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
Tel: (07) 3121101 ext. 2792
eMail：ytlin@kmu.edu.tw

YTLab Presents

Wet Lab vs Dry Lab

YJLab Presents

Molecular Docking

Molecular Docking

分子入塢

Handle Small Molecule

Molecular Docking

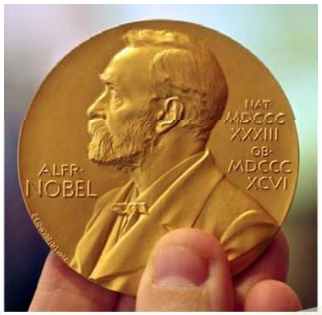
分子入塢

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

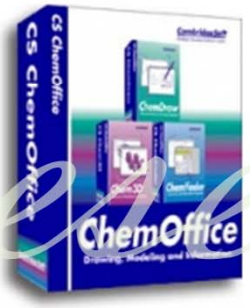
YTLab Presents

第一步:如何表達真實無誤的小分子在電腦裡?

YTLab Presents

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

Molecular Docking

Ying-Ting Lin | Contact

Molecular Docking

Experimental Protocols:	
Handle Small Molecule:	MolecularDocking_SmallMolecule
Handle Big Molecule:	MolecularDocking_BigMolecule
Handle Binding Pocket:	MolecularDocking_BindingPocket
Calculation of Molecular Docking:	MolecularDocking_Calculation

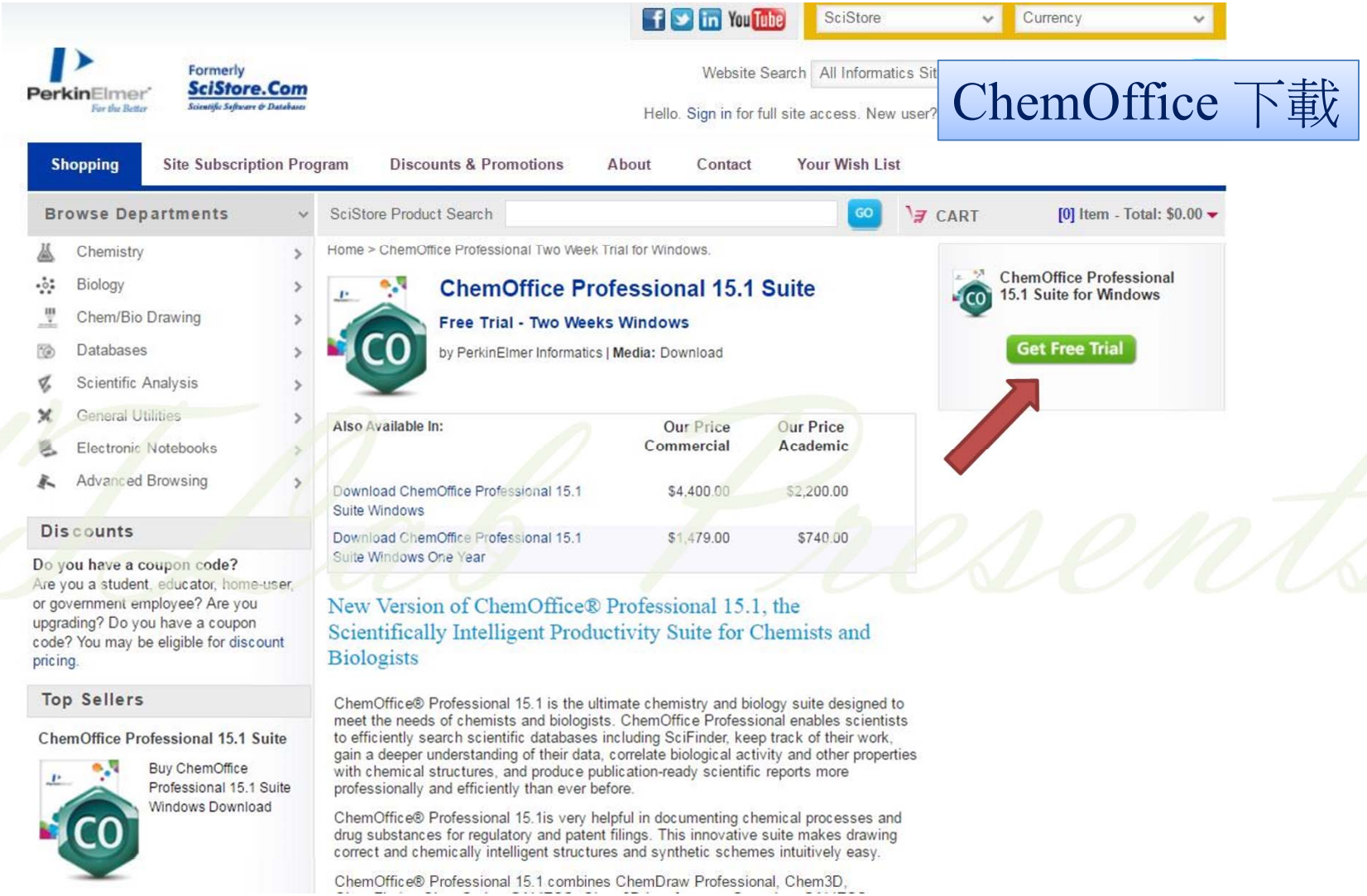
Computing Programs Installation:	
Molecular Editor:	ChemBioOffice (from SciStore)

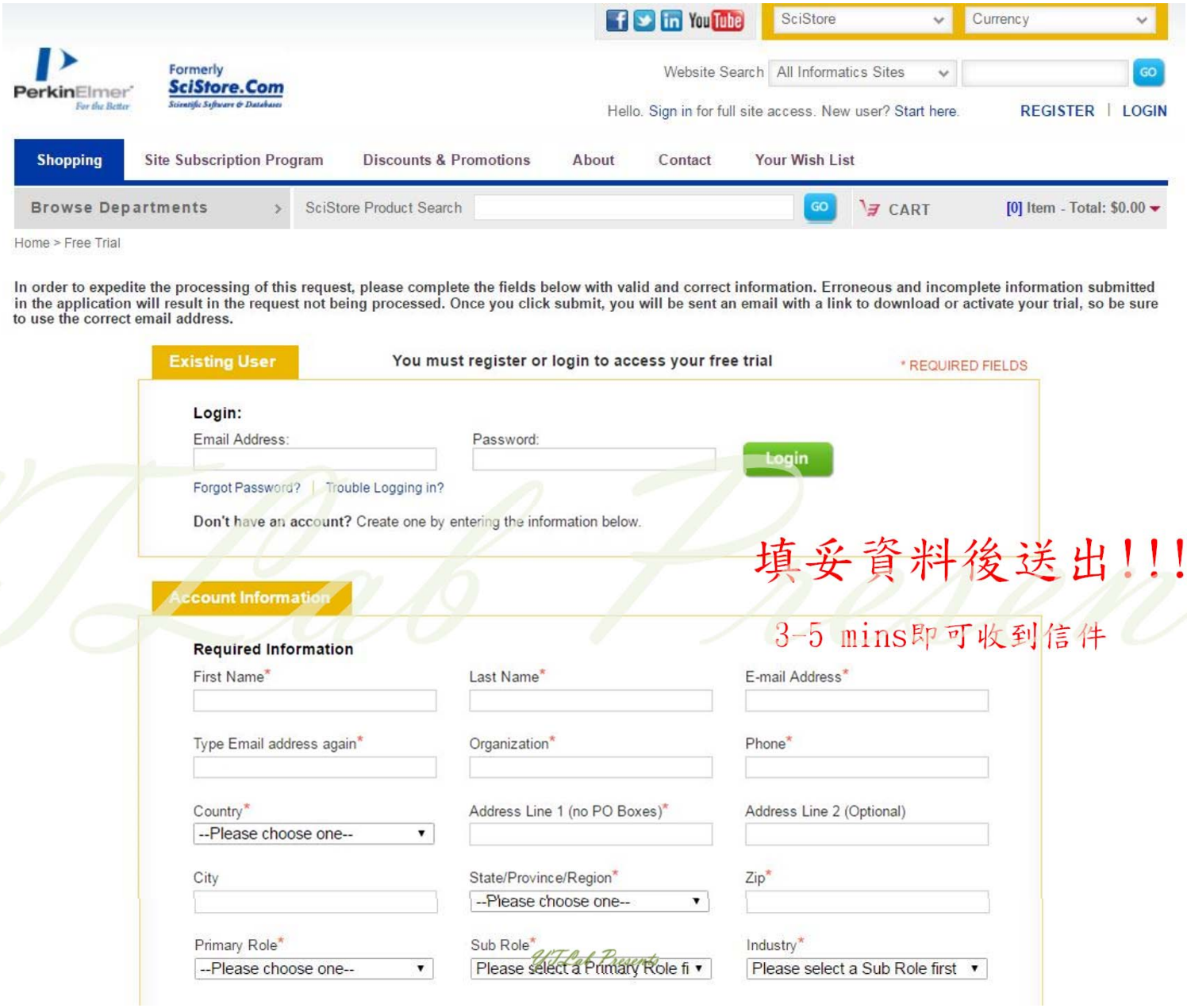
Other Installation:	
Protein Viewer:	Chimera (from UCSF Chimera)
Quamtum Chemistry:	MOPAC2012, libiomp5md.dll (from OpenMOPAC)

Report:
Hand in Your Report

YTLab Presents

ChemOffice 下載




SciStore
Currency
PerkinElmer
For the Better
Formerly
SciStore.Com
Scientific Software & Databases
Website Search
All Informatics Sites
GO
Hello. Sign in for full site access. New user? Start here.
REGISTER | LOGIN
Shopping
Site Subscription Program
Discounts & Promotions
About
Contact
Your Wish List
Browse Departments
SciStore Product Search
GO
CART
[0] Item - Total: $0.00
Home > Free Trial
In order to expedite the processing of this request, please complete the fields below with valid and correct information. Erroneous and incomplete information submitted in the application will result in the request not being processed. Once you click submit, you will be sent an email with a link to download or activate your trial, so be sure to use the correct email address.
Existing User
You must register or login to access your free trial
* REQUIRED FIELDS
Login:
Email Address:
Password:
Login
Forgot Password? | Trouble Logging in?
Don't have an account? Create one by entering the information below.
填妥資料後送出!!!
3-5 mins即可收到信件
Account Information
Required Information
First Name*
Last Name*
E-mail Address*
Type Email address again*
Organization*
Phone*
Country*
--Please choose one--
Address Line 1 (no PO Boxes)*
Address Line 2 (Optional)
City
State/Province/Region*
--Please choose one--
Zip*
Primary Role*
--Please choose one--
Sub Role*
Please select a Primary Role fi
Industry*
Please select a Sub Role first

第二封信件含有個人的serial number 及下載網址

寄件者: <informatics.customer_service@PERKINELMER.COM>
收件者: <u99022009@cc.kmu.edu.tw>
主旨: Your PerkinElmer Trial Order Information ECOM0291647

Dear yi-jing chuang,

Thank you for your order. This message contains information you will need to get started with your new purchase. Please save this mail for your records, as you may need this information again in the future.

Order Number: ECOM0291647

PRODUCTS & CODES

ChemBioOffice Ultra Trial Download Two Week 13

Quantity 1

Serial Number: 231-000168-5069

DOWNLOAD/ACCESS INSTRUCTIONS

To download your software and/or activate your subscription, please click on the link below (be sure it appears on one line so that it will work properly)

http://efulfillment.cambridgesoft.com/efulfillment/?GP=ECOM0291647&Cust=CHUANGYI-JING++&OrderLineID=561811

ACTIVATION INFORMATION

If your product requires activation, please use the serial number listed with your product name above. For additional information about how to activate your software, please visit:

http://perkinelmer.com/informatics/activation

NEED HELP?

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 :
http://www.perkinelmer.com/informatics/support/contact/

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

PerkinElmer
For the Better

Welcome ???

ChemBioOffice Ultra Trial Download Two Week 13

Windows

Quantity: 1

Click Here to Download Software - ChemBioOffice Ultra 13 Application

(Click on the link above, and proceed to save the file to your computer. Then see Installation Instructions.)

PerkinElmer
For the Better

Welcome ???

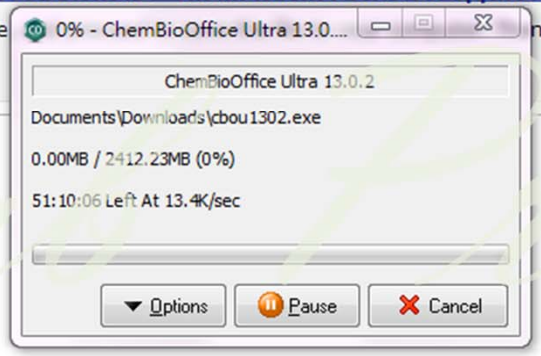
ChemBioOffice Ultra Trial Download Two Week 13

Windows

Quantity: 1

Click Here to Download Software - ChemBioOffice Ultra 13 Application

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



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For the Better

Welcome ???

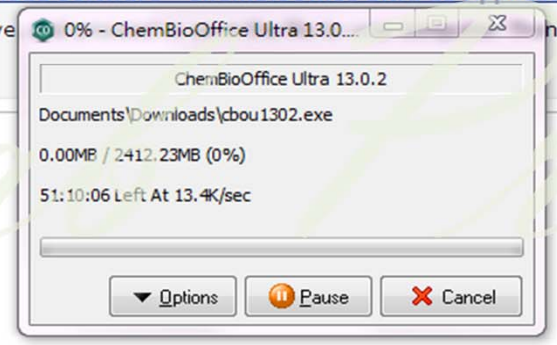
ChemBioOffice Ultra Trial Download Two Week 13

