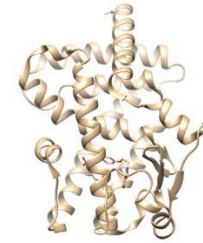




## 生物科技實驗



# 分子入塢 — (II) 準備大分子

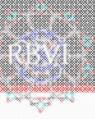
林盈廷副教授

實驗室：第一教學大樓 N1025室

Tel: (07) 3121101 ext. 2792

eMail : ytlin@kmu.edu.tw

*YTLab Presents*



Quick Links

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- Citing Chimera
- Contact Us

Recent Citations

Structures of *Mycobacterium smegmatis* 70S ribosomes in complex with HFE l-mRNA and P-RNA. 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):3626.

Malaria parasite translocon structure and mechanism of effector export. Ho CW, Beck UR *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 F102ed 4 receptor in a lipid-free state. Yang S, Wu Y *et al. Nature.* 2018 Aug 30;560(7720):666-670.

(Previously featured citations...)

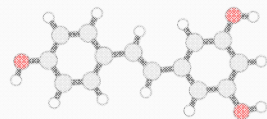
UCSF CHIMERA

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.

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...)

# Chimera

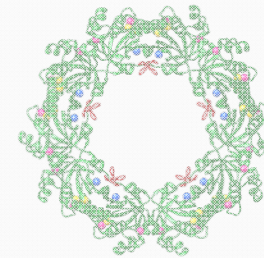
Gallery Sample

**Peroxioredoxin Wreath**

Peroxioredoxins 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...)



## Protein preparation

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

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**

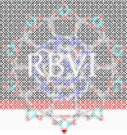
Chimera production release 1.13 is now available. See the [release notes](#) for what's new.

**June 2, 2018**

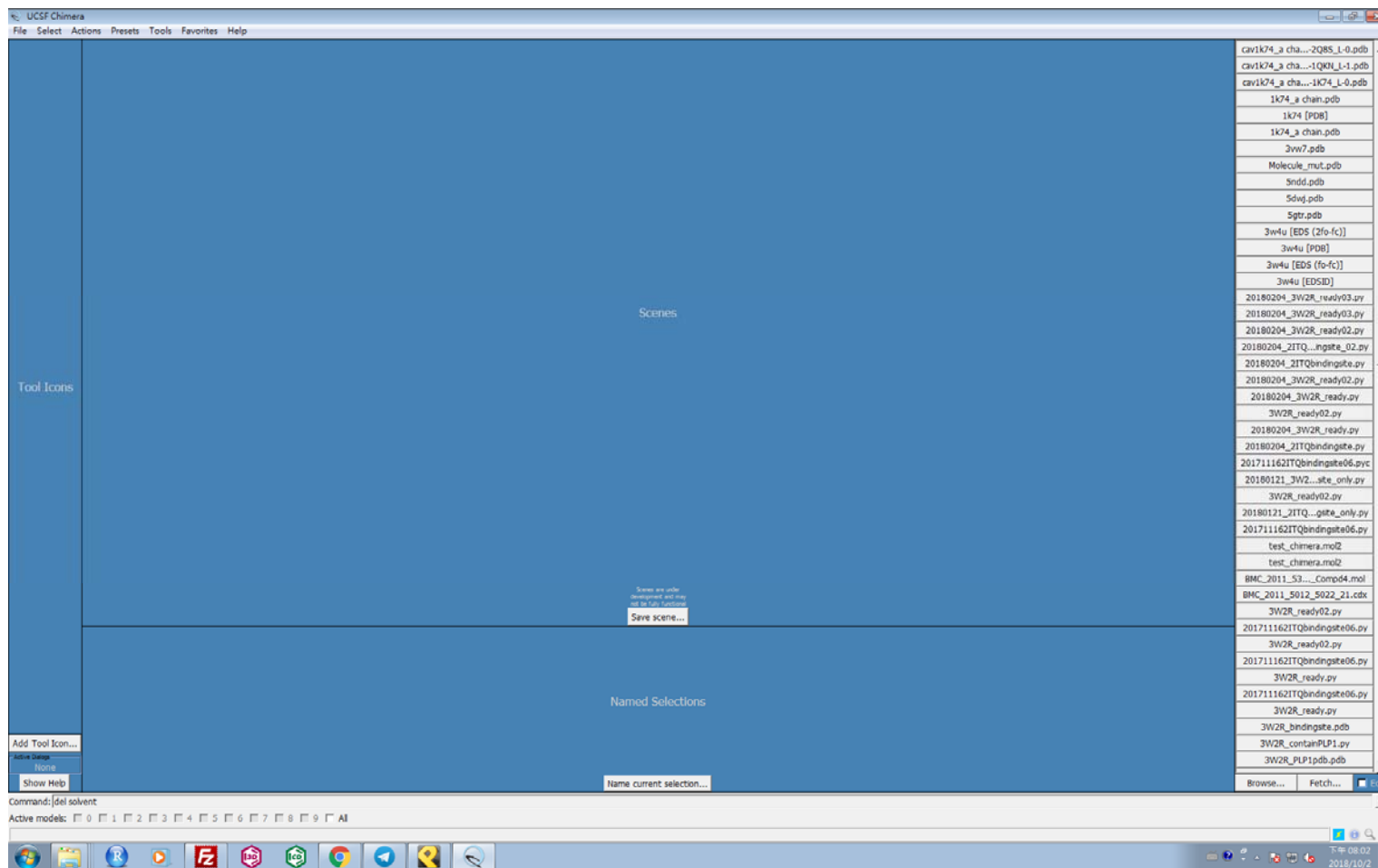
A production release candidate (version 1.13) is available. Please try it and report any problems. See the [release notes](#) for what's new.

(Previous news...)

Upcoming Events



# 操作步驟



步驟一：開啟Chimera軟體。



# 操作步驟

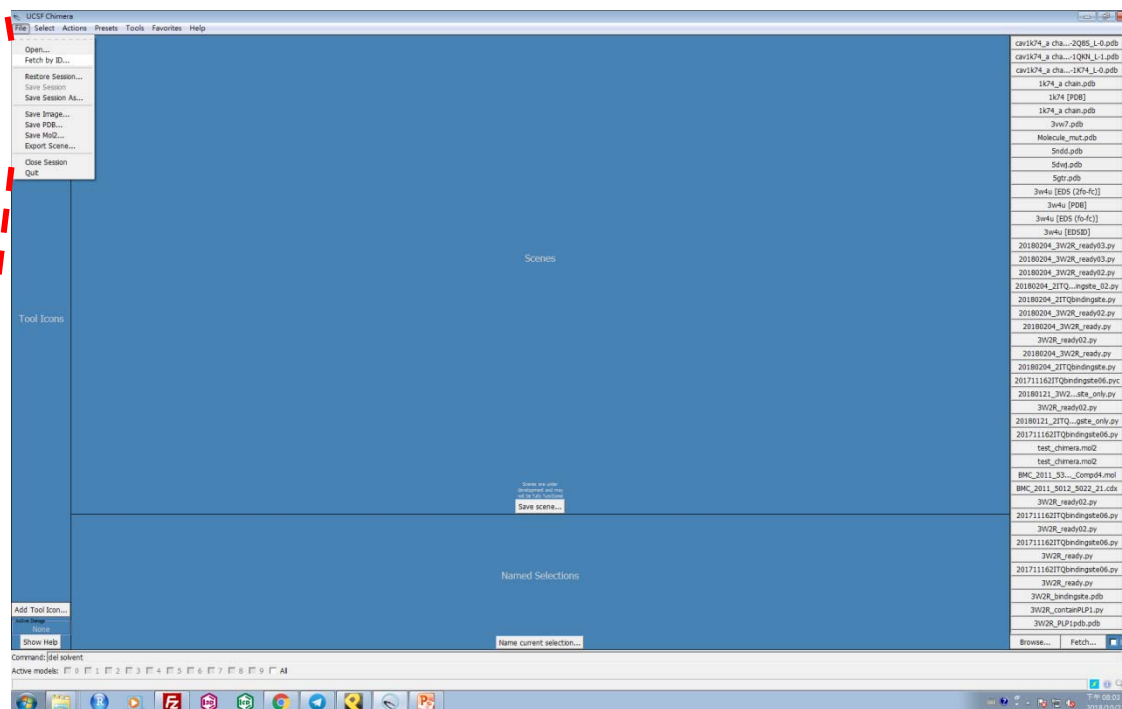
- Open...
- Fetch by ID...
- Restore Session...
- Save Session
- Save Session As...

