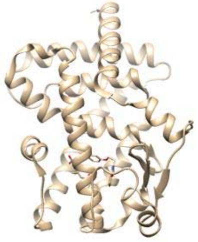
Biotechnology
Kaohsiung Medical University
高雄醫學大學 生物科技學系

生物科技實驗



分子入塢 — （II）準備大分子

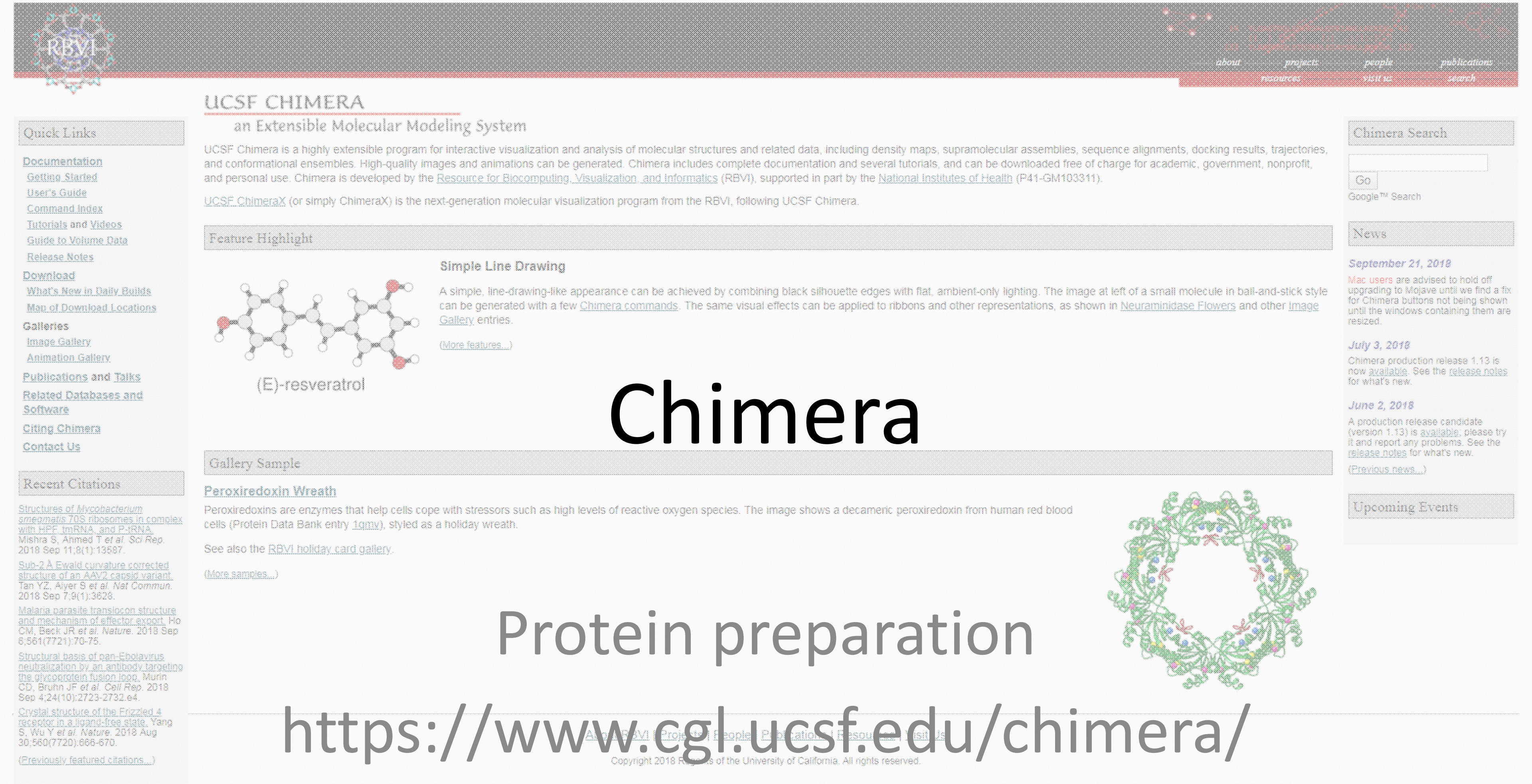
林盈廷副教授
實驗室：第一教學大樓 N1025室
Tel: (07) 3121101 ext. 2792
eMail：ytlin@kmu.edu.tw

YTLab Presents

Chimera

Protein preparation

https://www.cgl.ucsf.edu/chimera/



UCSF CHIMERA

an Extensible Molecular Modeling System

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, nonprofit, and personal use. Chimera is developed by the Resource for Biocomputing, Visualization, and Informatics (RBVI), supported in part by the National Institutes of Health (P41-GM103311).

UCSF ChimeraX (or simply ChimeraX) is the next-generation molecular visualization program from the RBVI, following UCSF Chimera.

Quick Links

- Documentation
  - Getting Started
  - User's Guide
  - Command Index
  - Tutorials and Videos
  - Guide to Volume Data
  - Release Notes
- Download
  - What's New in Daily Builds
  - Map of Download Locations
- Galleries
  - Image Gallery
  - Animation Gallery
- Publications and Talks
- Related Databases and Software
- Citing Chimera
- Contact Us

Feature Highlight

(E)-resveratrol

Simple Line Drawing

A simple, line-drawing-like appearance can be achieved by combining black silhouette edges with flat, ambient-only lighting. The image at left of a small molecule in ball-and-stick style can be generated with a few Chimera commands. The same visual effects can be applied to ribbons and other representations, as shown in Neuraminidase Flowers and other Image Gallery entries.

(More features...)

Gallery Sample

Peroxiredoxin Wreath

Peroxiredoxins are enzymes that help cells cope with stressors such as high levels of reactive oxygen species. The image shows a decameric peroxiredoxin from human red blood cells (Protein Data Bank entry 1qmv), styled as a holiday wreath.

See also the RBVI holiday card gallery.

(More samples...)

Recent Citations

Structures of *Mycobacterium smegmatis* 70S ribosomes in complex with HPF, tmRNA, and P-tRNA. Mishra S, Ahmed T *et al. Sci Rep.* 2018 Sep 11;8(1):13587.

Sub-2 Å Ewald curvature corrected structure of an AAV2 capsid variant. Tan YZ, Aiyer S *et al. Nat Commun.* 2018 Sep 7;9(1):3628.

Malaria parasite translocon structure and mechanism of effector export. Ho CM, Beck JR *et al. Nature.* 2018 Sep 6;561(7721):70-75.

Structural basis of pan-Ebolavirus neutralization by an antibody targeting the glycoprotein fusion loop. Murin CD, Bruhn JF *et al. Cell Rep.* 2018 Sep 4;24(10):2723-2732.e4.

Crystal structure of the Frizzled 4 receptor in a ligand-free state. Yang S, Wu Y *et al. Nature.* 2018 Aug 30;560(7720):666-670.

(Previously featured citations...)

Chimera Search

Go

Google™ Search

News

September 21, 2018

Mac users are advised to hold off upgrading to Mojave until we find a fix for Chimera buttons not being shown until the windows containing them are resized.

July 3, 2018

Chimera production release 1.13 is now available. See the release notes for what's new.