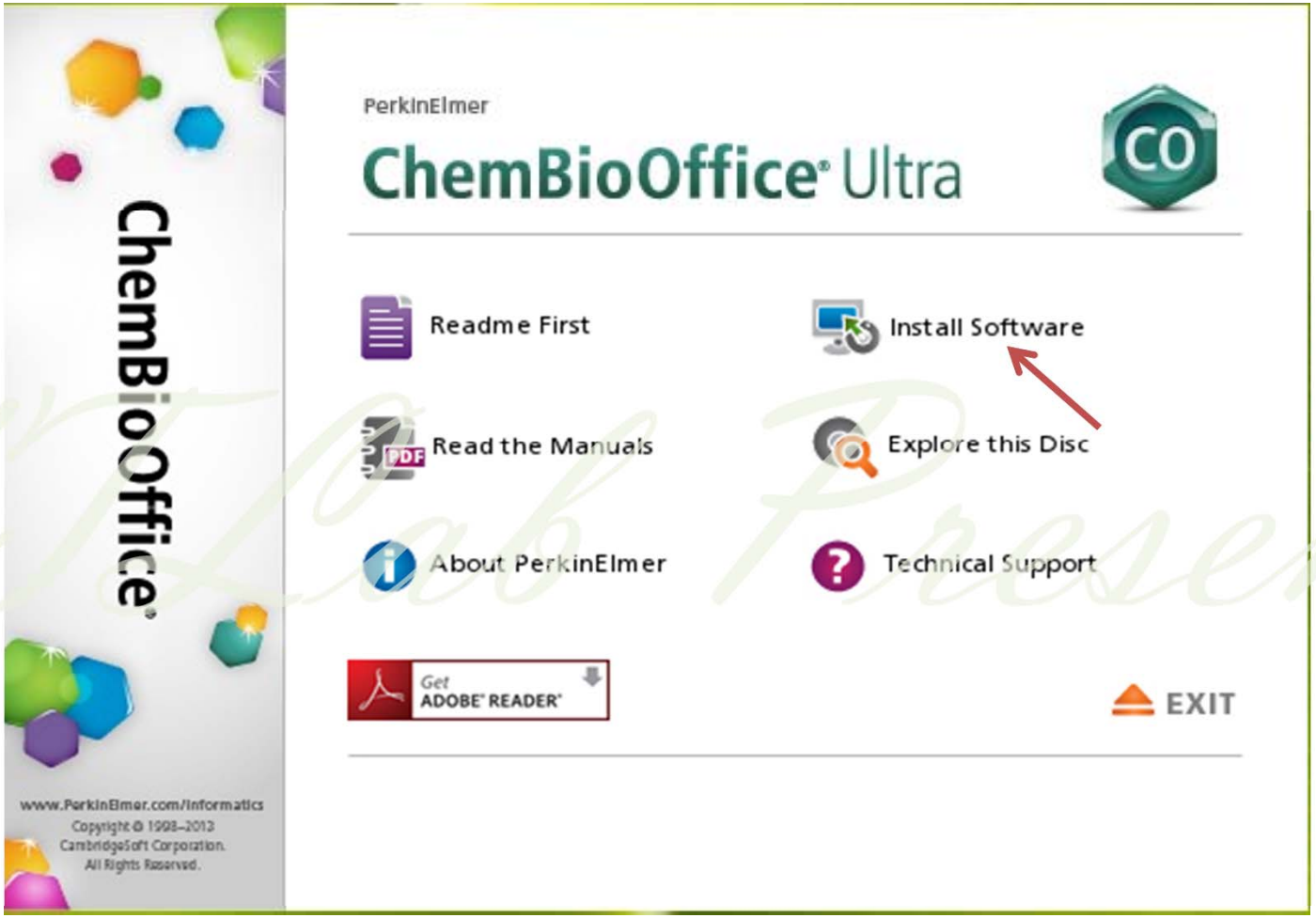
Windows

Quantity: 1

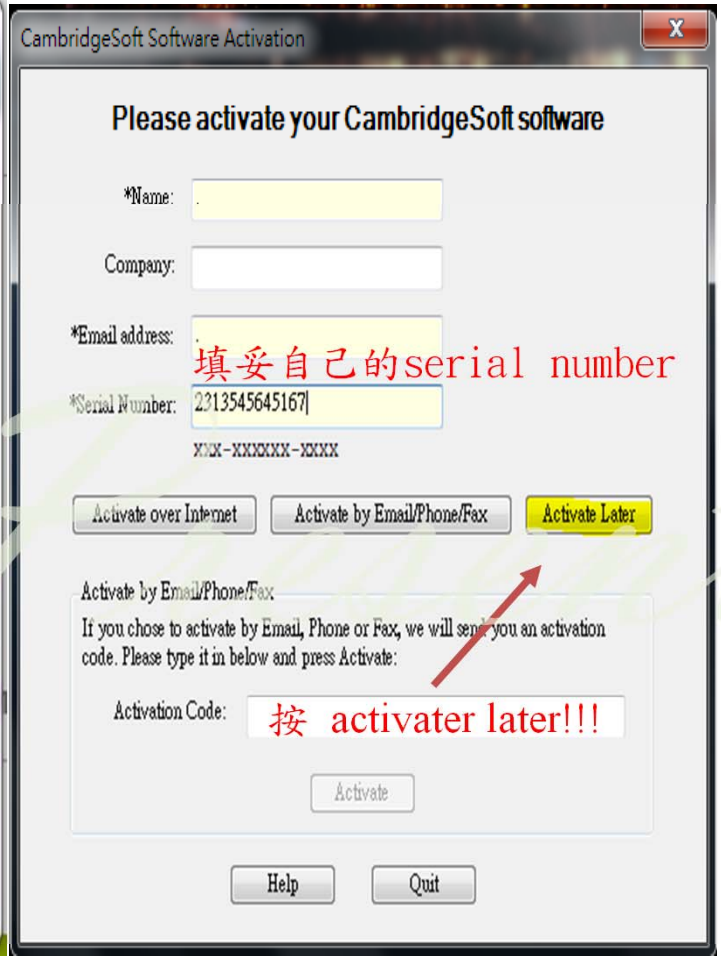
Click Here to Download Software - ChemBioOffice Ultra 13 Application

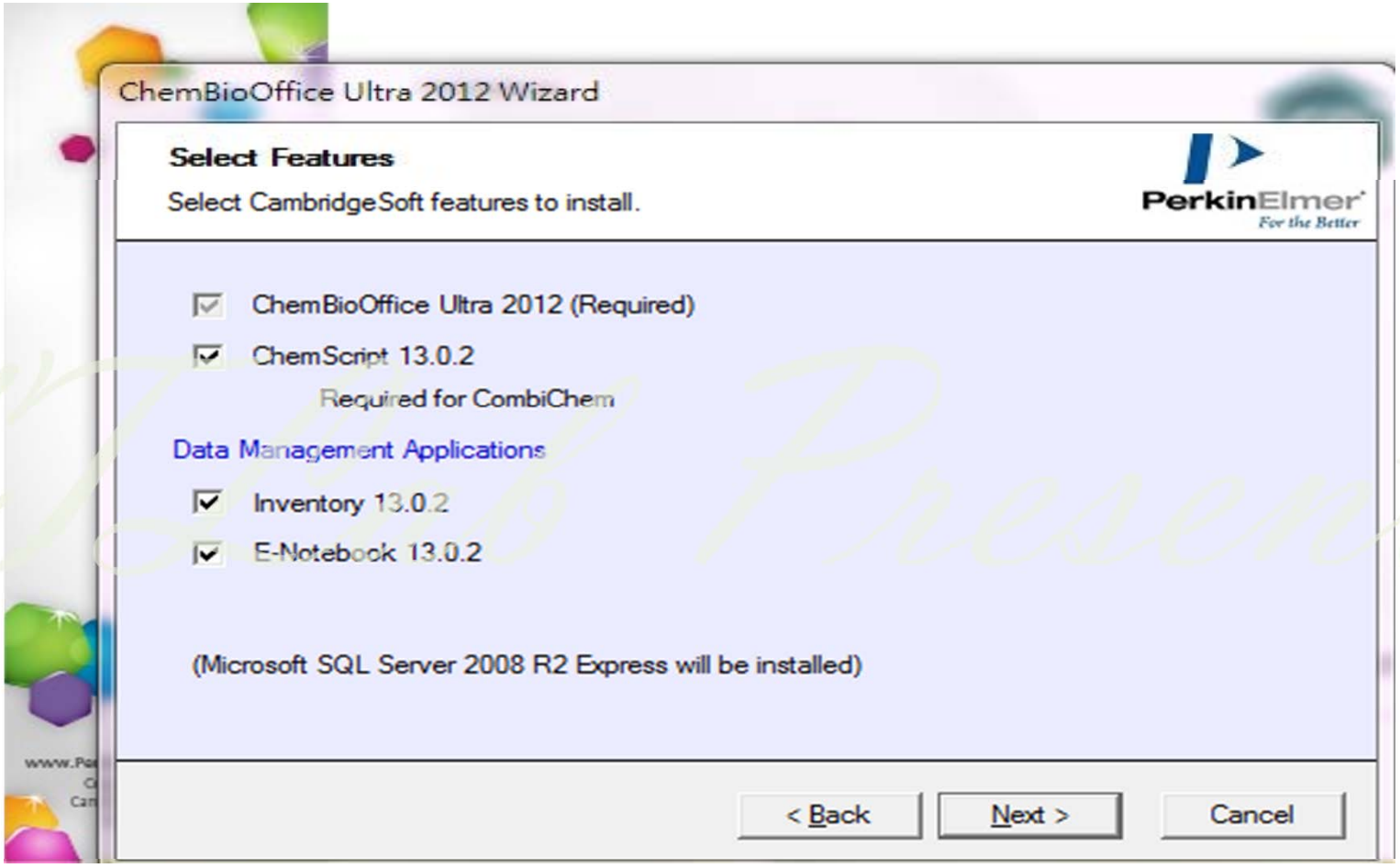
(Click on the link above ... see Installation Instructions.)

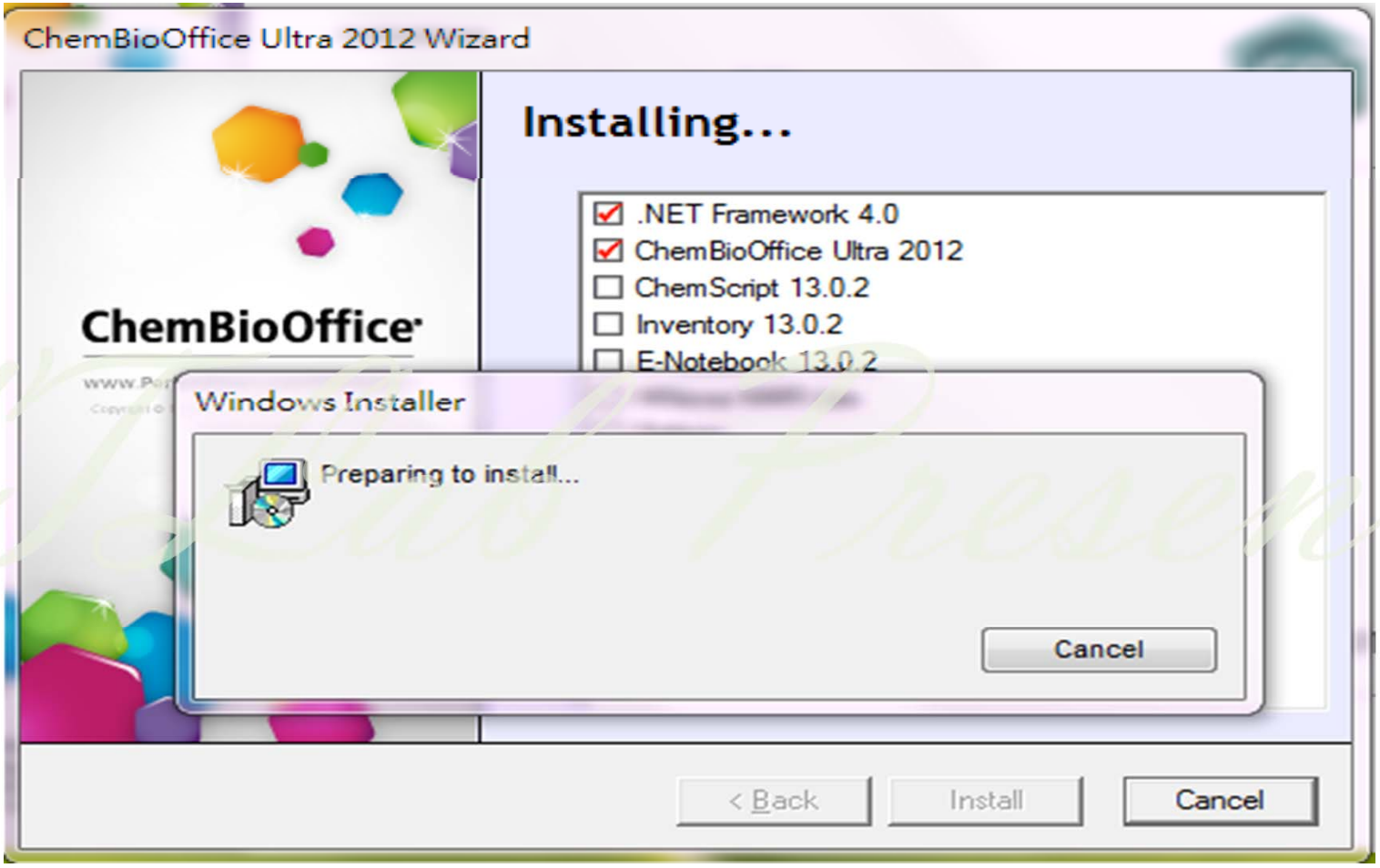


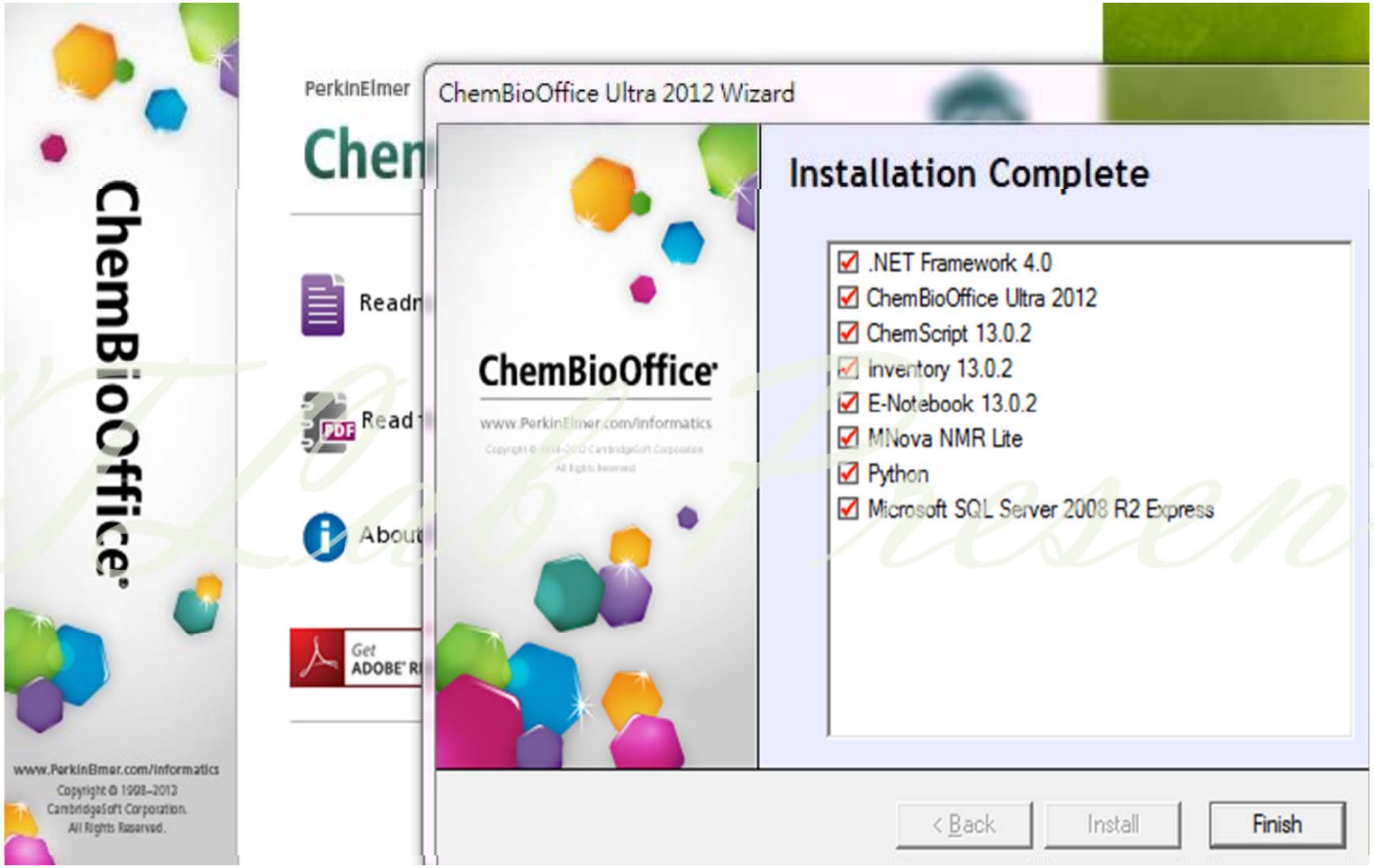



ChemBioOffice Ultra 2012 Wizard
Welcome to the ChemBioOffice Ultra 2012 Wizard
ChemBioOffice
Please wait while the wizard prepares the system for installation...
NOTE: Users with personal firewalls installed on their system will need to temporarily disable them. Firewalls may be reactivated after the installation is complete.
Next >
Cancel


CambridgeSoft Software Activation
Please activate your CambridgeSoft software
*Name:
Company:
*Email address:
填妥自己的serial number
*Serial Number:
2313545645167
xxx-xxxxxx-xxxx
Activate over Internet
Activate by Email/Phone/Fax
Activate Later
Activate by Email/Phone/Fax
If you chose to activate by Email, Phone or Fax, we will send you an activation code. Please type it in below and press Activate:
Activation Code:
按 activater later!!!
Activate
Help
Quit

