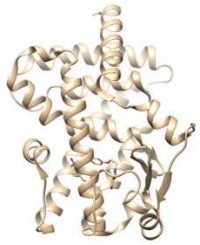
生物科技實驗



分子入塢 —（III）執行分子入塢

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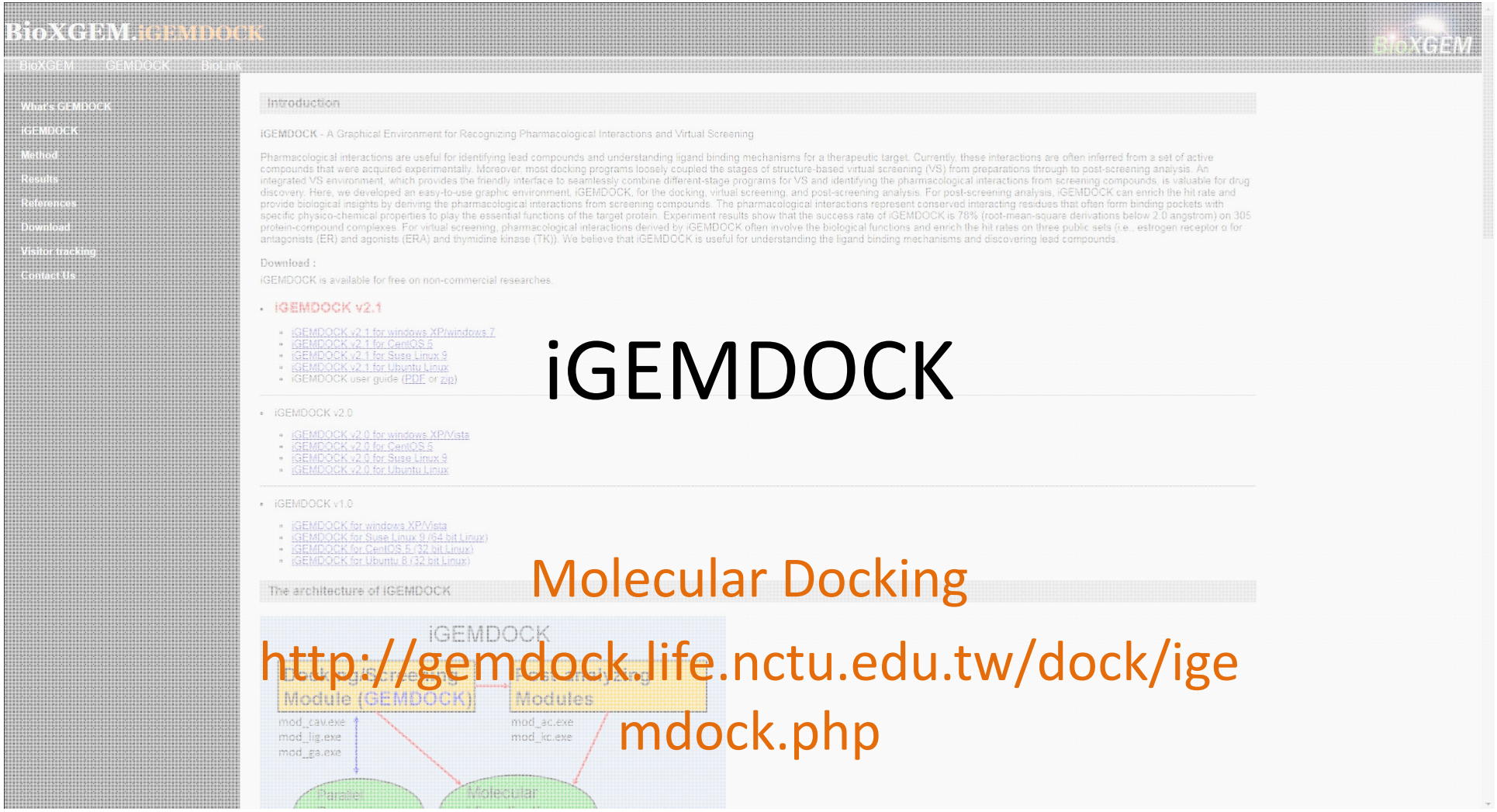
實驗室：第一教學大樓 N1025室
Tel: (07) 3121101 ext. 2792
eMail：ytlin@kmu.edu.tw

YTLab Presents

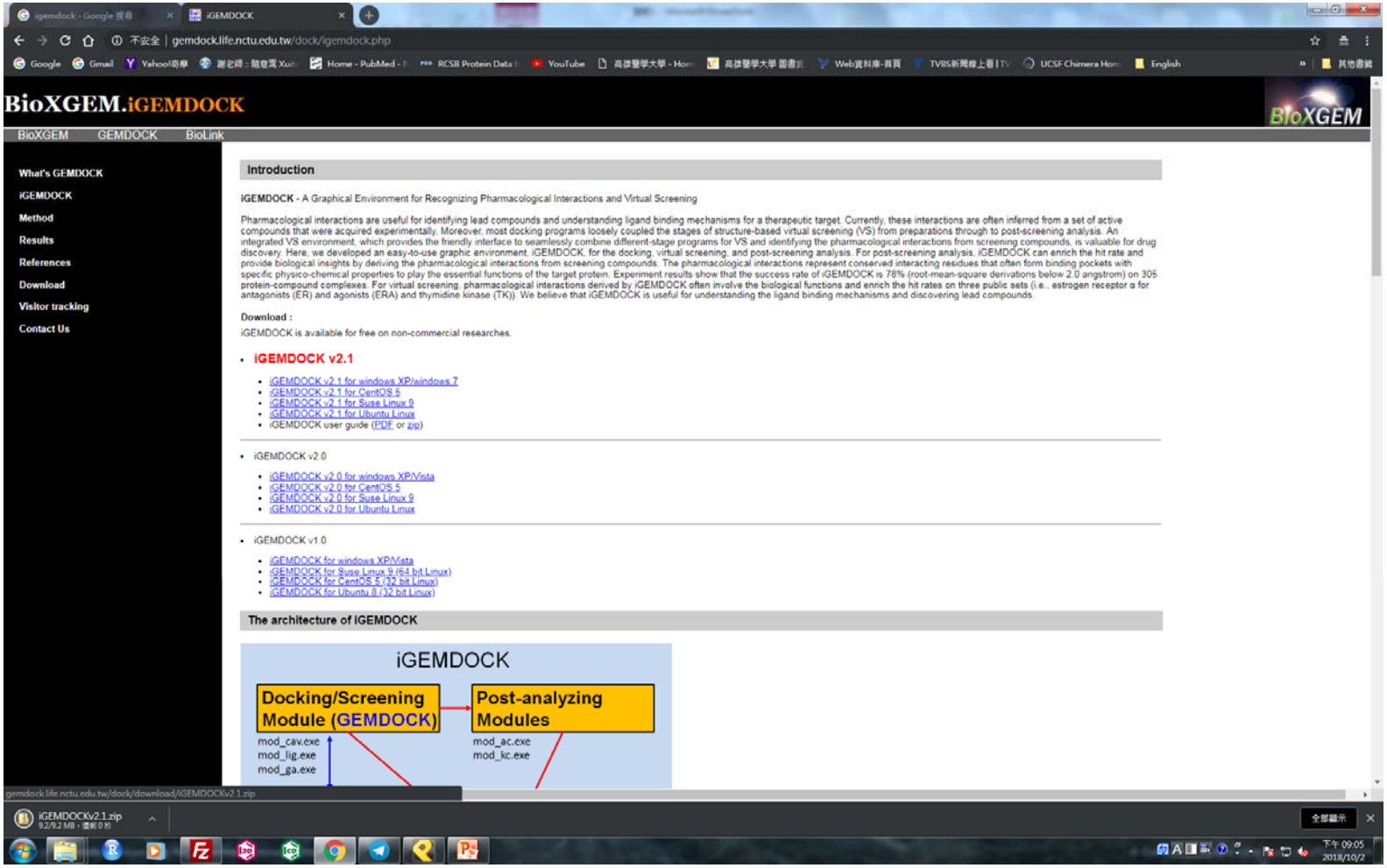


iGEMDOCK

Molecular Docking

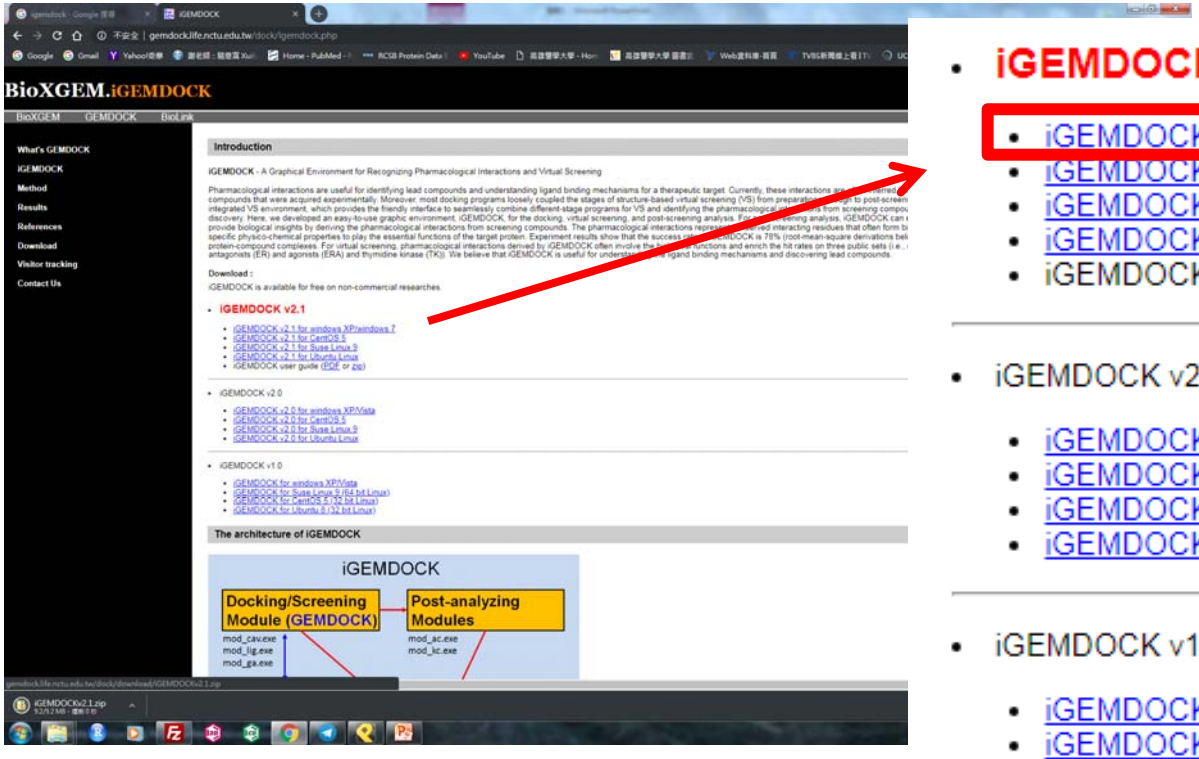
http://gemdock.life.nctu.edu.tw/dock/igemdock.php