June 2, 2018

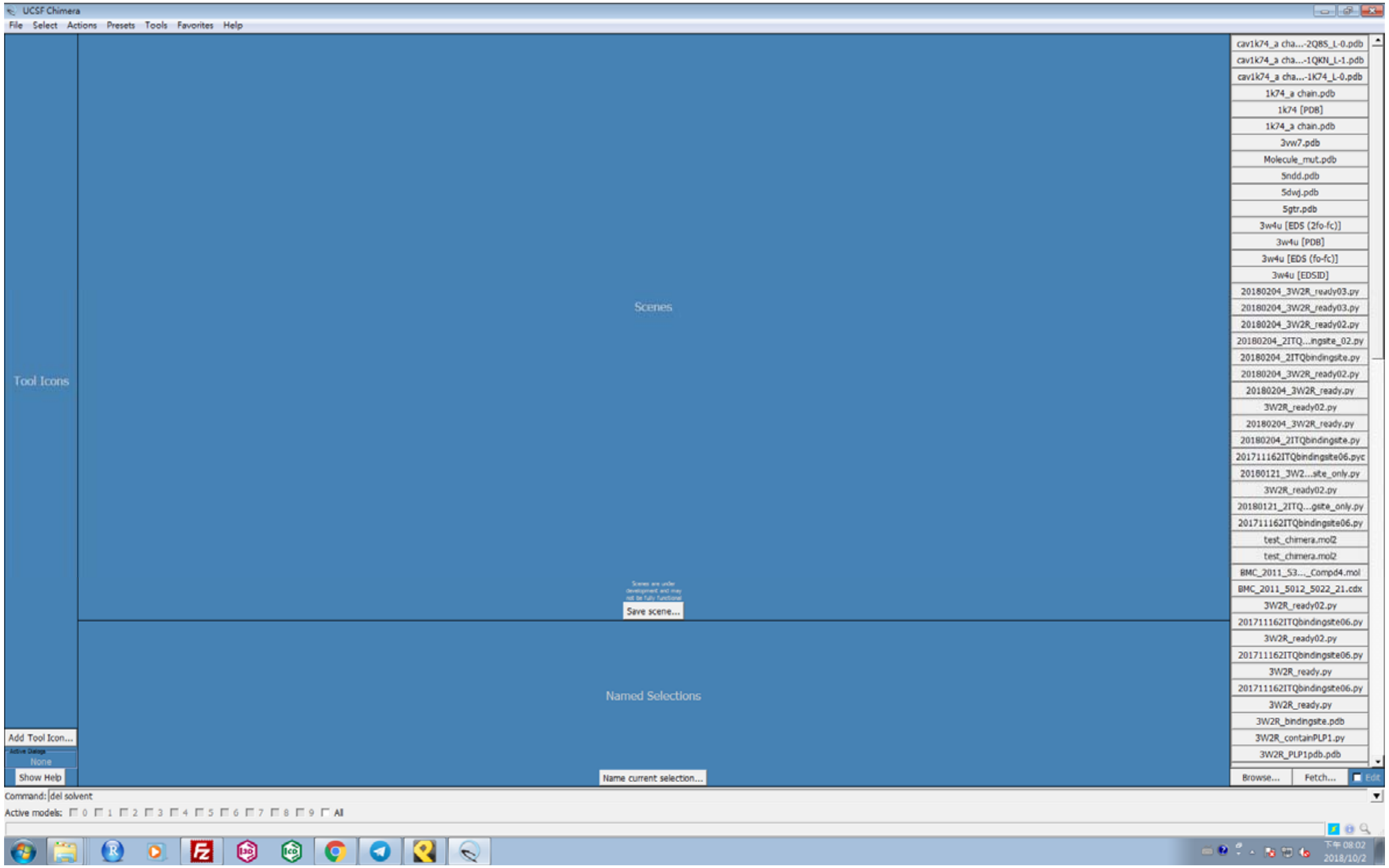
A production release candidate (version 1.13) is available; please try it and report any problems. See the release notes for what's new.

(Previous news...)