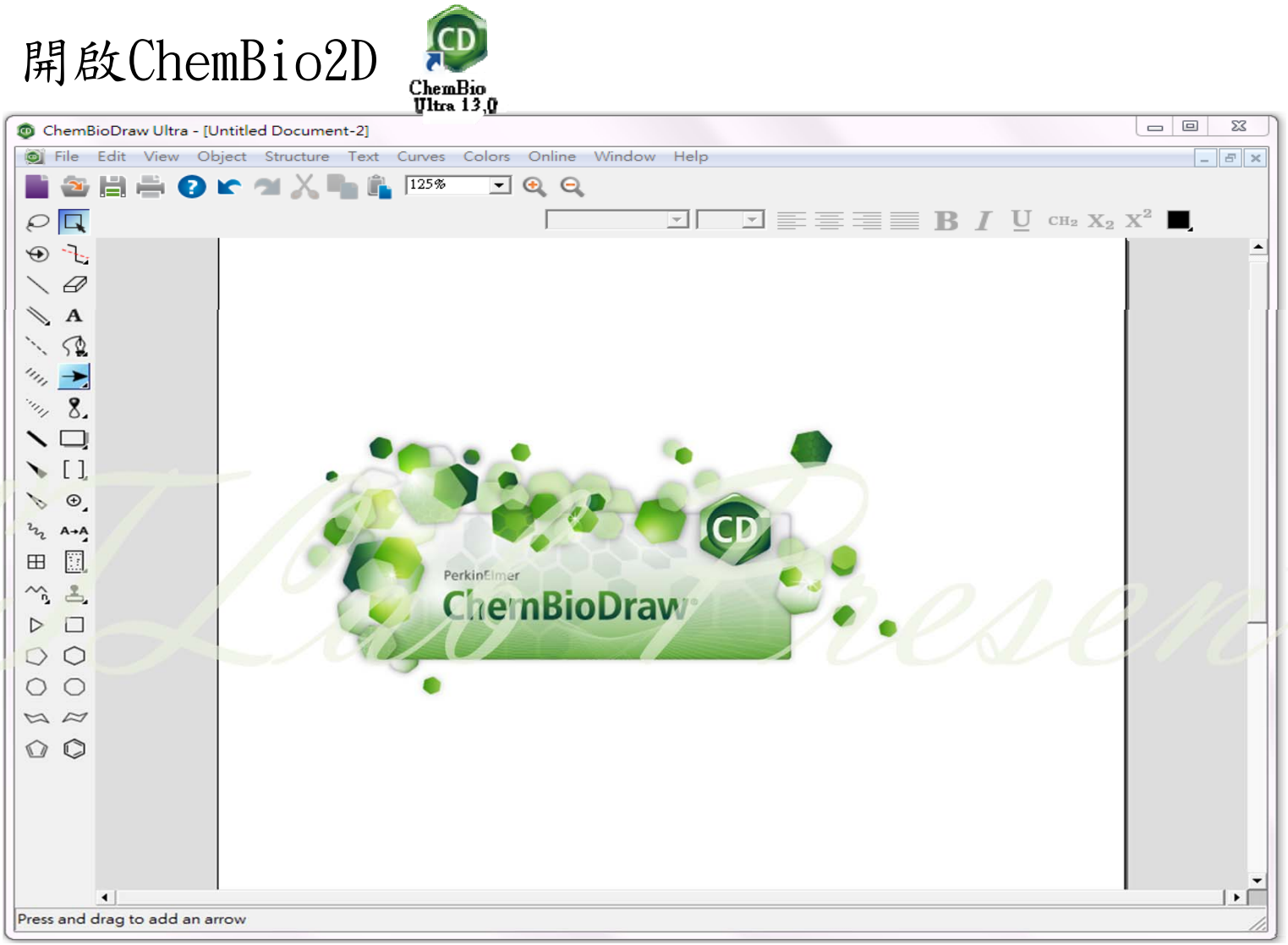




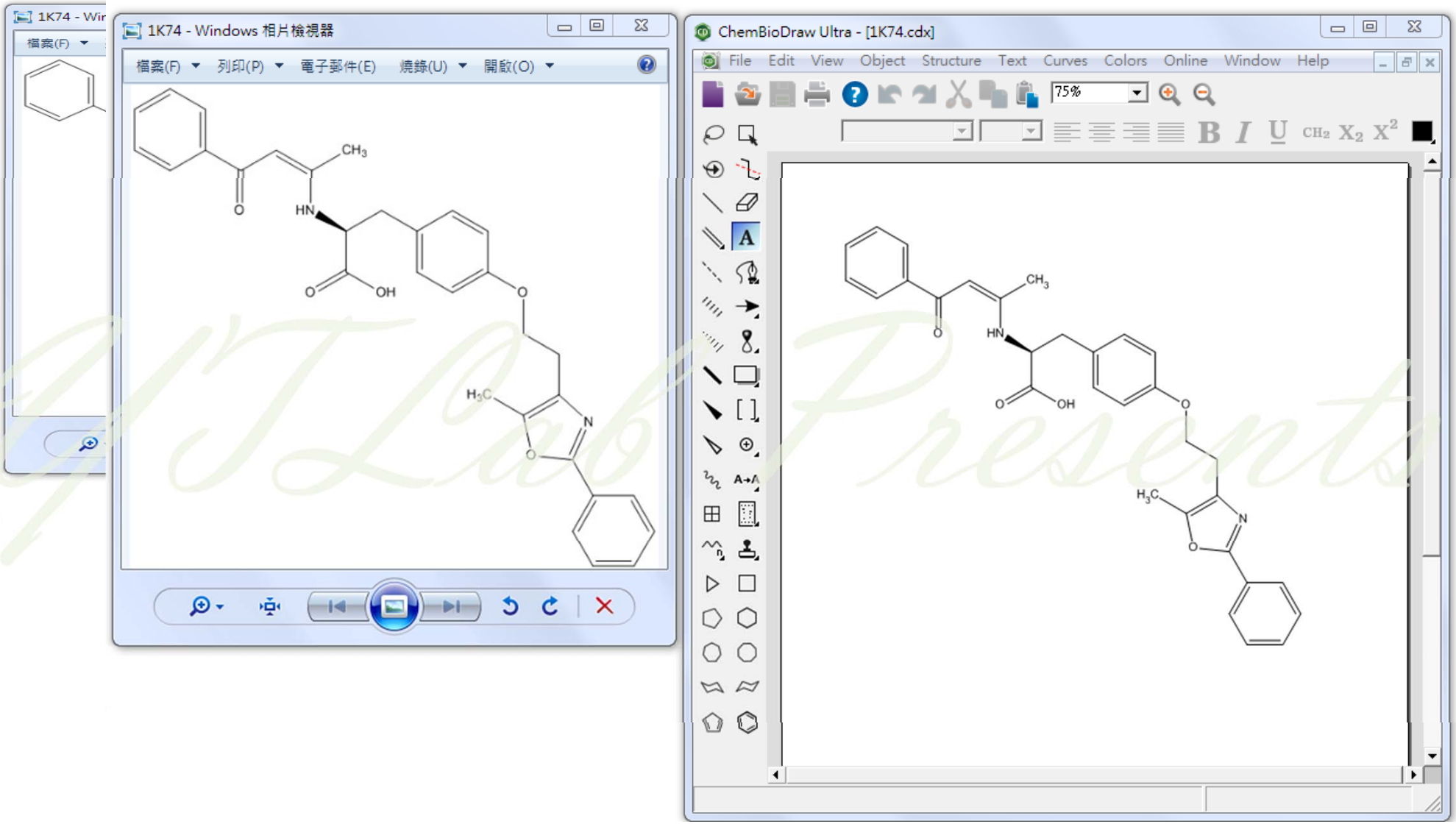


安裝完畢!

開啟ChemBio2D



依樣畫葫蘆


1K74 - Windows 相片檢視器
檔案(F) 列印(P) 電子郵件(E) 燒錄(U) 開啟(O)
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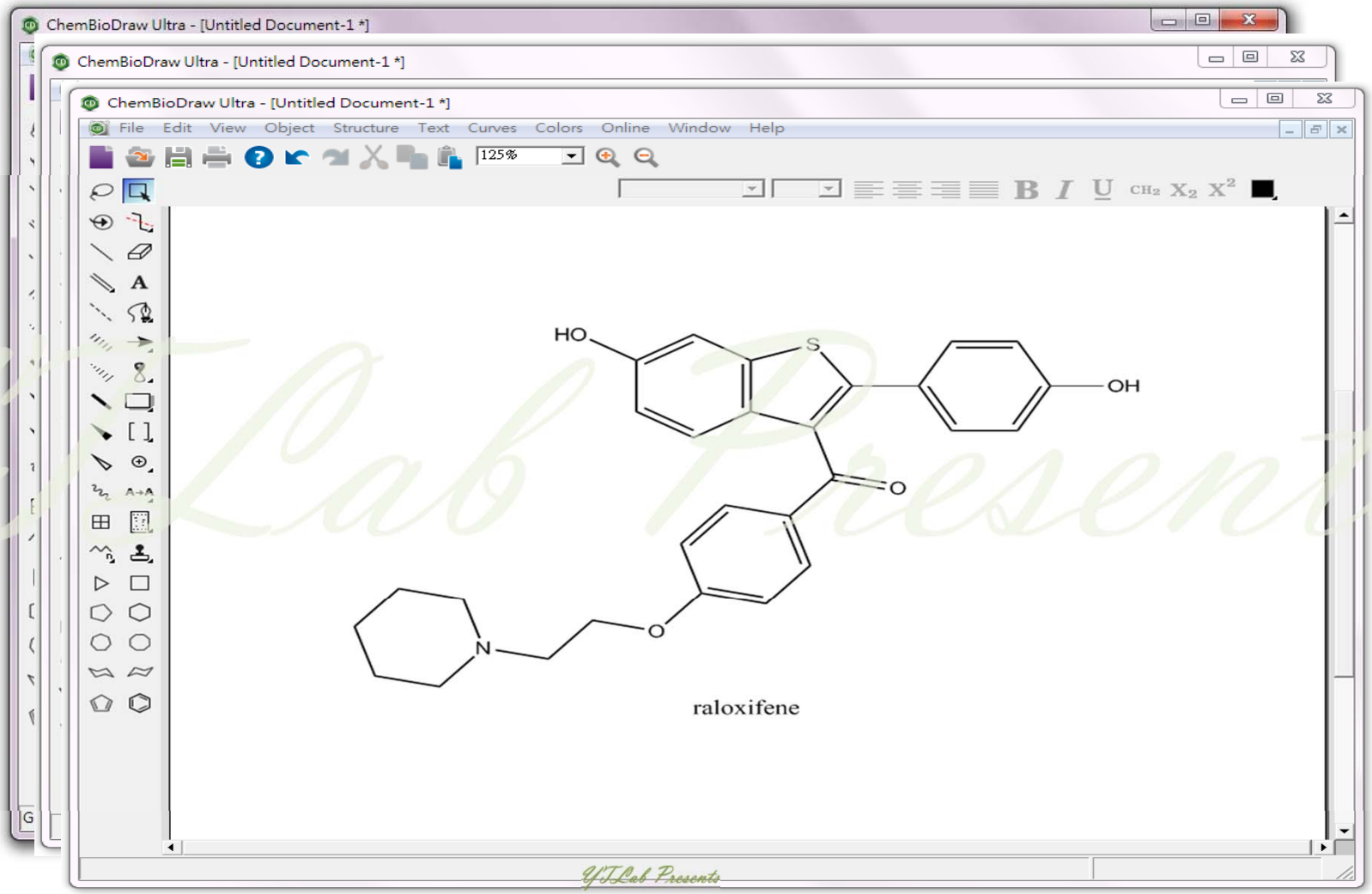
File Edit View Object Structure Text Curves Colors Online Window Help
75%

Structure➔ name to structure



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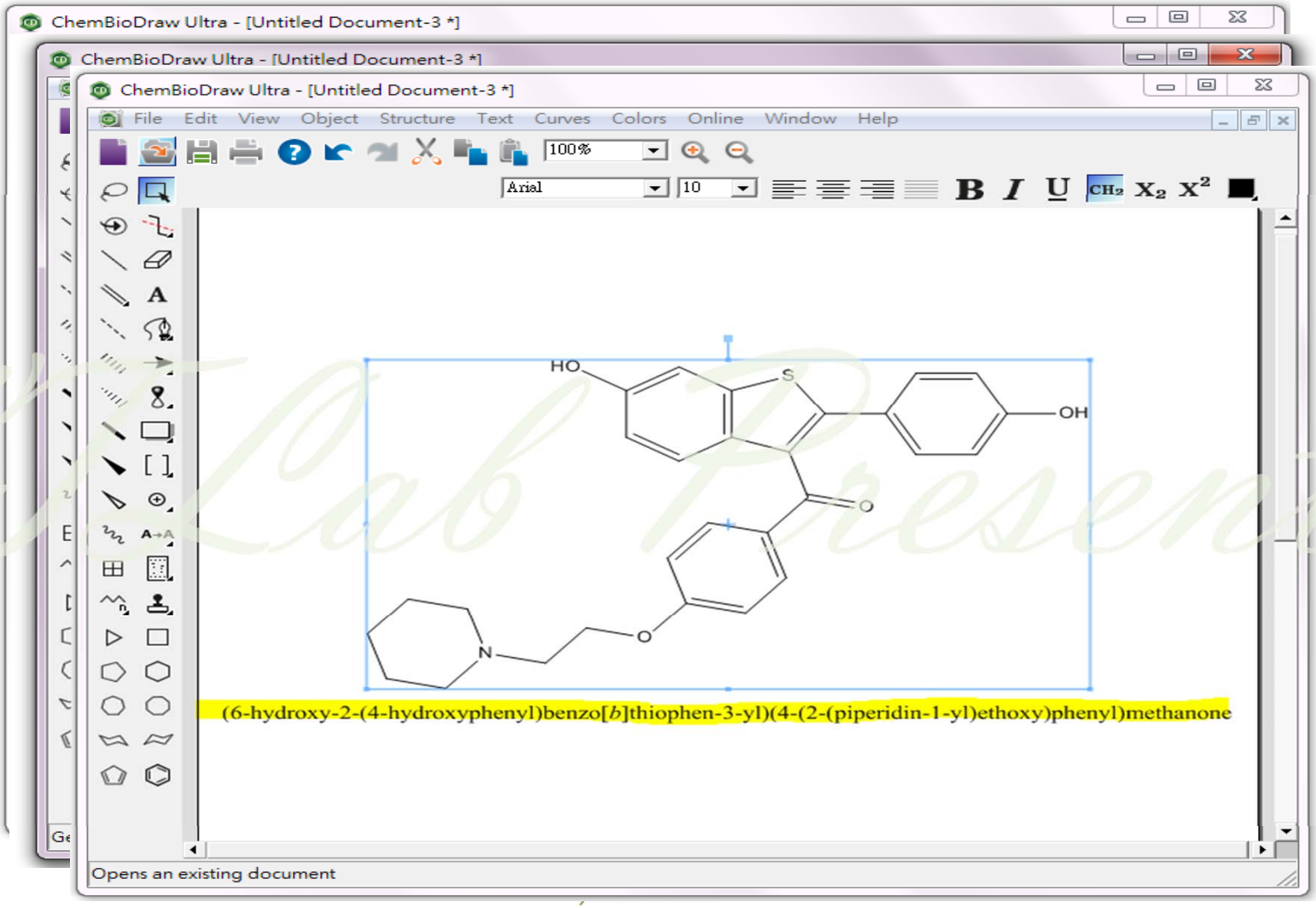
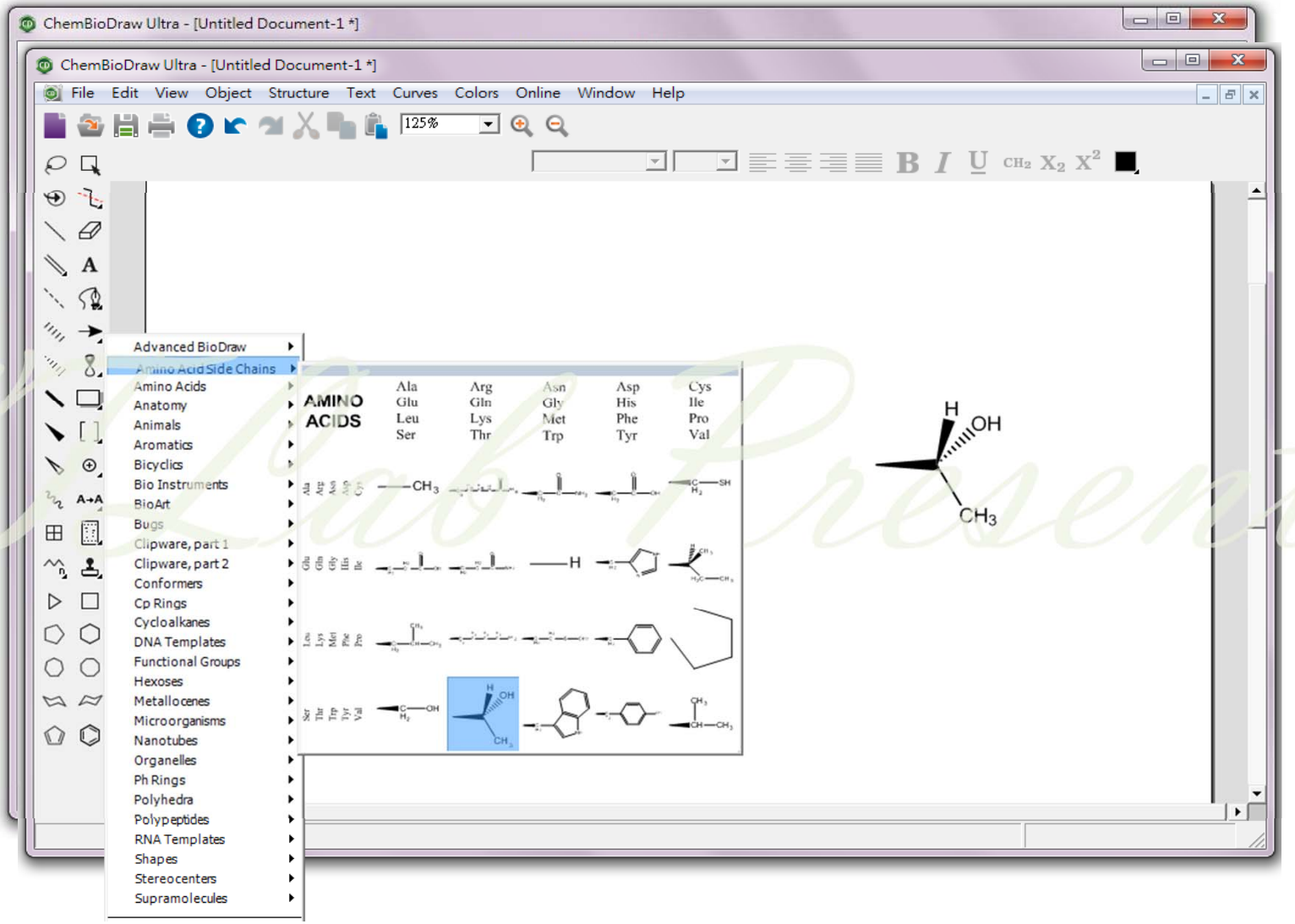
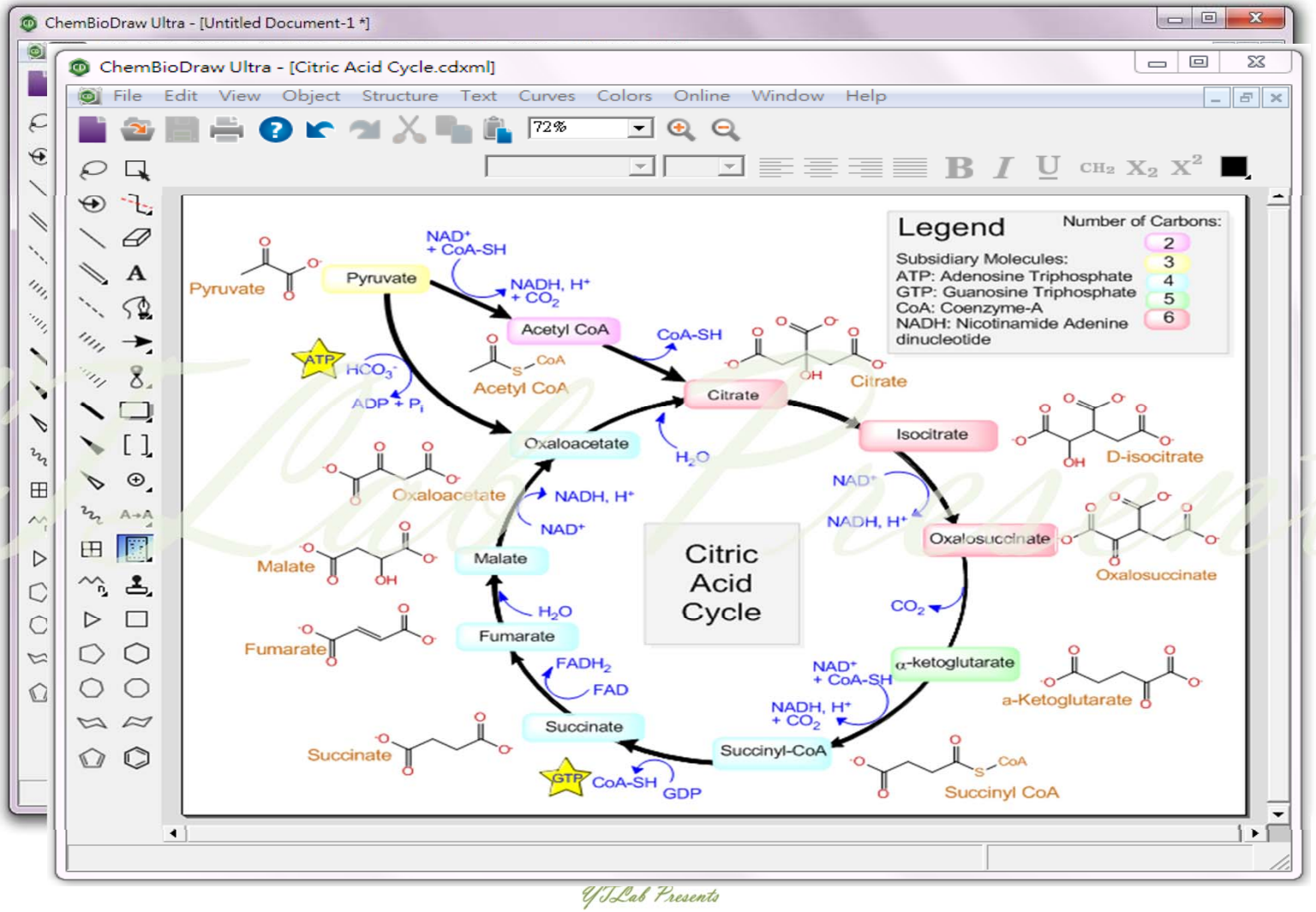