操作步驟



步驟一：到iGEMDOCK網站

操作步驟



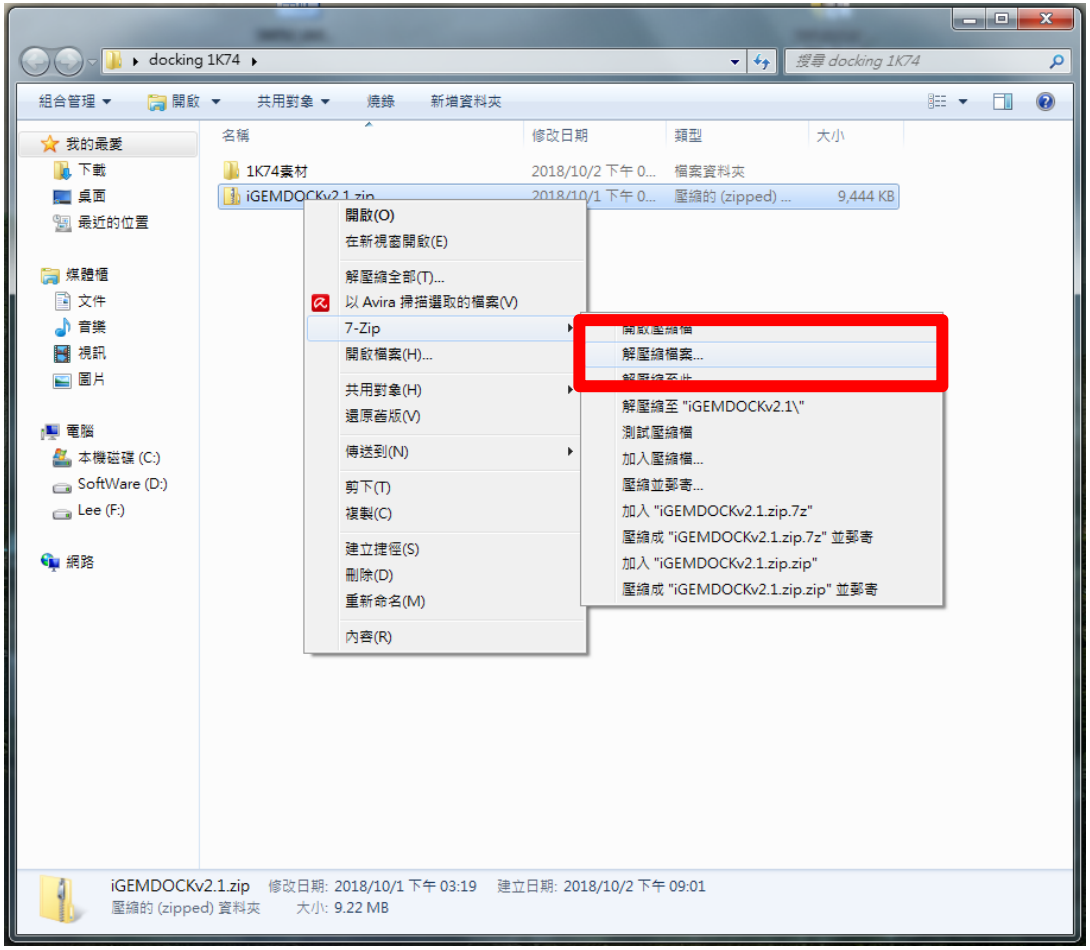
- **iGEMDOCK v2.1**
  - iGEMDOCK v2.1 for windows XP/windows 7
  - iGEMDOCK v2.1 for CentOS 5
  - iGEMDOCK v2.1 for Suse Linux 9
  - iGEMDOCK v2.1 for Ubuntu Linux
  - iGEMDOCK user guide (PDF or zip)

- iGEMDOCK v2.0
  - iGEMDOCK v2.0 for windows XP/Vista
  - iGEMDOCK v2.0 for CentOS 5
  - iGEMDOCK v2.0 for Suse Linux 9
  - iGEMDOCK v2.0 for Ubuntu Linux

- iGEMDOCK v1.0
  - iGEMDOCK for windows XP/Vista
  - iGEMDOCK for Suse Linux 9 (64 bit Linux)
  - iGEMDOCK for CentOS 5 (32 bit Linux)
  - iGEMDOCK for Ubuntu 8 (32 bit Linux)

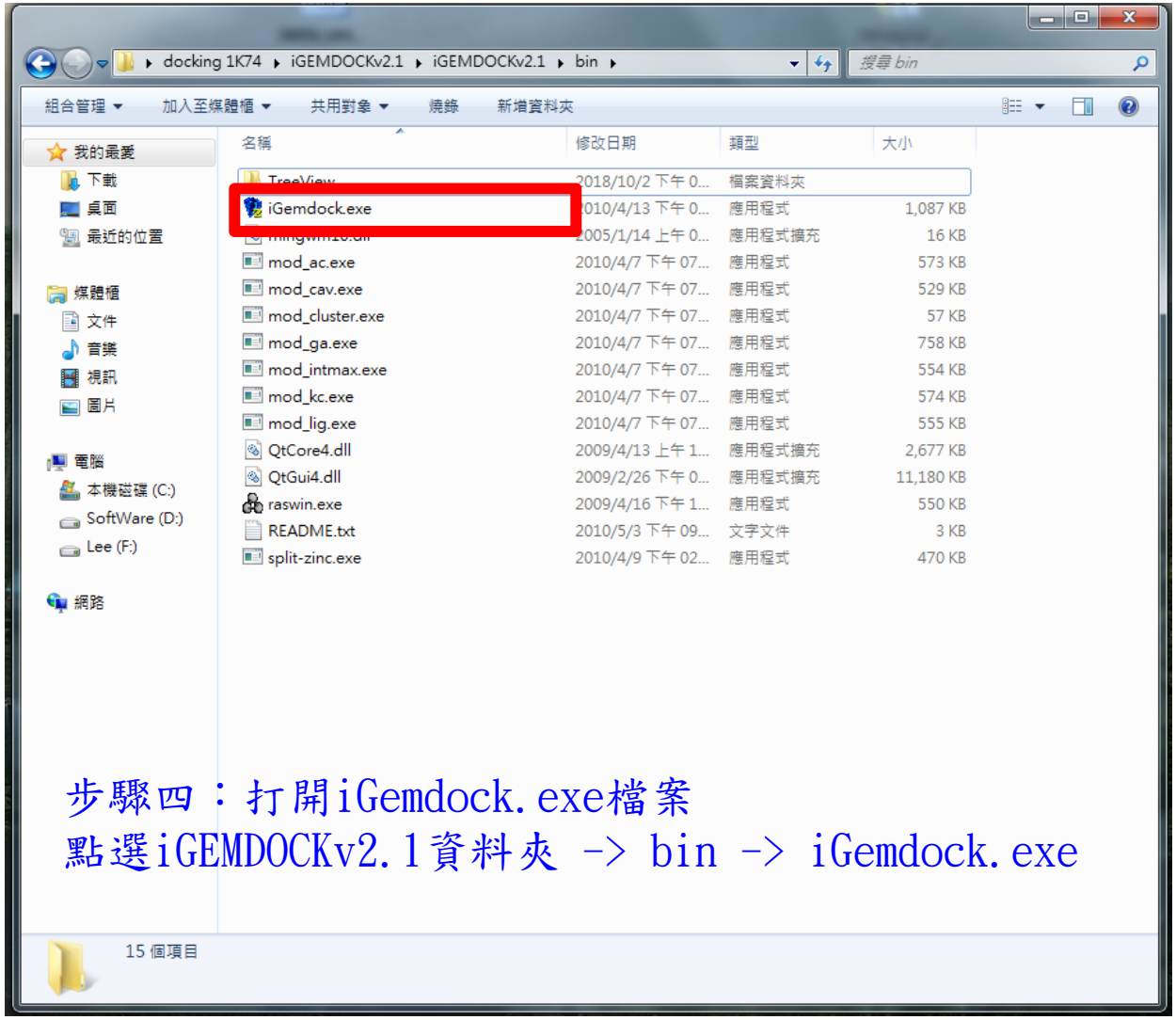
步驟二：下載iGWMDOCK軟體 v2.1 for windows XP/windows 7

