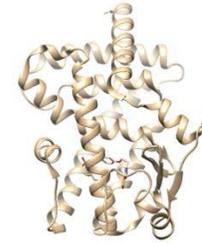




生物科技實驗



分子入塢 — (II) 準備大分子

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YTLab Presents



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](#)

Recent Citations

Structures of *Mycobacterium smegmatis* 70S ribosomes in complex with HFE, tmRNA, 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.

[\(Previously featured citations...\)](#)

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

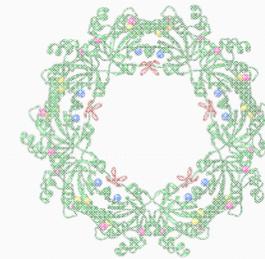
Gallery Sample

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](#).

[\(More samples...\)](#)



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

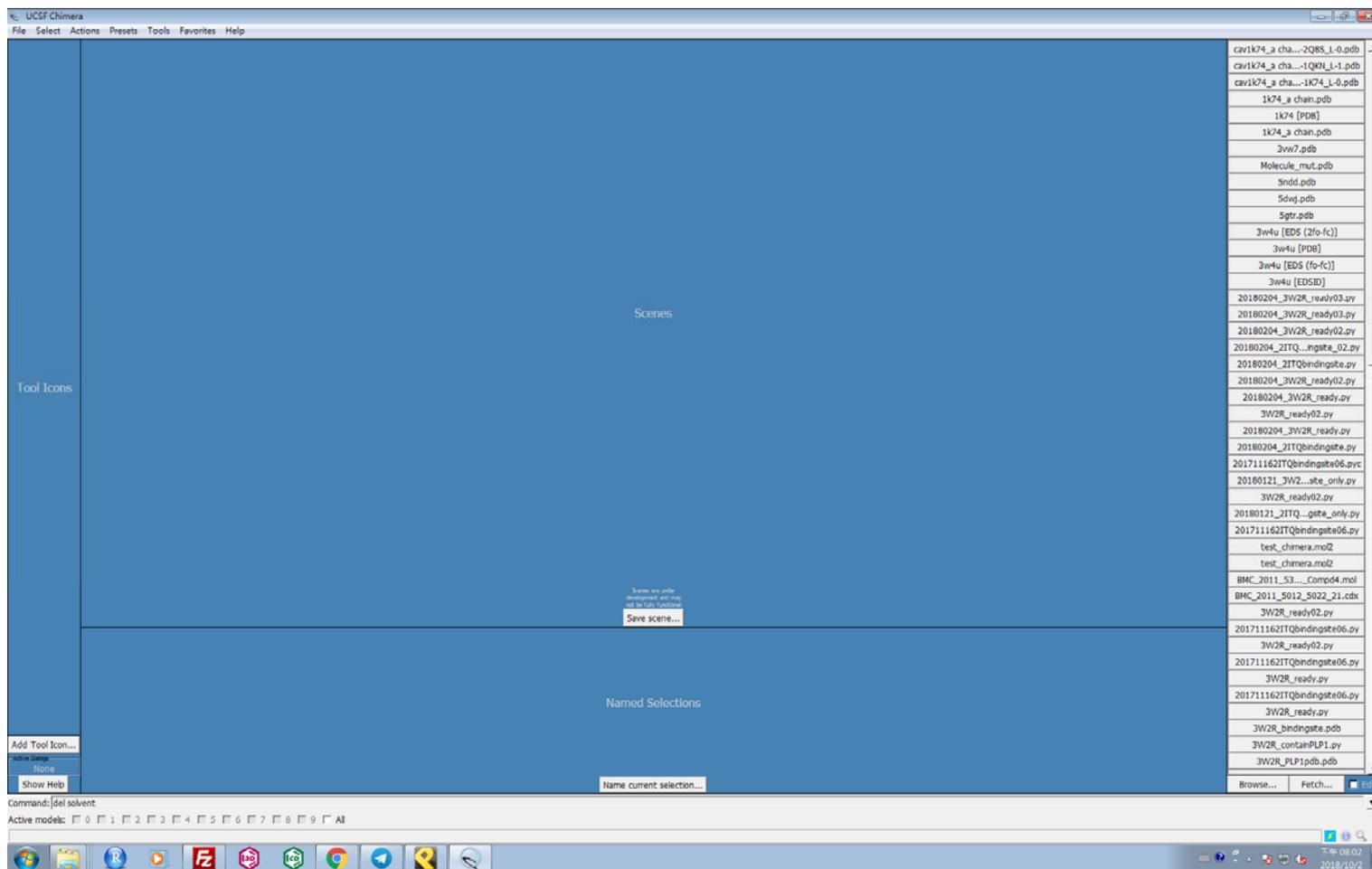
A production release candidate (version 1.13) is available. Please try it and report any problems. See the [release notes](#) for what's new.

[\(Previous news...\)](#)

Upcoming Events



操作步驟

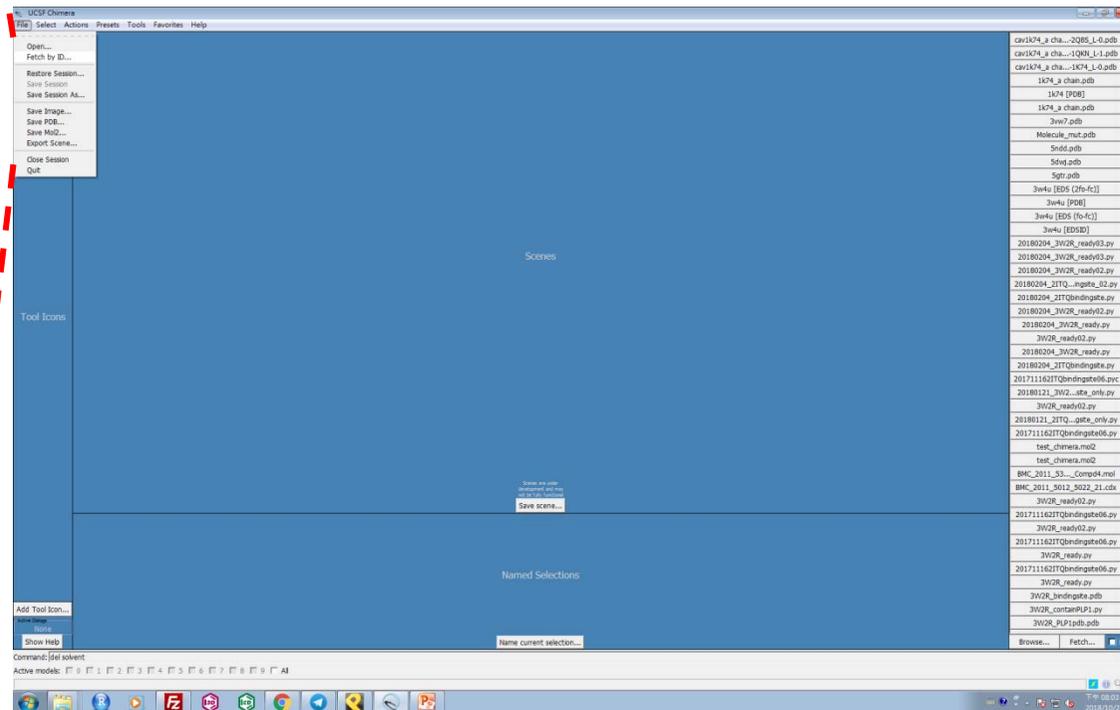


步驟一：開啟Chimera軟體。



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

1.