---

- Save Image...
- Save PDB...
- Save Mol2...
- Export Scene...

---

- Close Session
- Quit

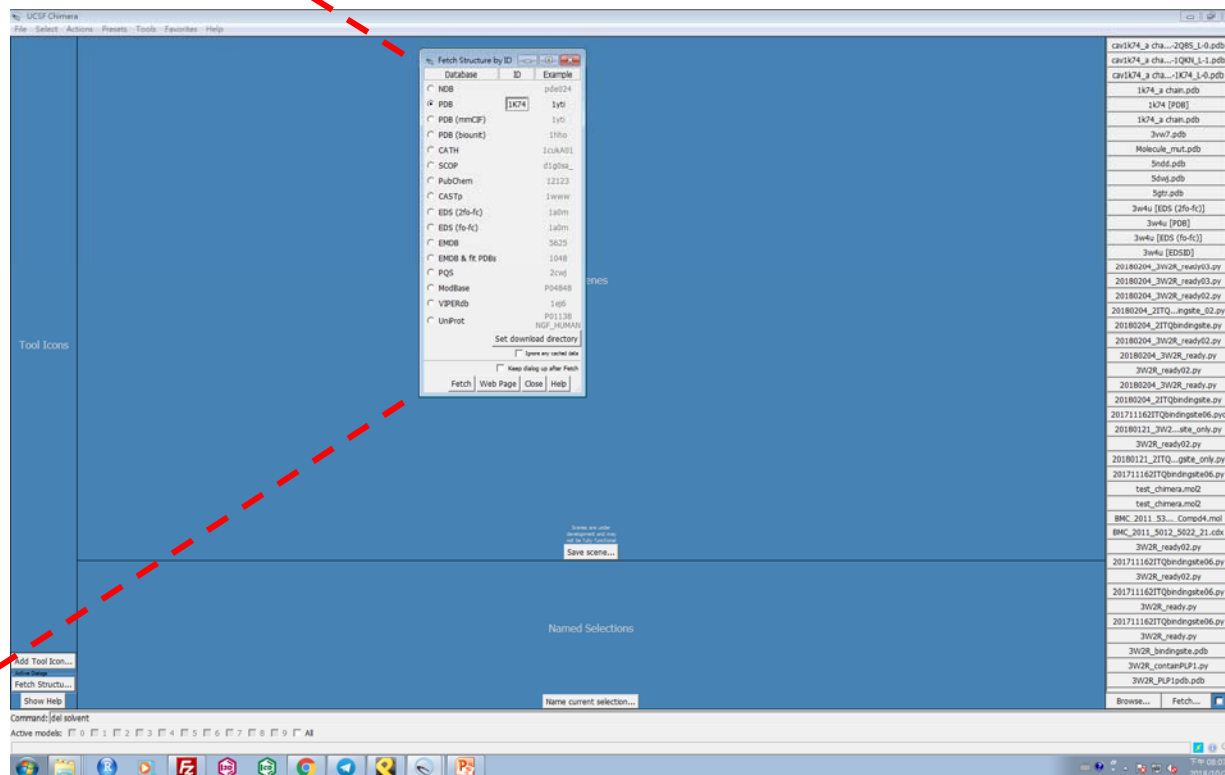
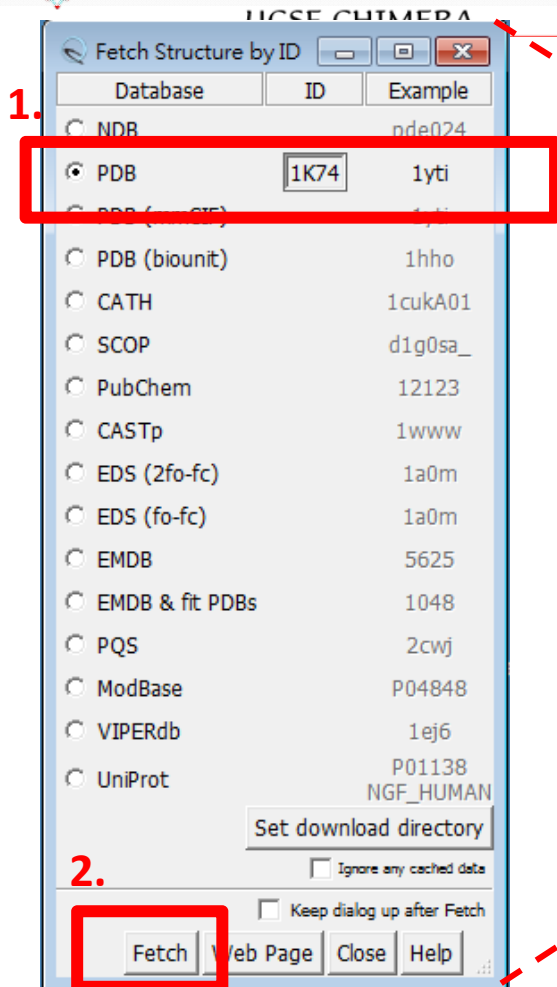