操作步驟



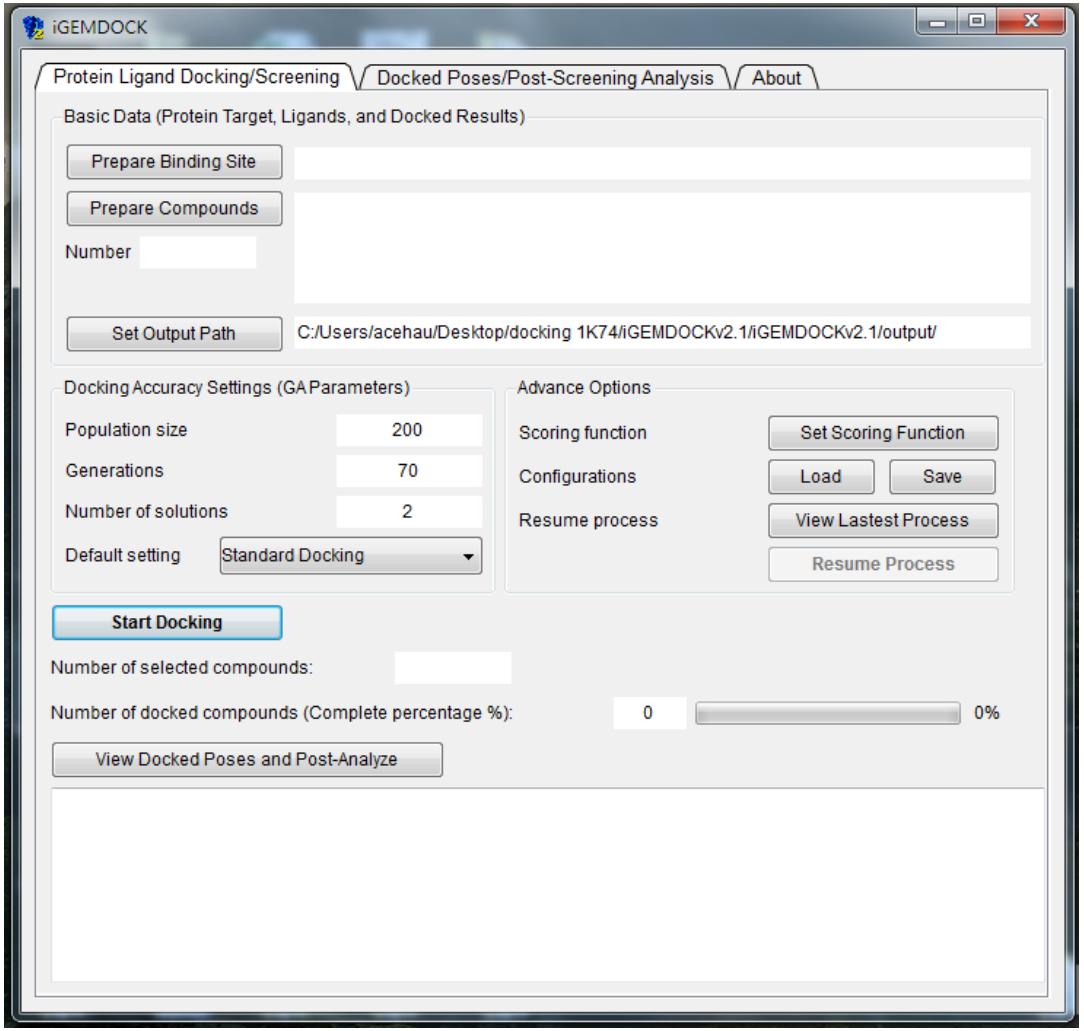
步驟三：按右鍵，解壓縮iGEMDOCKv2.1.zip壓縮檔。

操作步驟



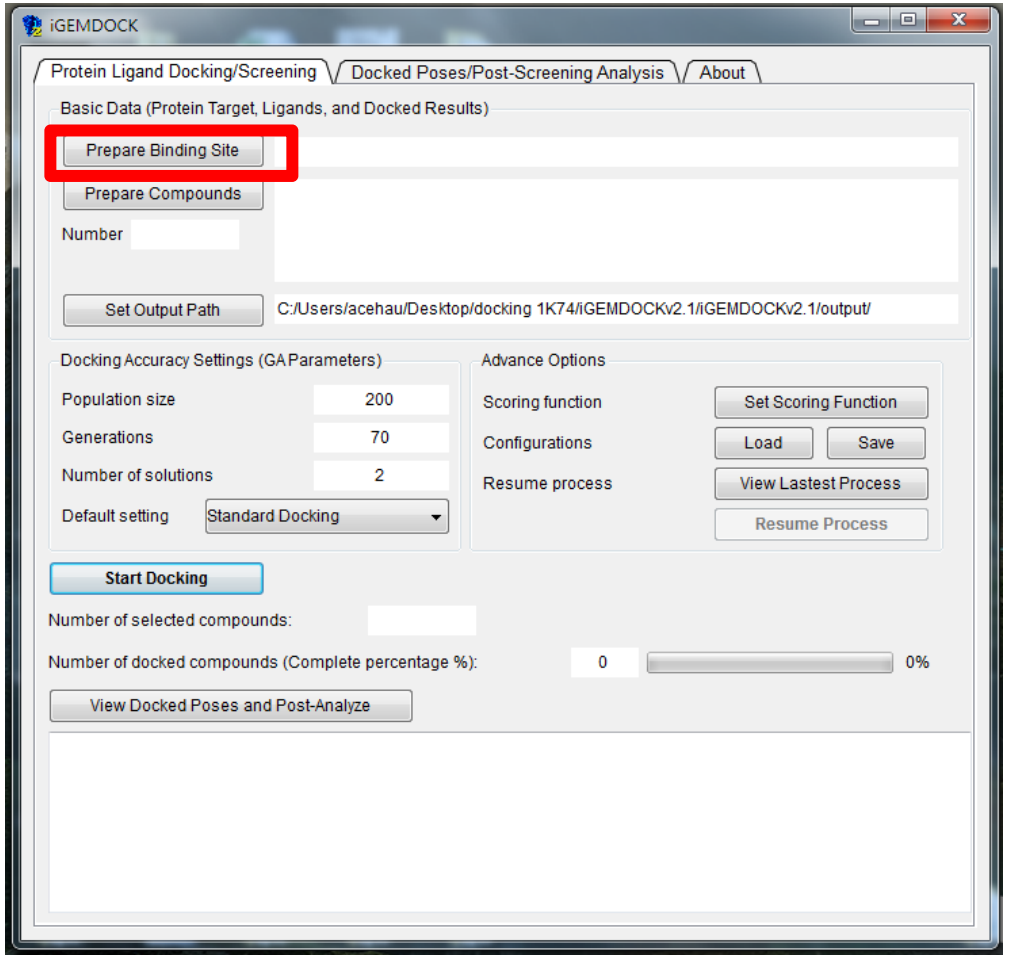
步驟四：打開iGemdock.exe檔案
點選iGEMDOCKv2.1資料夾 -> bin -> iGemdock.exe