Upcoming Events

About RBVI | Projects | People | Publications | Resources | Visit Us

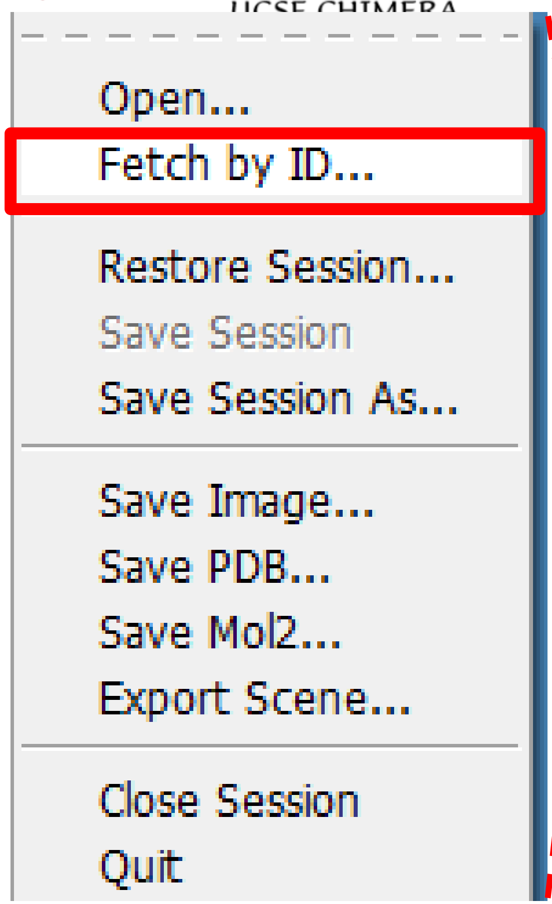
操作步驟

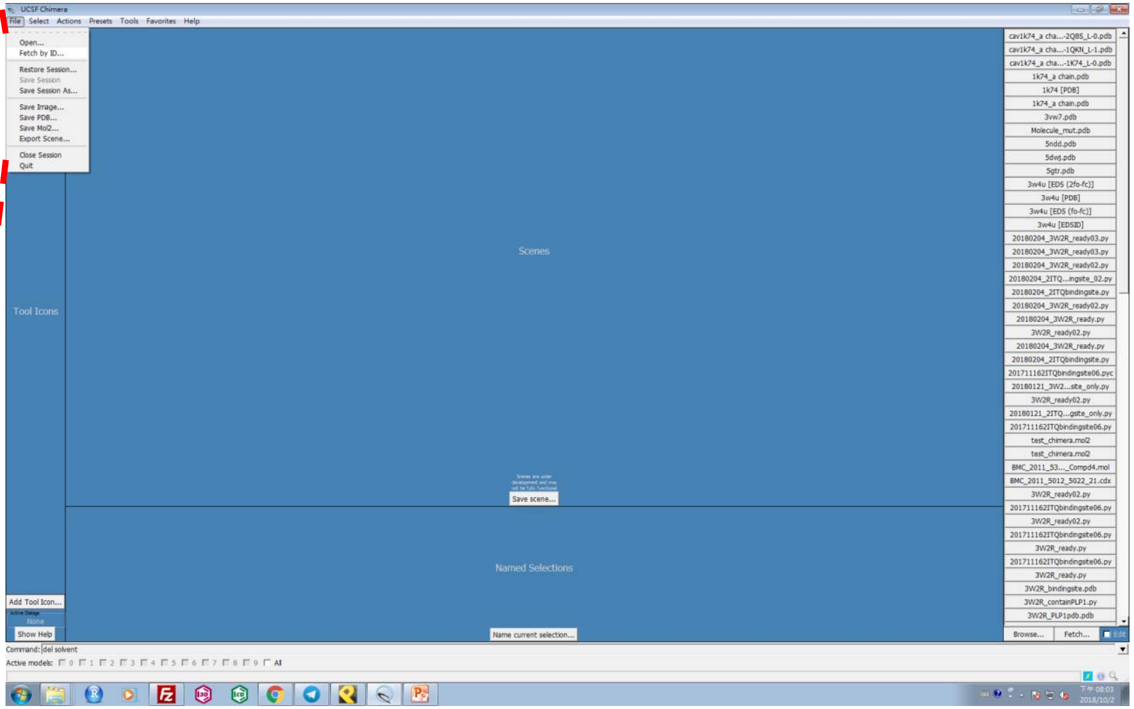


Command: del solvent

步驟一：開啟Chimera軟體。

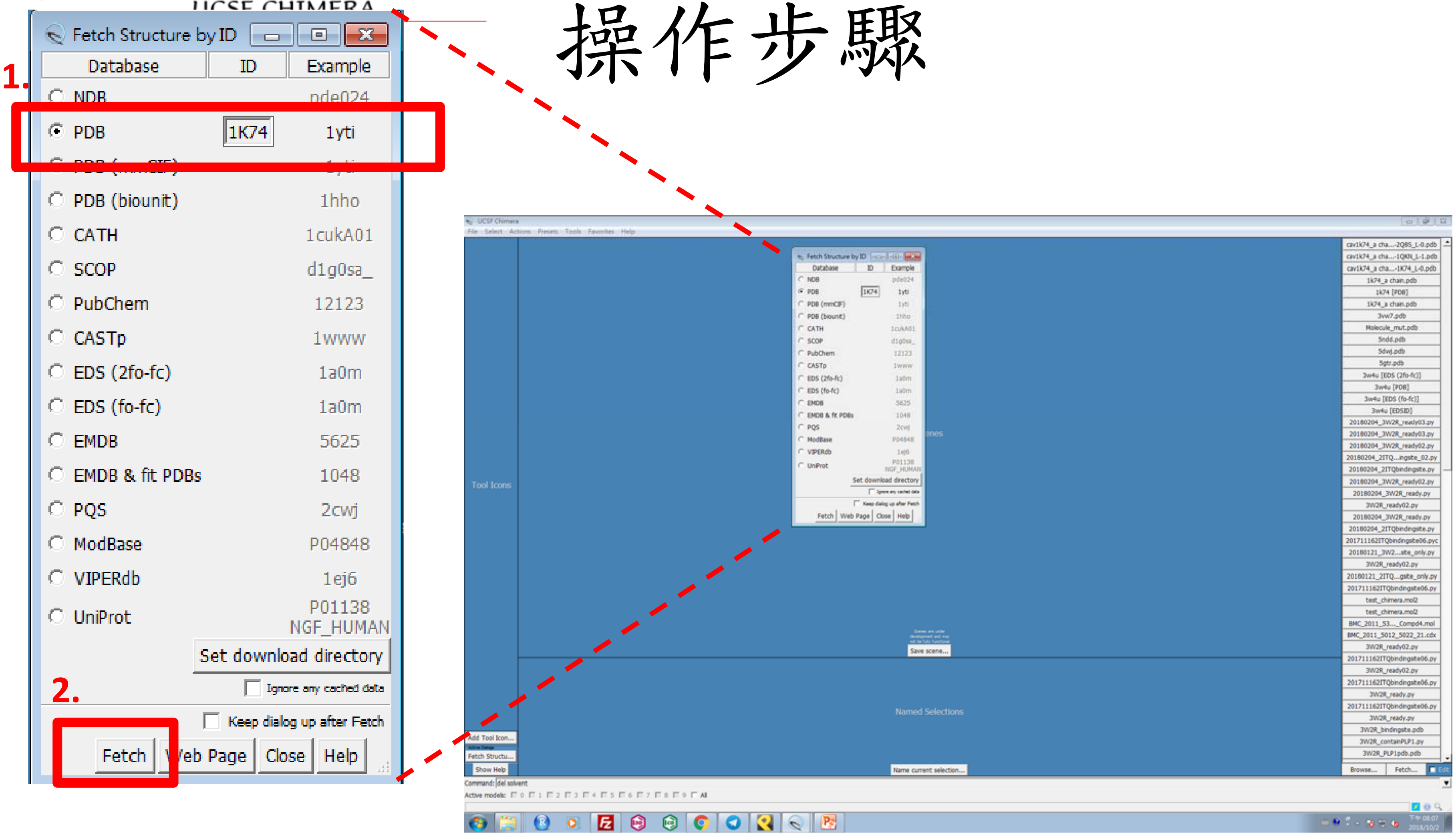
操作步驟





步驟二：
下載蛋白資訊，在視窗右上方點選File -> Fetch by ID

操作步驟



Database	ID	Example
○ NDB		pde024
● PDB	1K74	1yti
○ PDB (mmCIF)		1yti
○ PDB (biounit)		1hho
○ CATH		1cukA01
○ SCOP		d1g0sa_
○ PubChem		12123
○ CASTp		1www
○ EDS (2fo-fc)		1a0m
○ EDS (fo-fc)		1a0m
○ EMDB		5625
○ EMDB & fit PDBs		1048
○ PQS		2cwj
○ ModBase		P04848
○ VIPERdb		1ej6
○ UniProt		P01138 NGF_HUMAN