步驟二：

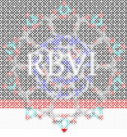
下載蛋白資訊，在視窗右上方點選File -> Fetch by ID



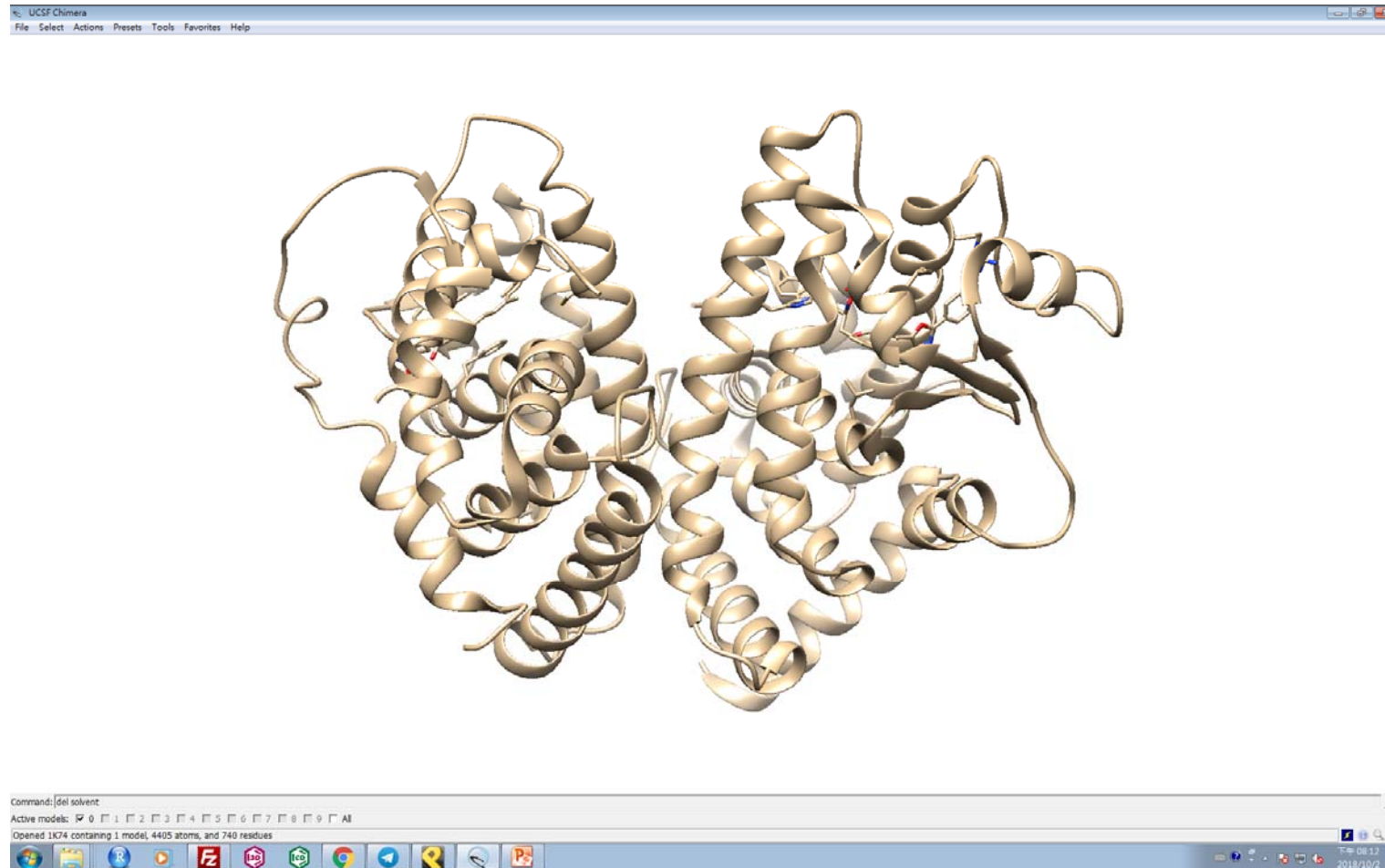
# 操作步驟



步驟三：  
在PDB選項中輸入蛋白質代號：1K74，並按下Fetch紐。



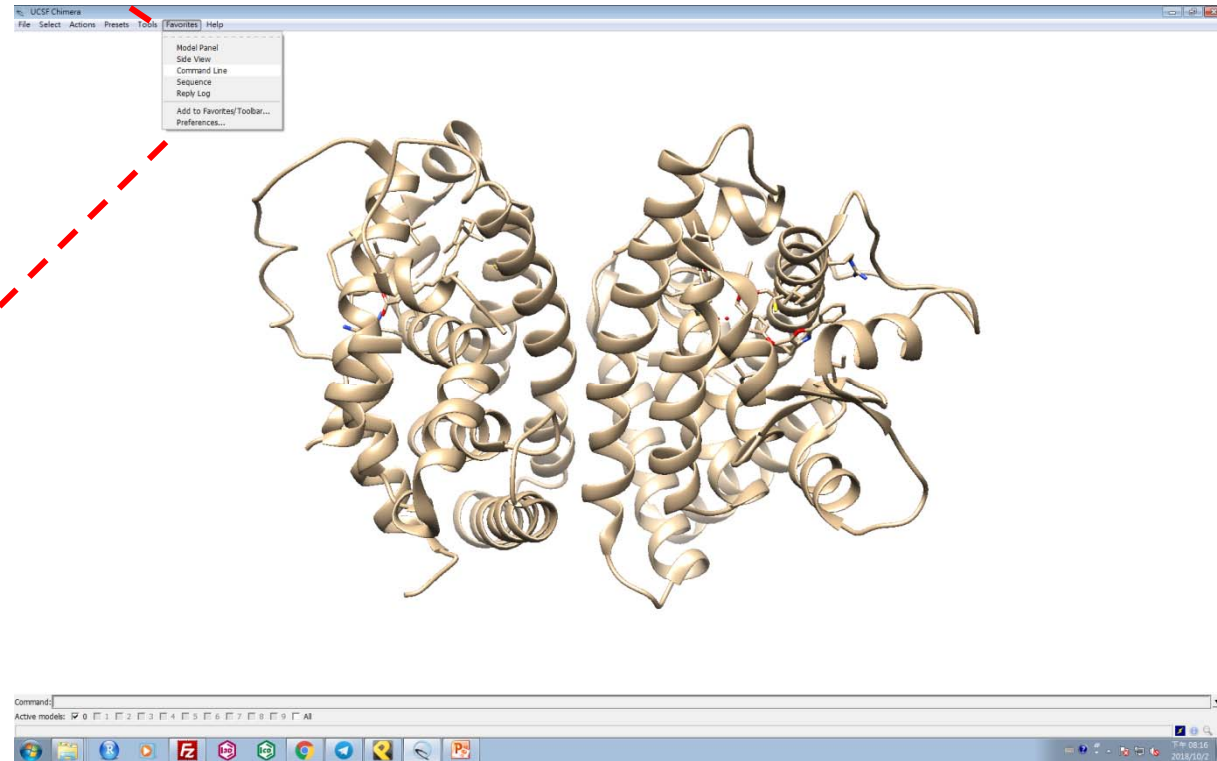
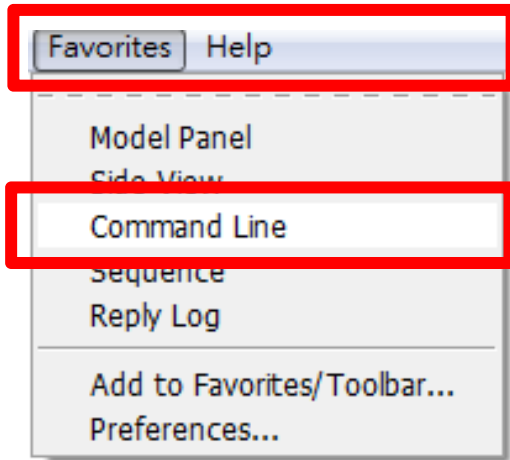
# 操作步驟