操作步驟



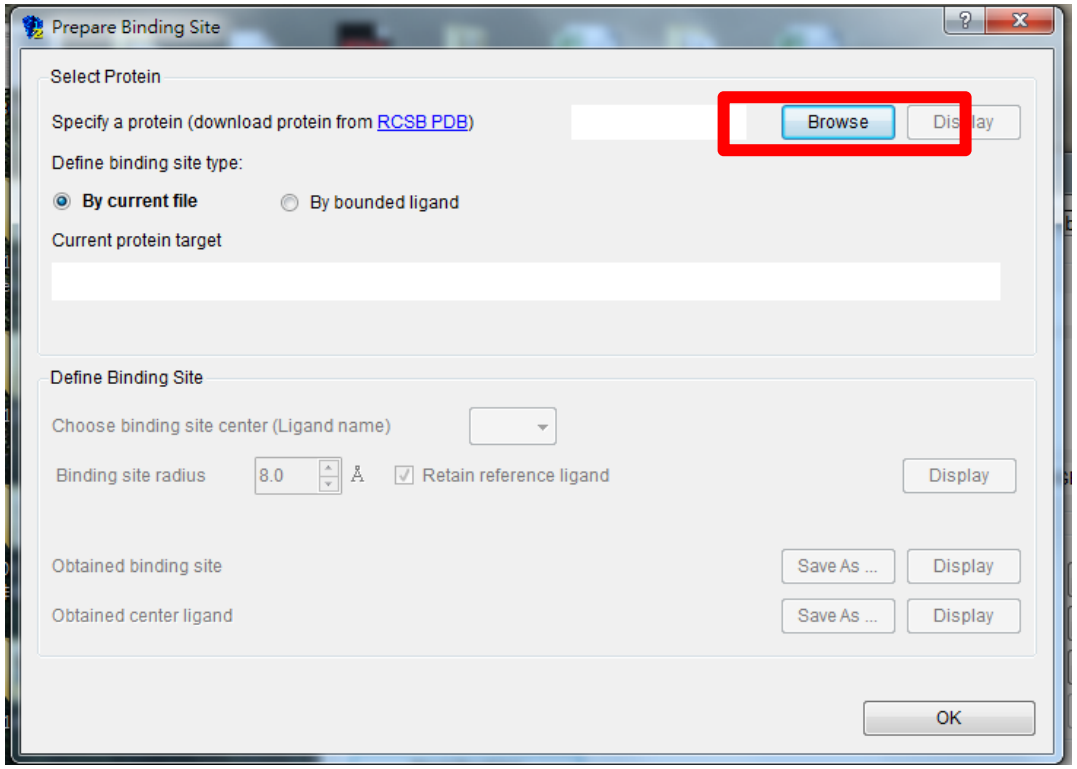
此為iGEMDOCK程式介面

操作步驟



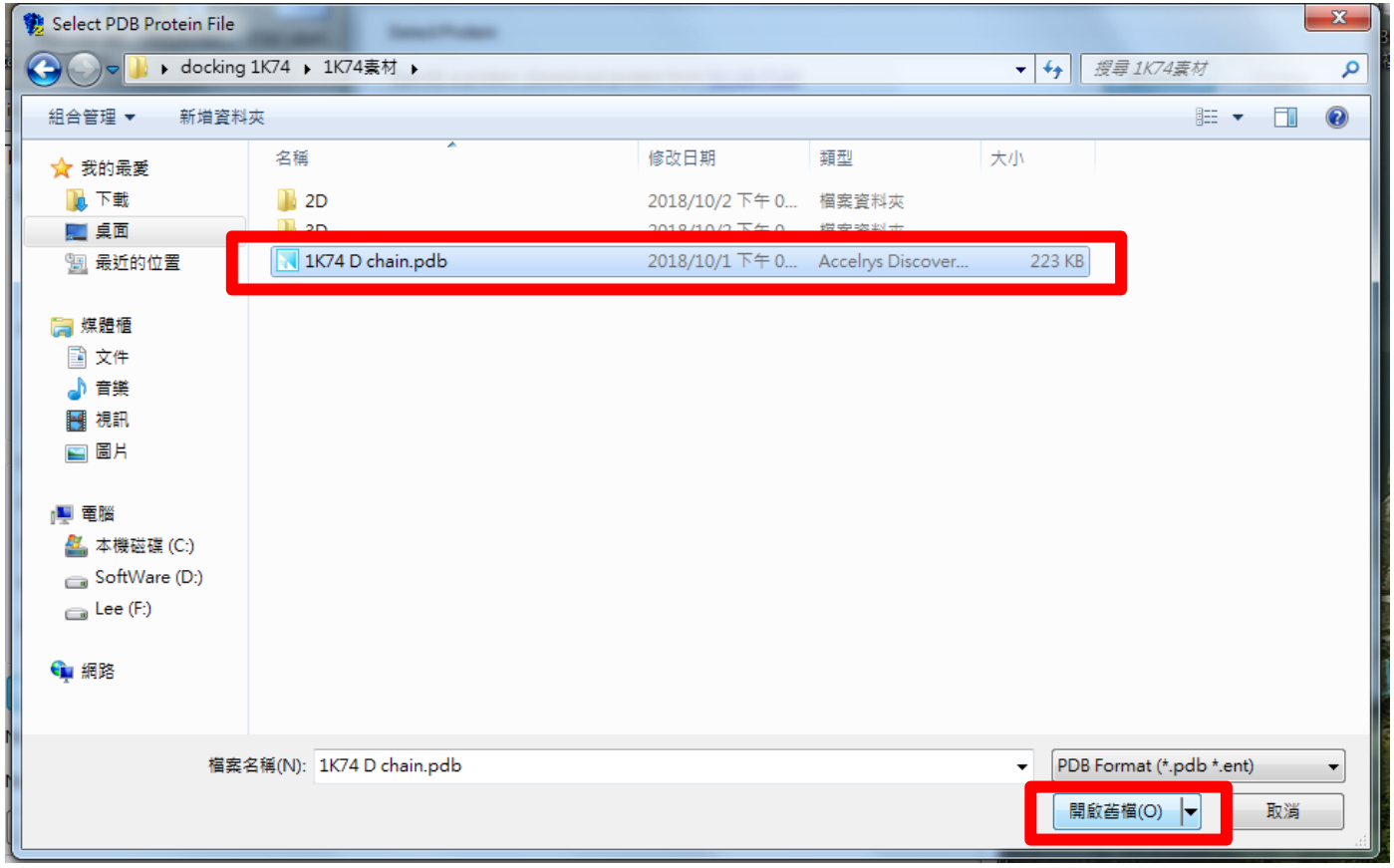
步驟四：按下Prepare Binding Site

操作步驟



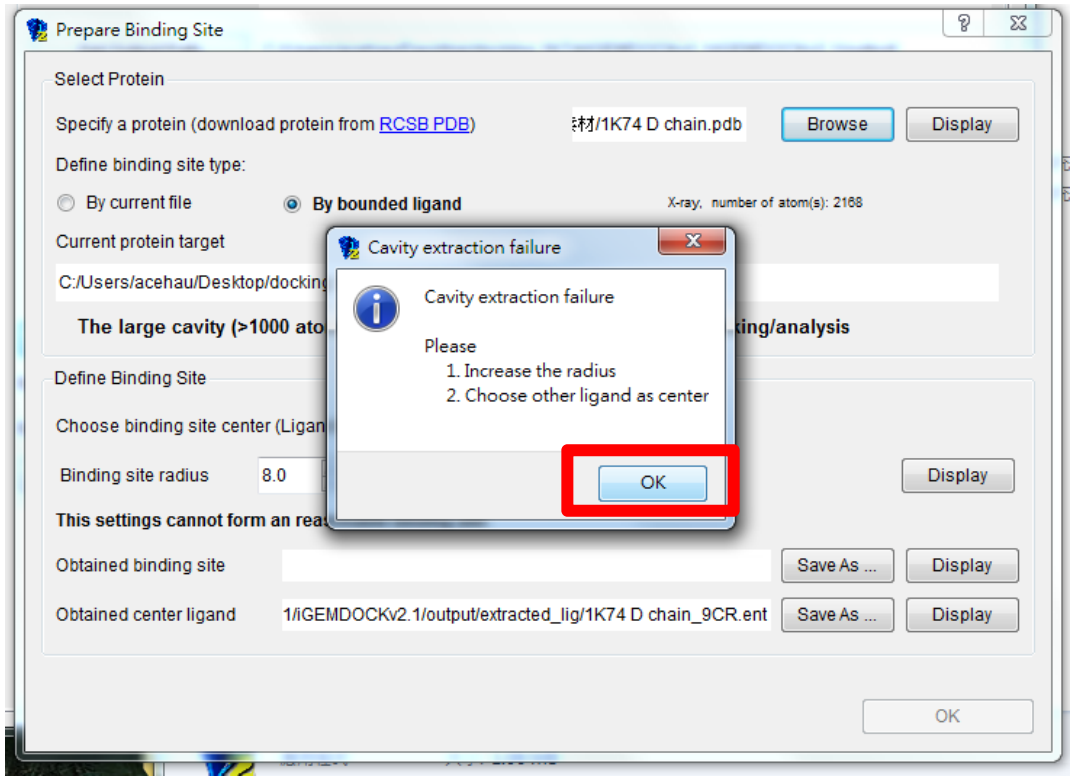
步驟五：按下Browse

操作步驟



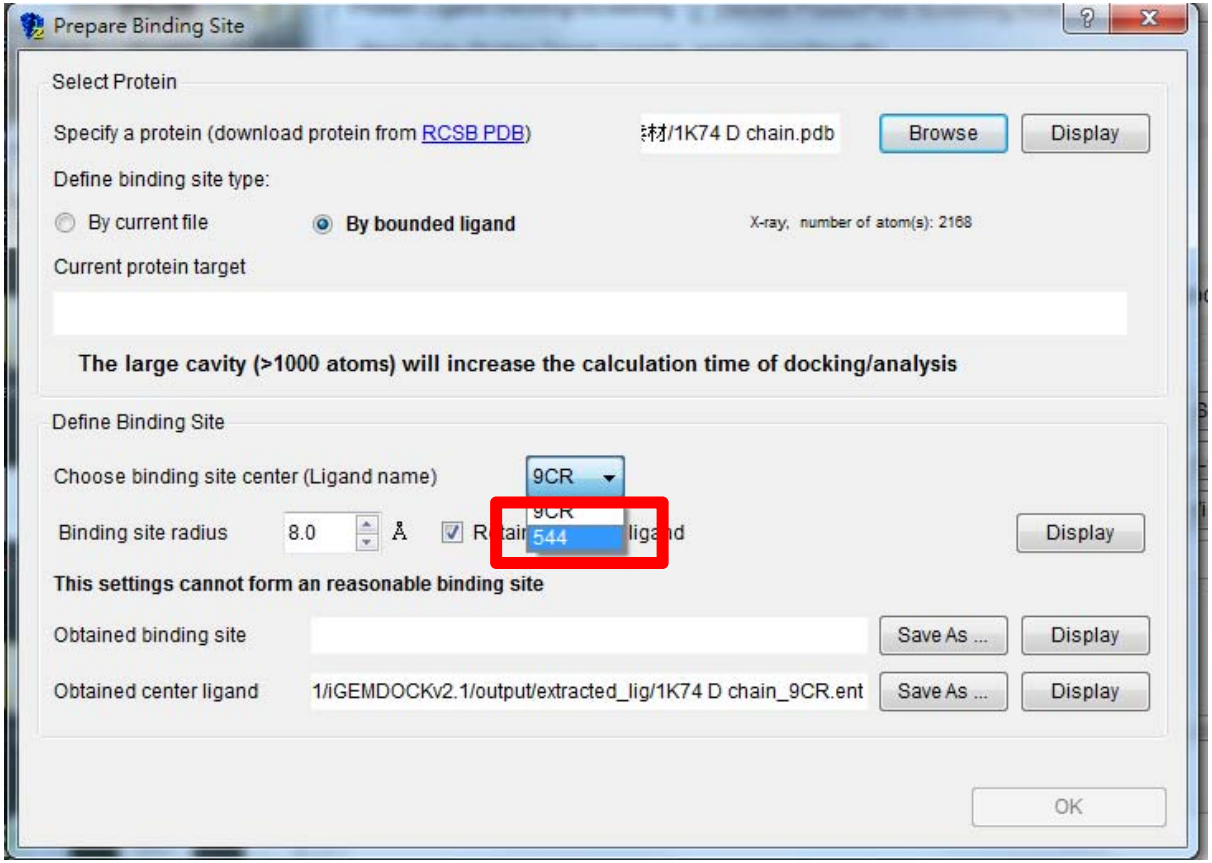
步驟六：找到先前存放好的蛋白質檔案，並開啟

操作步驟



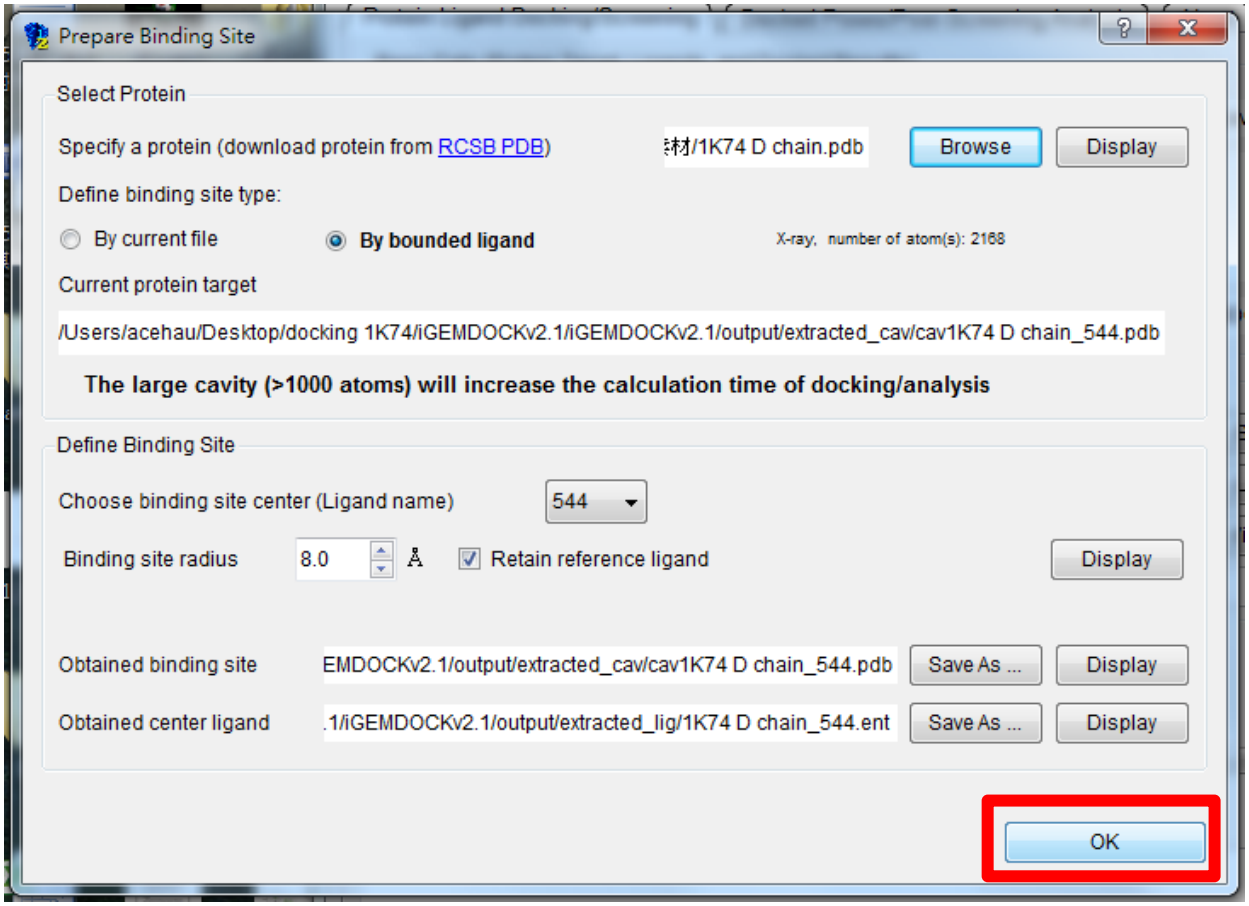
步驟七：程式會出現設定binding site的提醒視窗，按下OK即可

操作步驟



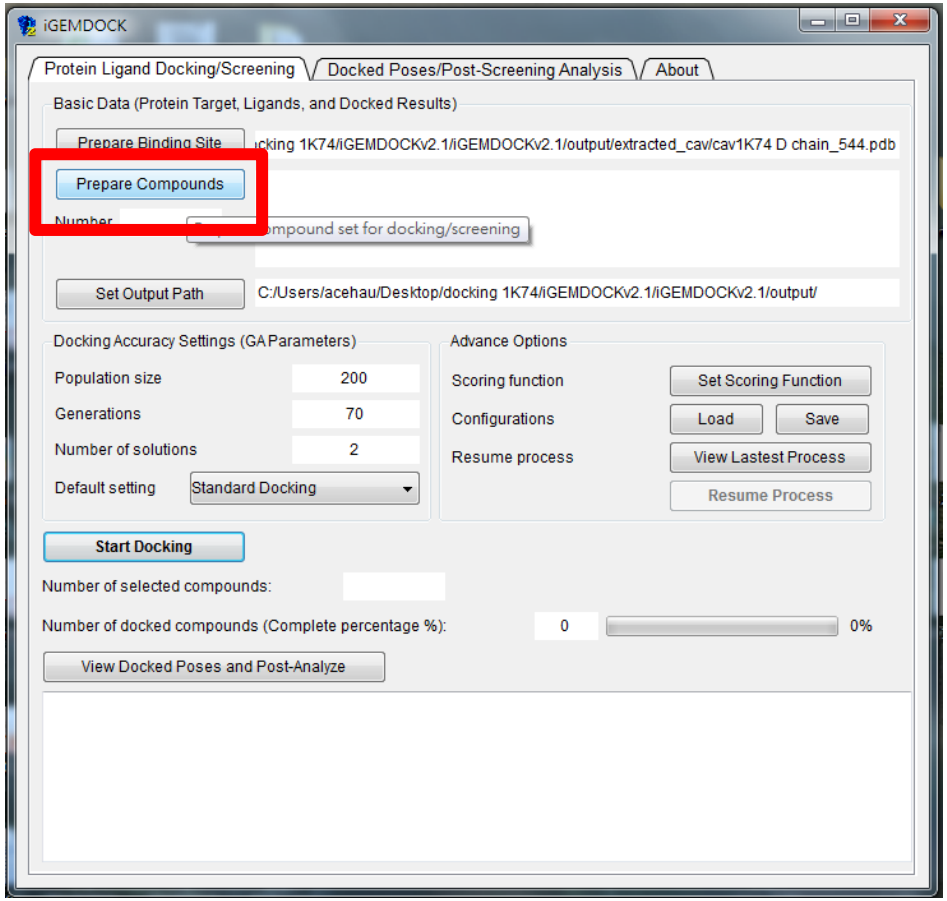
步驟八：選擇ligand 544 8Å範圍作為binding site

操作步驟



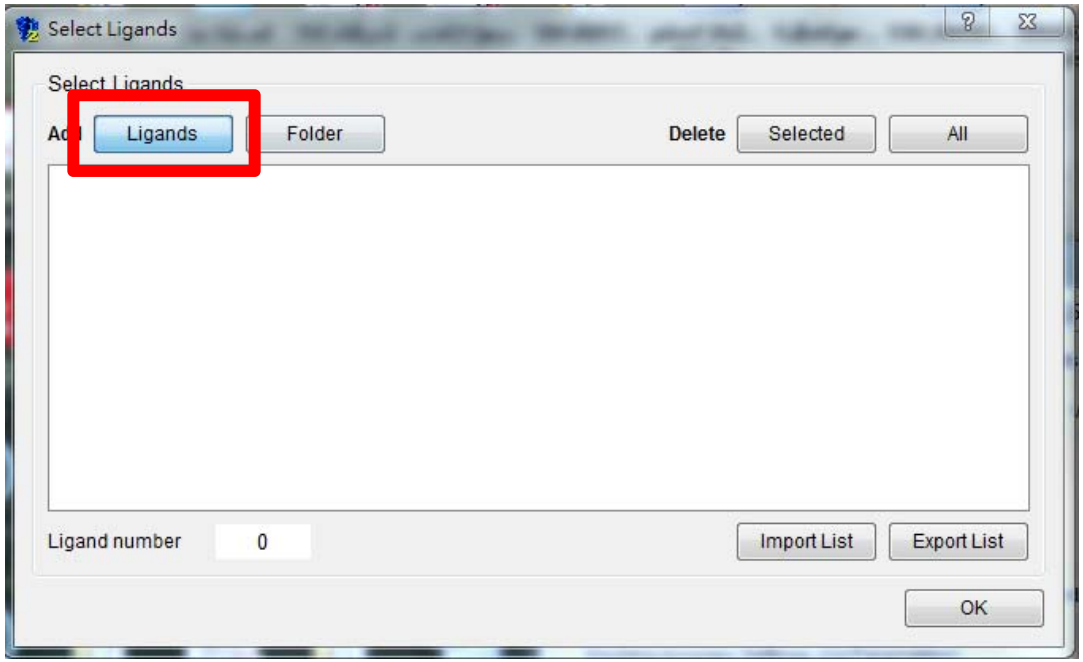
步驟九：設定好後，點選OK

操作步驟



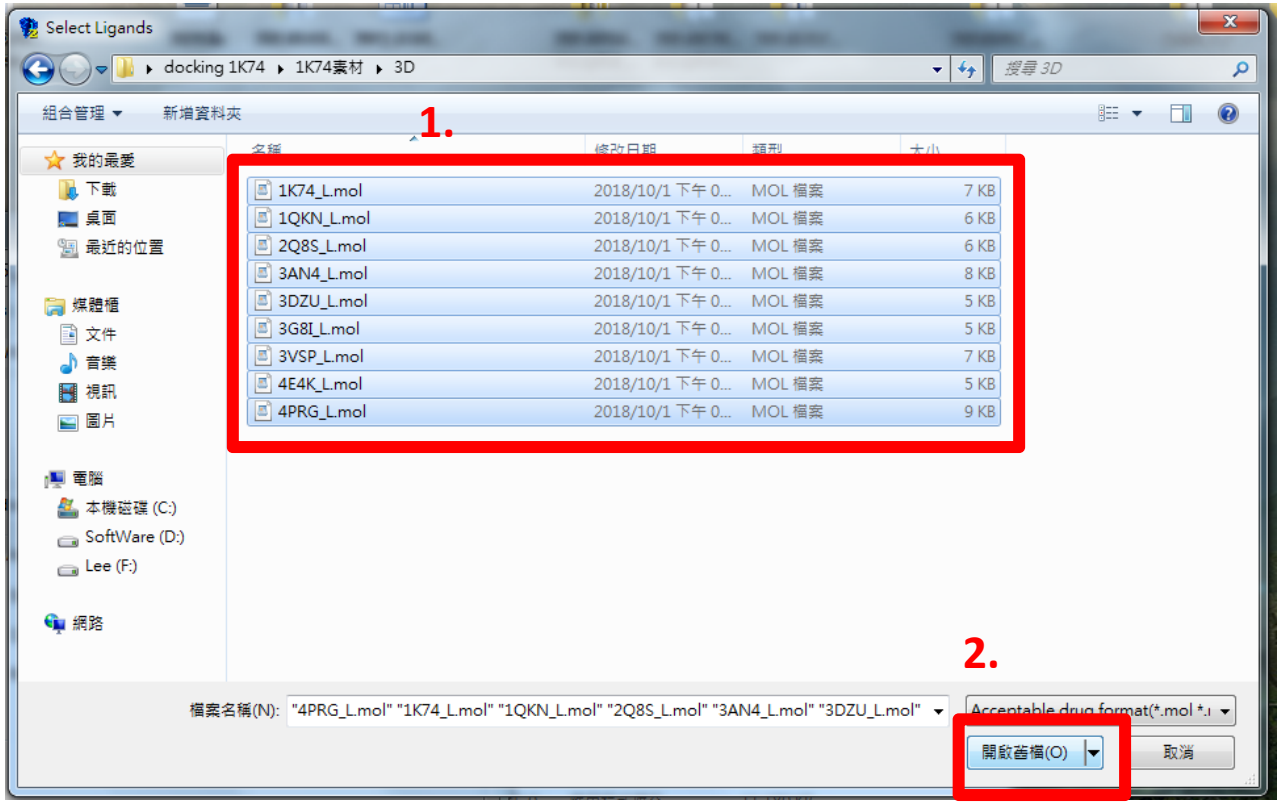