Database	ID	Example
<input type="radio"/> NDR		nde024
<input checked="" type="radio"/> PDB	1K74	1yti
<input type="radio"/> PDB (biounit)		1hho
<input type="radio"/> CATH		1cukA01
<input type="radio"/> SCOP		d1g0sa_
<input type="radio"/> PubChem		12123
<input type="radio"/> CASTp		1www
<input type="radio"/> EDS (2fo-fc)		1a0m
<input type="radio"/> EDS (fo-fc)		1a0m
<input type="radio"/> EMDB		5625
<input type="radio"/> EMDB & fit PDBs		1048
<input type="radio"/> PQS		2cwj
<input type="radio"/> ModBase		P04848
<input type="radio"/> VIPERdb		1ej6
<input type="radio"/> UniProt		P01138 NGF_HUMAN

Set download directory

Ignore any cached data

Keep dialog up after Fetch

Fetch Web Page Close Help

2.

UCSF Chimera

File Select Actions Present Tools Favorites Help

Fetch Structure by ID

Database	ID	Example
<input type="radio"/> NDR		nde024
<input checked="" type="radio"/> PDB	1K74	1yti
<input type="radio"/> PDB (biounit)		1hho
<input type="radio"/> CATH		1cukA01
<input type="radio"/> SCOP		d1g0sa_
<input type="radio"/> PubChem		12123
<input type="radio"/> CASTp		1www
<input type="radio"/> EDS (2fo-fc)		1a0m
<input type="radio"/> EDS (fo-fc)		1a0m
<input type="radio"/> EMDB		5625
<input type="radio"/> EMDB & fit PDBs		1048
<input type="radio"/> PQS		2cwj
<input type="radio"/> ModBase		P04848
<input type="radio"/> VIPERdb		1ej6
<input type="radio"/> UniProt		P01138 NGF_HUMAN

Set download directory

Ignore any cached data

Keep dialog up after Fetch

Fetch Web Page Close Help

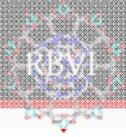
Named Selections

Command: [del] solvent

Active models: [0] [1] [2] [3] [4] [5] [6] [7] [8] [9] [A]

Time: 08:07 2018/2/02

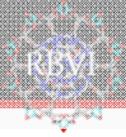
步驟三：
在PDB選項中輸入蛋白質代號：1K74，並按下Fetch紐。



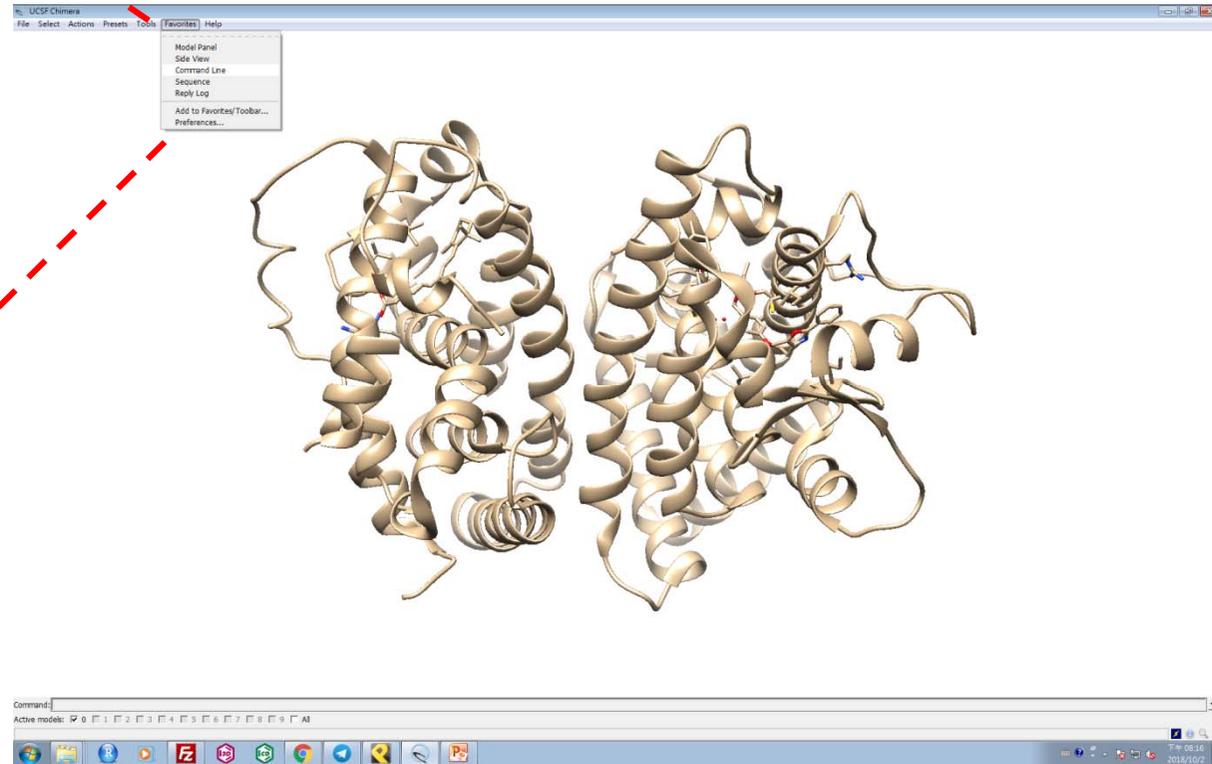
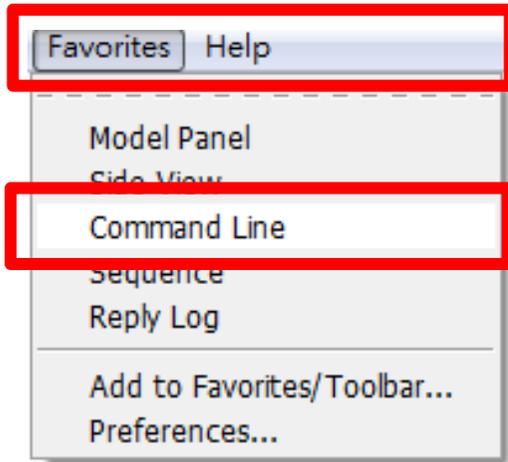
操作步驟



