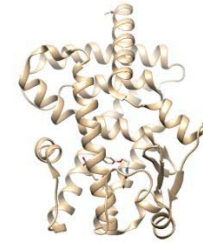




## 生物科技實驗



# 分子入塢 — (III) 執行分子入塢

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*YTLab Presents*

What's iGEMDOCK

iGEMDOCK

Method

Results

References

Download

Visitor tracking

Contact Us

Introduction

iGEMDOCK - A Graphical Environment for Recognizing Pharmacological Interactions and Virtual Screening

Pharmacological interactions are useful for identifying lead compounds and understanding ligand binding mechanisms for a therapeutic target. Currently, these interactions are often inferred from a set of active compounds that were acquired experimentally. Moreover, most docking programs loosely coupled the stages of structure-based virtual screening (VS) from preparations through to post-screening analysis. An integrated VS environment, which provides the friendly interface to seamlessly combine different-stage programs for VS and identifying the pharmacological interactions from screening compounds, is valuable for drug discovery. Here, we developed an easy-to-use graphic environment, iGEMDOCK, for the docking, virtual screening, and post-screening analysis. For post-screening analysis, iGEMDOCK can enrich the hit rate and provide biological insights by deriving the pharmacological interactions from screening compounds. The pharmacological interactions represent conserved interacting residues that often form binding pockets with specific physico-chemical properties to play the essential functions of the target protein. Experiment results show that the success rate of iGEMDOCK is 78% (root-mean-square derivations below 2.0 angstrom) on 305 protein-compound complexes. For virtual screening, pharmacological interactions derived by iGEMDOCK often involve the biological functions and enrich the hit rates on three public sets (i.e., estrogen receptor  $\alpha$  for antagonists (ER) and agonists (ERA) and thymidine kinase (TK)). We believe that iGEMDOCK is useful for understanding the ligand binding mechanisms and discovering lead compounds.

Download :

iGEMDOCK is available for free on non-commercial researches.

• 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

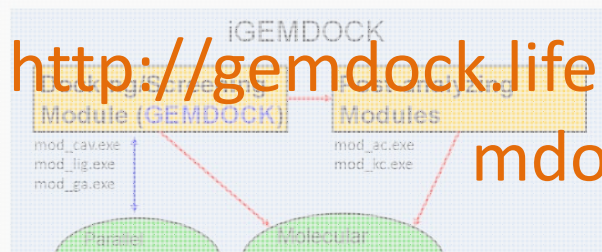
- [iGEMDOCK v2.0 for windows XP/Vista](#)
- [iGEMDOCK v2.0 for CentOS 5](#)
- [iGEMDOCK v2.0 for Suse Linux 9](#)
- [iGEMDOCK v2.0 for Ubuntu Linux](#)

• 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](#)