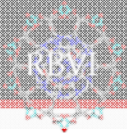
步驟四：此為成功下載蛋白質結構的畫面。



# 操作步驟



步驟五：  
在視窗上方點選Favorites -> Command Line



# 操作步驟

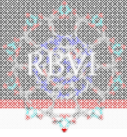


步驟六：

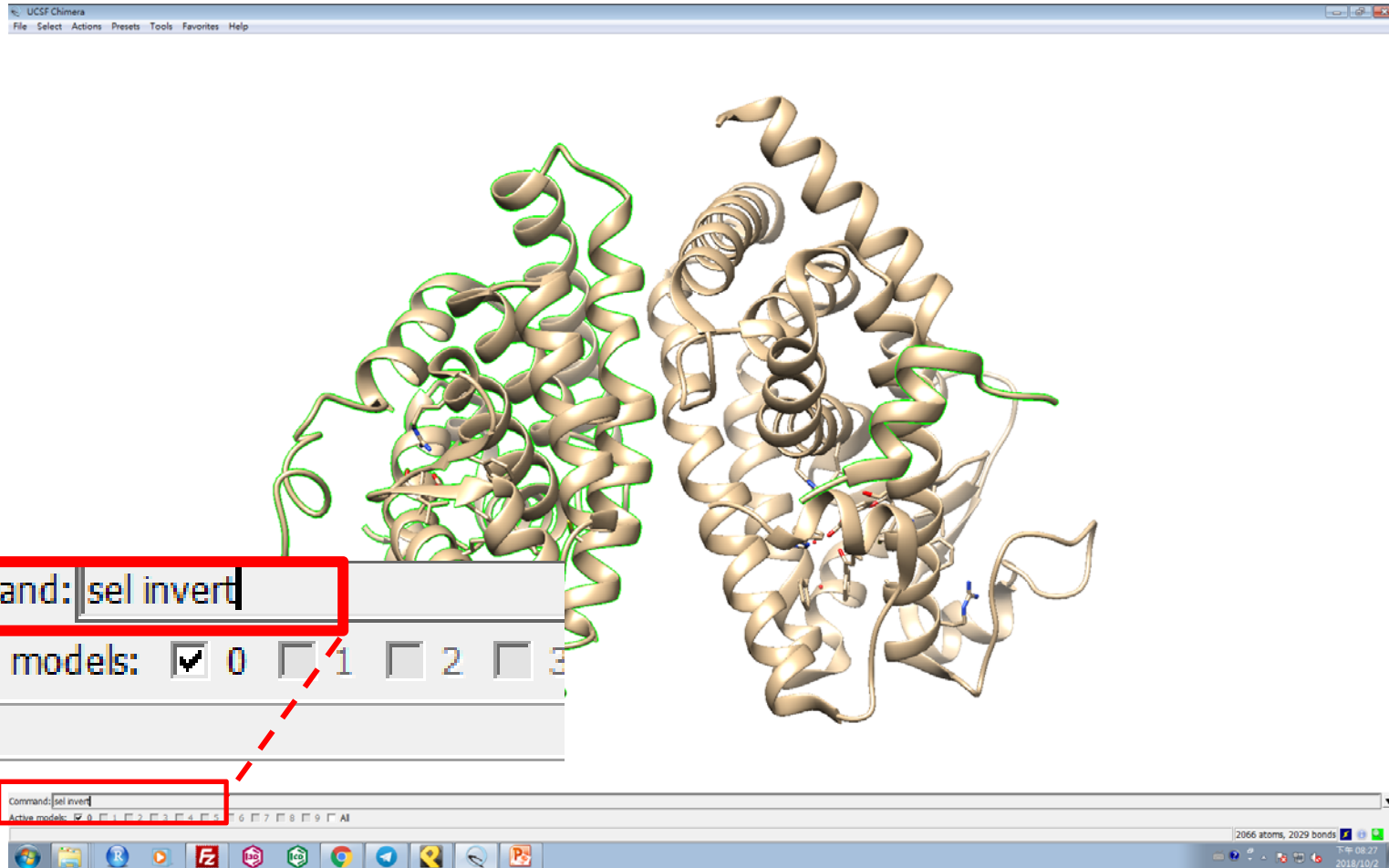
在下方Command列輸入指令：`sel :.d`，

按下Enter後D chain會被綠色外框框起來