步驟三：
在PDB選項中輸入蛋白質代號：1K74，並按下Fetch鈕。

操作步驟

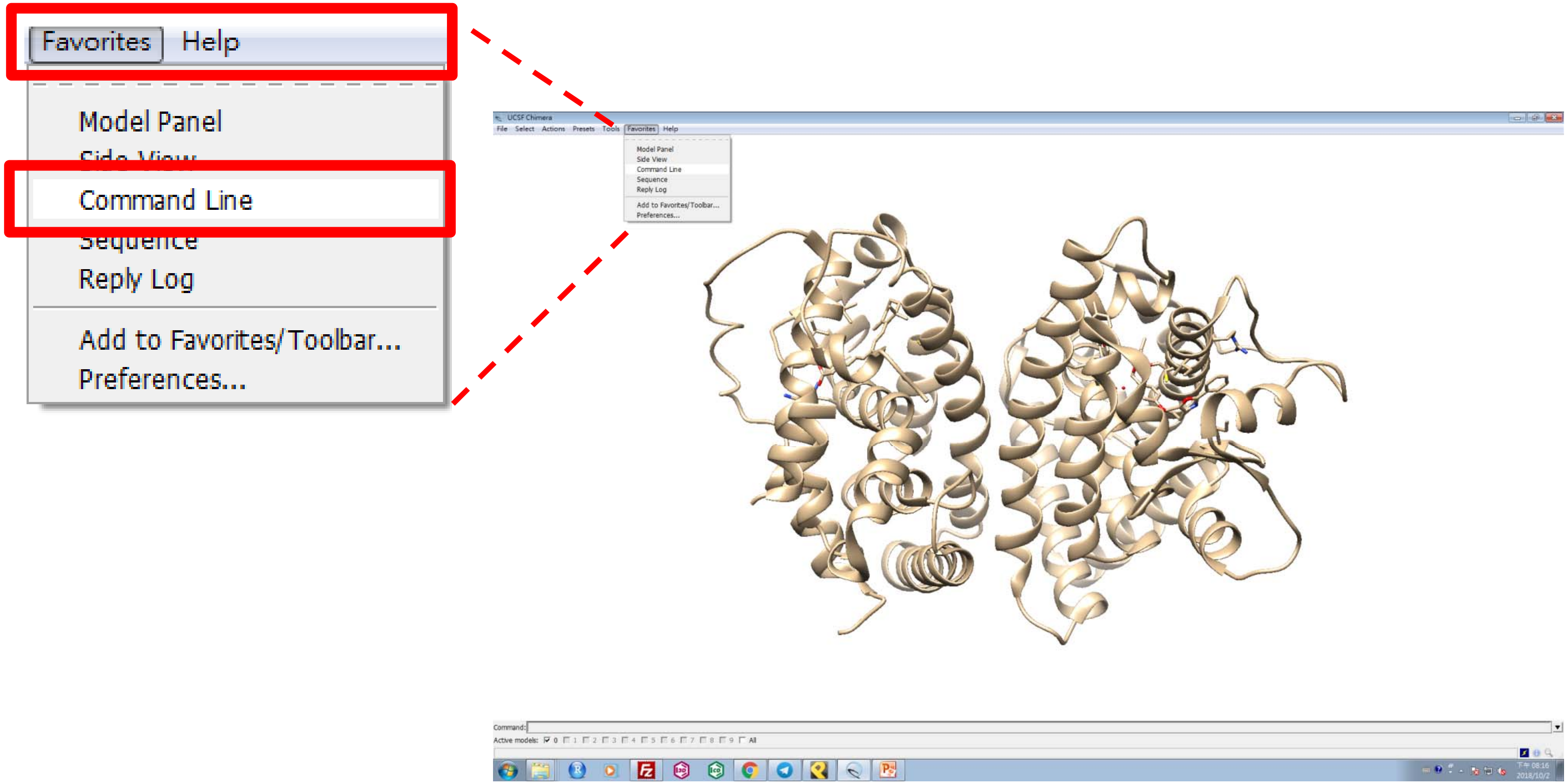
```
Command: del solvent
```

Active models: ☑ 0 ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ All

Opened 1K74 containing 1 model, 4405 atoms, and 740 residues

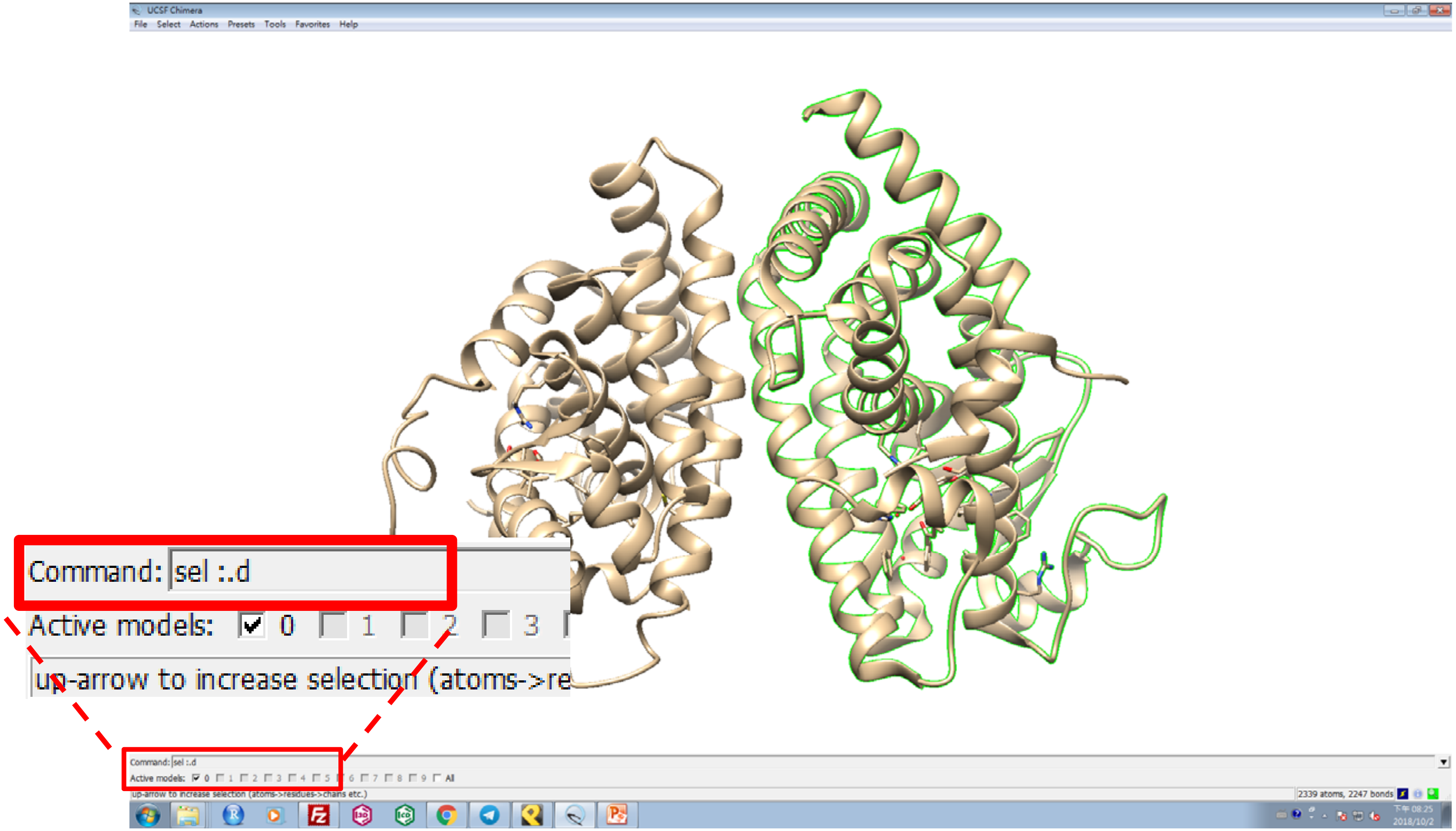
步驟四：此為成功下載蛋白質結構的畫面。

操作步驟



步驟五：
在視窗上方點選Favorites -> Command Line

操作步驟



```
Command: sel :.d
Active models: ☑ 0 ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ All
up-arrow to increase selection (atoms->residues->chains etc.)
2339 atoms, 2247 bonds
```