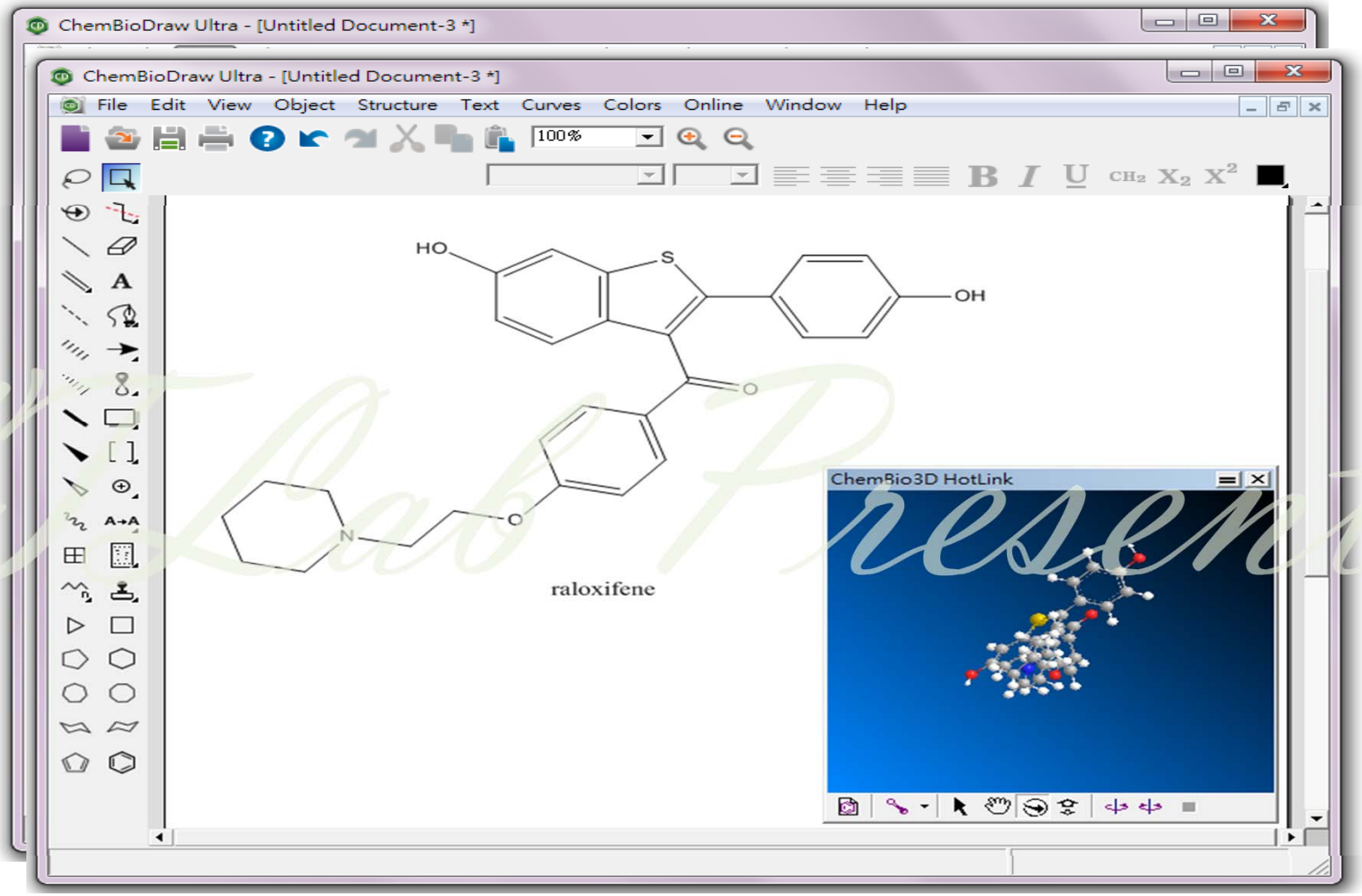
Templates


ChemBioDraw Ultra - [Untitled Document-1 *]
File Edit View Object Structure Text Curves Colors Online Window Help
125%
Advanced BioDraw
Amino Acid Side Chains
Amino Acids
Anatomy
Animals
Aromatics
Bicyclics
Bio Instruments
BioArt
Bugs
Clipware, part 1
Clipware, part 2
Conformers
Cp Rings
Cycloalkanes
DNA Templates
Functional Groups
Hexoses
Metallocenes
Microorganisms
Nanotubes
Organelles
Ph Rings
Polyhedra
Polypeptides
RNA Templates
Shapes
Stereocenters
Supramolecules
AMINO ACIDS
Ala Arg Asn Asp Cys
Glu Gln Gly His Ile
Leu Lys Met Phe Pro
Ser Thr Trp Tyr Val
H
OH
CH3