步驟十：按下Prepare Compounds，載入要計算的小分子

操作步驟



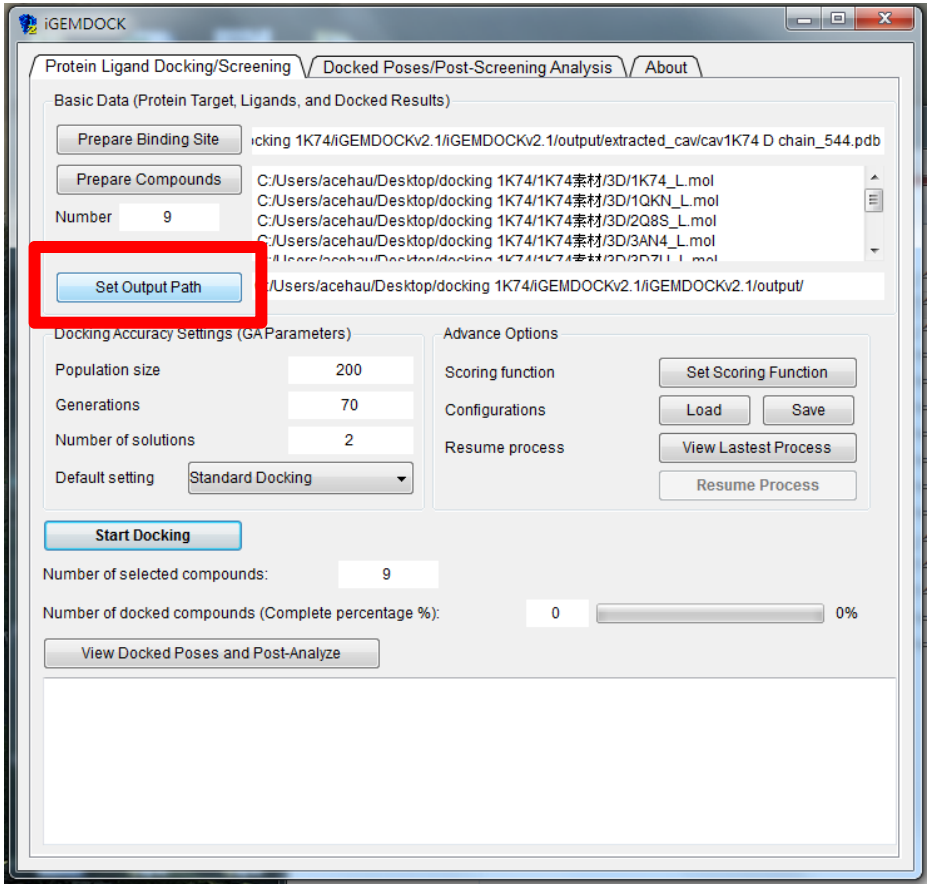
步驟十一：按下Ligands鈕

操作步驟



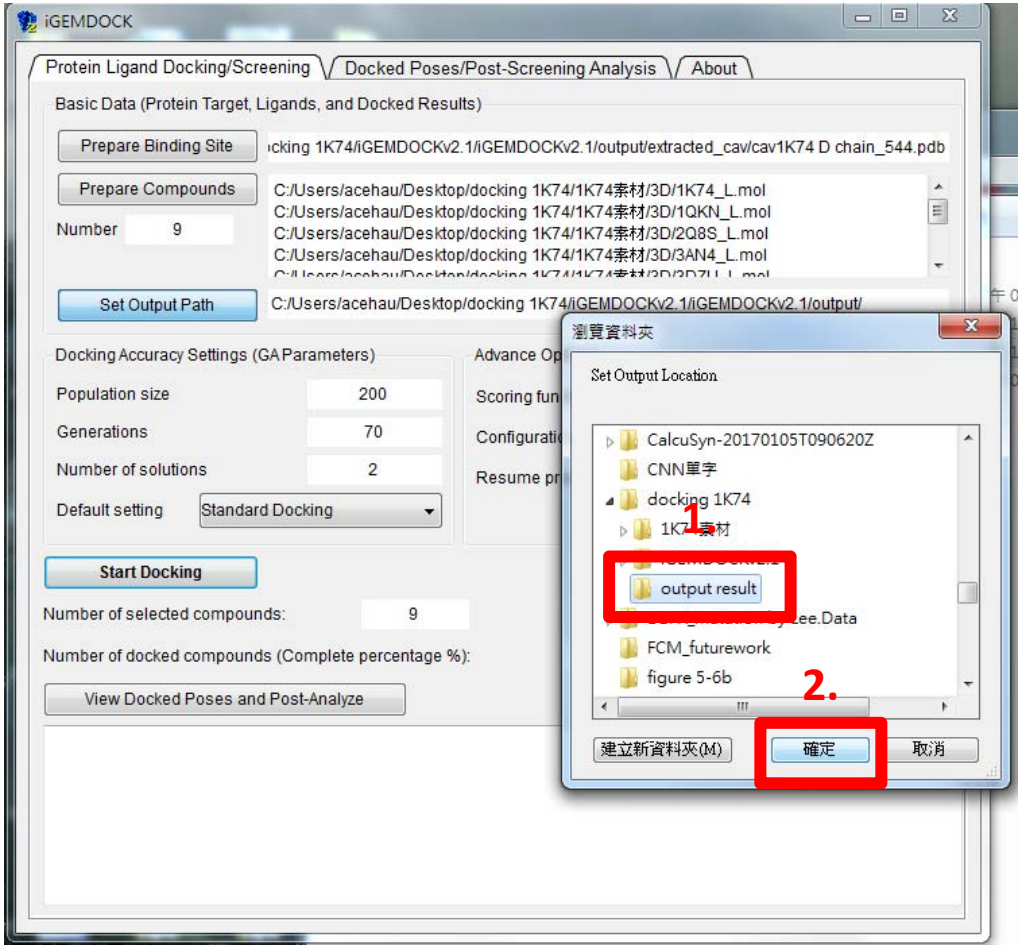
步驟十二：1. 選擇要計算的小分子 2. 按下「開啟舊檔」開啟檔案

操作步驟



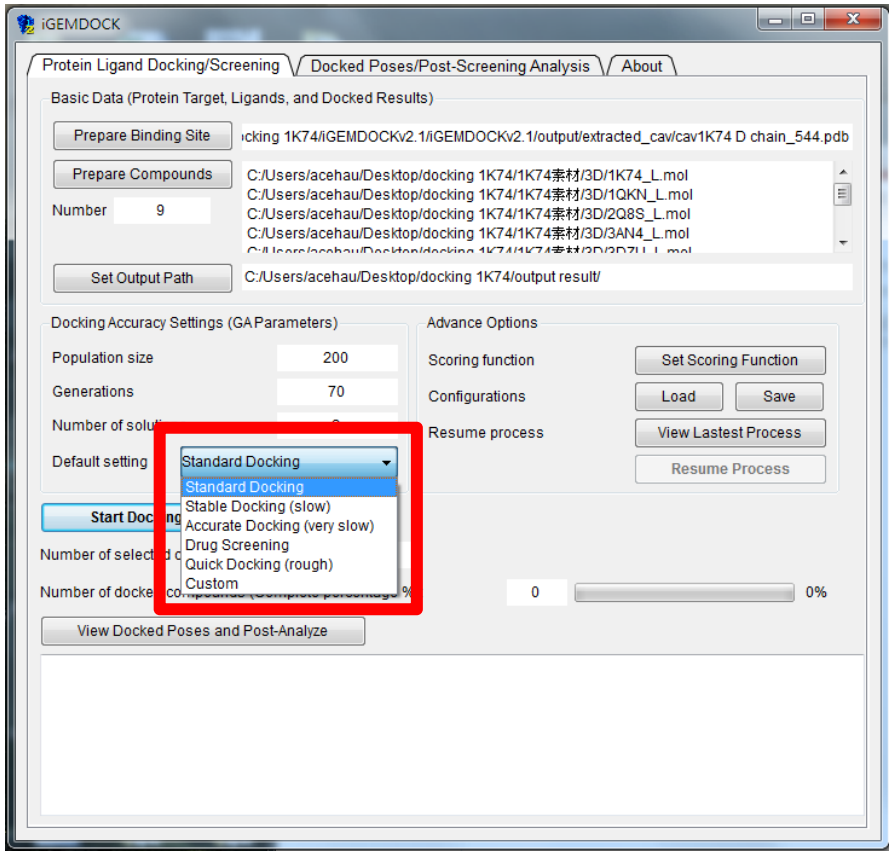
步驟十三：按下Set Output Path

操作步驟



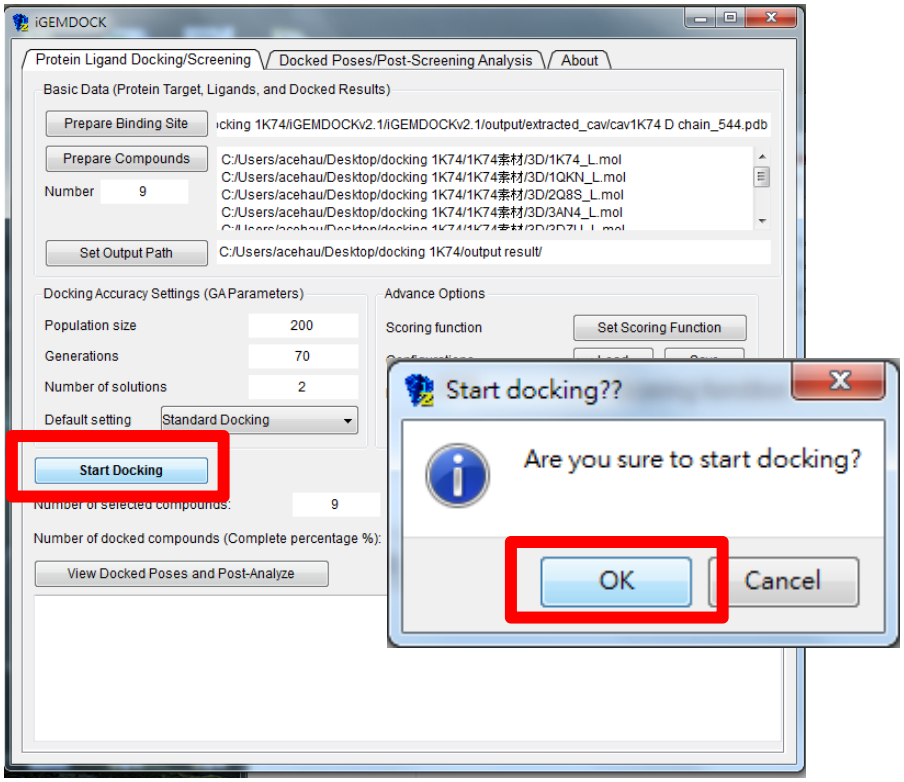
步驟十四：1.選擇要存放的資料夾 2.按下「確定」完成設定

操作步驟



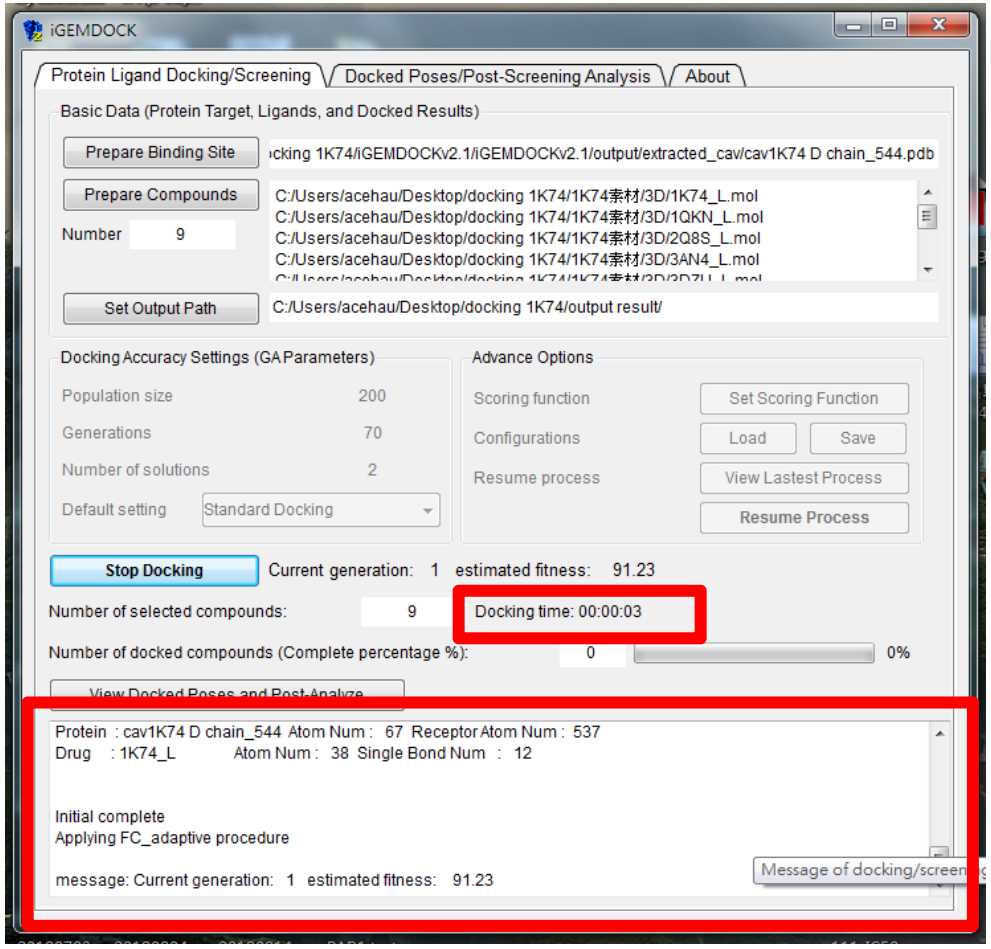
步驟十五：在Default setting的地方，選擇你要的計算模式

操作步驟



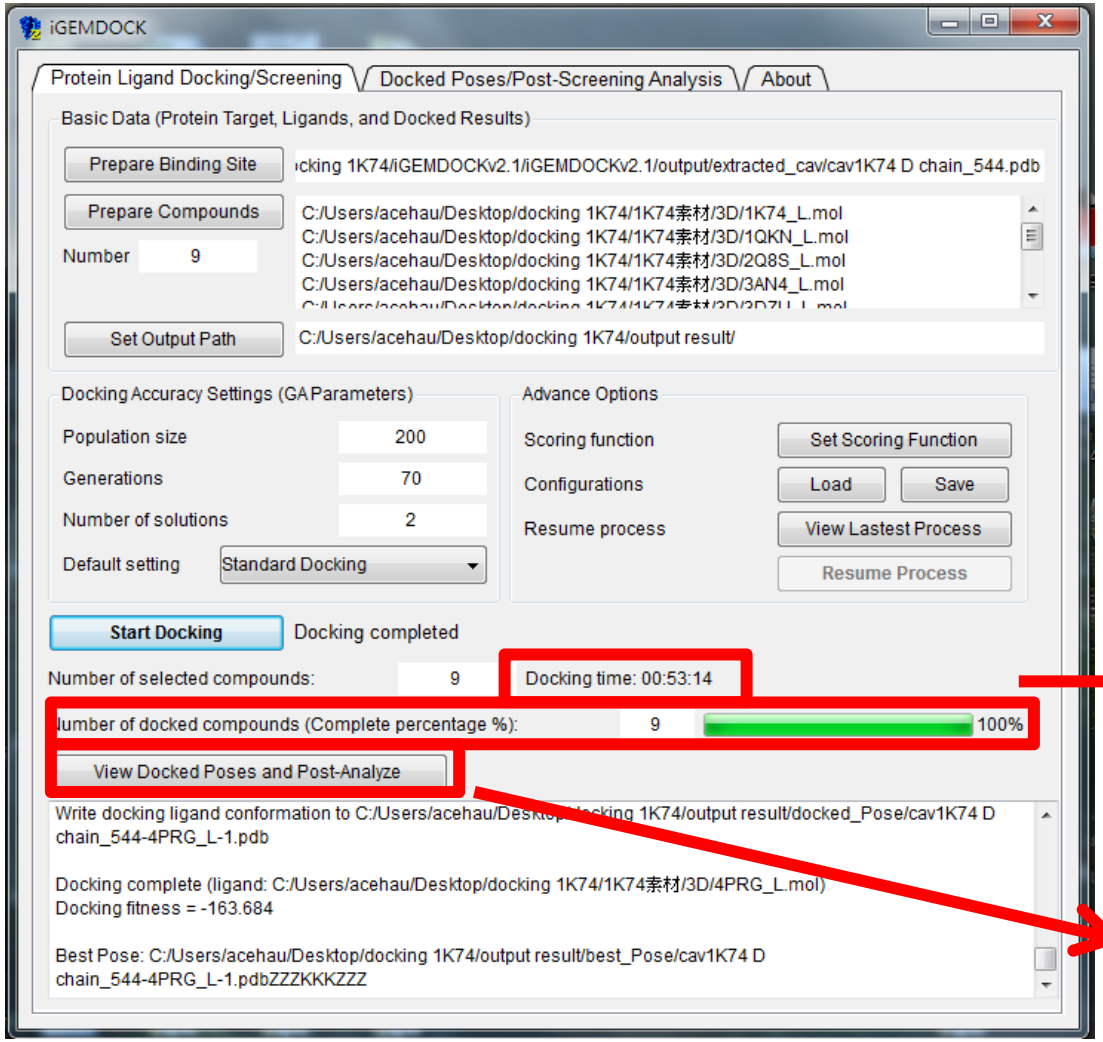
步驟十六：最後按下Start Docking，並在確認視窗中按下OK開始計算。

操作步驟



步驟十七：完成上述步驟後，可以在Docking time的地方看到計算執行的時間，以及在下方區塊看到執行狀況。