步驟六：
在下方Command列輸入指令：sel :.d，
按下Enter後D chain會被綠色外框框起來

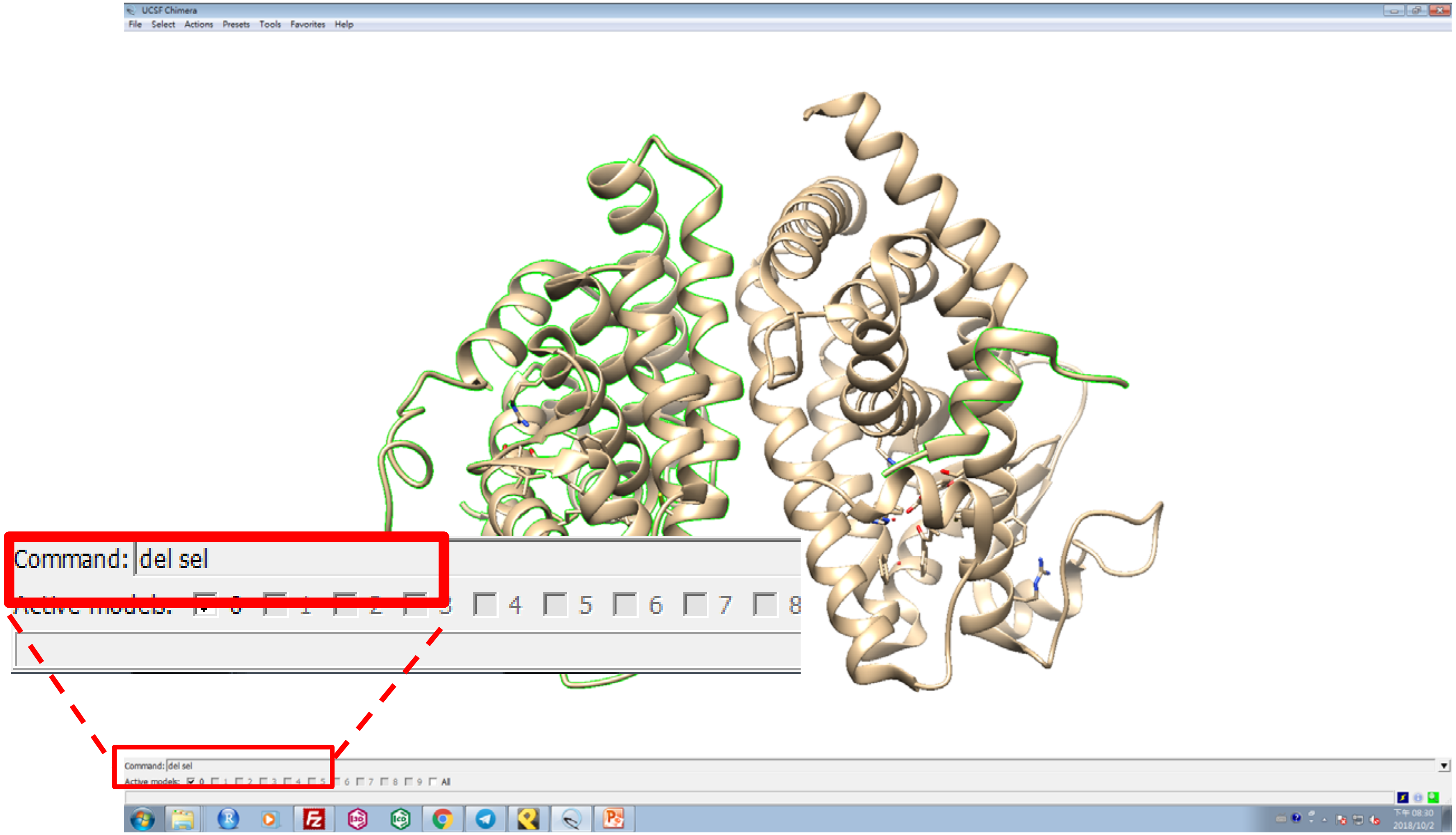
操作步驟

Command: sel invert

Active models: ☑ 0 ☐ 1 ☐ 2 ☐ 3

步驟七：在下方Command列輸入指令：sel invert，
按下Enter後D chain以外的部分會被綠色外框框起來

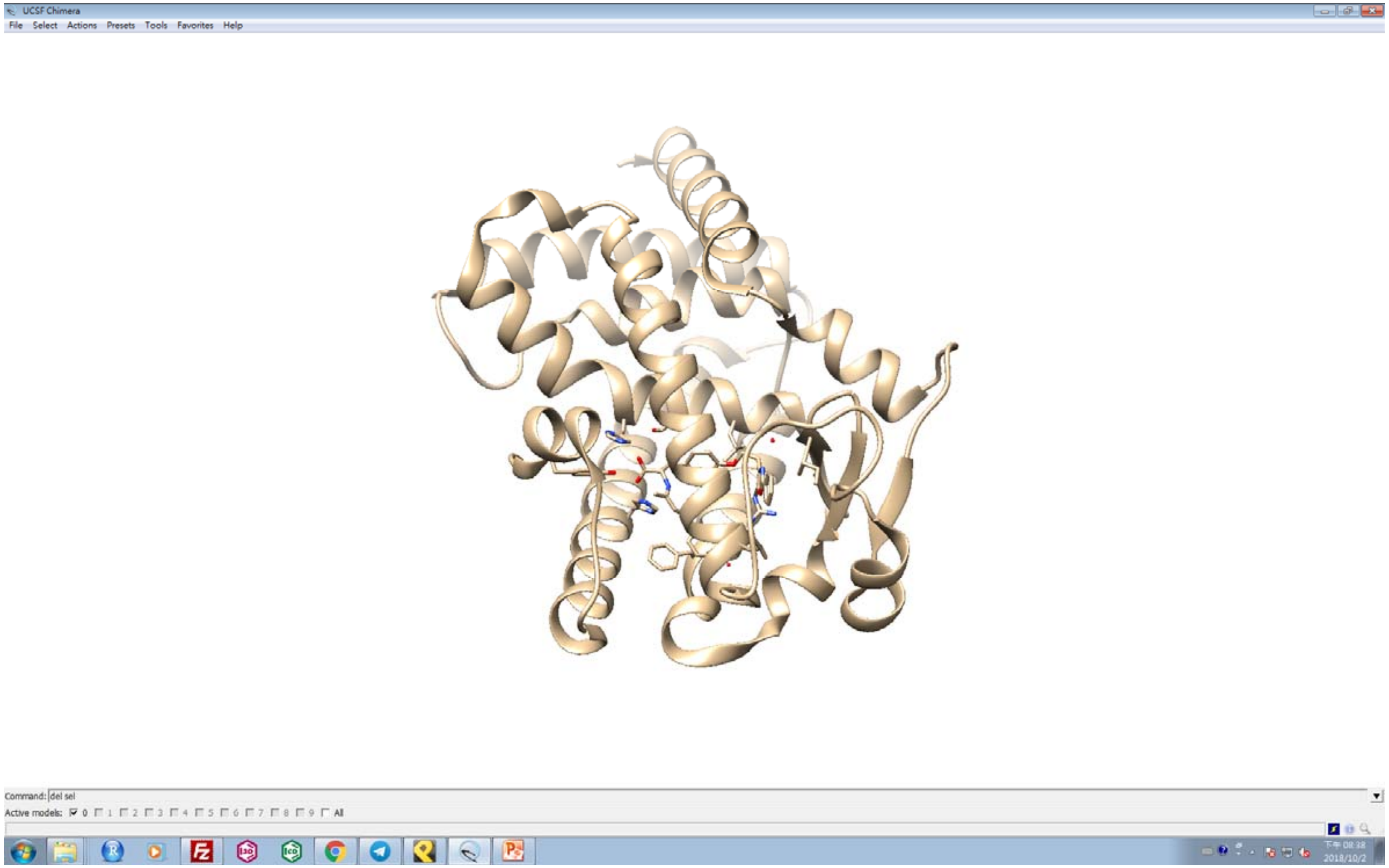
操作步驟



Command: del sel

步驟八：在下方Command列輸入指令：del sel

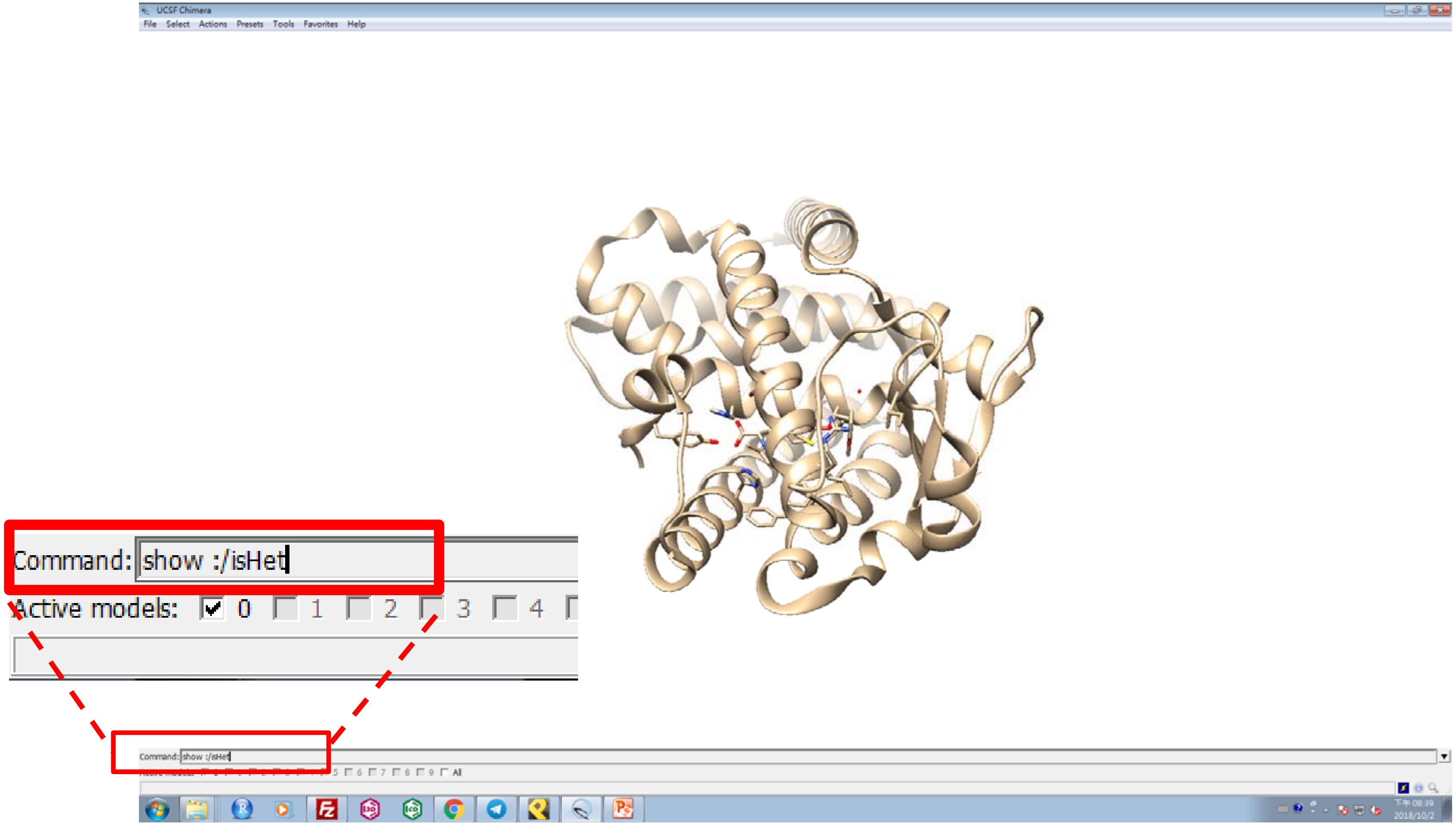
操作步驟



```
Command: del sel
Active models: ☑ 0 ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ All
```