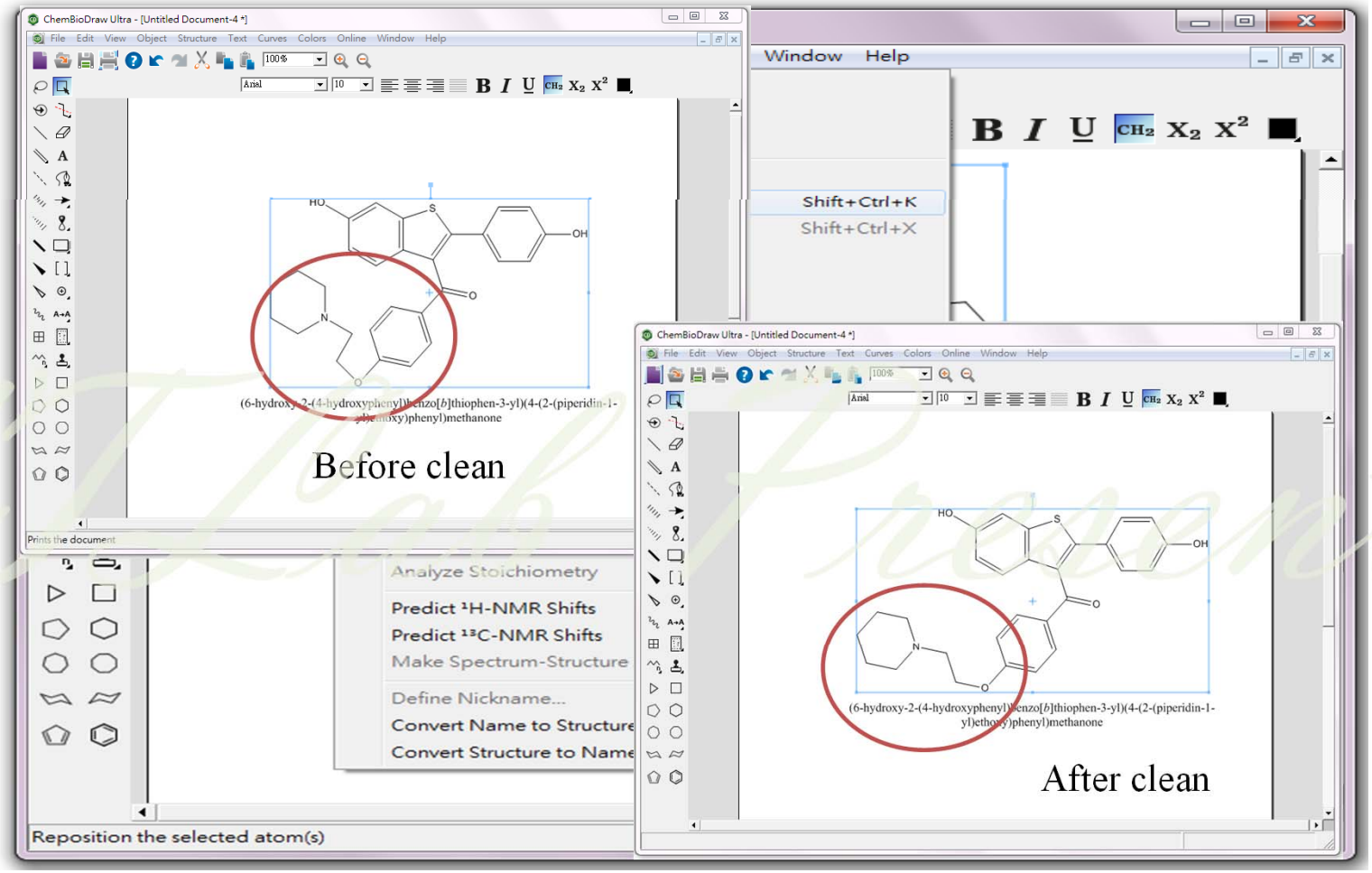
sample　　舉手加分:請試著說明citric acid cycle



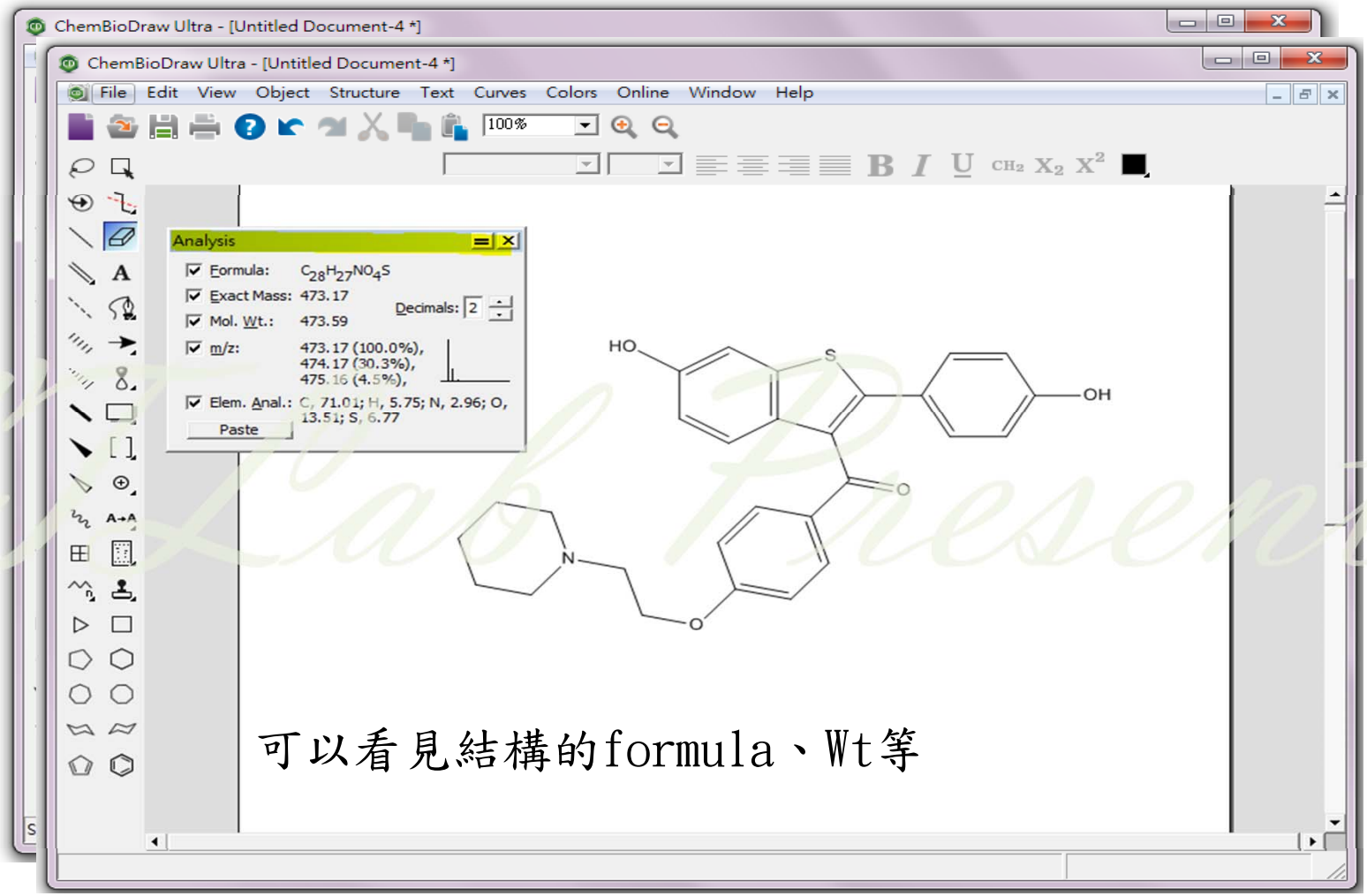
Chem3D Preview



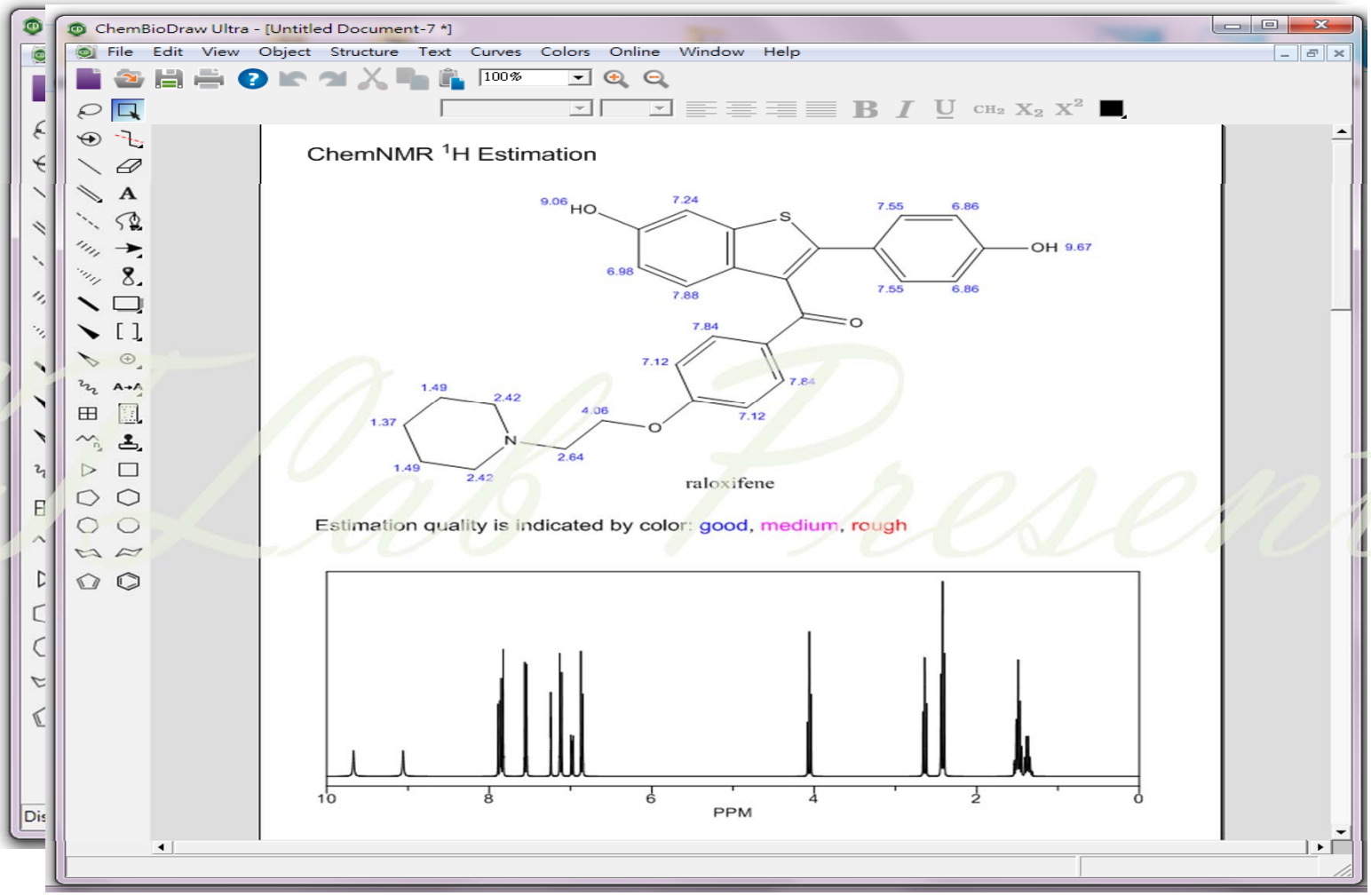
Structure ➔ clean up structure



Analysis window



Structure ➔ predict H-NMR Shifts



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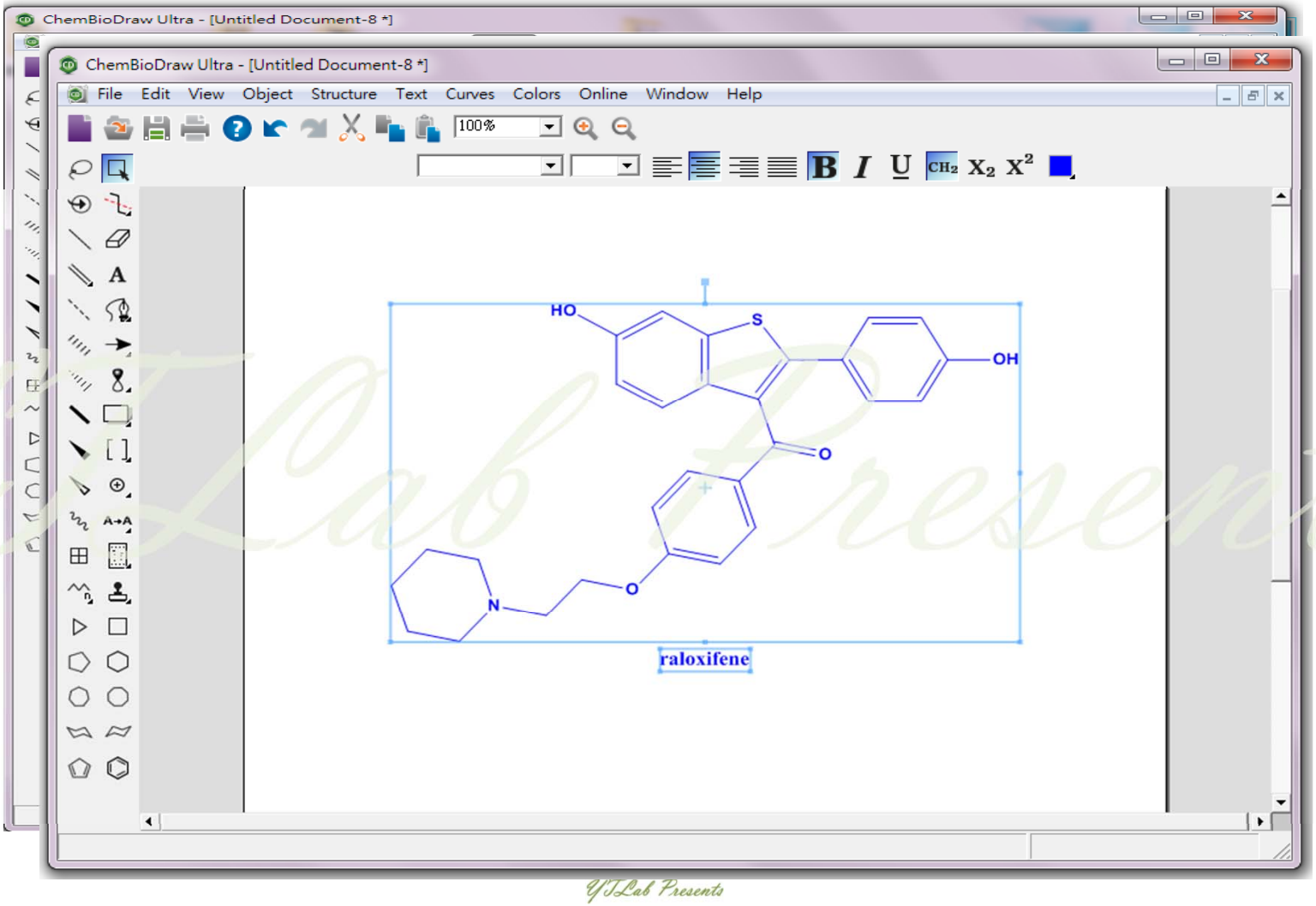
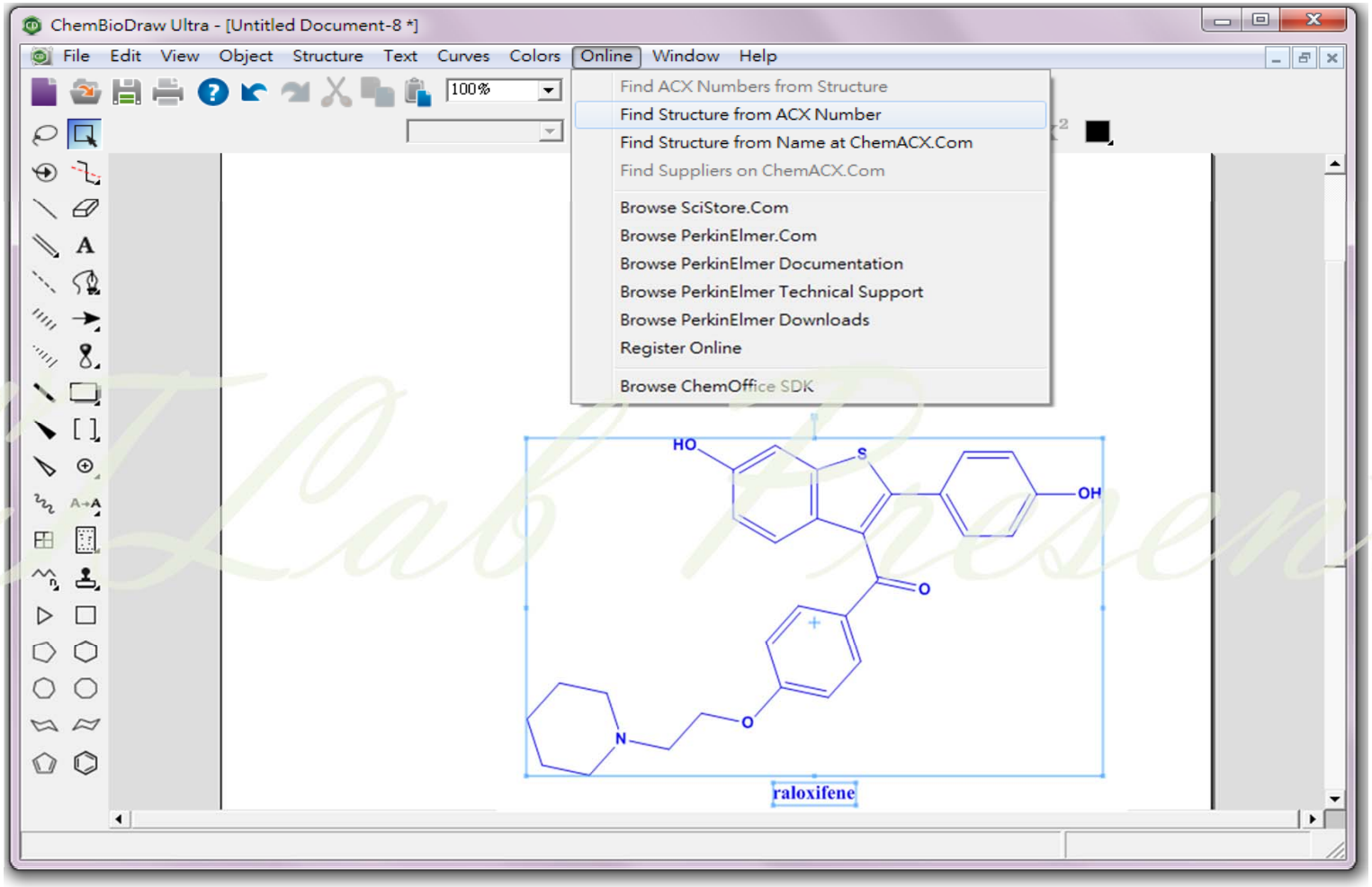
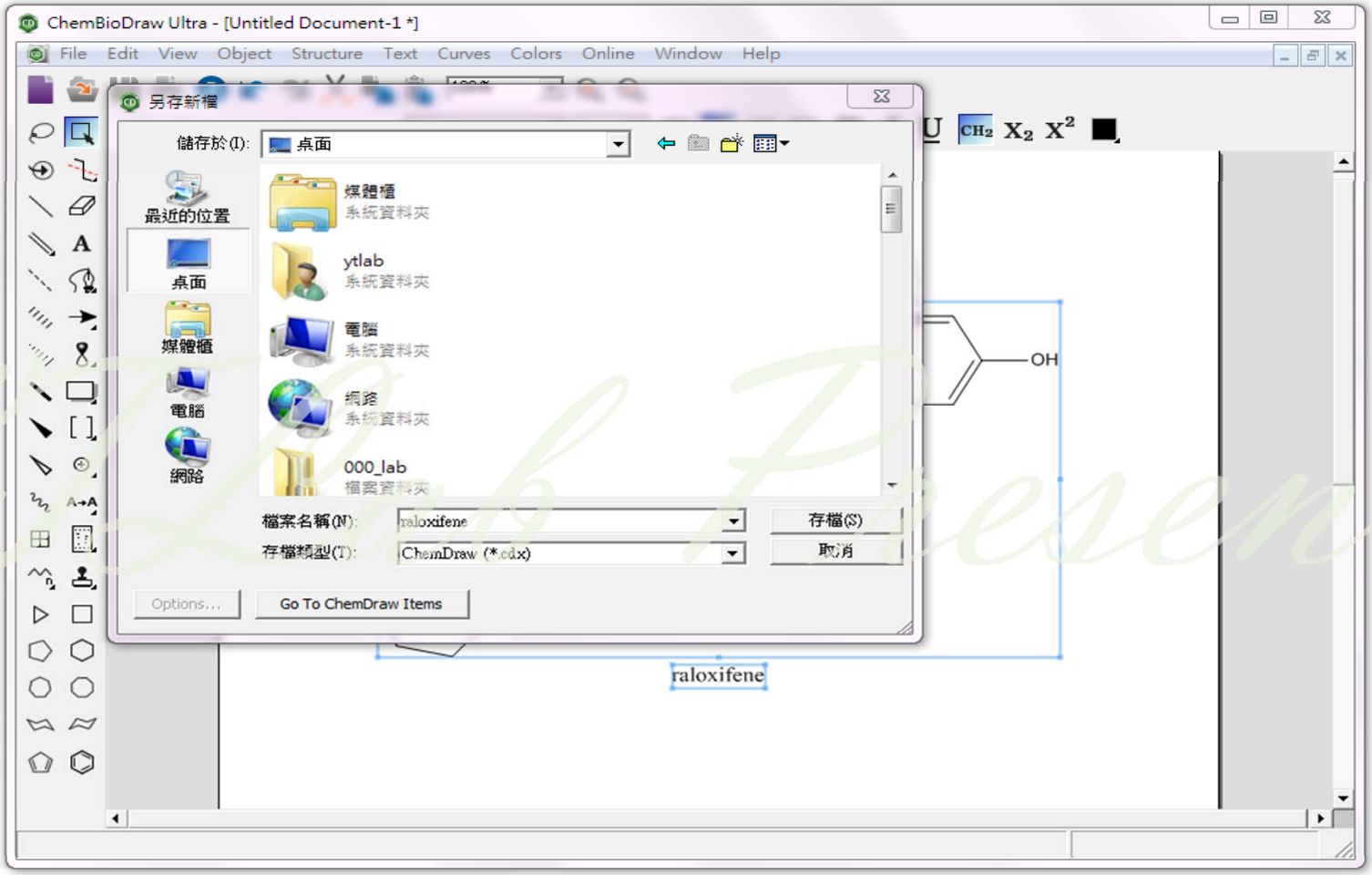


Online=> Find Structure from ACX Number



Save as➔ 選取.cdx檔

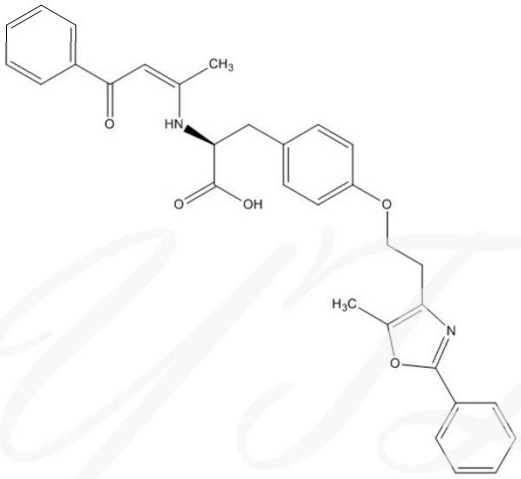


Experment 1：

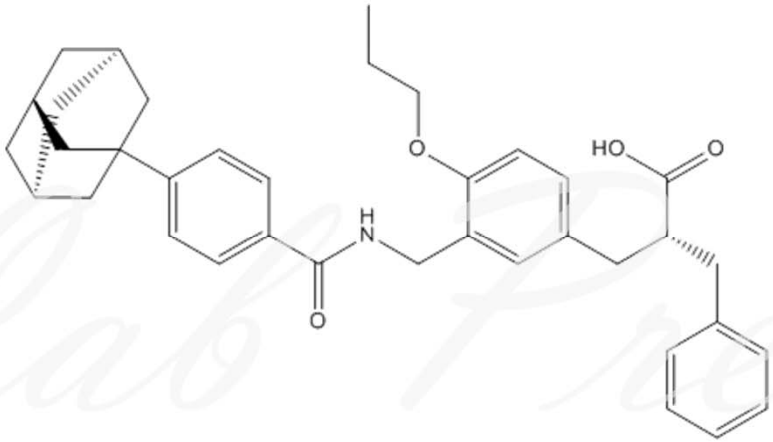
以ChemDraw畫出下列三種Group(共九個)，

並標記其化合物ID，存檔(.cdx)以備下星期上課使用。

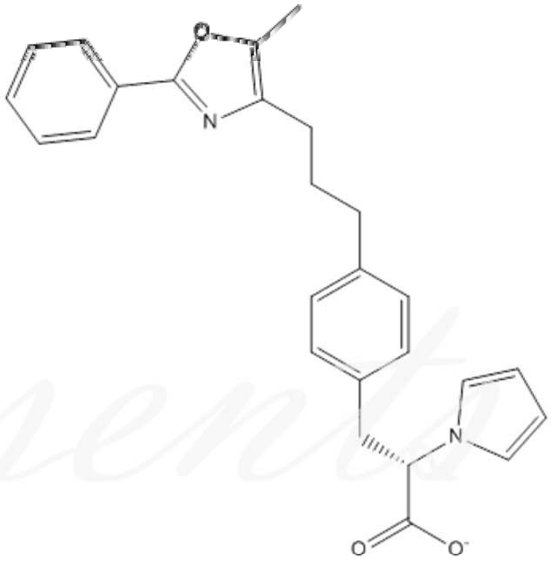
Group 1 :