操作步驟

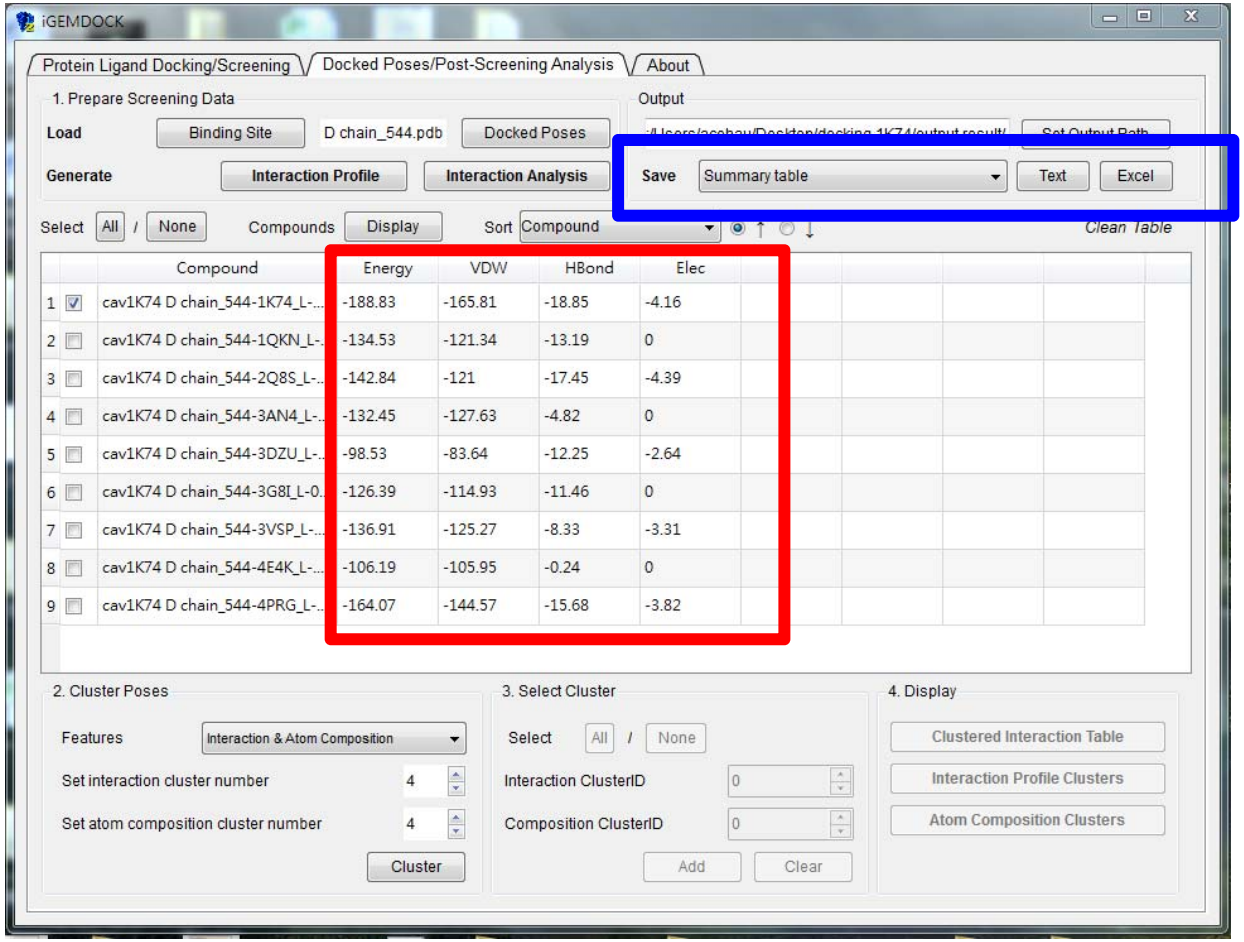


經過一個小時的計算，終於計算出結果了！

步驟十八：按下View Docked Poses and Post-Analyze觀看結果

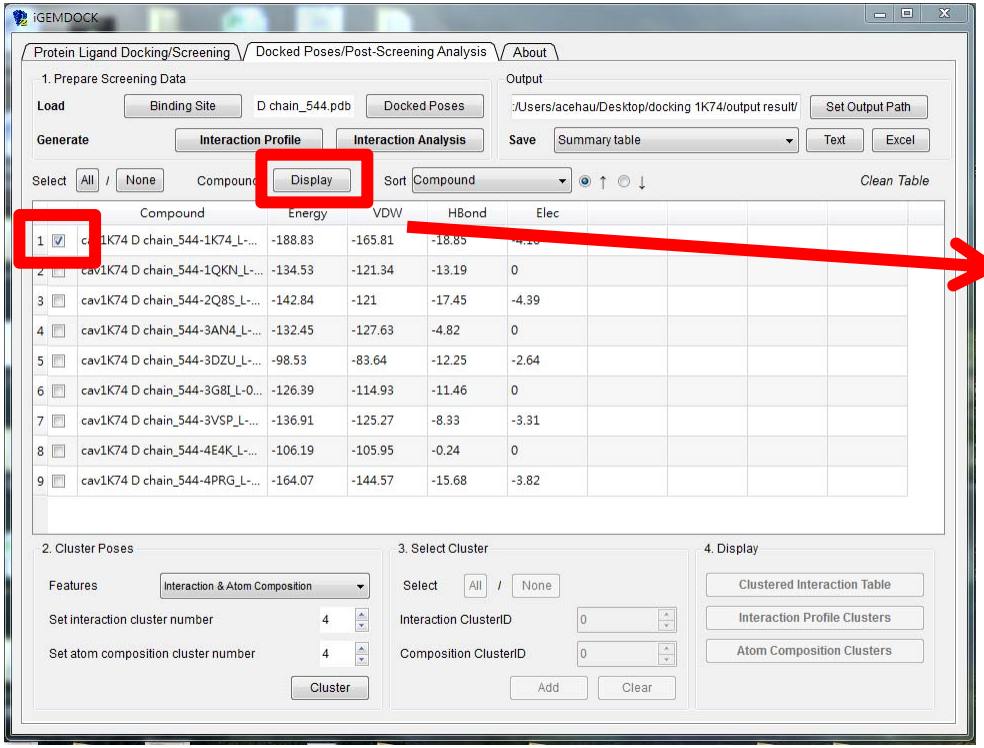
操作步驟

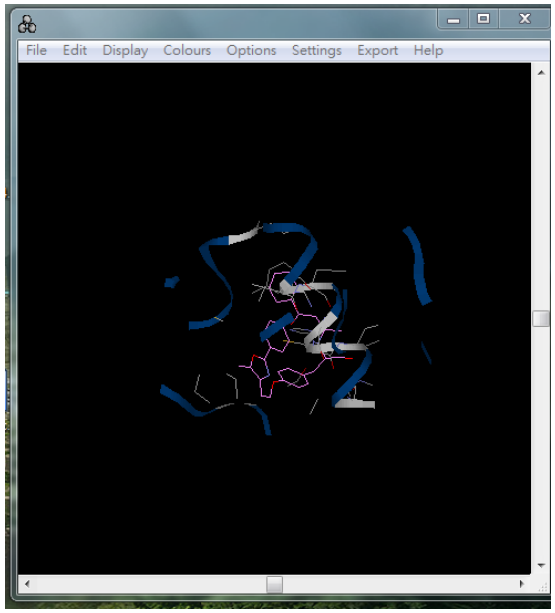
紅色框框中，記錄著計算出來的能量分數。



步驟十九：在Save的部分點選Excel按鈕，將記錄的能量狀況已Excel檔的方式儲存。

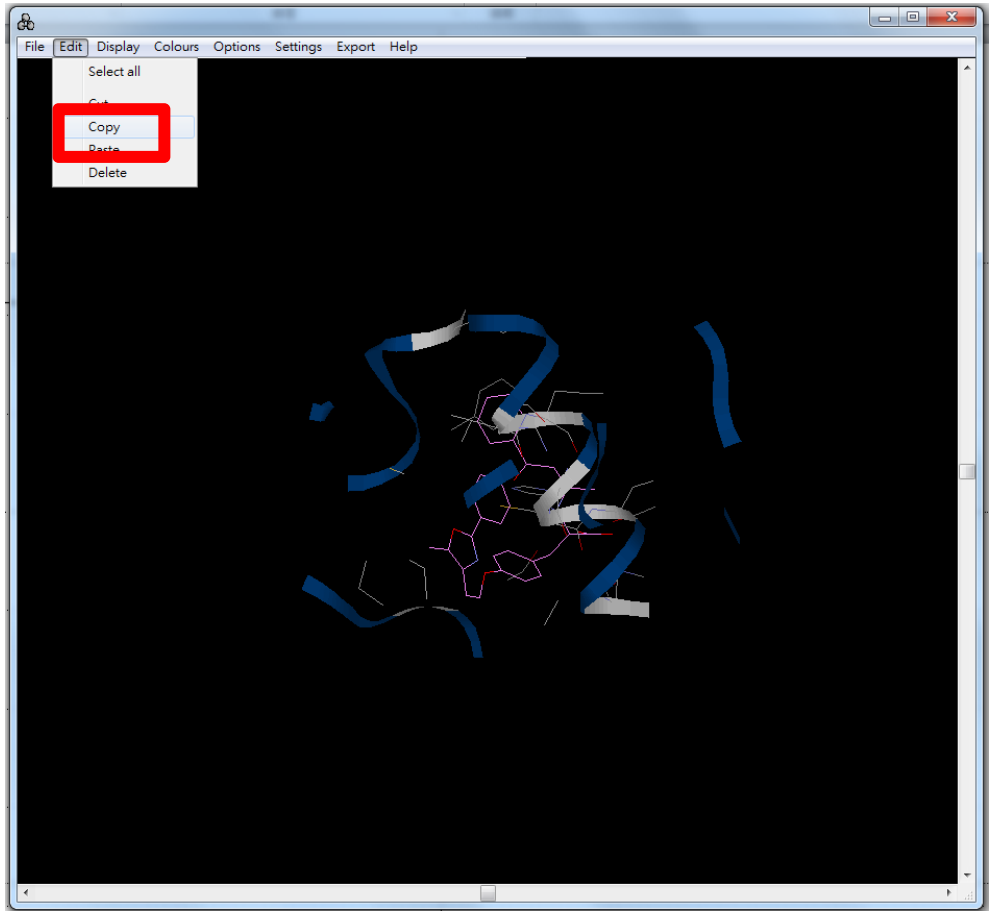
操作步驟





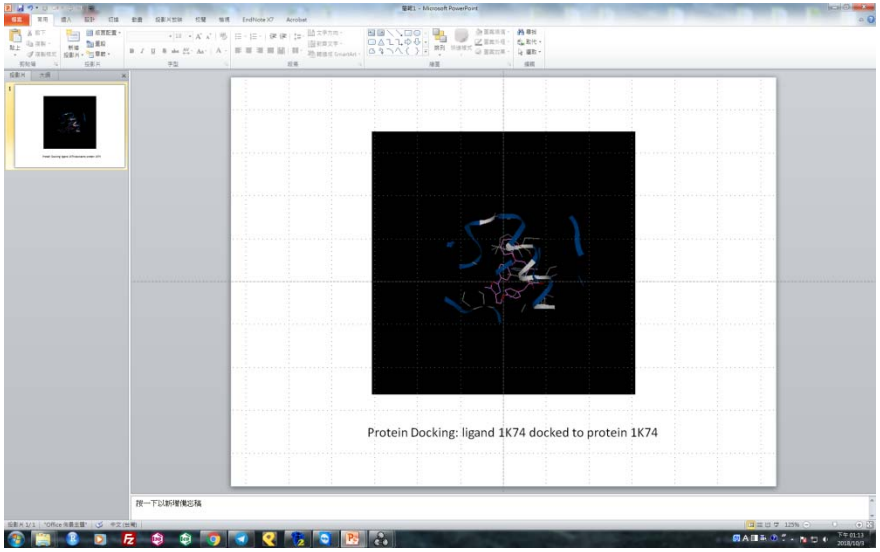
步驟二十：點選要觀看的結果，按下Display鍵後，3D結構會顯示在新視窗中。

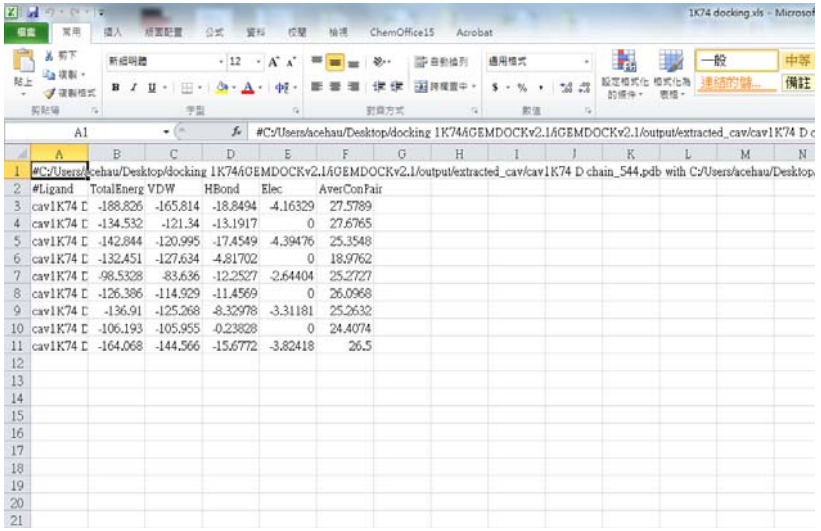
操作步驟



步驟二十一：在3D結構視窗中，點選Edit -> Copy，將binding結果狀況貼上powerpoint檔做記錄。

操作步驟