步驟九：按下Enter後D chain以外的部分會被刪除，只保留D chain

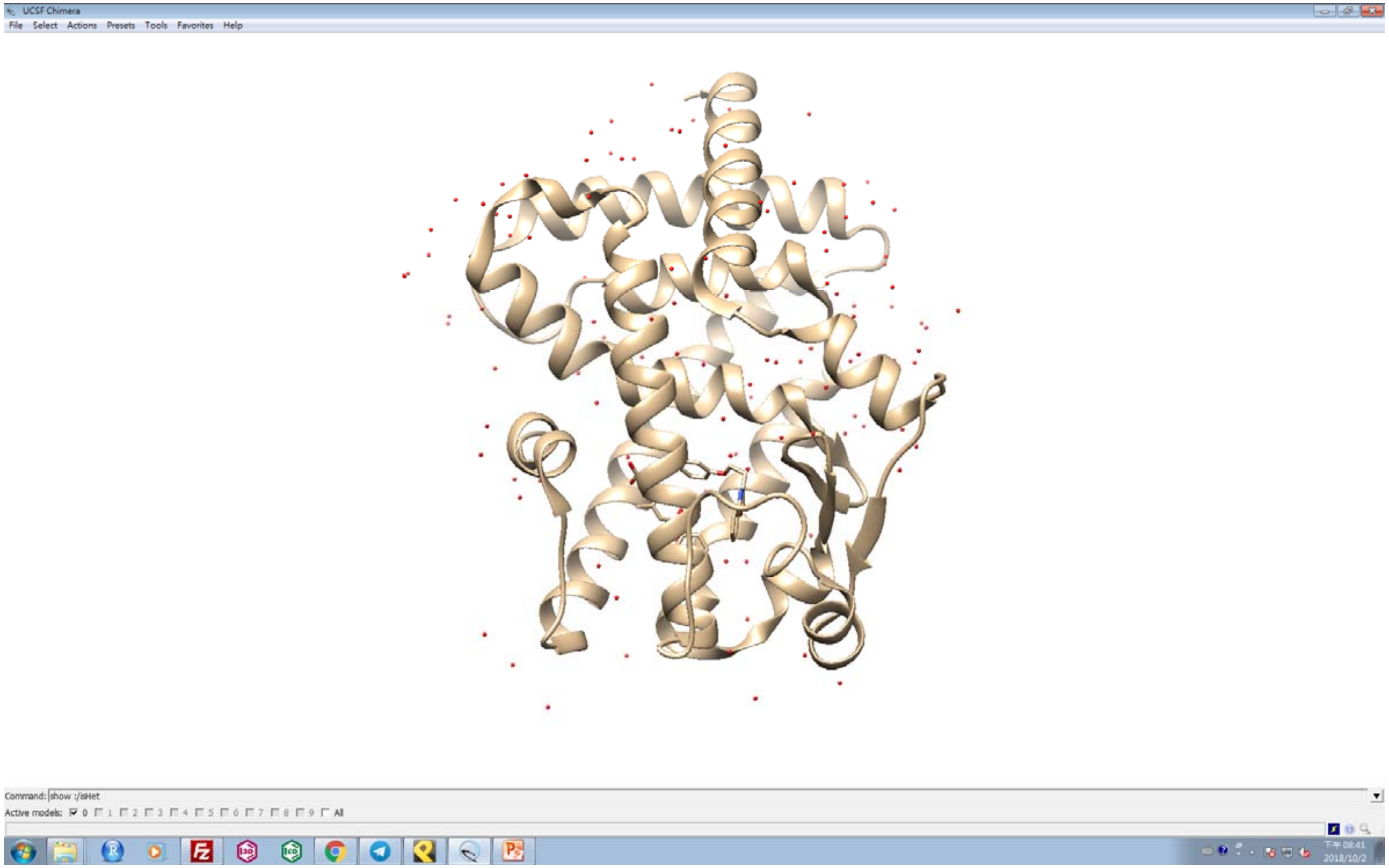
操作步驟



Command: show :/isHet

步驟十：在下方Command列輸入指令：show :/isHet

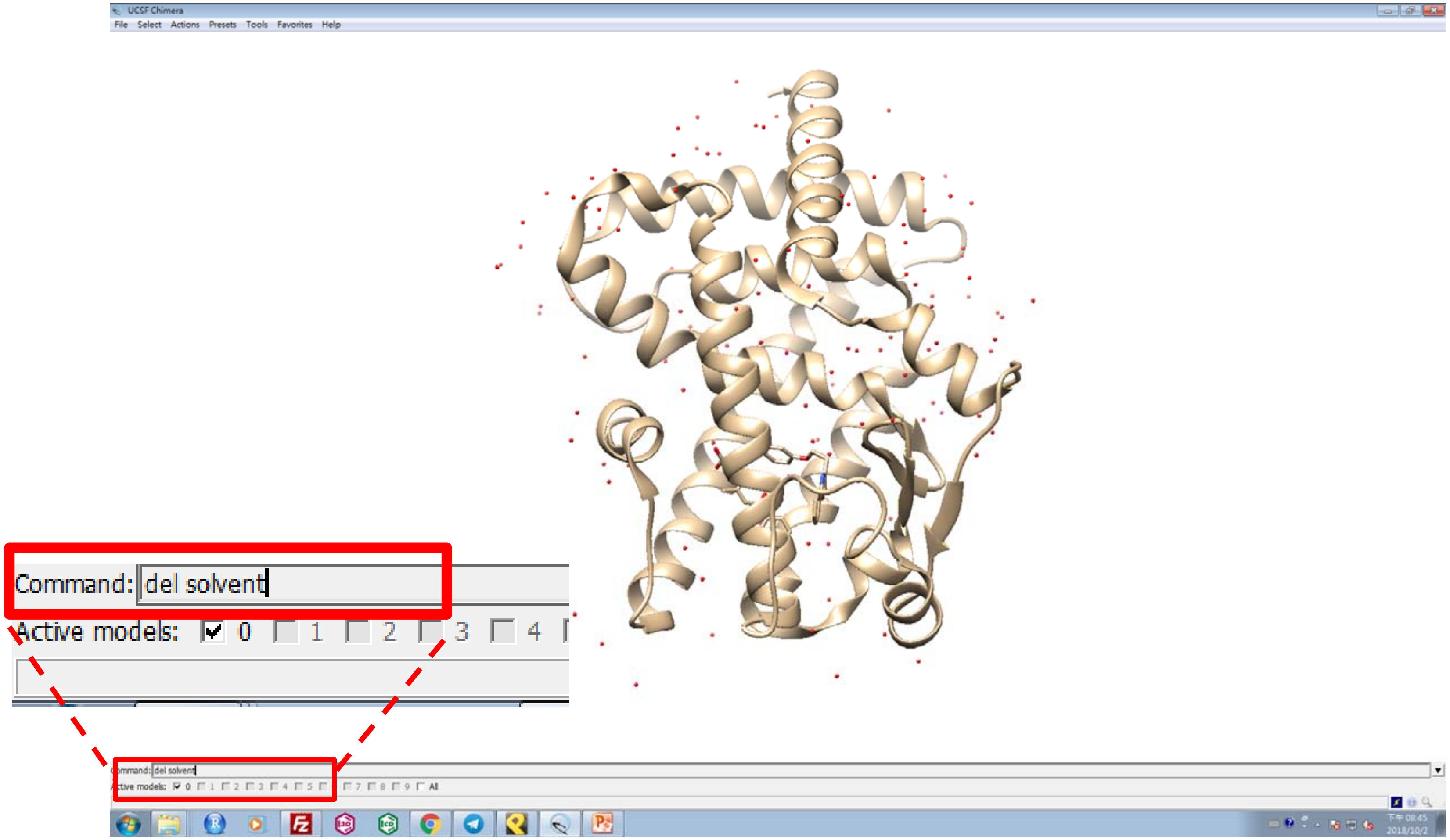
操作步驟



Command: show :/isHet

按下Enter後除了蛋白質之外的物質，皆會以原子、分子的形式顯示出來，有人知道途中紅色圓點是什麼嗎？

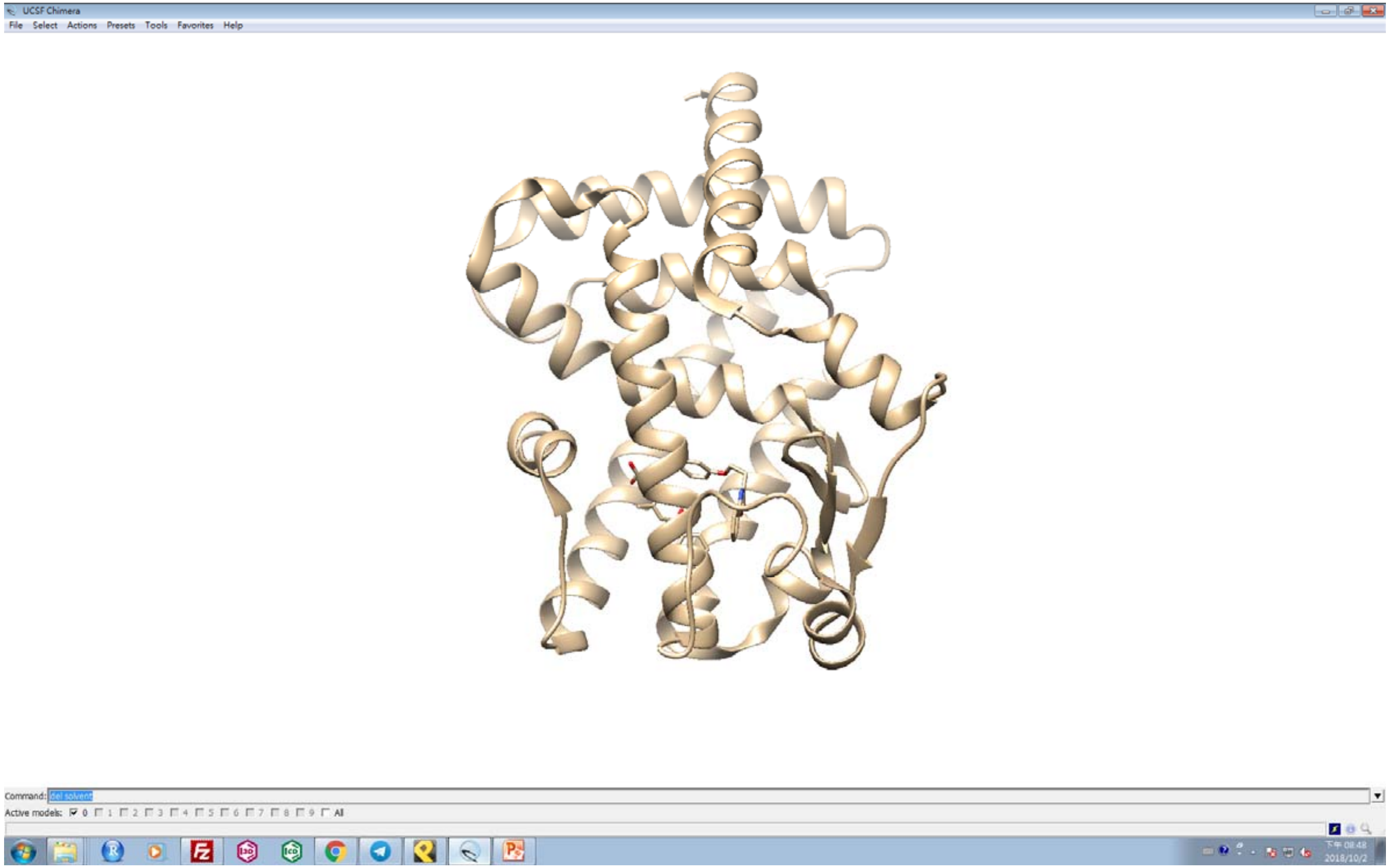
操作步驟



Command: del solvent