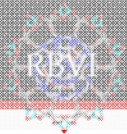




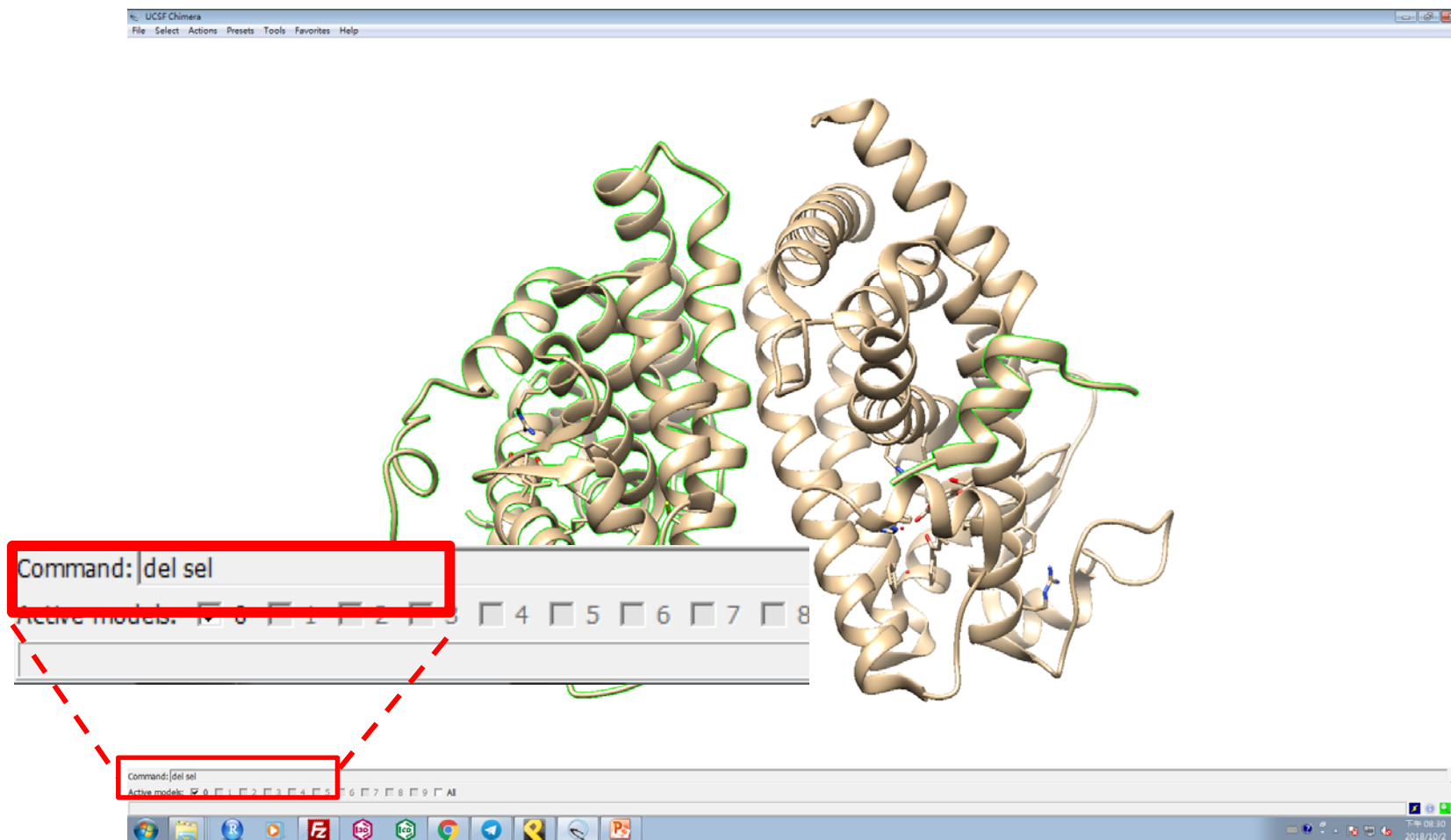
# 操作步驟



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



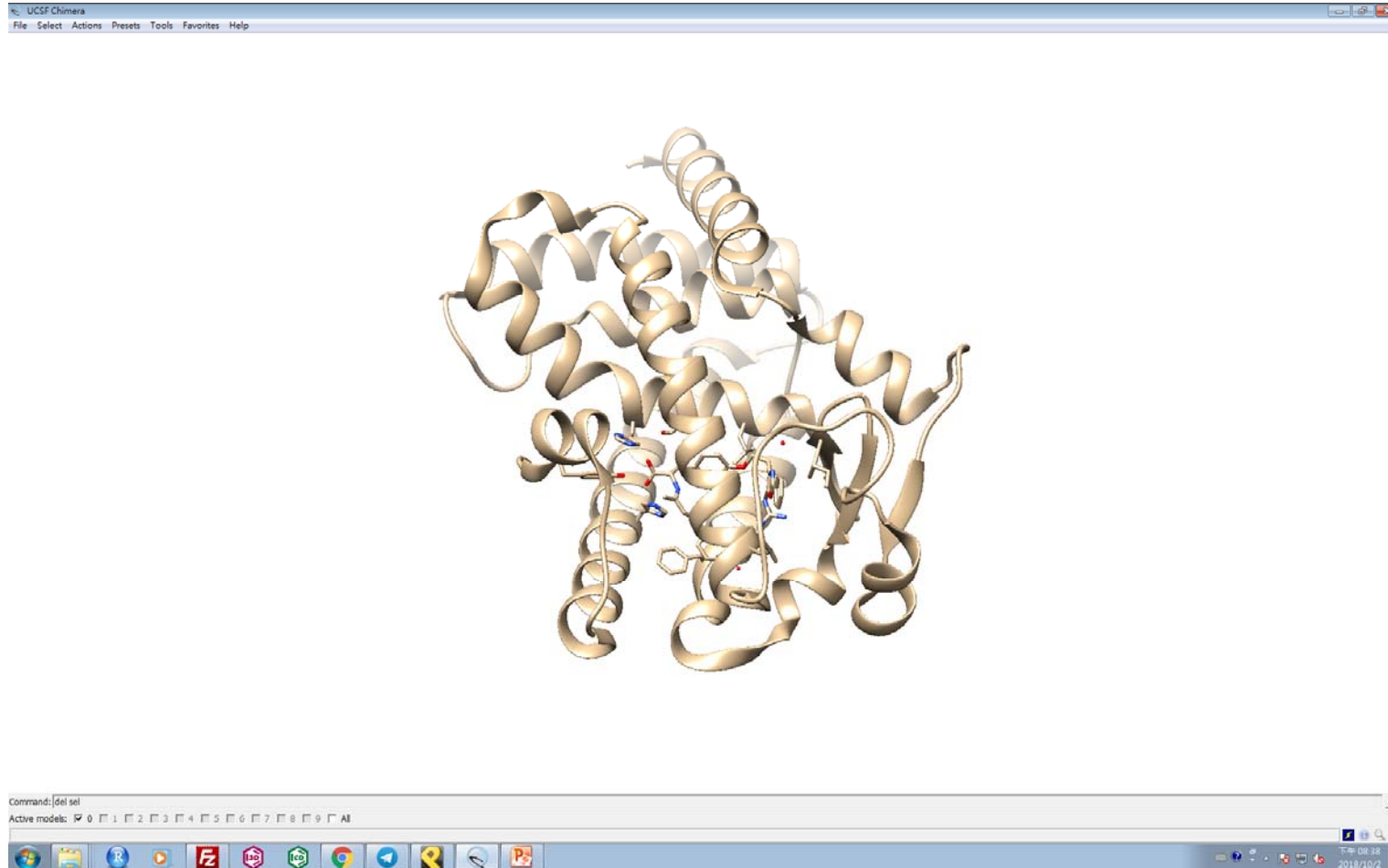
# 操作步驟



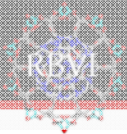