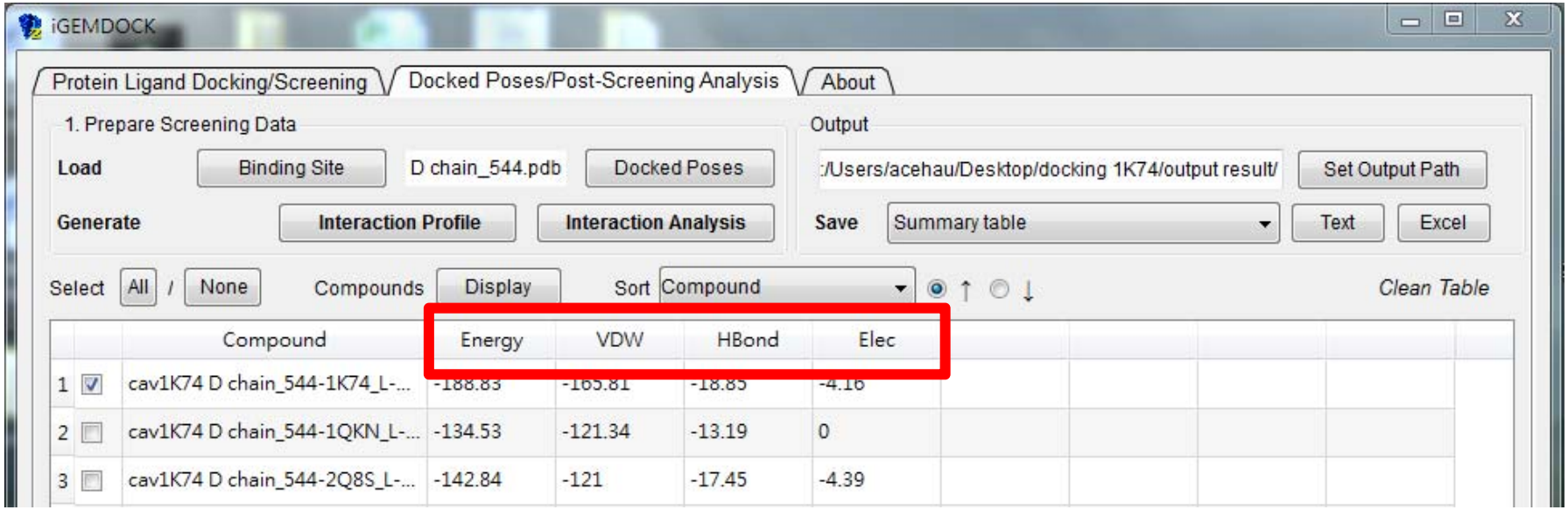


	A	B	C	D	E	F
1	#C:/Users/acehau/Desktop/docking 1K74/iGEMDOCKv2.1/iGEMDOCKv2.1/output/extracted_cav/cav1K74 D chain_544.pdb with C:/Users/acehau/Desktop/					
2	#Ligand	TotalEnerg	VDW	HBond	Elec	AverConPair
3	cav1K74 D	-188.826	-165.814	-18.8494	-4.16329	27.5789
4	cav1K74 D	-134.532	-121.34	-13.1917	0	27.6765
5	cav1K74 D	-142.844	-120.995	-17.4549	-4.39476	25.3548
6	cav1K74 D	-132.451	-127.634	-4.81702	0	18.9762
7	cav1K74 D	-98.5328	-83.636	-12.2527	-2.64404	25.2727
8	cav1K74 D	-126.386	-114.929	-11.4569	0	26.0968