# iGEMDOCK

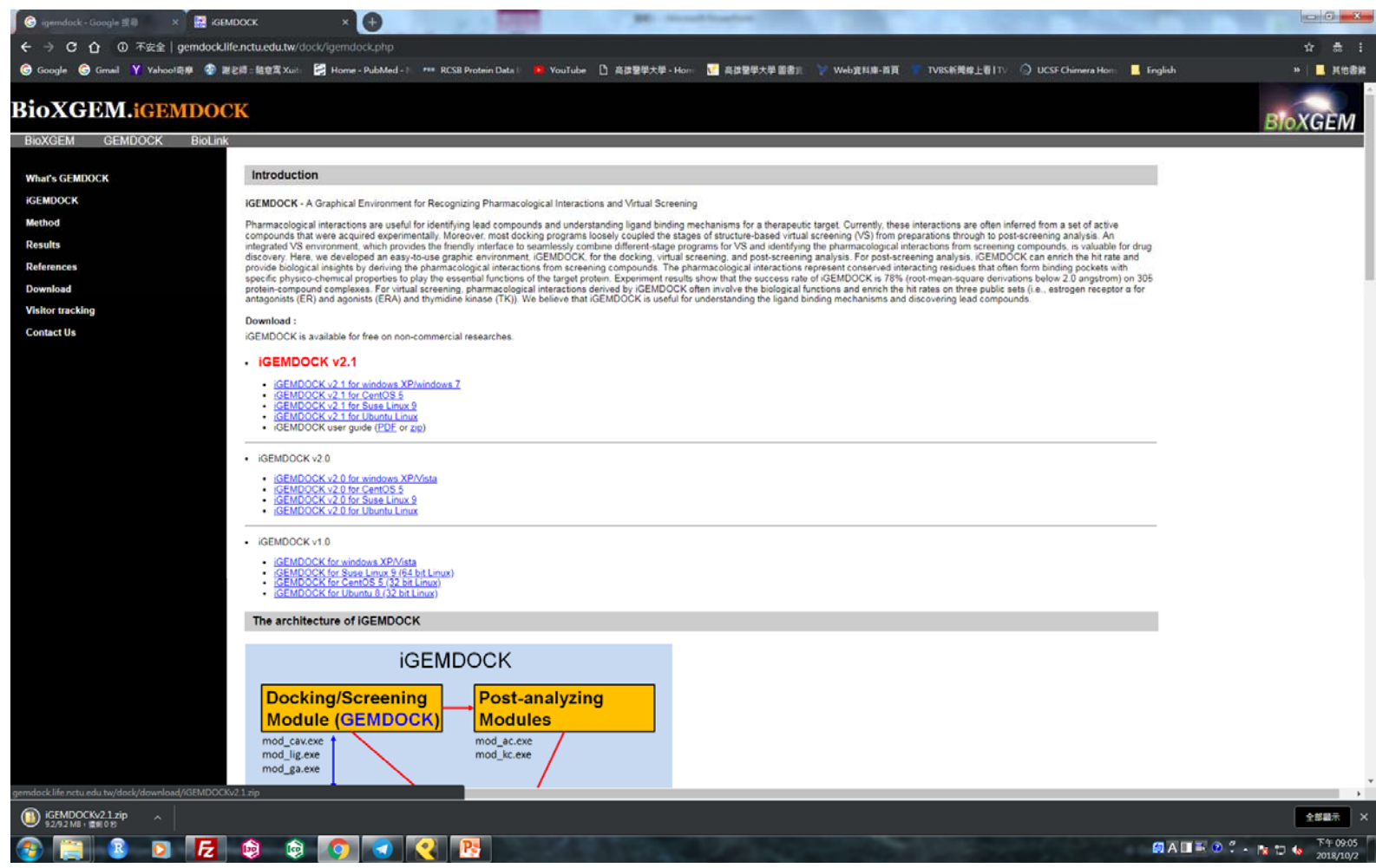
The architecture of iGEMDOCK



## Molecular Docking

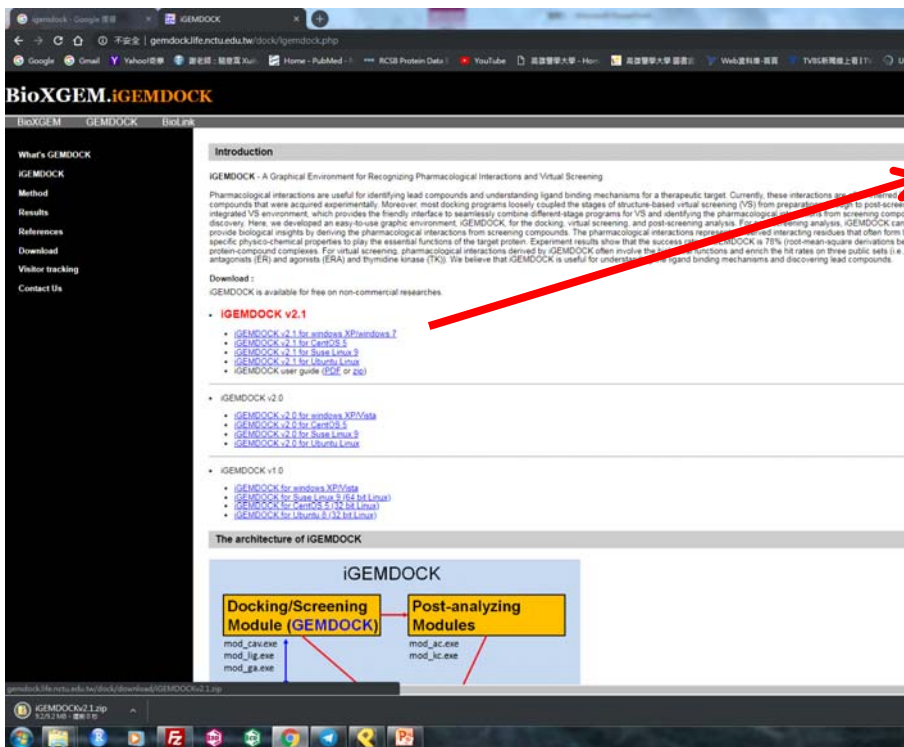
<http://gemdock.life.nctu.edu.tw/dock/igemdock.php>