步驟十一：在下方Command列輸入指令：del solvent，
刪除蛋白質、小分子以外的溶劑。

操作步驟

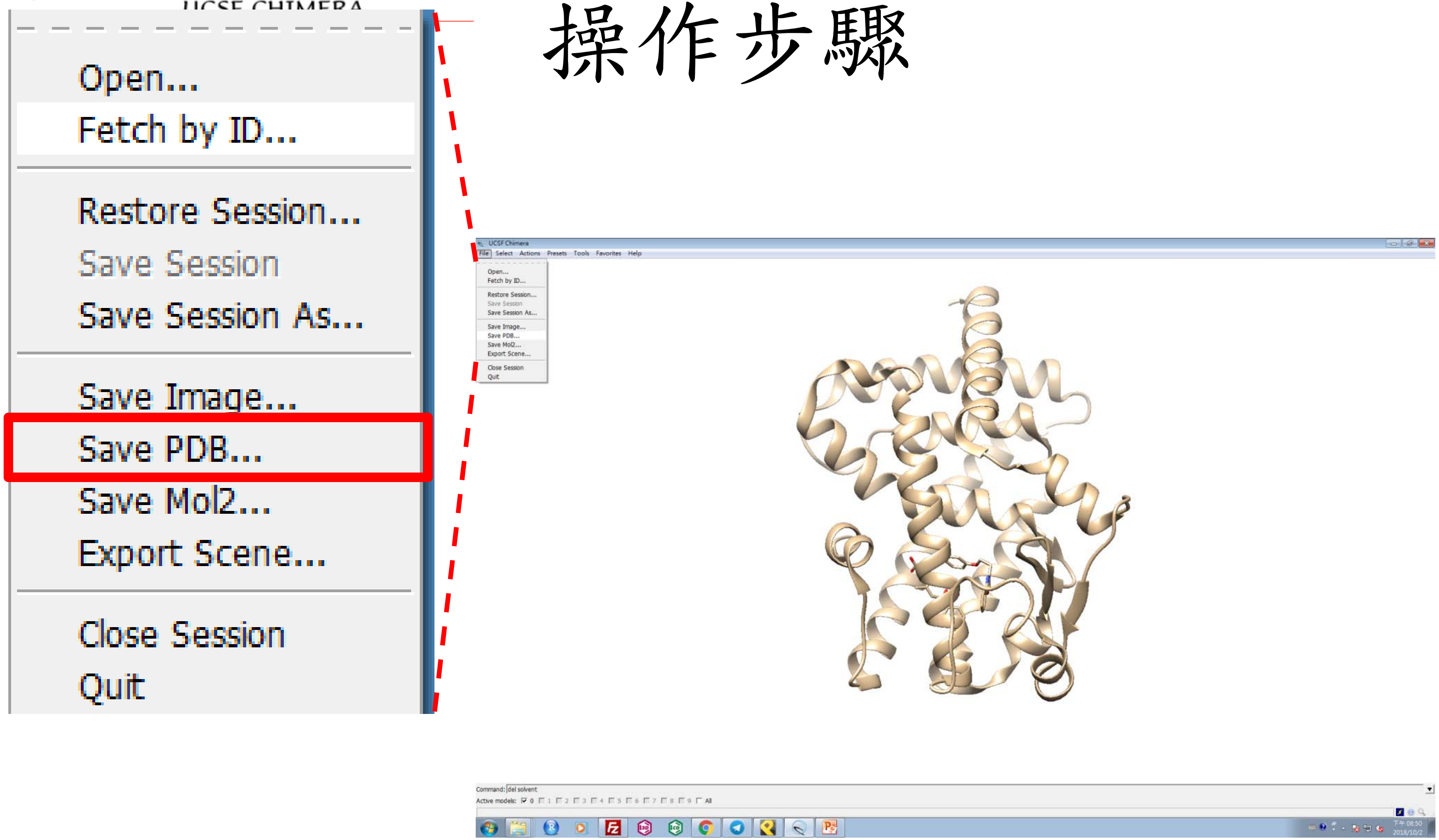


```
Command: del solvent
```

Active models: ☑ 0 ☐ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ All

按下Enter後，蛋白質、小分子之外的物質，皆會被刪除。
準備蛋白質的步驟大致上就完成了。

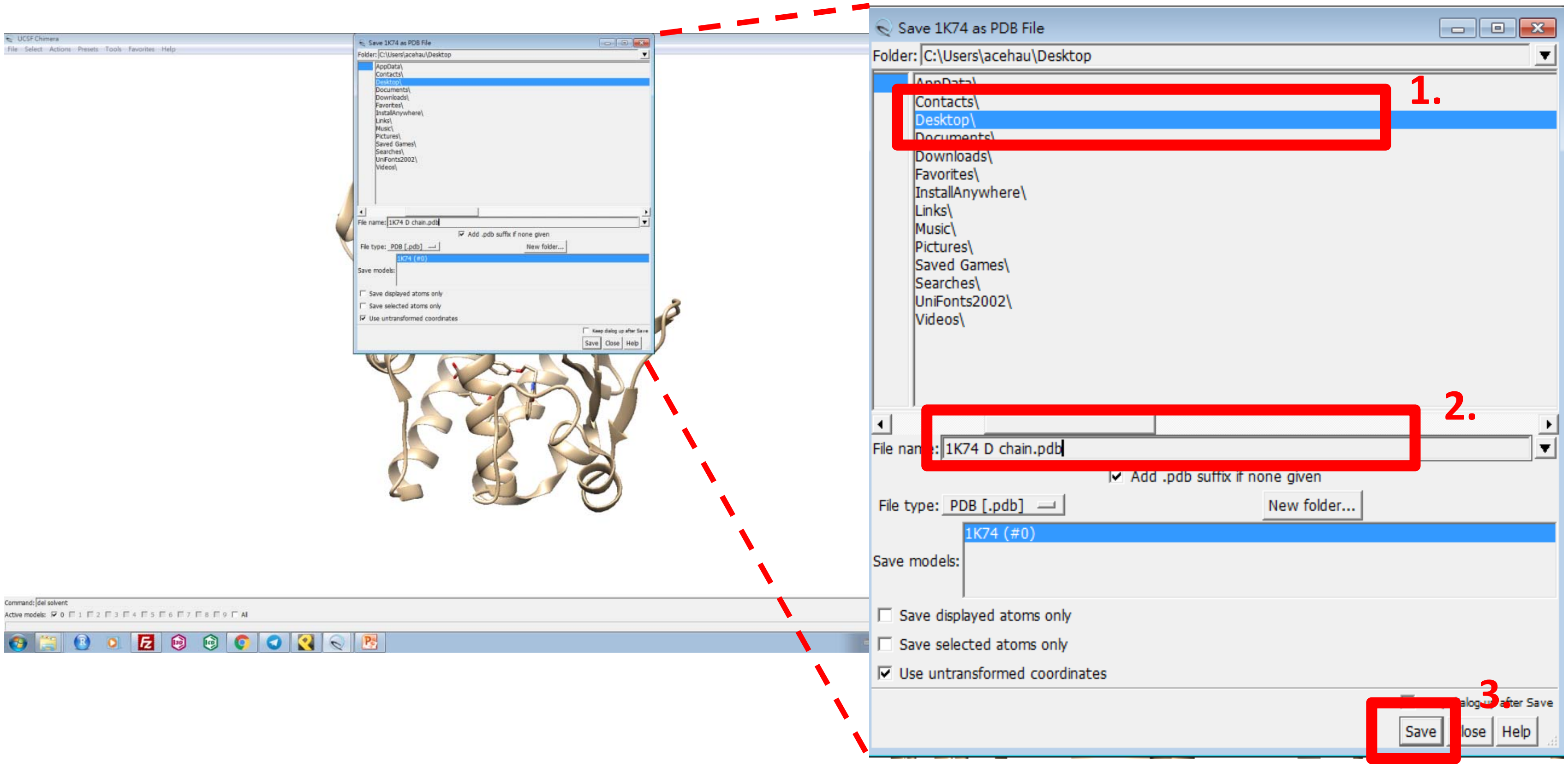
操作步驟



Command: del solvent

步驟十二：
儲存蛋白資訊，在視窗右上方點選File -> Save PDB，
點選完後會出現儲存檔案的視窗。

操作步驟



Save 1K74 as PDB File

Folder: C:\Users\acehau\Desktop

File name: 1K74 D chain.pdb

☑ Add .pdb suffix if none given

File type: PDB [.pdb]

Save models: 1K74 (#0)

☐ Save displayed atoms only

☐ Save selected atoms only

☑ Use untransformed coordinates

步驟十三：
1.點選要儲存蛋白質的路徑 2.輸入檔案名稱並加上檔案類型副檔名.pdb
3.按下右下角Save鍵儲存

完成以上步驟，今天要用到的蛋白質就已經準備好了。