9	cav1K74 D	-136.91	-125.268	-8.32978	-3.31181	25.2632
10	cav1K74 D	-106.193	-105.955	-0.23828	0	24.4074
11	cav1K74 D	-164.068	-144.566	-15.6772	-3.82418	26.5

步驟二十二：完成檔案儲存後，實驗就算完成了。

結報Q&A

- Q1：分析結果視窗中的Energy、VDW、Hbond、Elec是什麼？該依據哪個來挑選小分子候選子(compound candidate)？



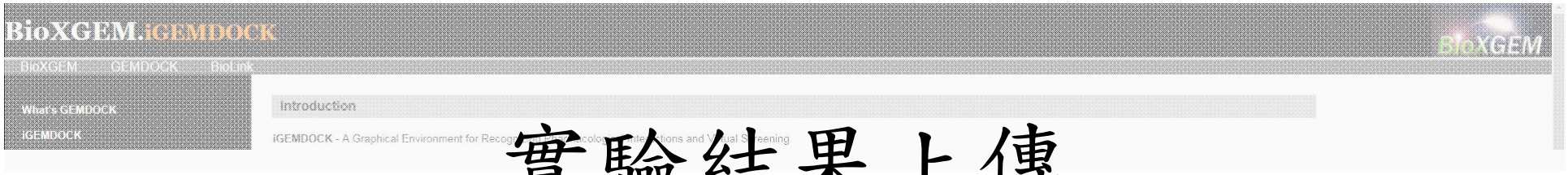
結報Q&A

- Q2：哪個小分子最有開發藥物的潛能？請回答，並將各個小分子後續藥物開發潛能進行排序。

ex. Compound 2。 Compound 2 > Compound 3 > Compound 7…

結報Q&A

- Q3：以今天的分子入塢的實驗速度，一萬個小分子，多久電腦會執行完畢？



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)

祝大家實驗順利！

Wish you have a successful experiment in cyberspace.