# 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 \(PDF or zip\)](#)

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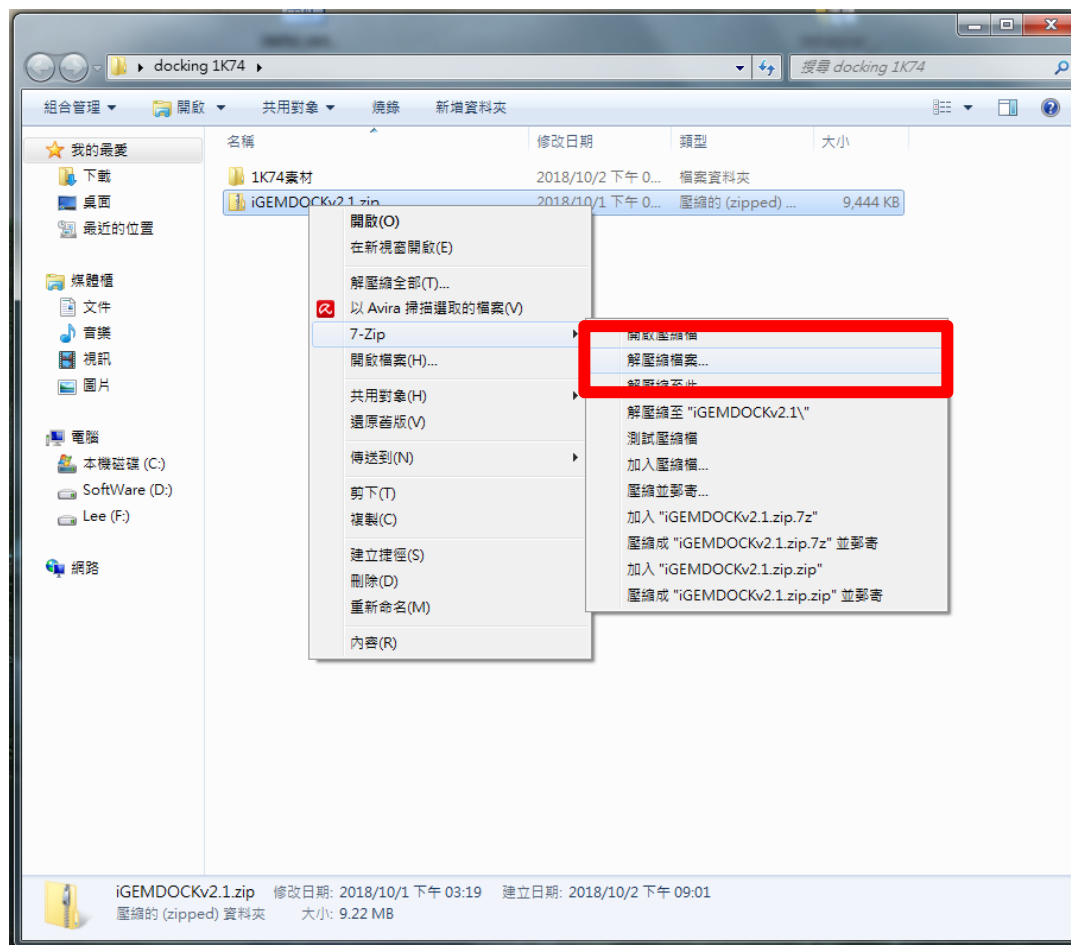
- iGEMDOCK v2.0
  - [iGEMDOCK v2.0 for windows XP/Vista](#)
  - [iGEMDOCK v2.0 for CentOS 5](#)
  - [iGEMDOCK v2.0 for Suse Linux 9](#)
  - [iGEMDOCK v2.0 for Ubuntu Linux](#)

