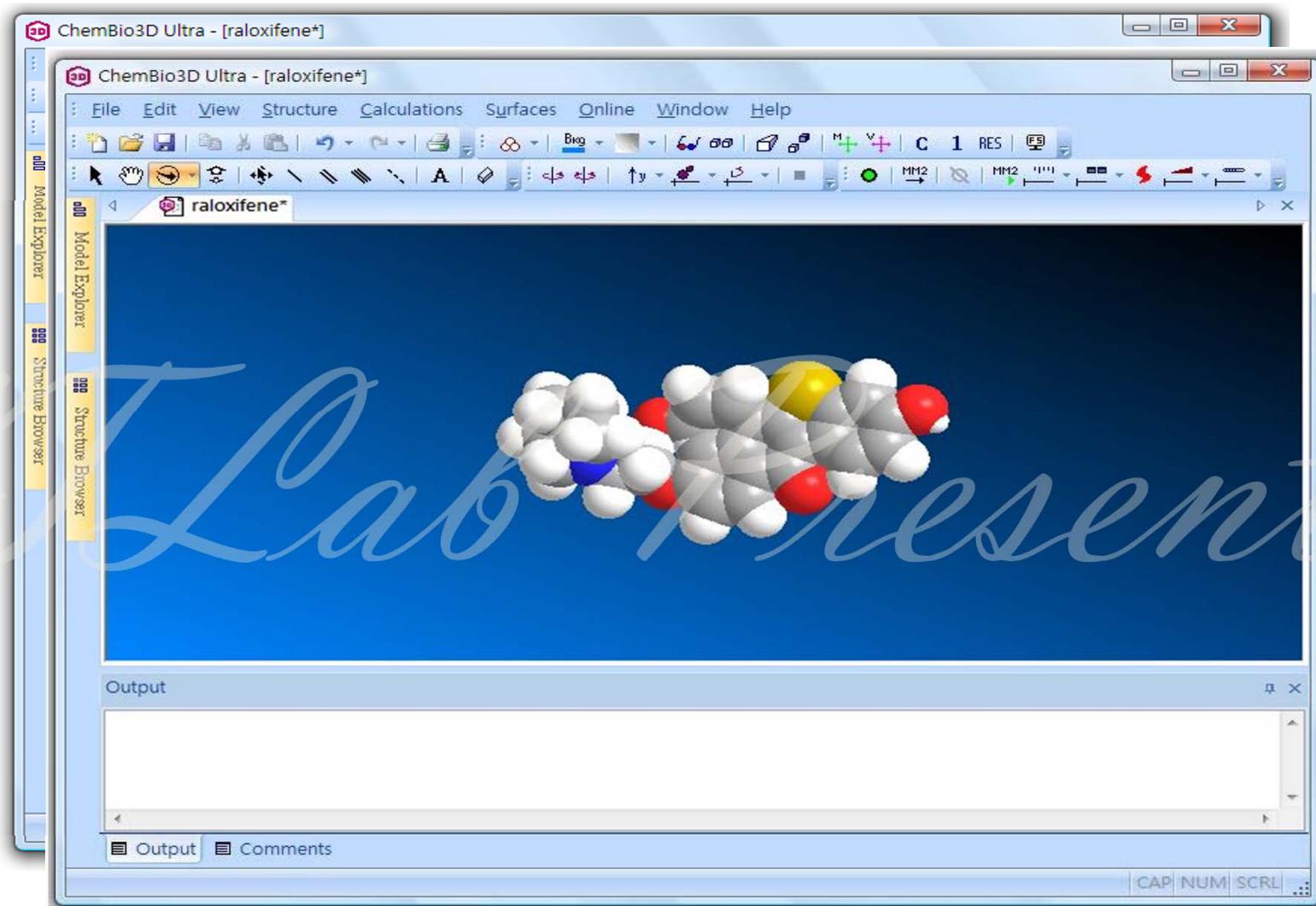
Stereo → 嘗試用鬥雞眼看出立體結構



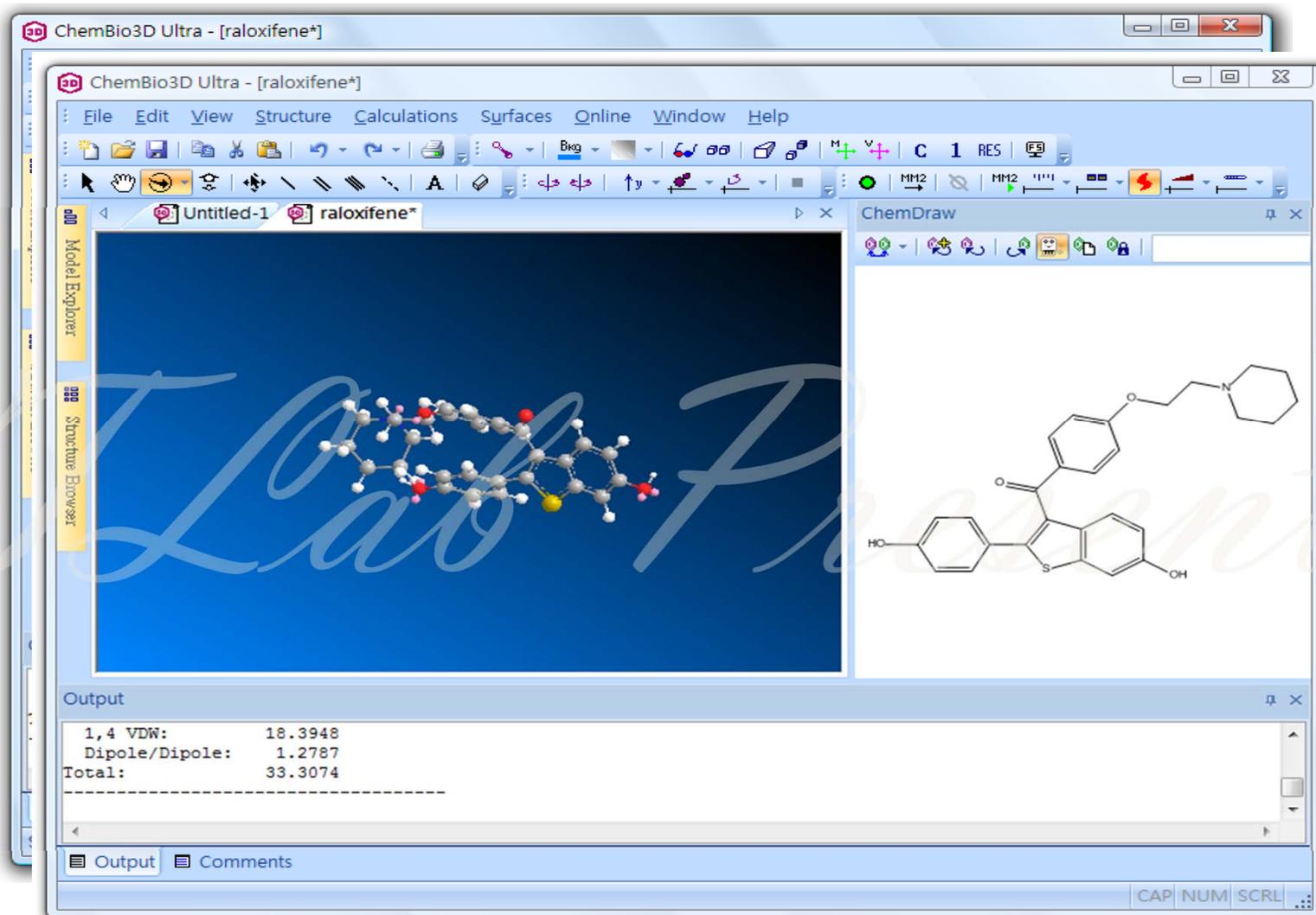
View → Demo ⇒ Spin



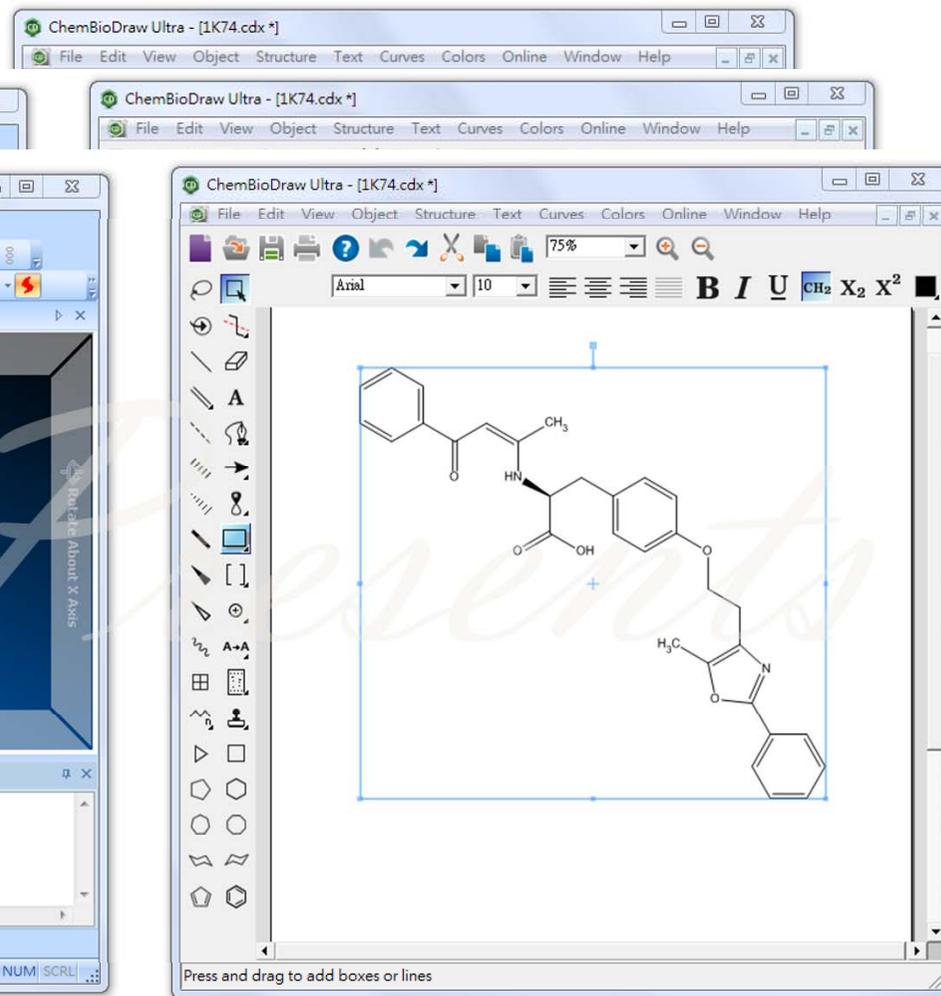