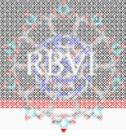
步驟四：此為成功下載蛋白質結構的畫面。



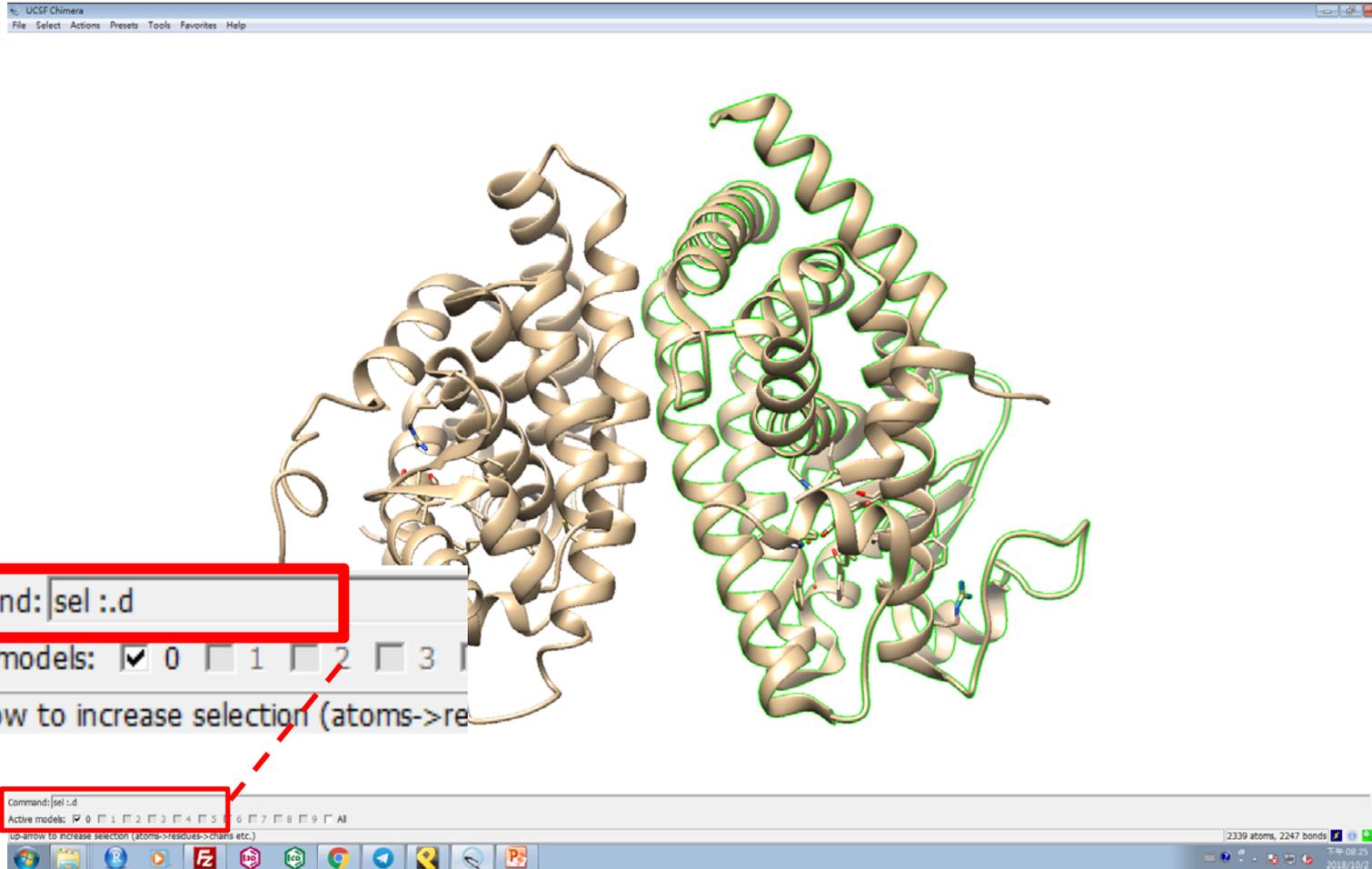
操作步驟



步驟五：
在視窗上方點選Favorites -> Command Line



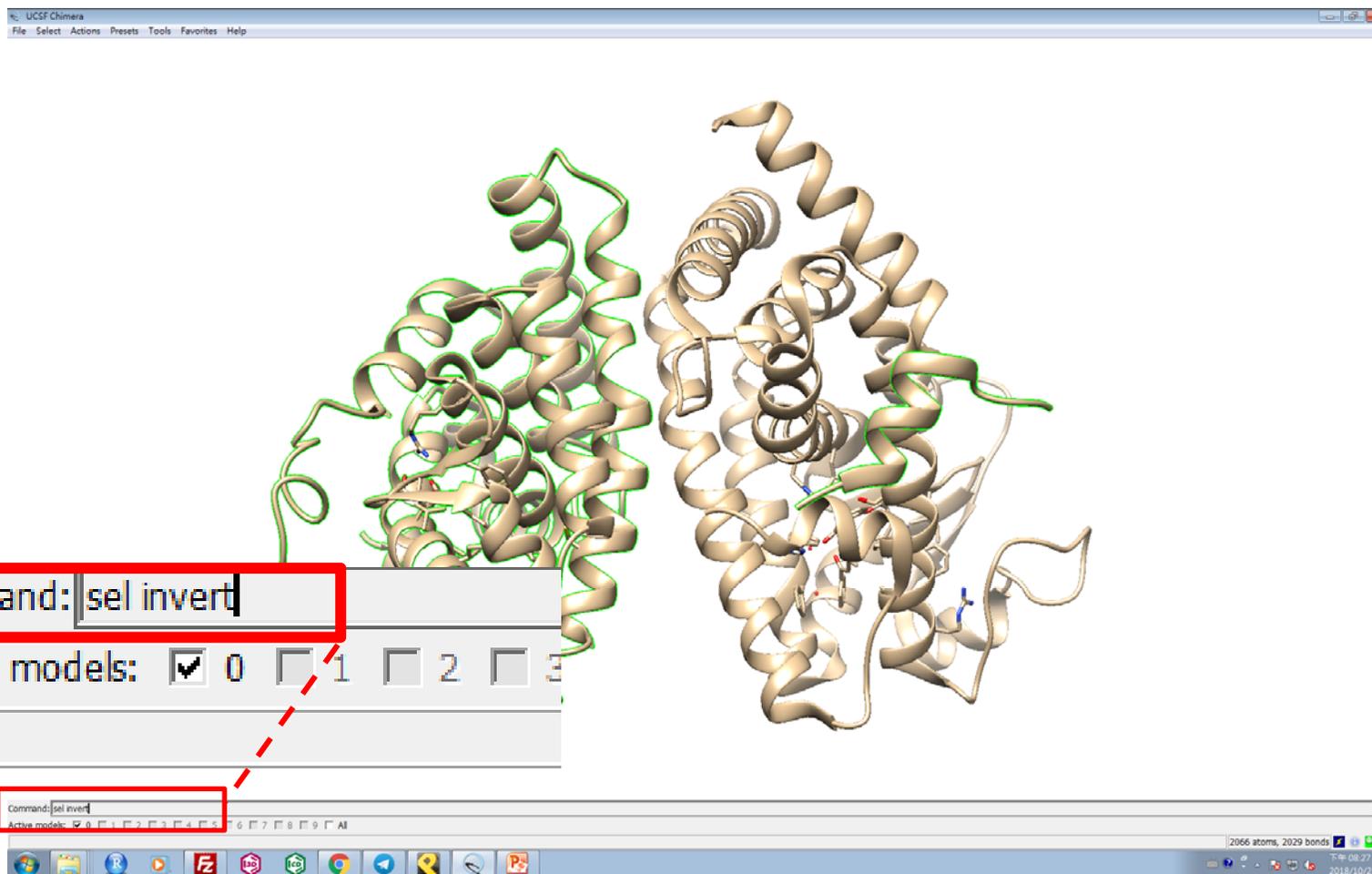
操作步驟



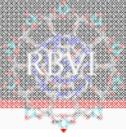