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- 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 \(32 bit Linux\)](#)

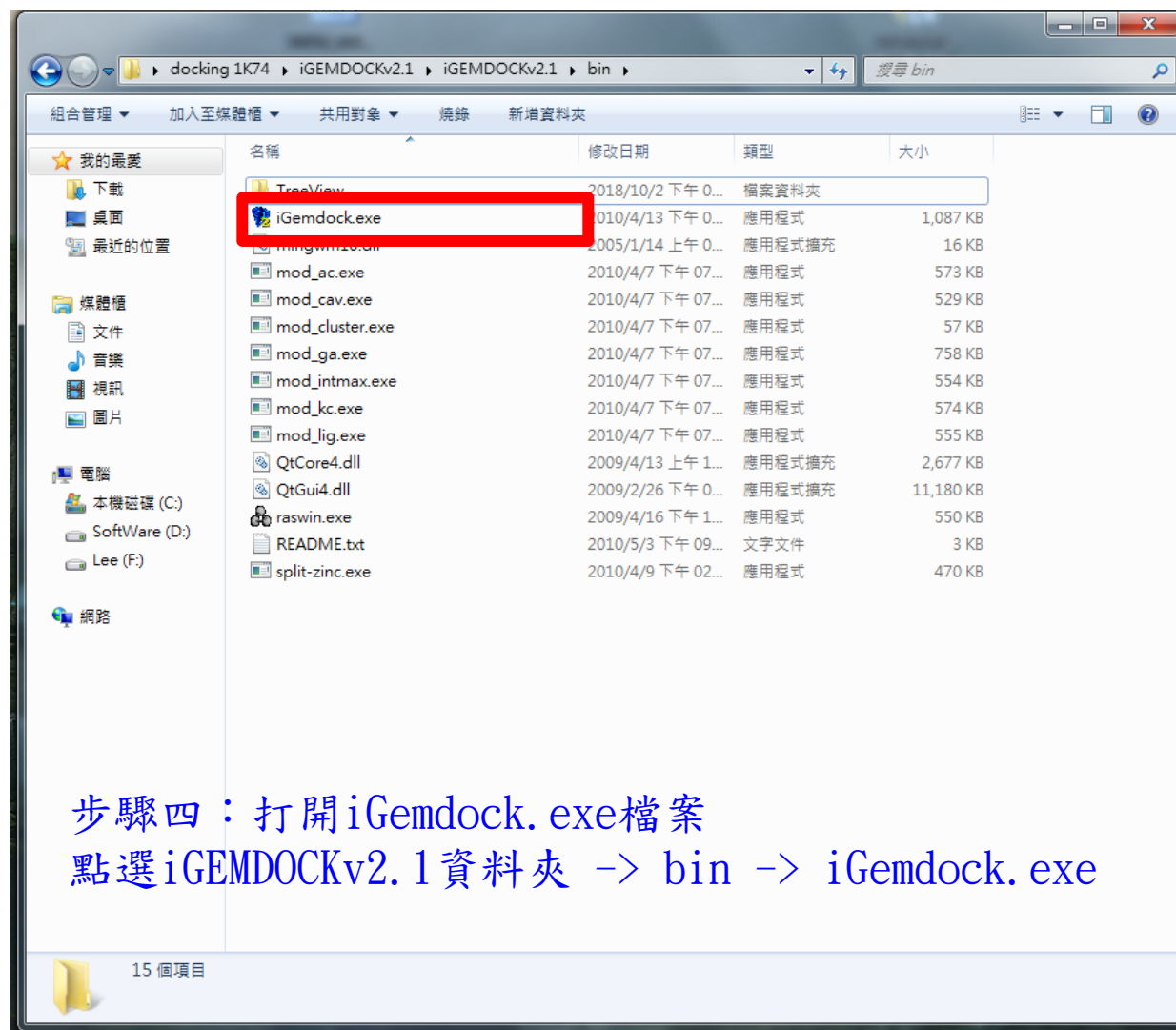
步驟二：下載iGEMDOCK軟體 v2.1 for windows XP/windows 7