步驟八：在下方Command列輸入指令：`del sel`



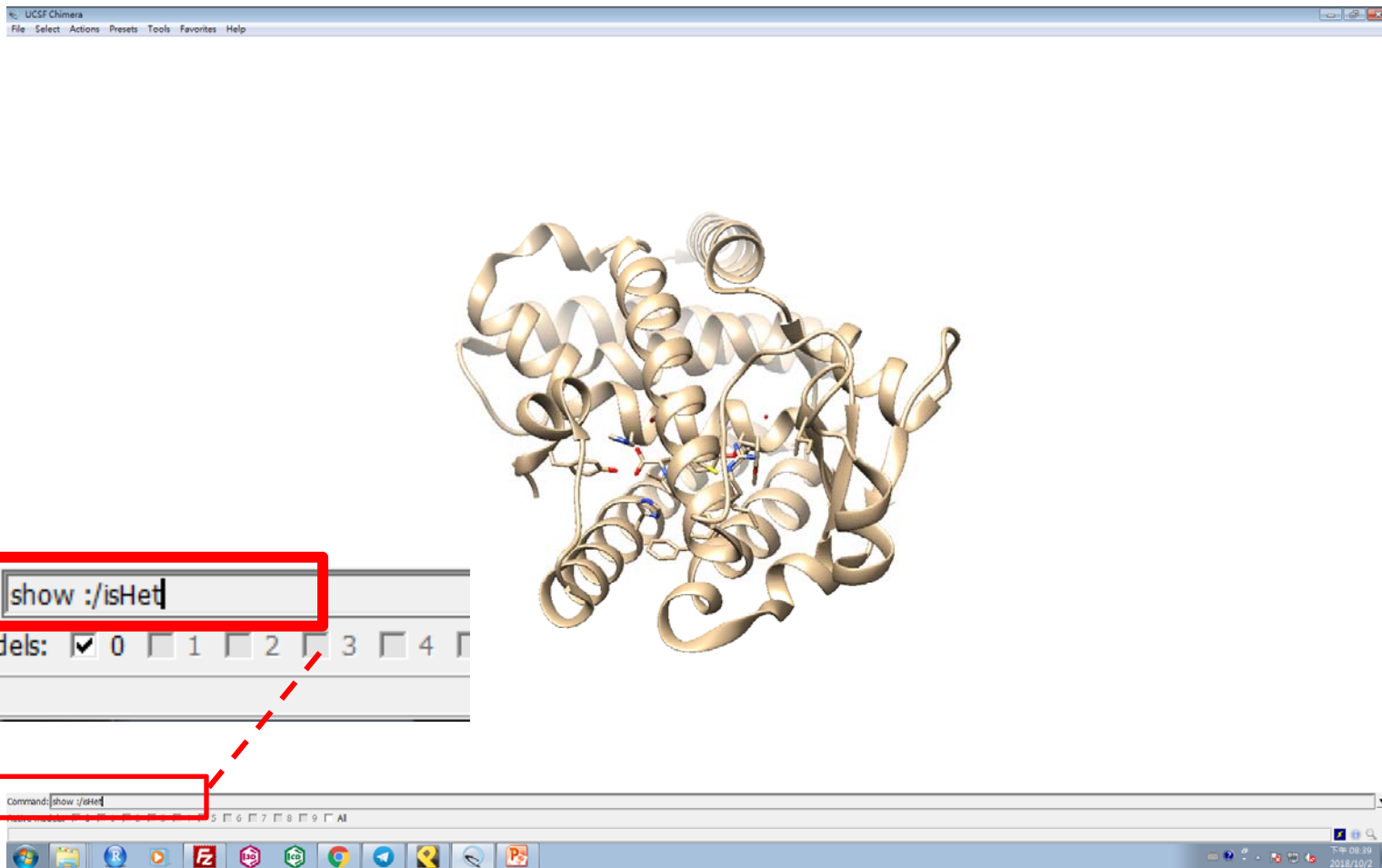
# 操作步驟



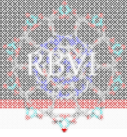
步驟九：按下Enter後D chain以外的部分會被刪除，只保留D chain



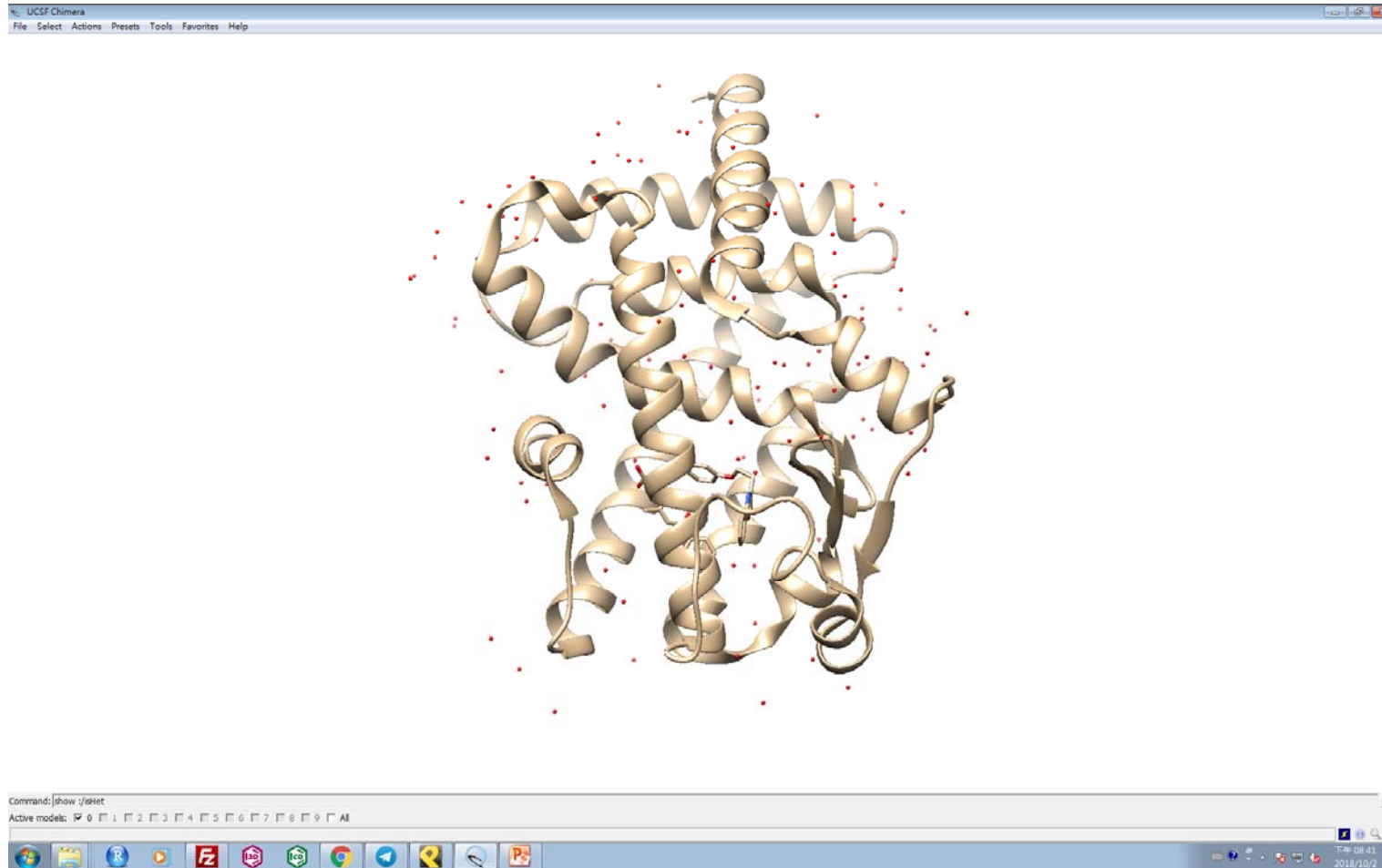
# 操作步驟



步驟十：在下方Command列輸入指令：`show :/isHet`