步驟六：
在下方Command列輸入指令：`sel :.d`，
按下Enter後D chain會被綠色外框框起來



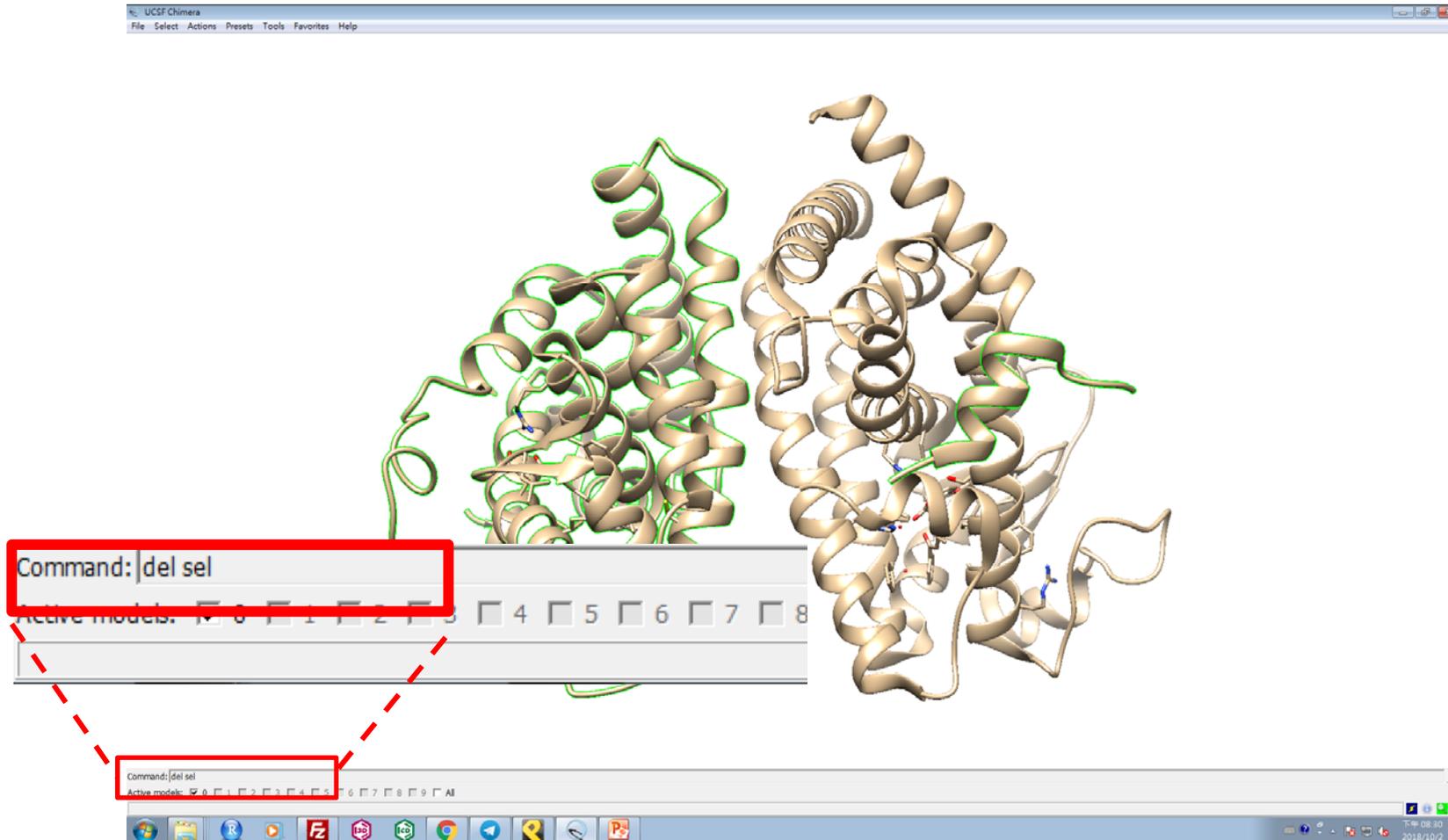
操作步驟



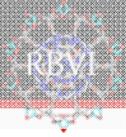
步驟七：在下方Command列輸入指令：`sel invert`，
按下Enter後D chain以外的部分會被綠色外框框起來