1K74_L

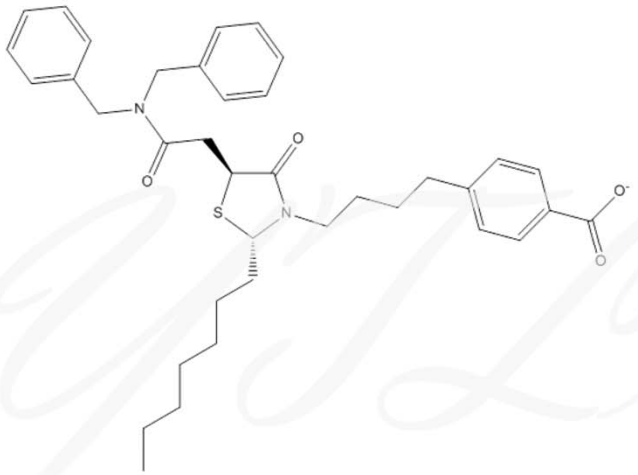


3AN4_L

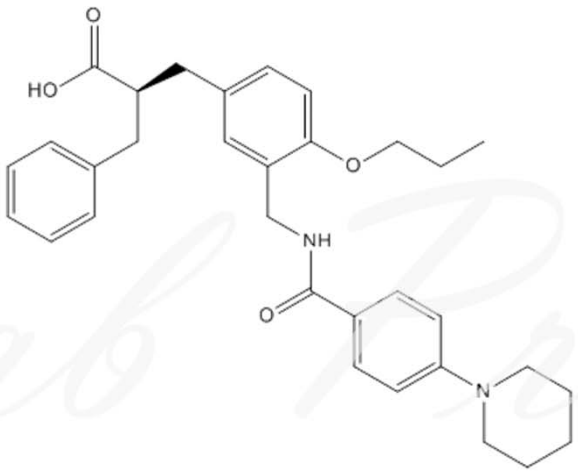


2Q8S_L

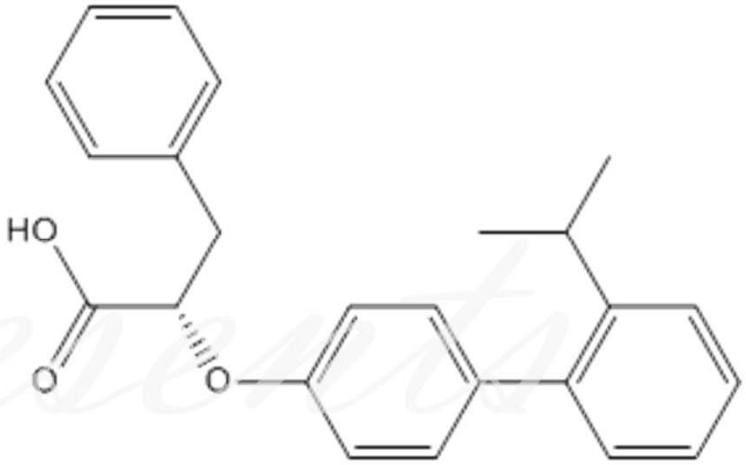
Group 2 :



4PRG_L

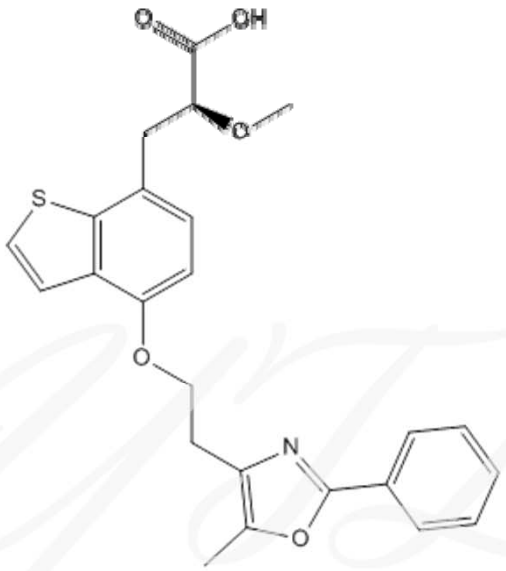


3VSP_L

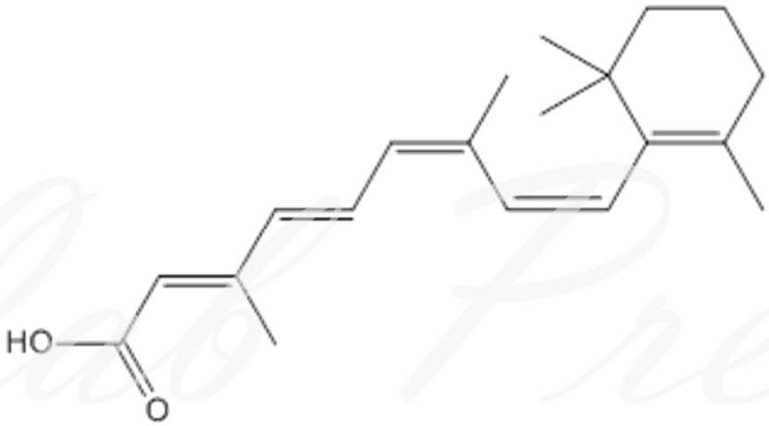


4E4K_L

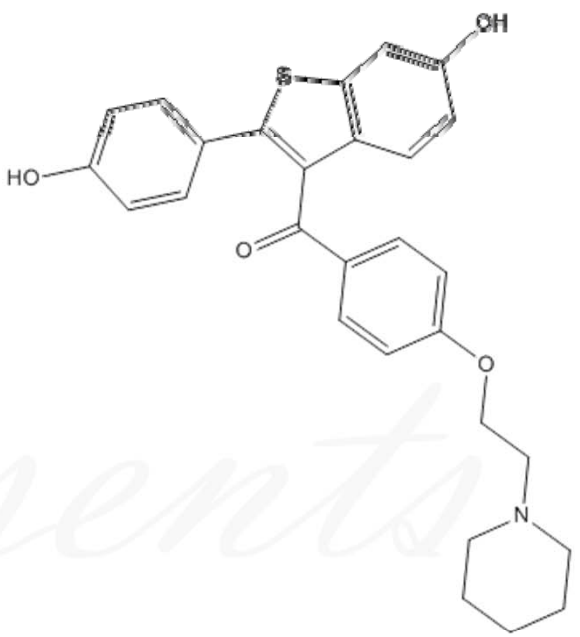
Group 3 :



3G8I_L



3DZU_L



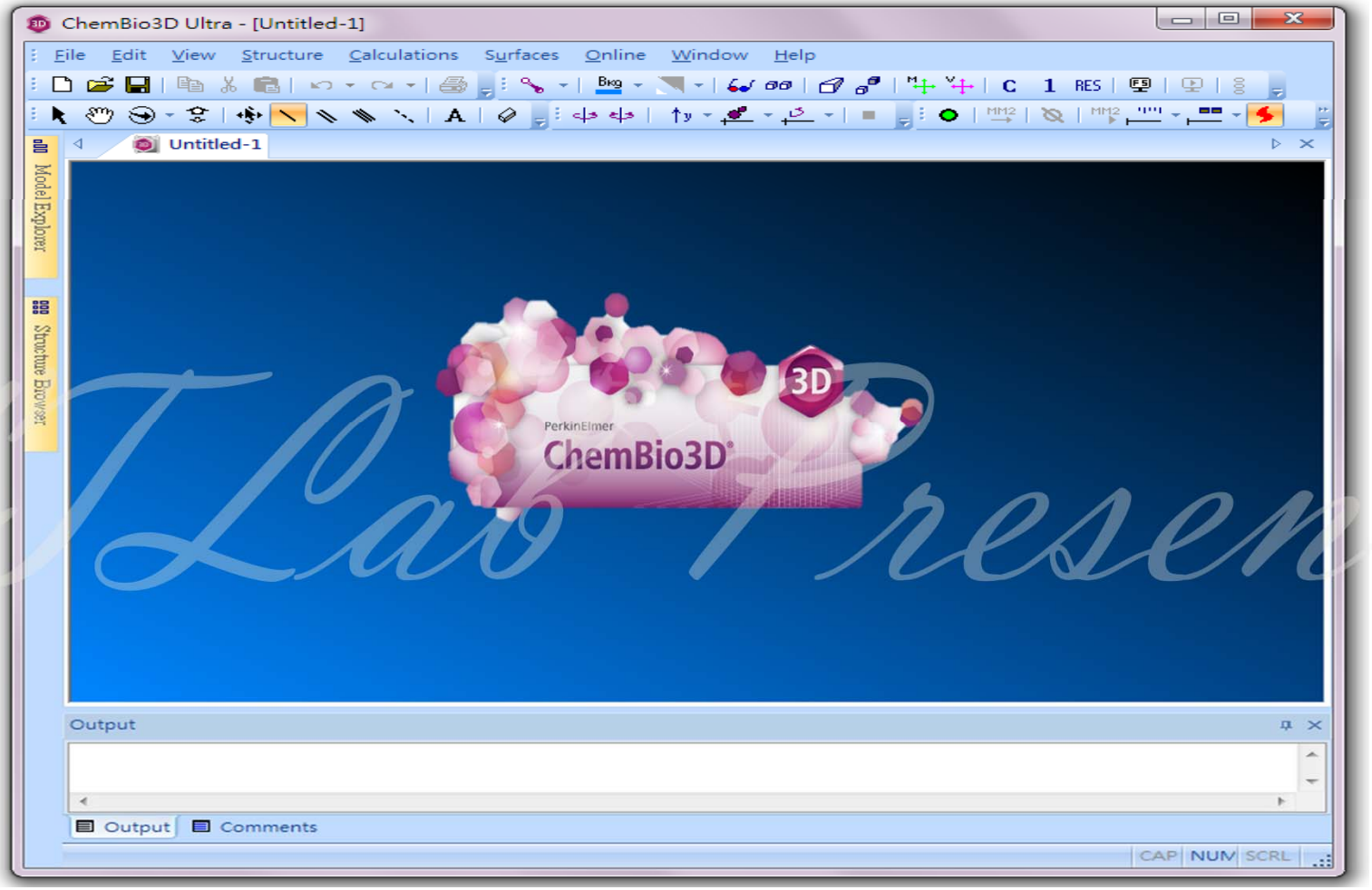
1QKN_L

開一個目錄到桌面上

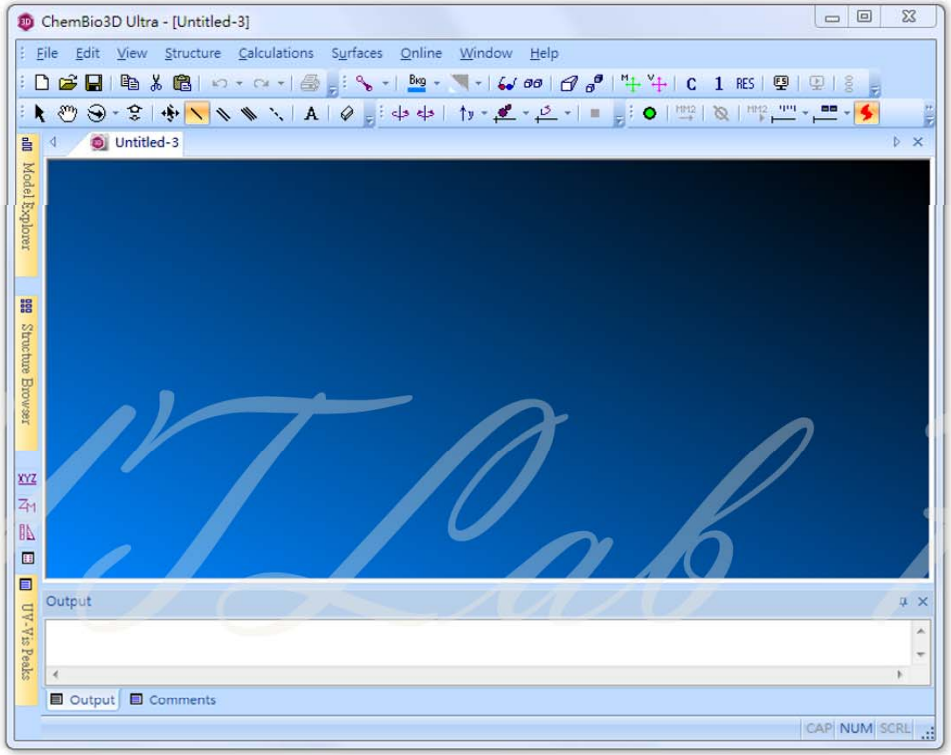
- 目錄名稱:
  (例) 20171012_MolecularDockingI_1060220168_林盈廷_01