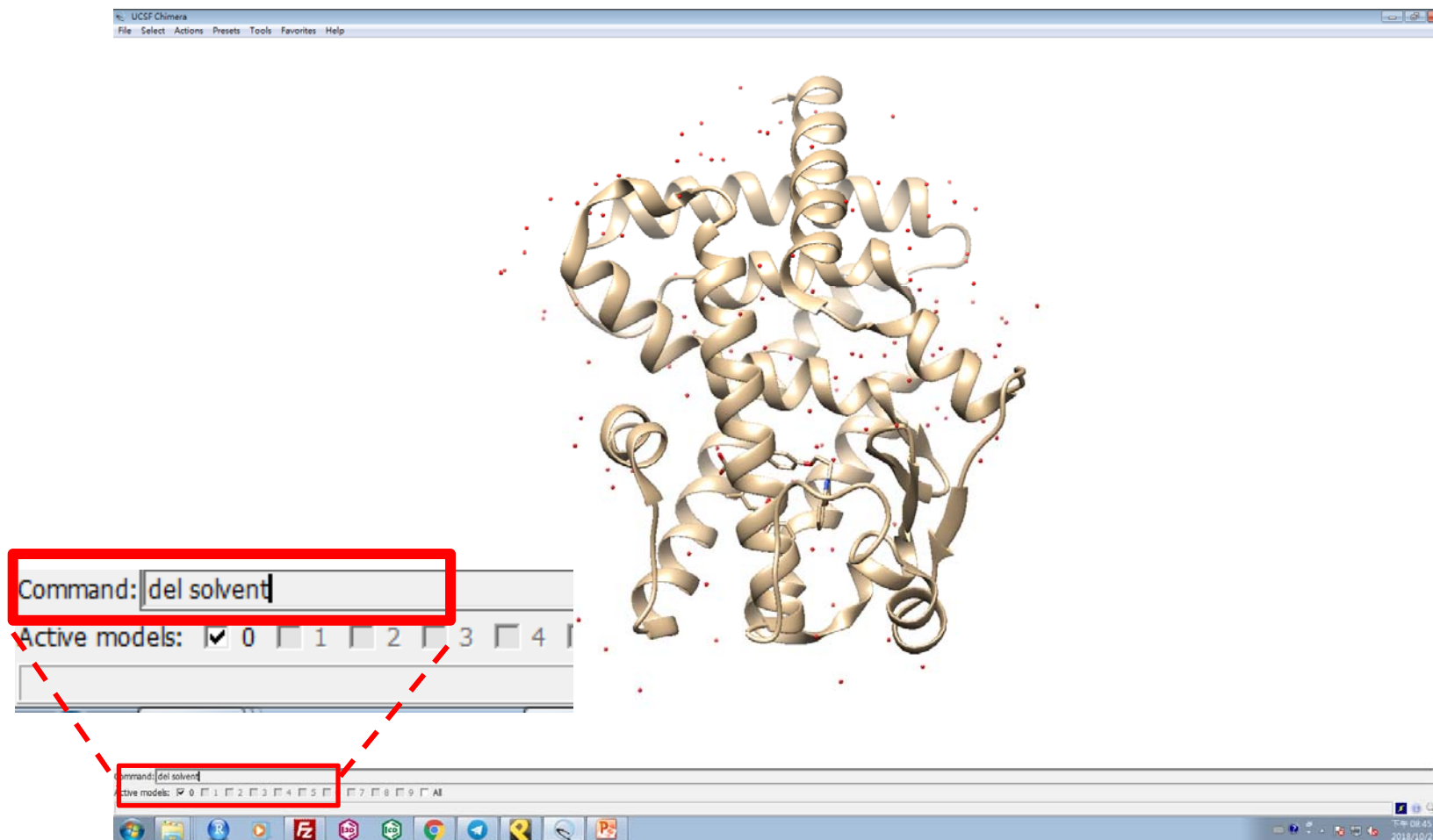
# 操作步驟



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？



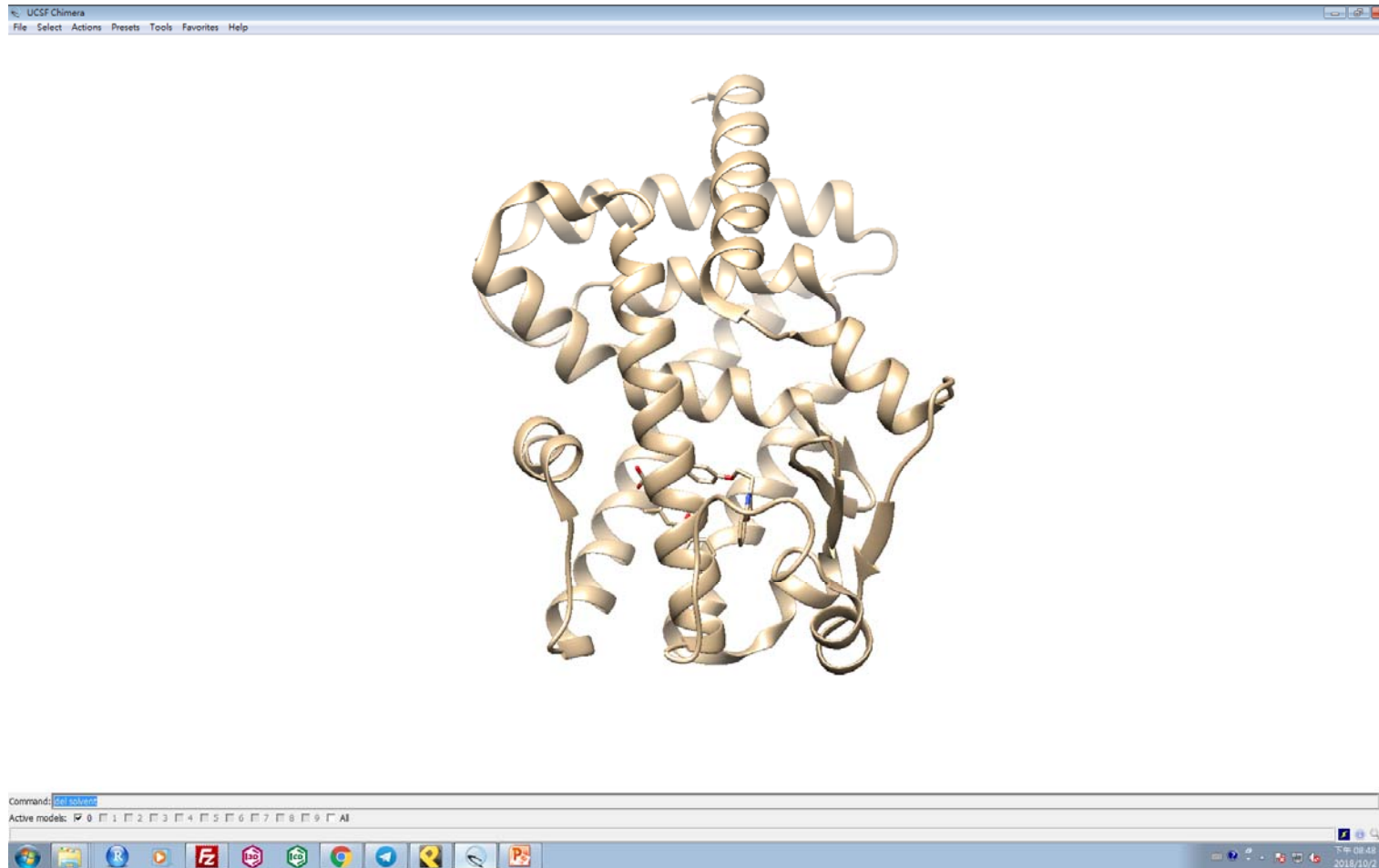
# 操作步驟



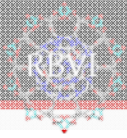
步驟十一：在下方Command列輸入指令：[del solvent](#)，刪除蛋白質、小分子以外的溶劑。