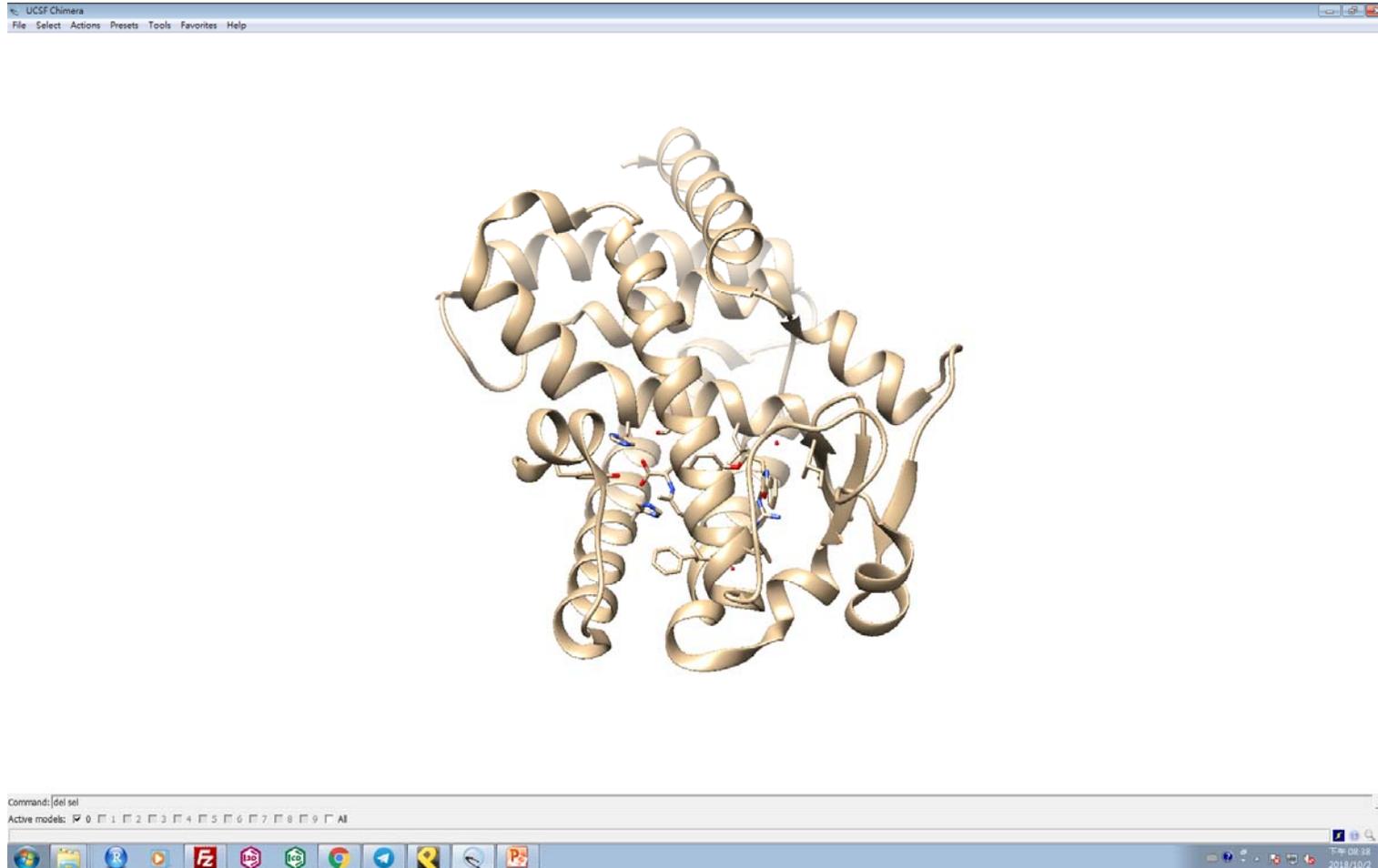
操作步驟



步驟八：在下方Command列輸入指令：`del sel`



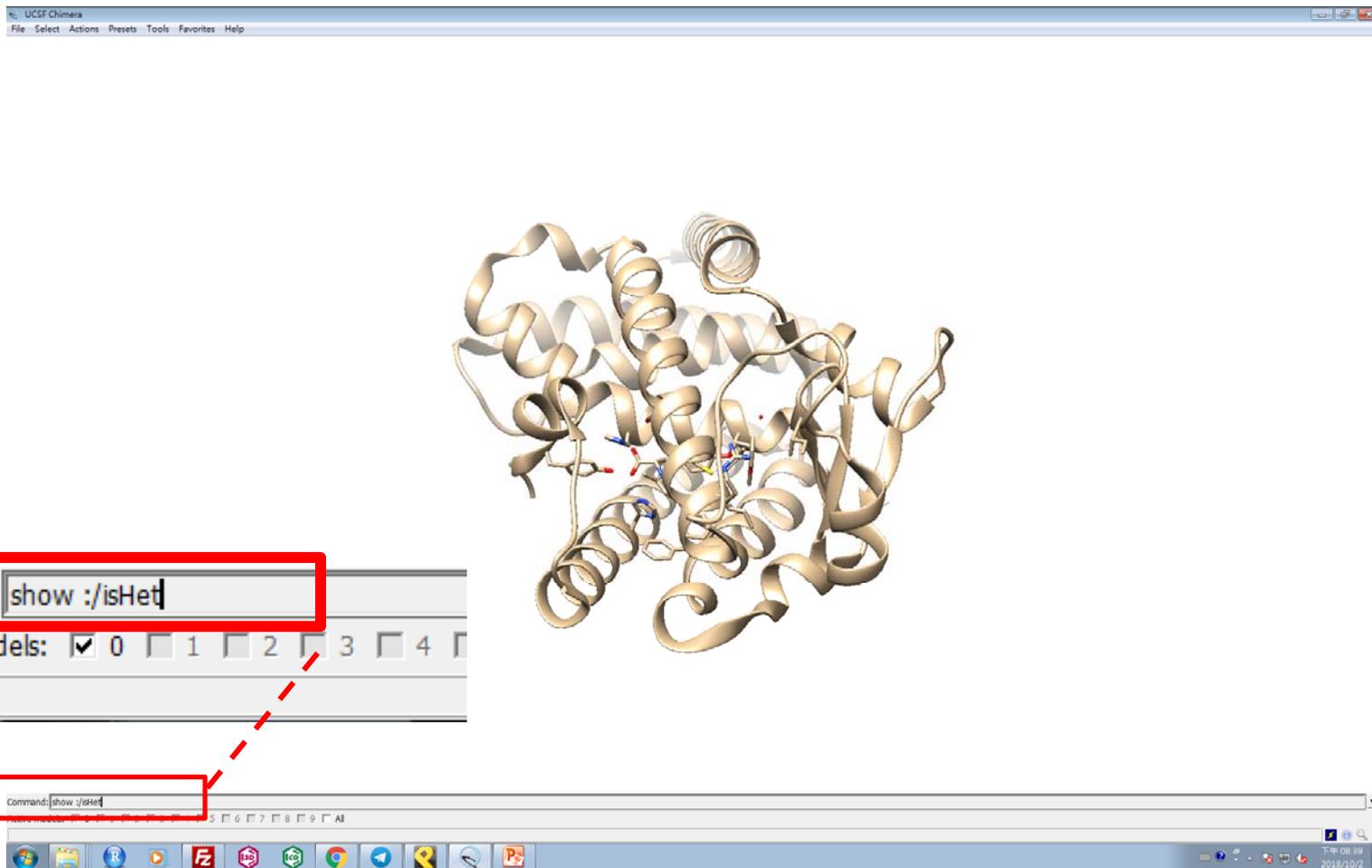
操作步驟



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



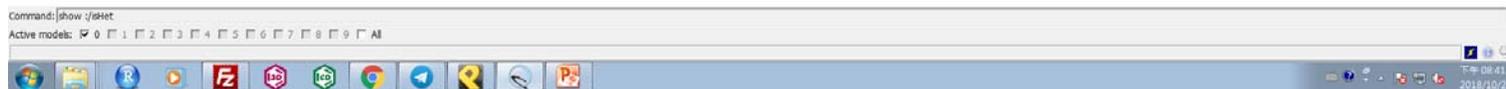