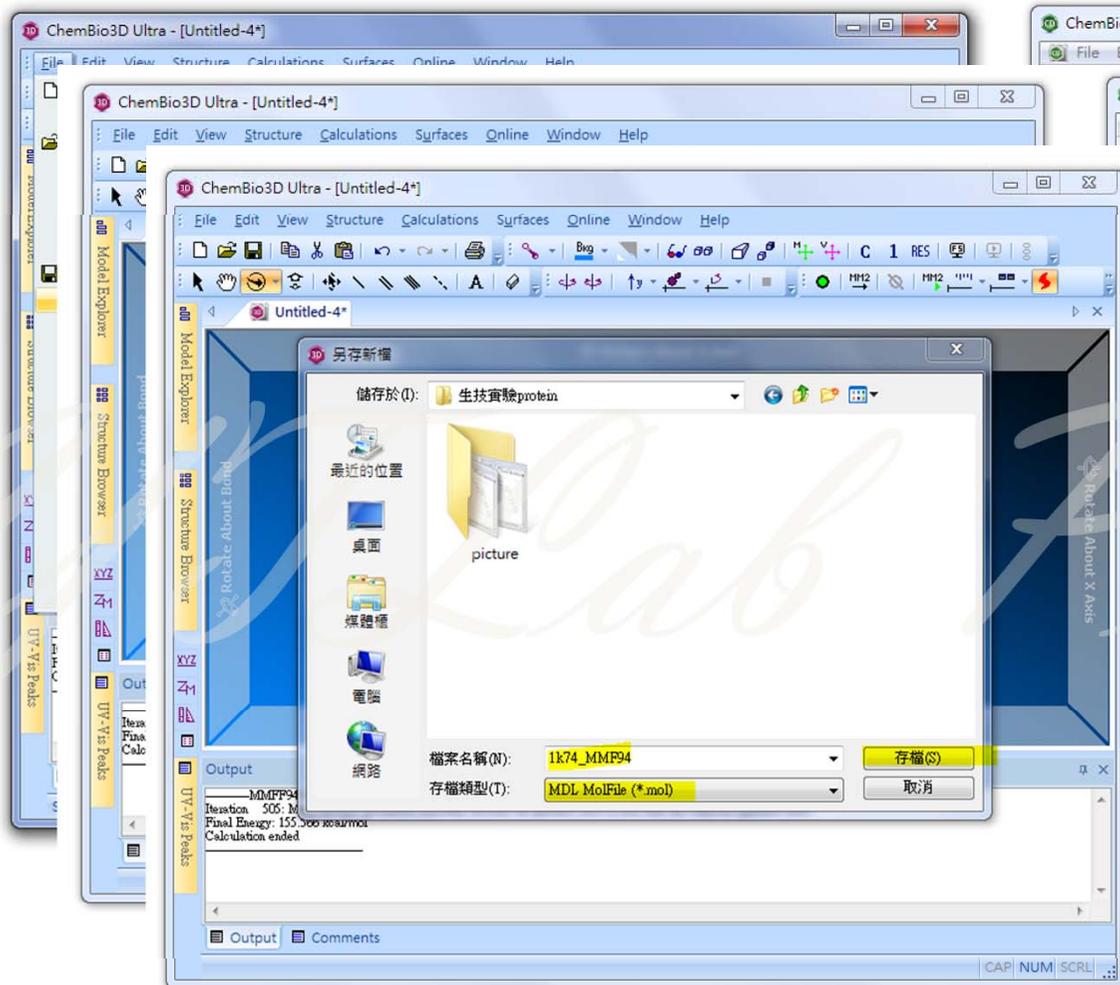
## Display Mode



View → ChemDraw Panel



Save as → 選取.mol檔



Experiment 2 :

計算已畫出九個小分子，求取 MMFF94 能量之最小值，  
並存檔成.mol檔，以備下次上課使用。

## 實驗討論（寫在word檔內）：

- Q: 從二度空間的小分子，轉換成三度空間的小分子，用了那個計算理論？那九個小分子三度空間的形狀合理嗎？量量鍵長鍵角？（提示：用ChemBio3D 的功能）
- Q: 何謂分子力學（MM）？此建立真實小分子在電腦內的實驗用了哪些分子力學？
- Q: 今年(2013)三位諾貝爾獎得主，究竟把可哪些類型的實驗帶到電腦網路世界來執行，找出來瞭解及討論。（舉例說明）

# 壓縮目錄到桌面上

- 壓縮檔名稱：  
(例) 20181102\_MolecularDockingI\_1060220168\_林盈廷\_01.rar



# 實驗結果上傳

- 第一天：2D、3D小分子檔案
- 第二天：分數excel檔、word(回答Q&A、圖片記錄)

Wish you have a successful experiment in cyberspace.