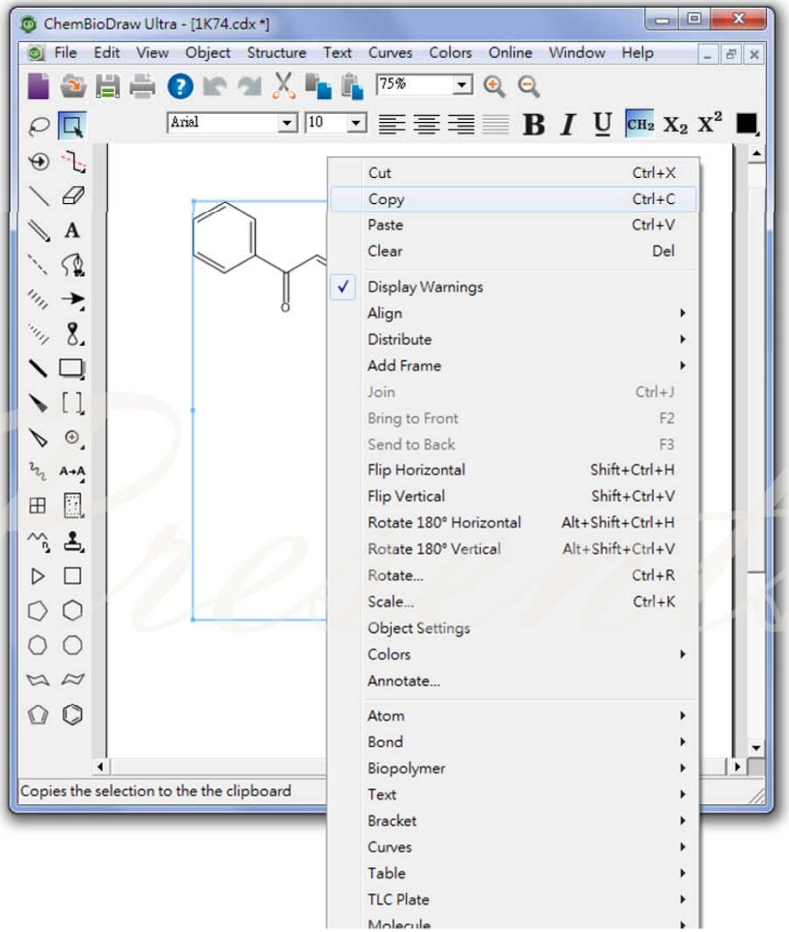
所有實驗用檔案 cdx, mol, word 放進去;
用來交今日實驗報告

開啟Chem3D

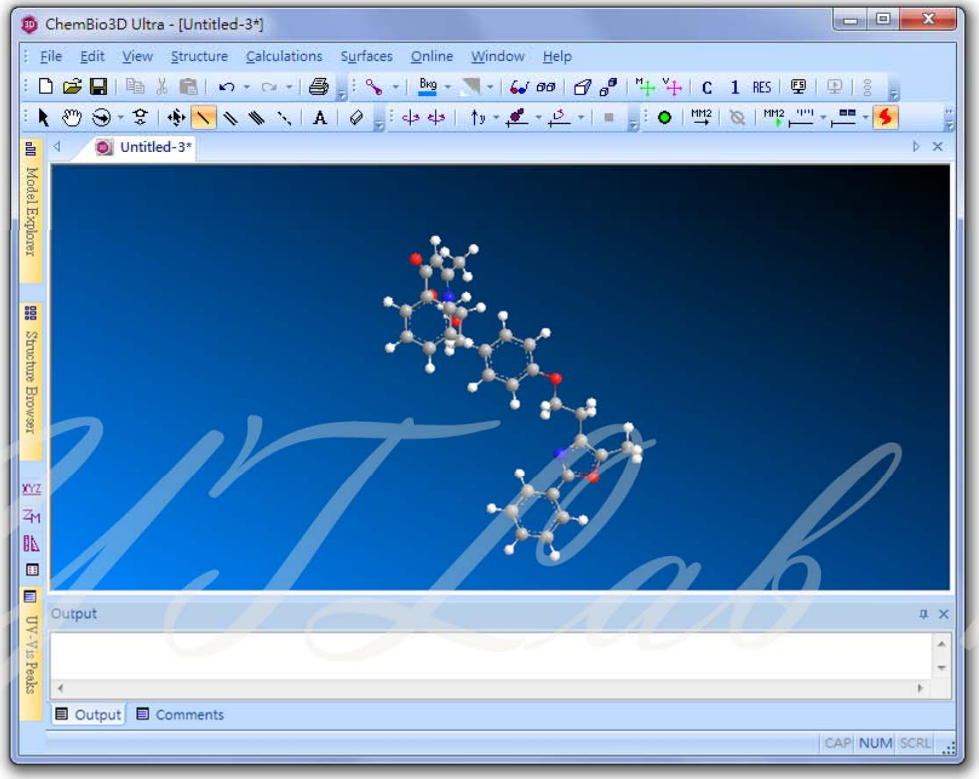


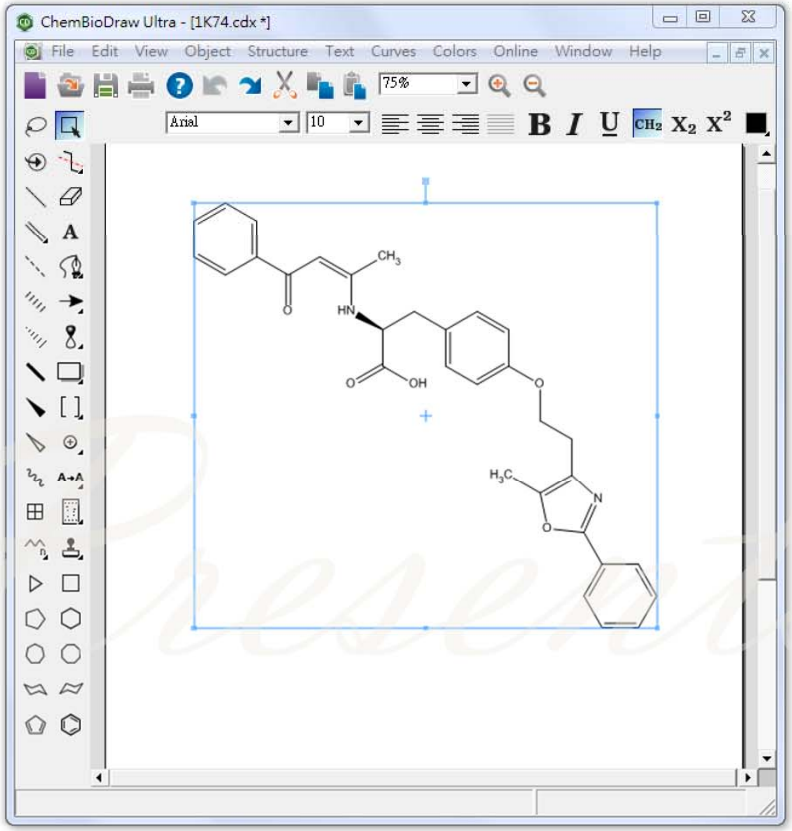
將化合物copy進Chem3D



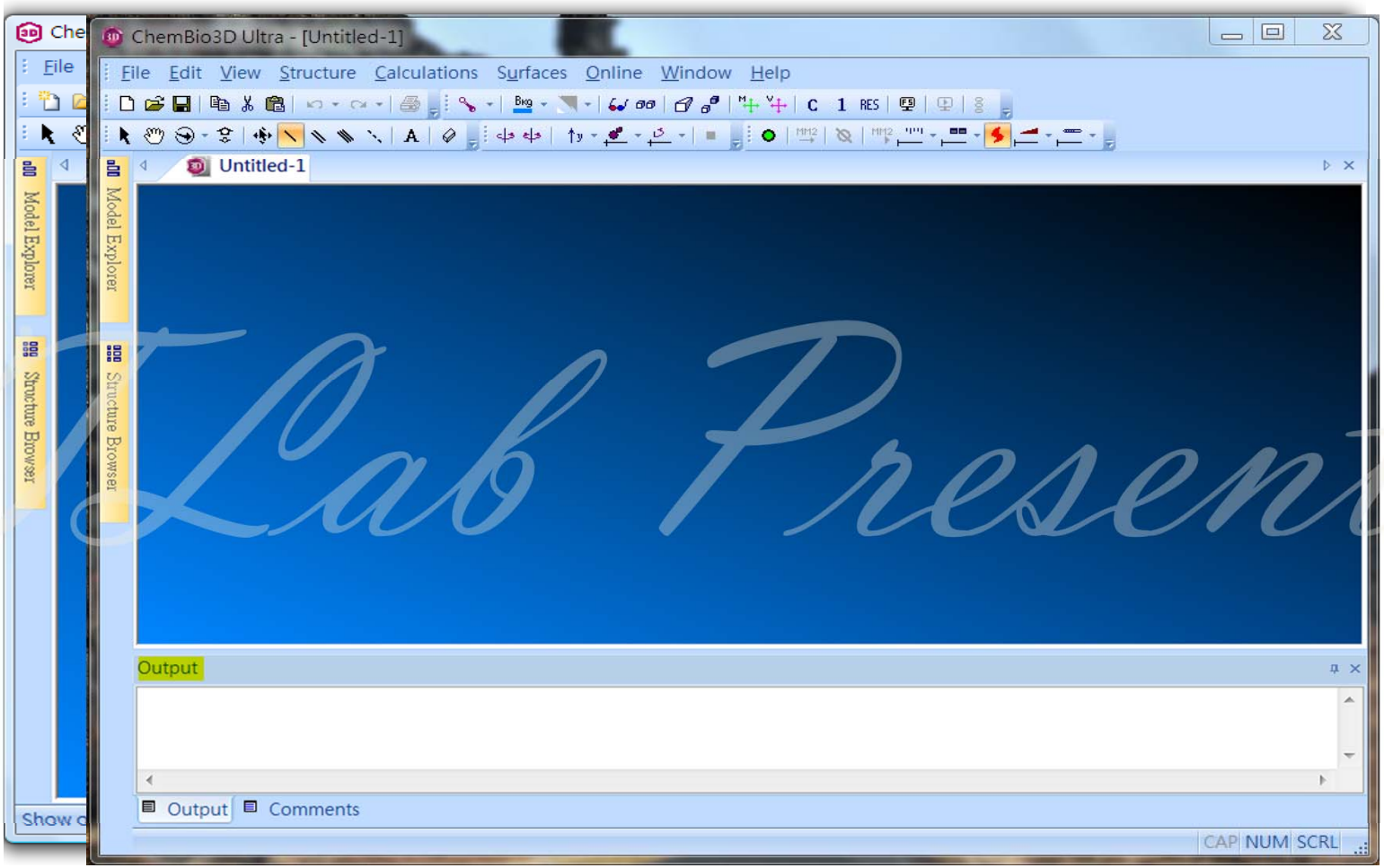


將化合物copy進Chem3D

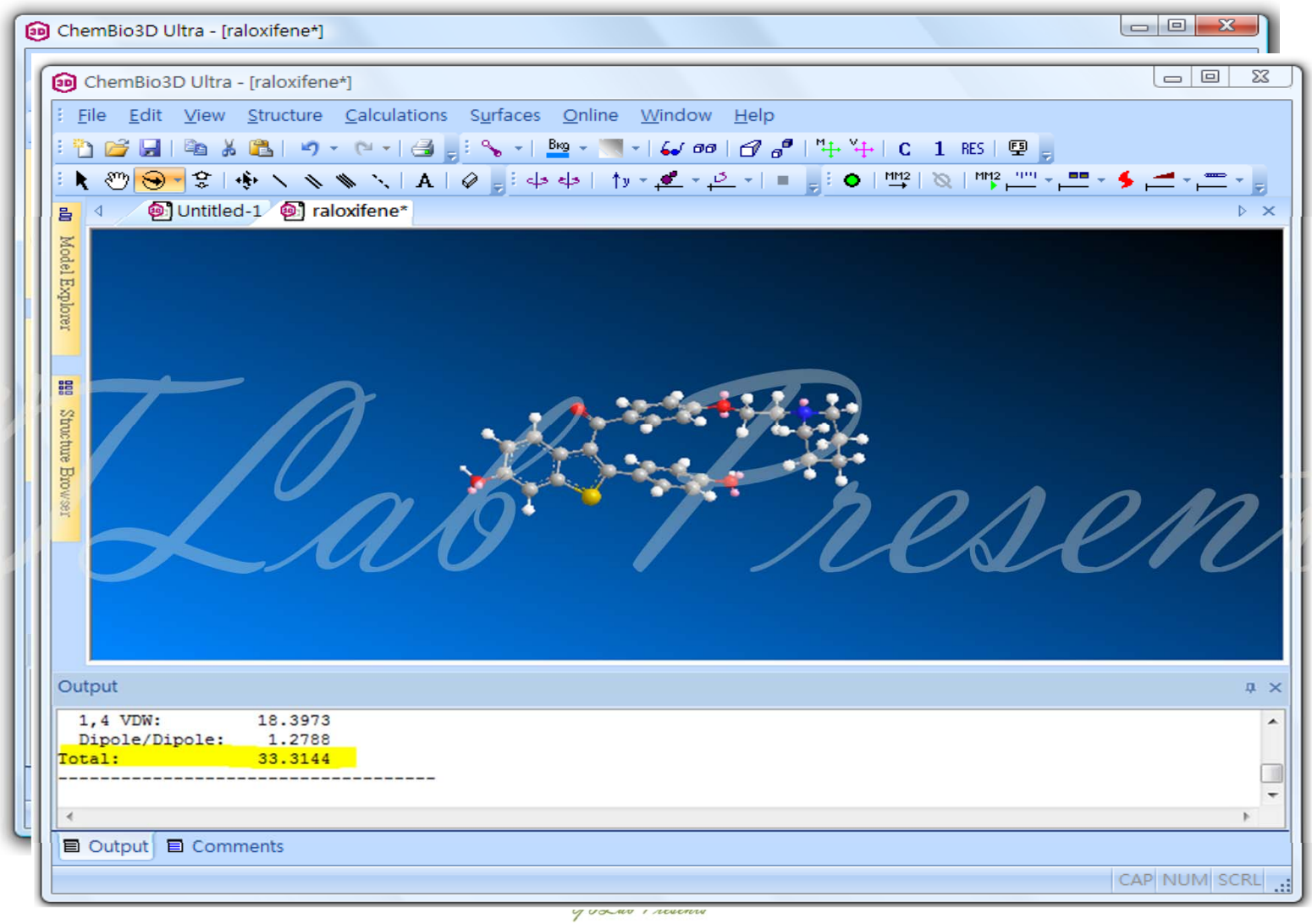




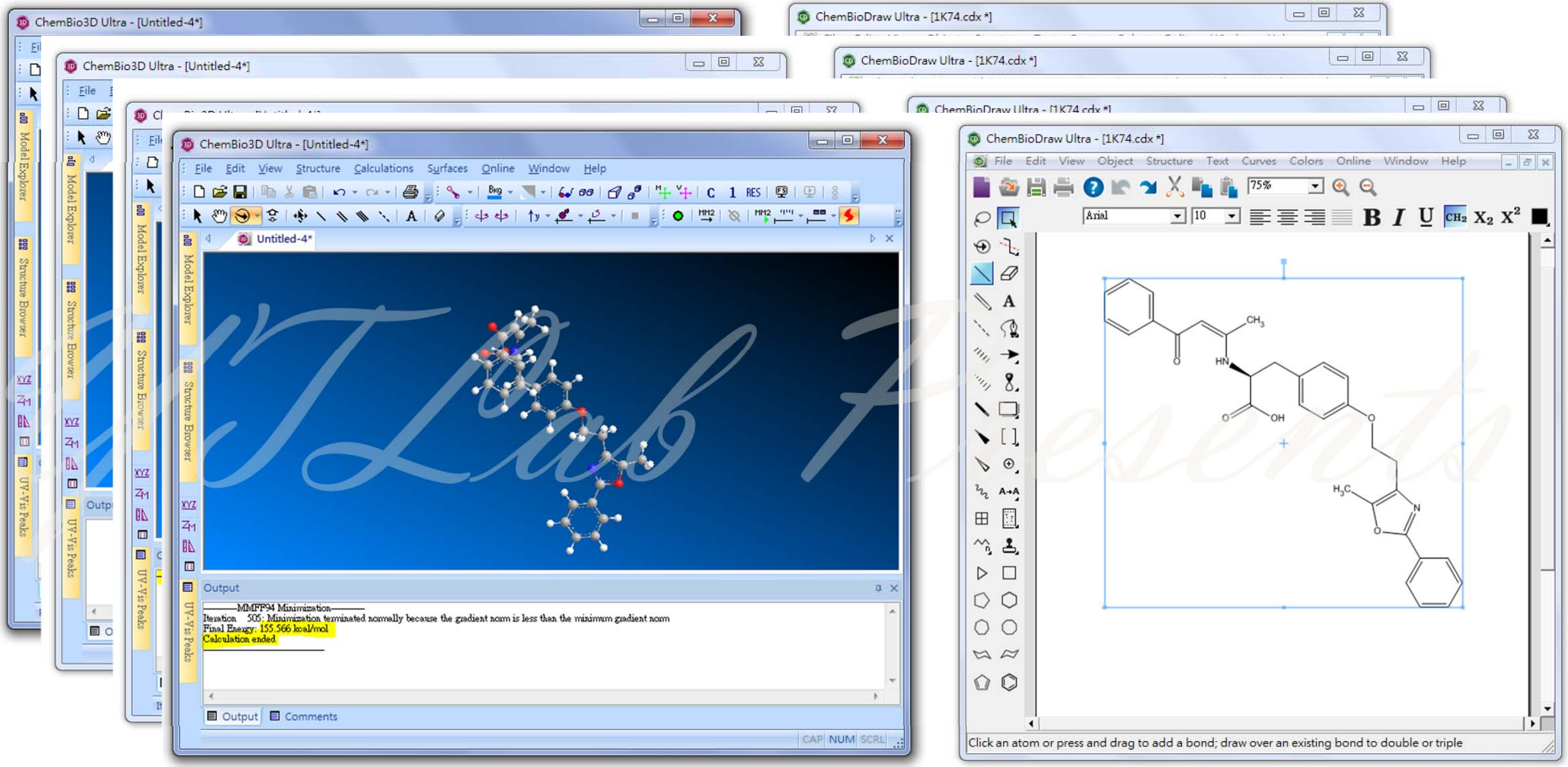
選取 View中 Output Box



MM2 Minimize



MMFF94 Minimize



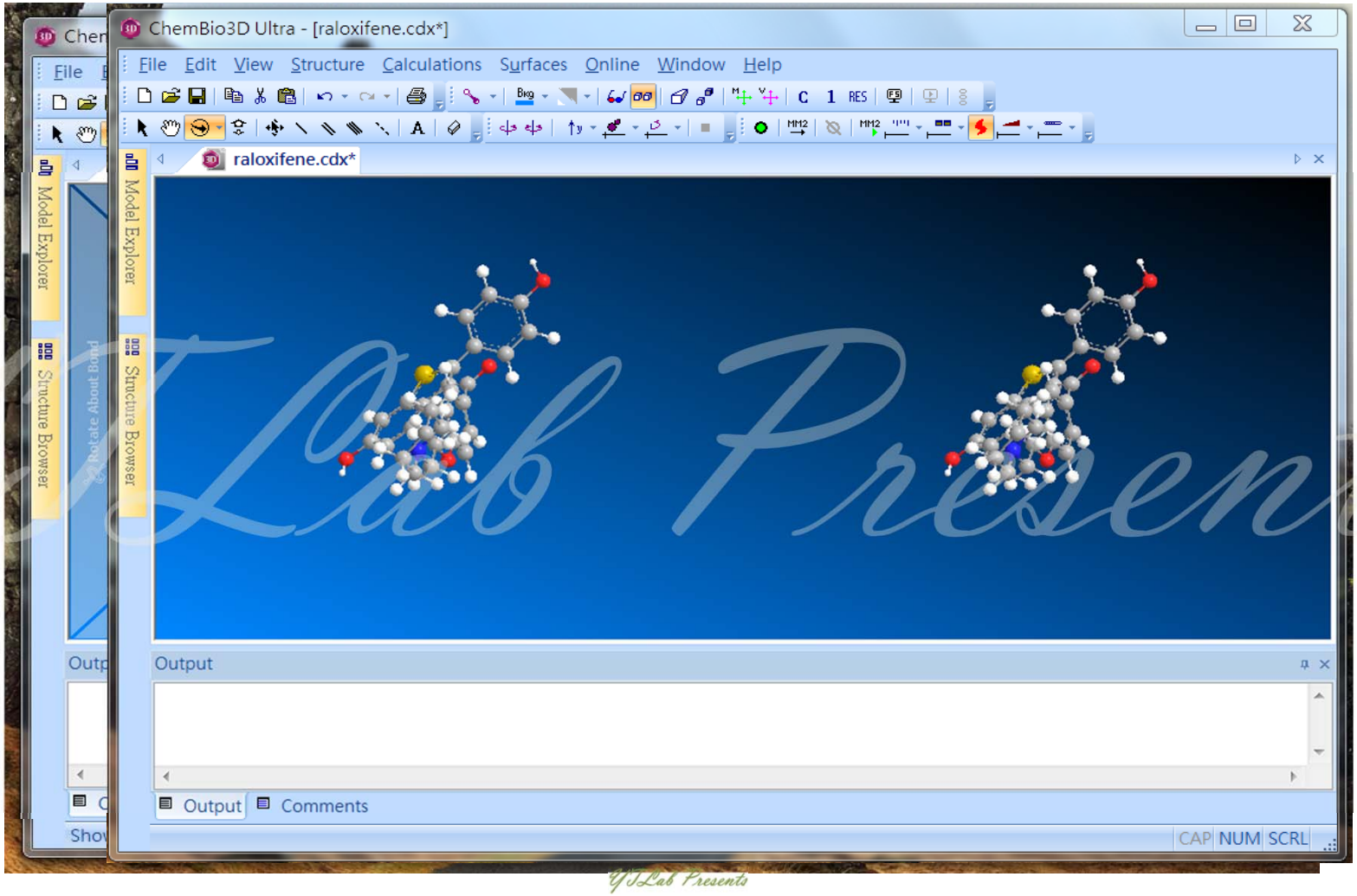
Molecular mechanics