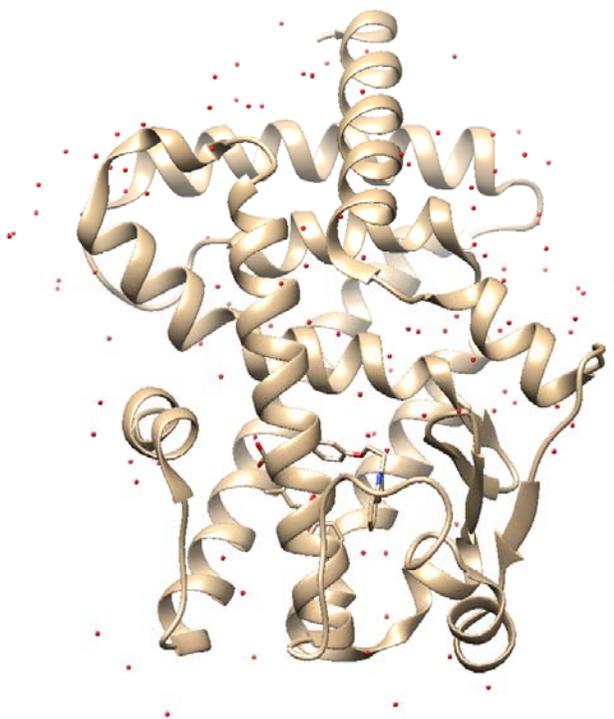
操作步驟



步驟十：在下方Command列輸入指令：`show :/isHet`



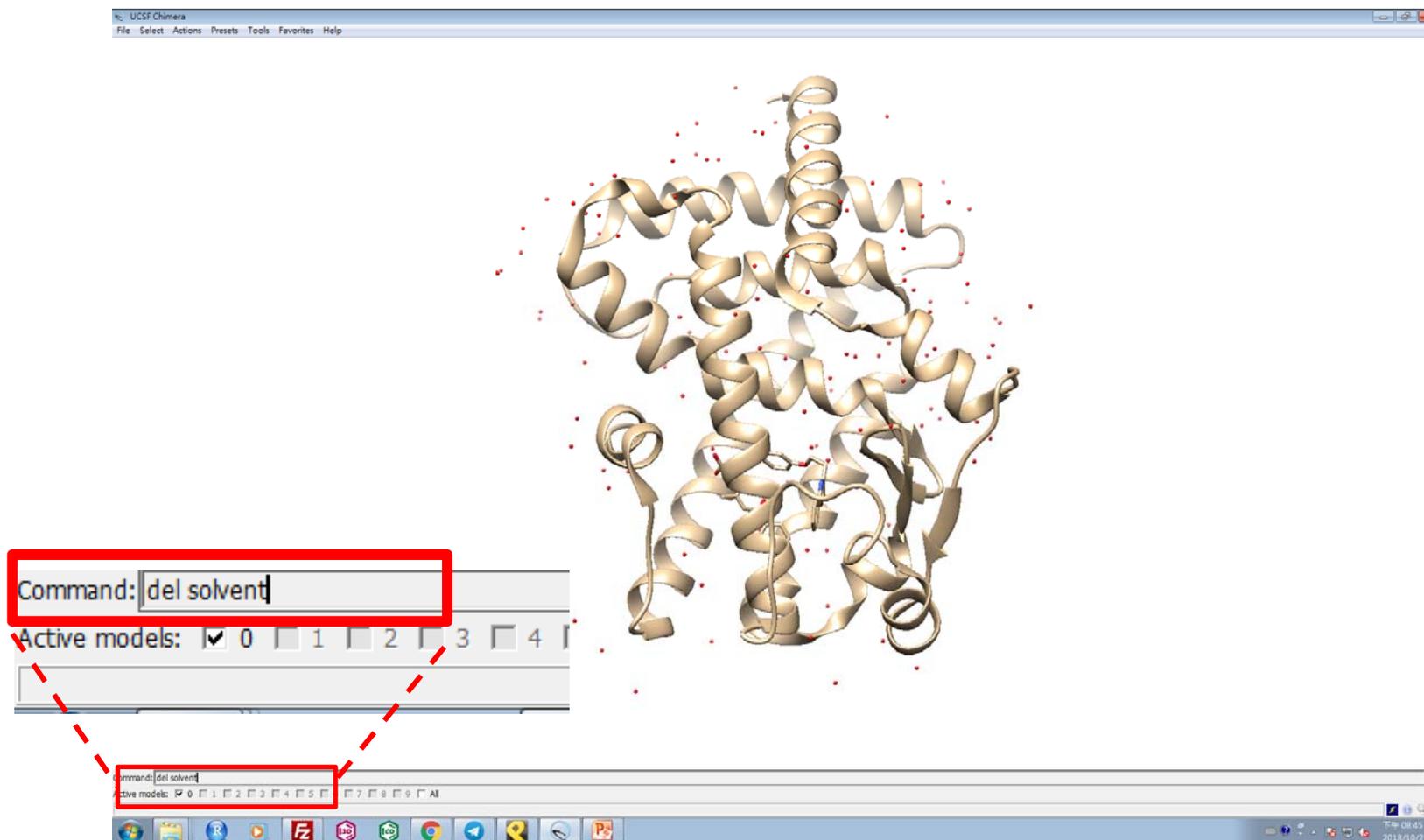
操作步驟



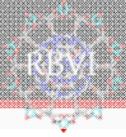
按下Enter後除了蛋白質之外的物質，皆會以原子、分子的形式顯示出來，有人知道途中紅色圓點是什麼嗎？