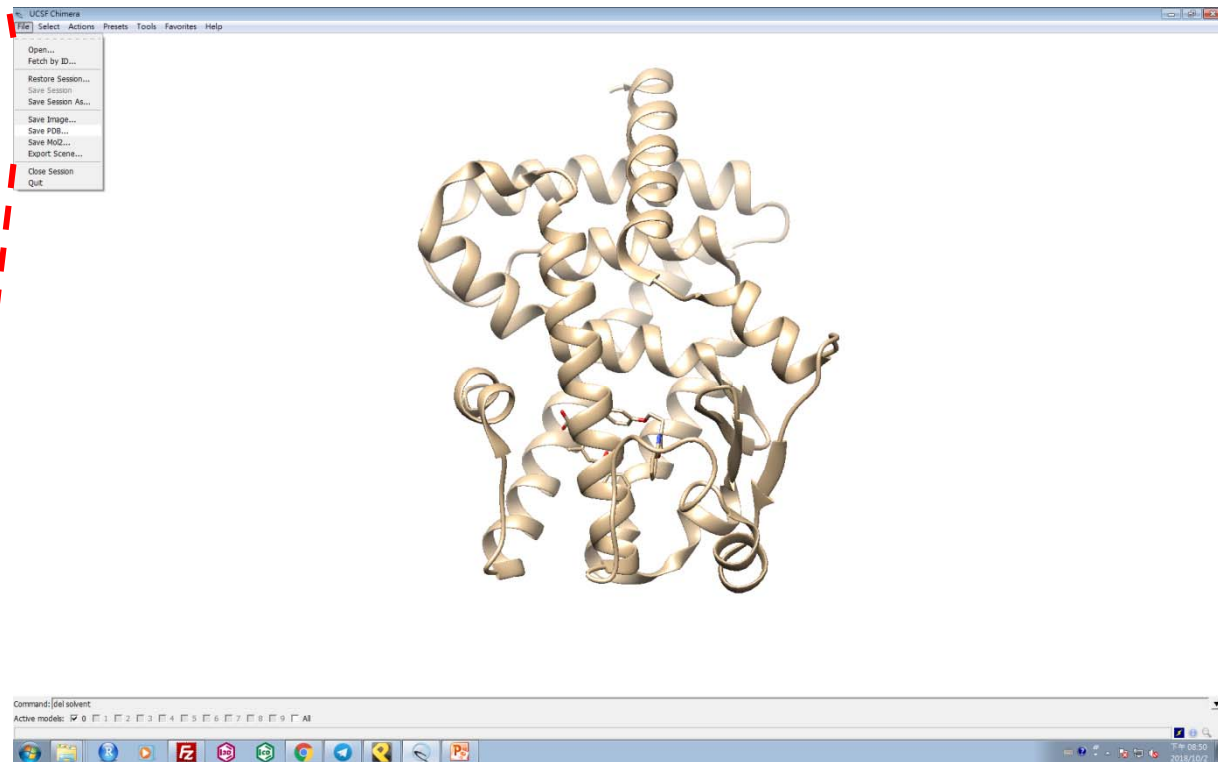
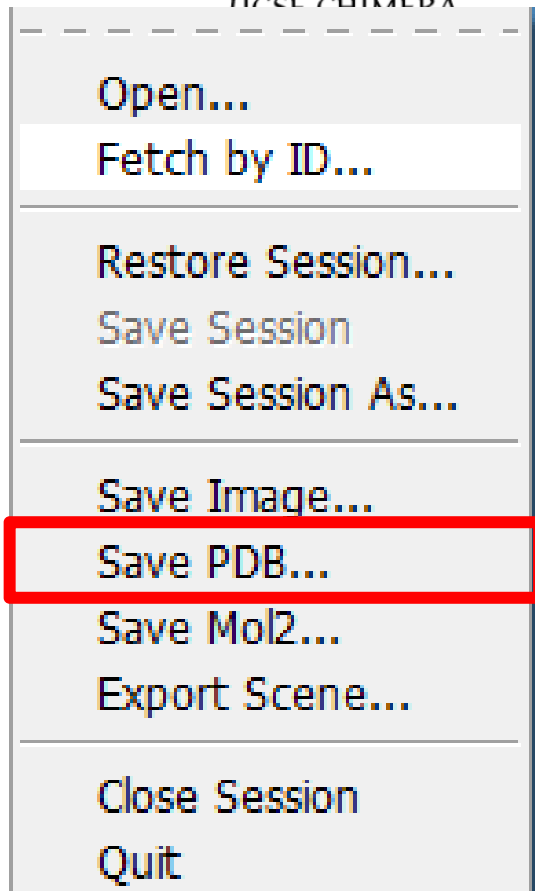
# 操作步驟



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。

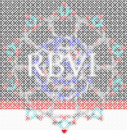


# 操作步驟

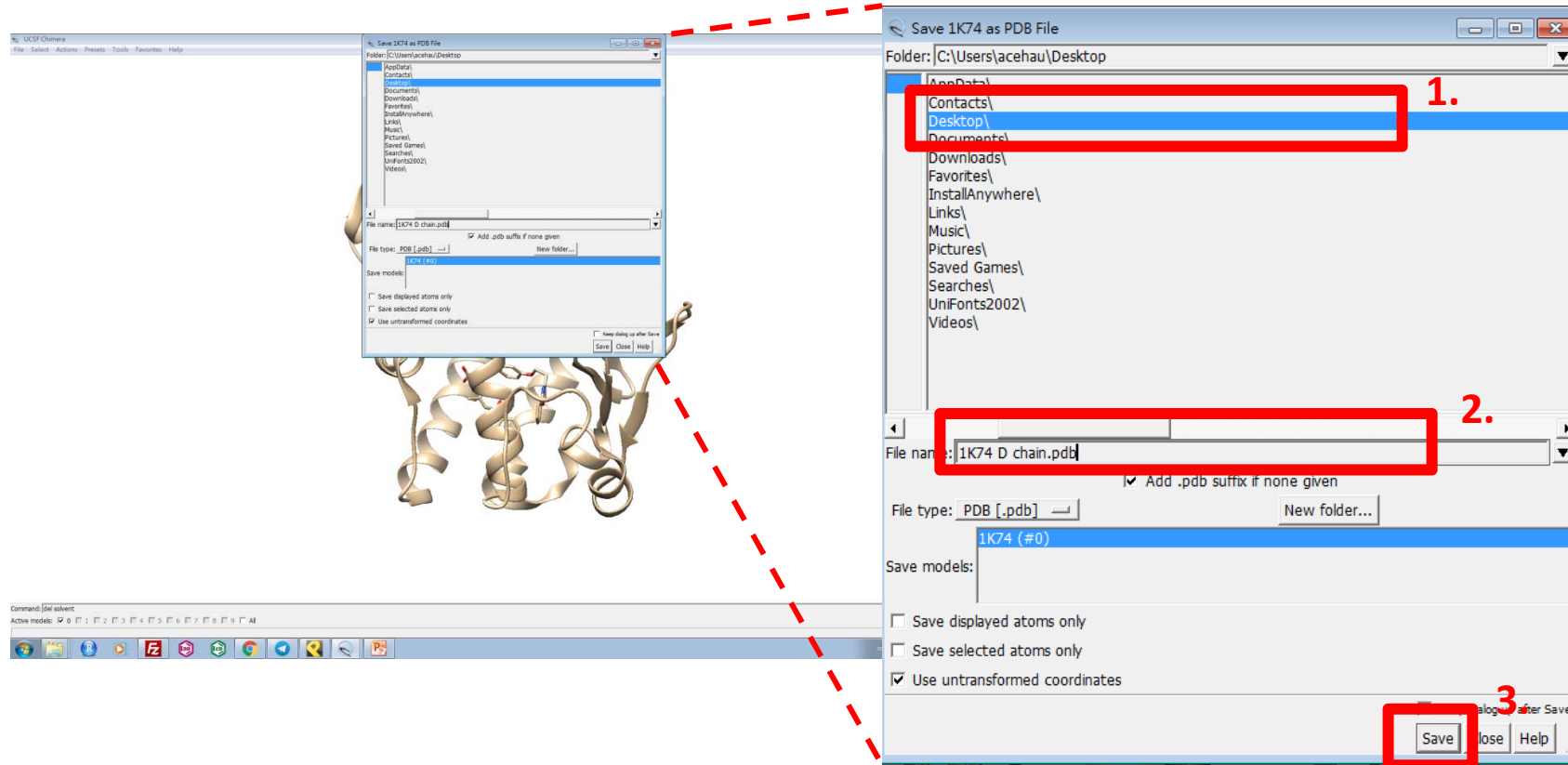


步驟十二：  
儲存蛋白資訊，在視窗右上方點選File -> Save PDB，  
點選完後會出現儲存檔案的視窗。



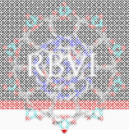


# 操作步驟



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。