http://en.wikipedia.org/wiki/Molecular_mechanics

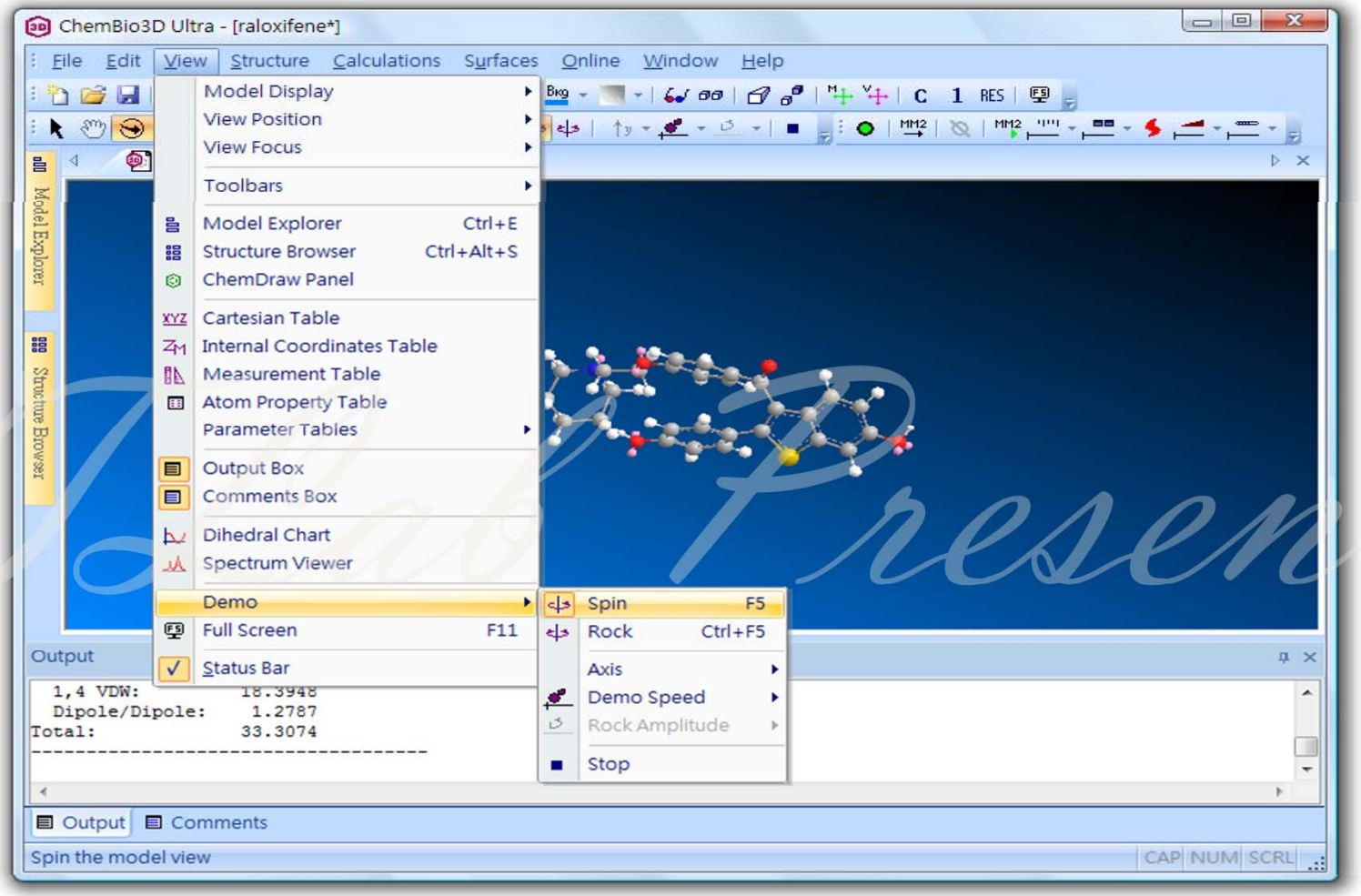
Molecular dynamics

http://en.wikipedia.org/wiki/Molecular_dynamics

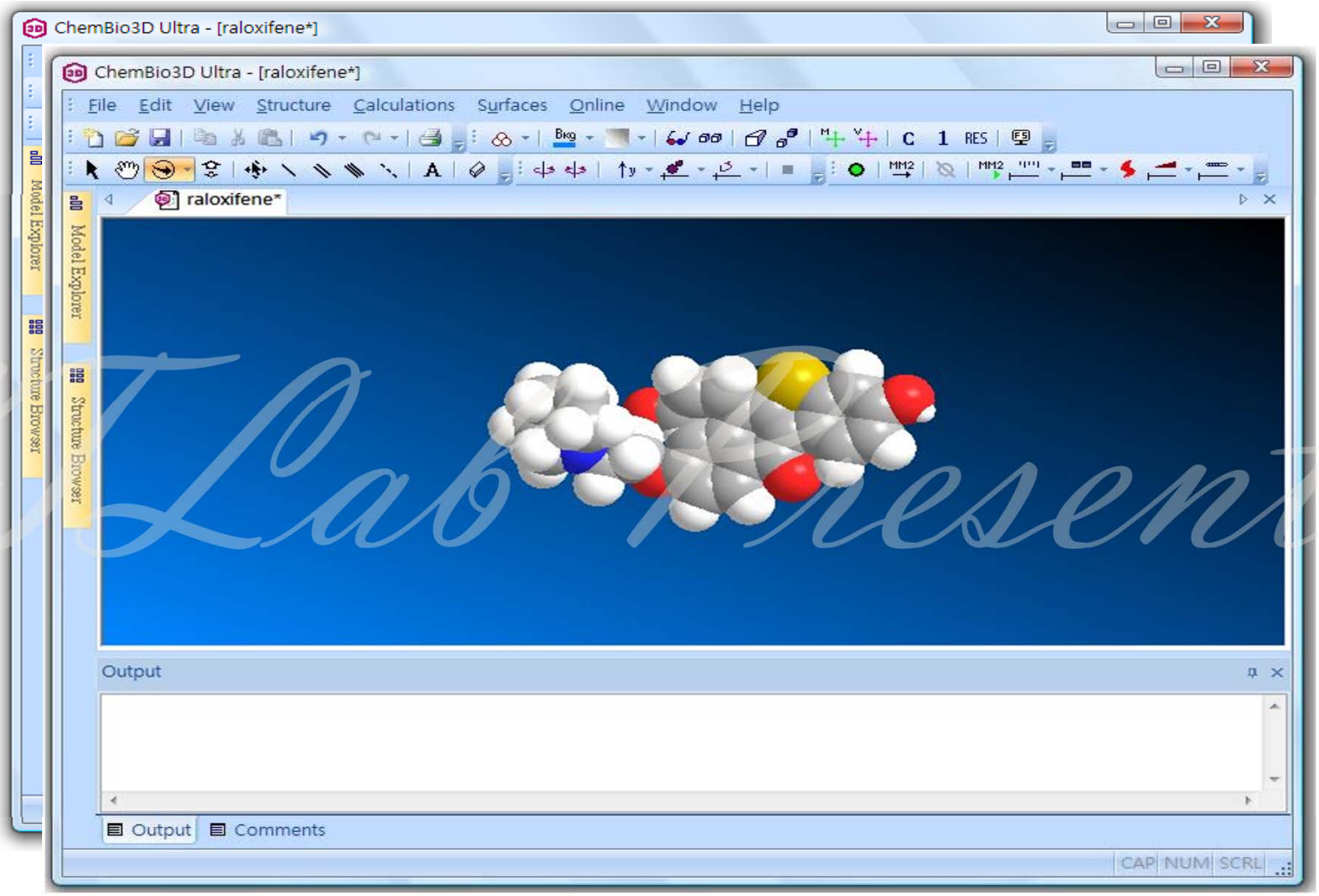
Stereo➔嘗試用鬥雞眼看出立體結構



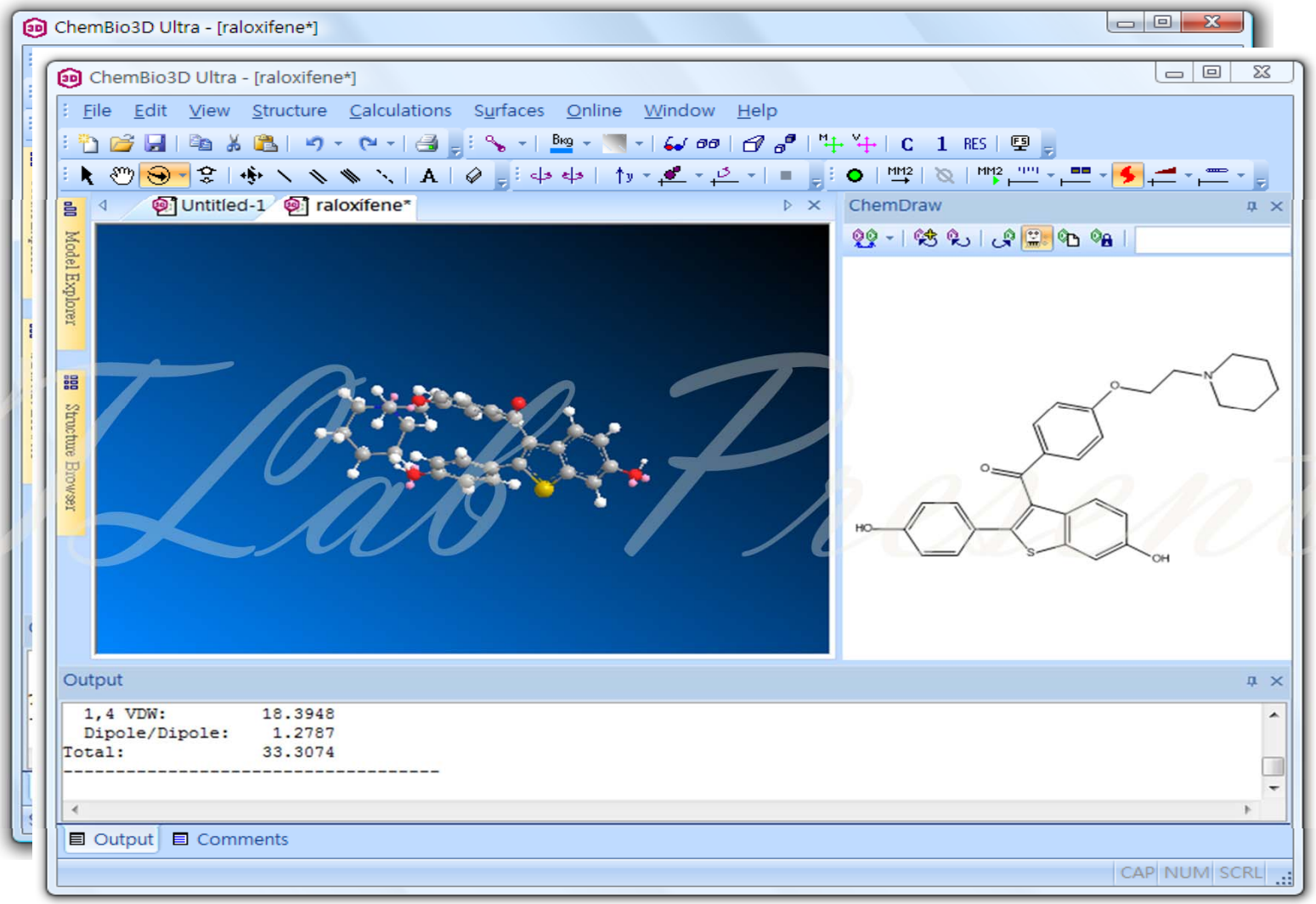
View➔Demo=>Spin



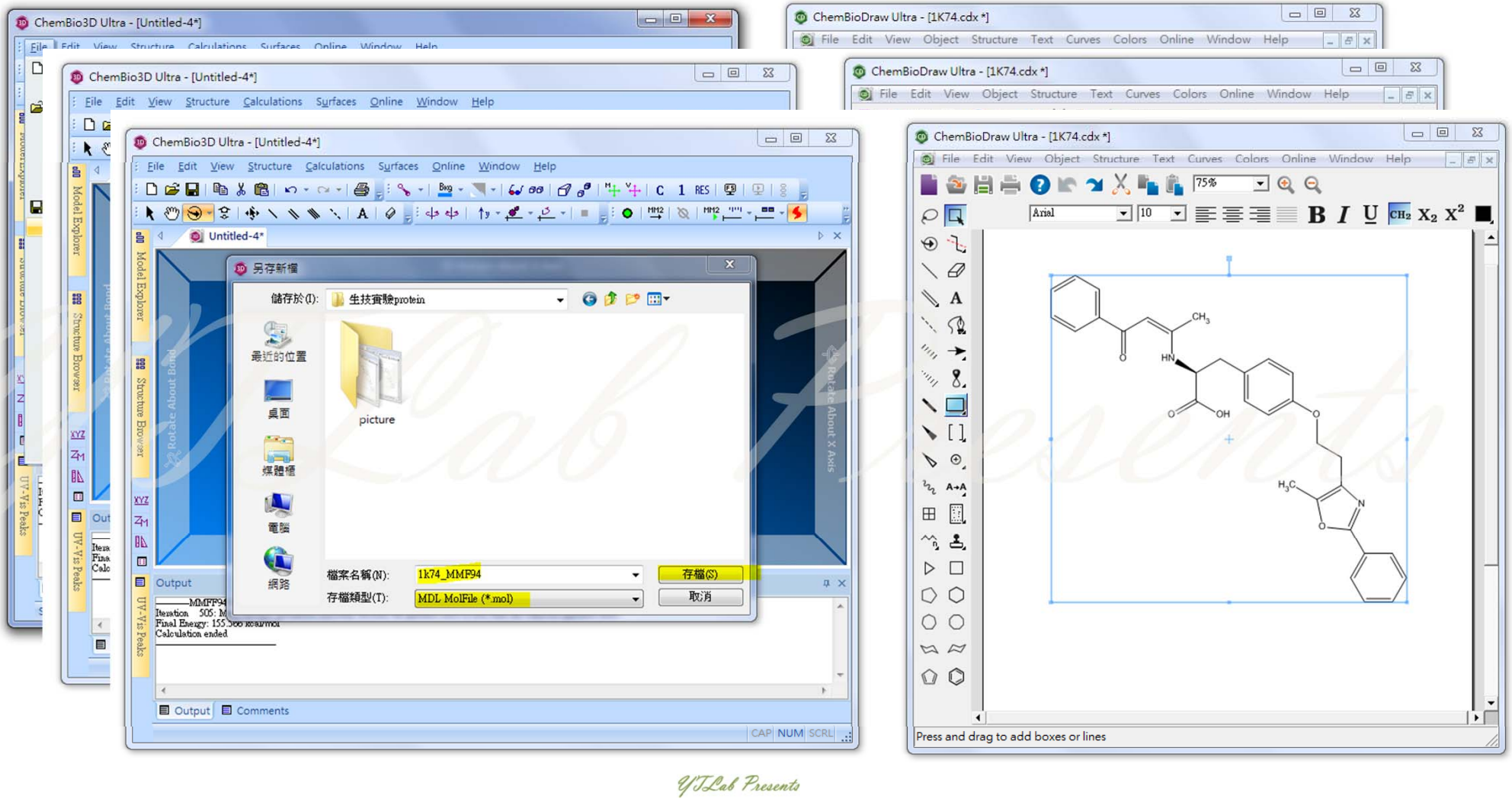
Display Mode



View ➔ ChemDraw Panel



Save as➔ 選取.mol檔



Experment 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.