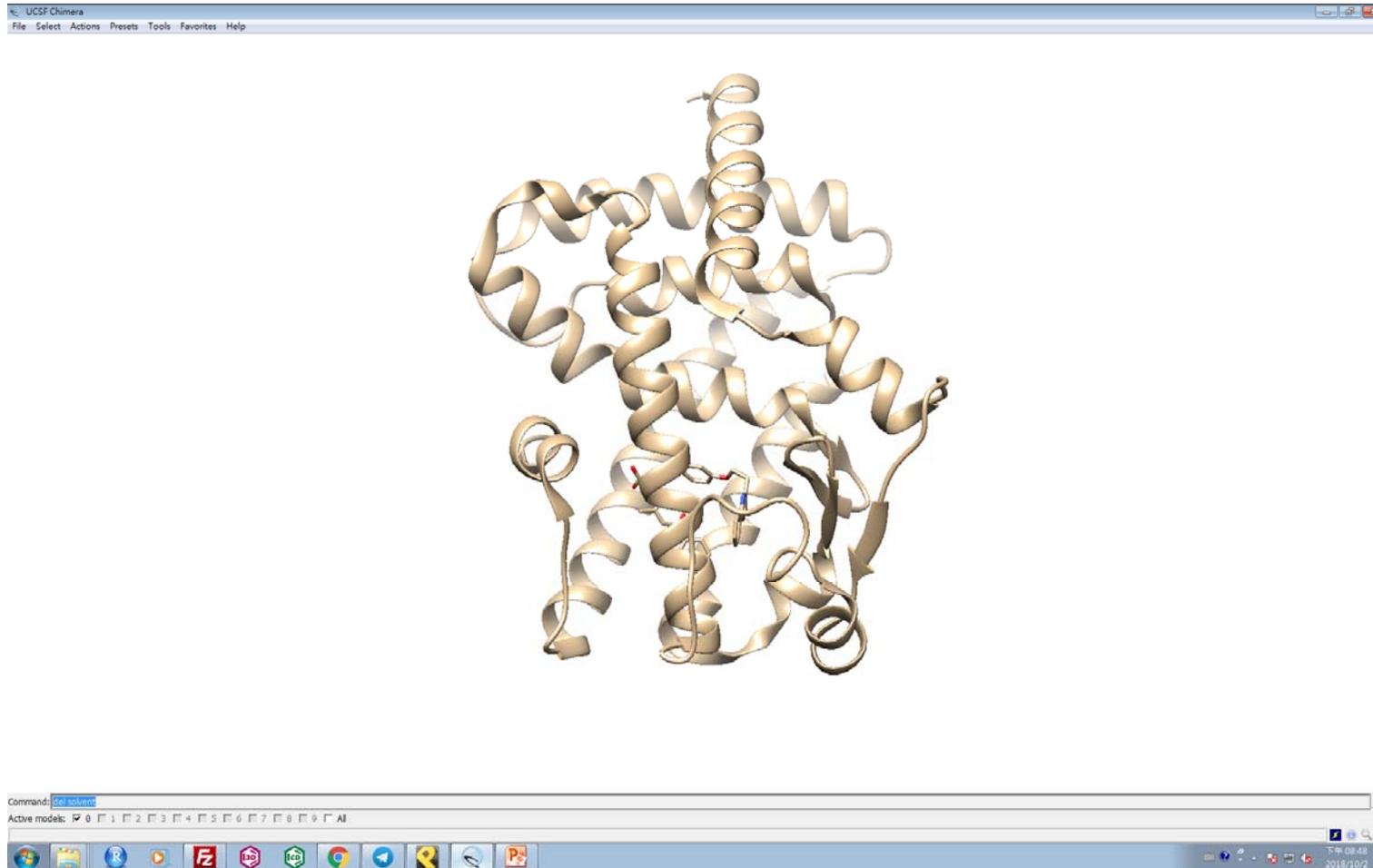
操作步驟



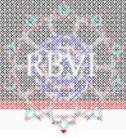
步驟十一：在下方Command列輸入指令：`del solvent`，刪除蛋白質、小分子以外的溶劑。



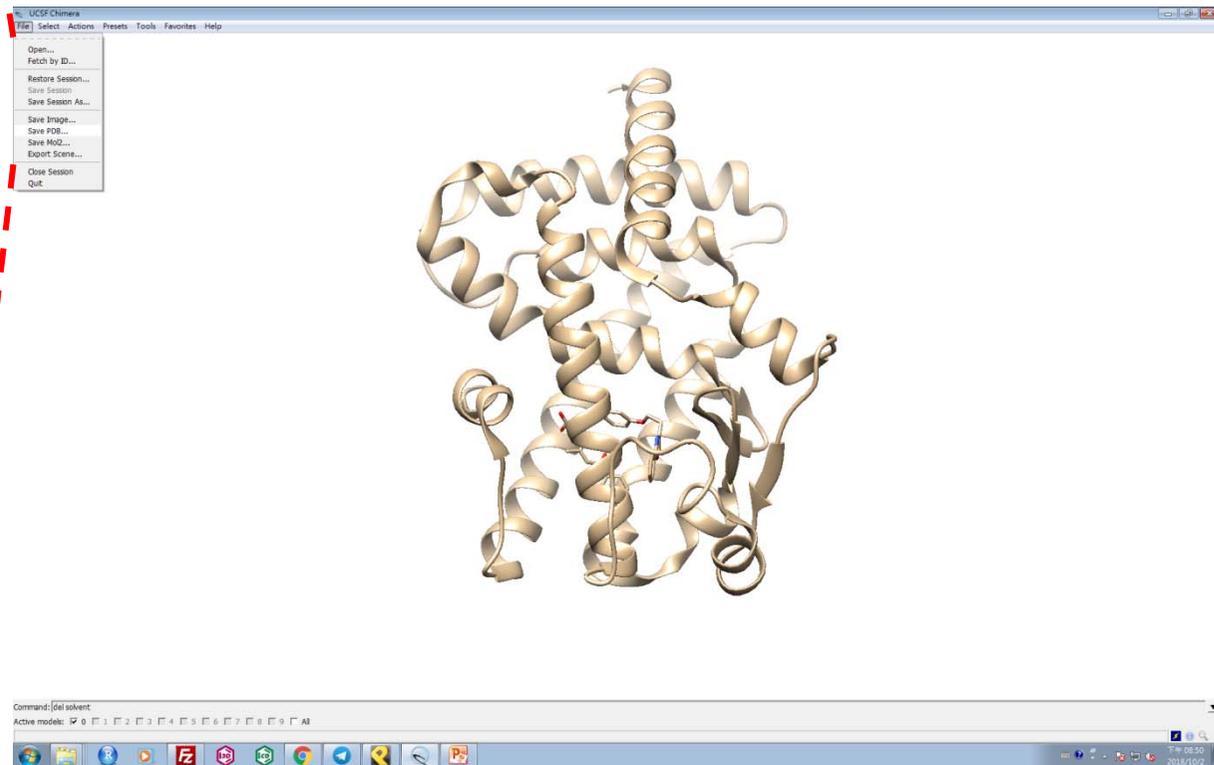
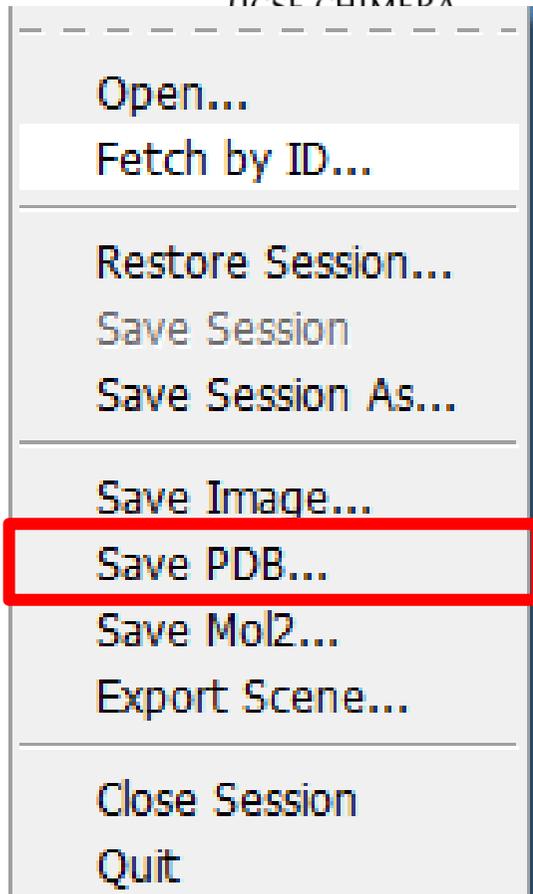
操作步驟



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。

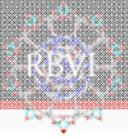


操作步驟

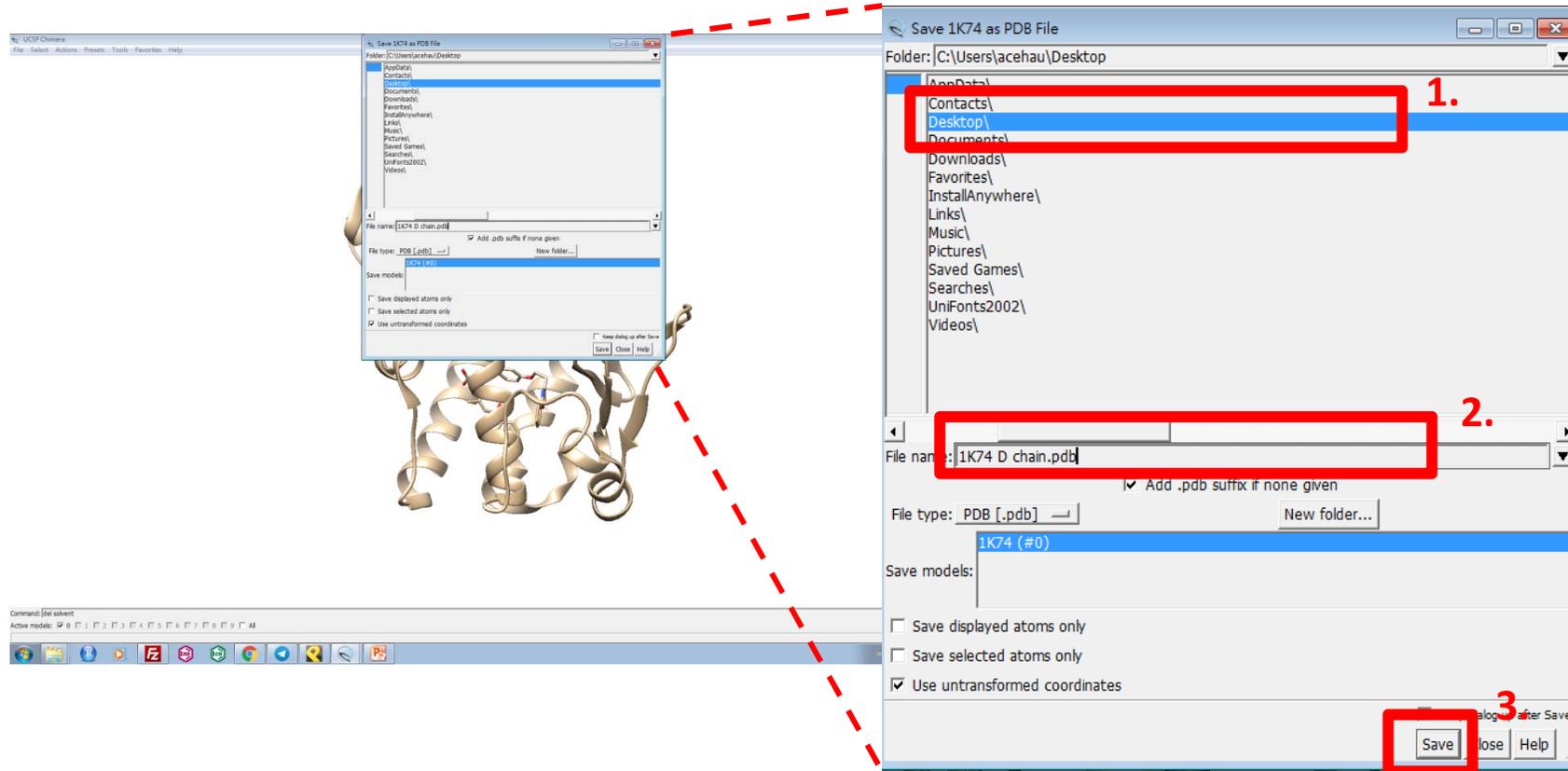


步驟十二：

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。

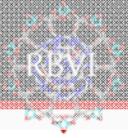


操作步驟



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。