# 操作步驟



步驟三：按右鍵，解壓縮iGEMDOCKv2.1.zip壓縮檔。

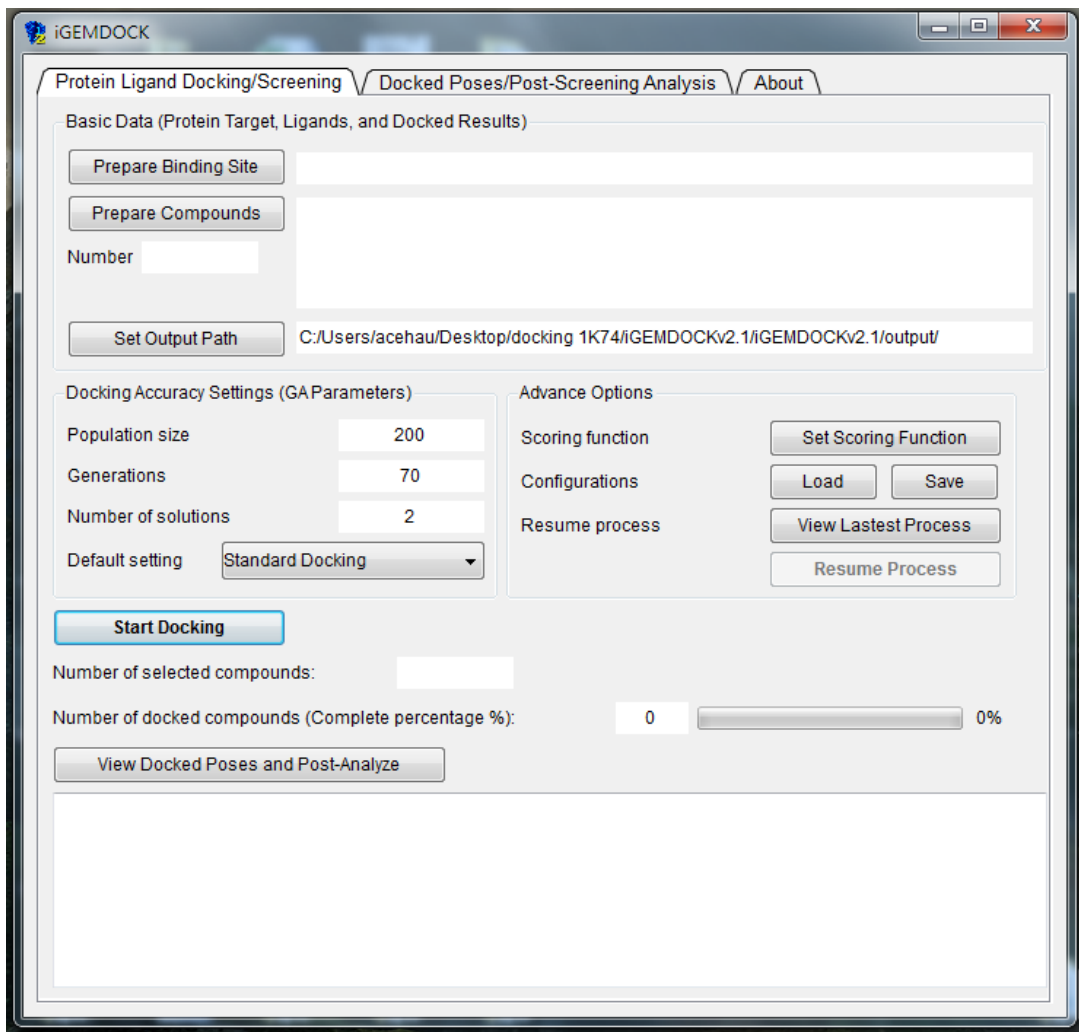
# 操作步驟



步驟四：打開iGemdock.exe檔案

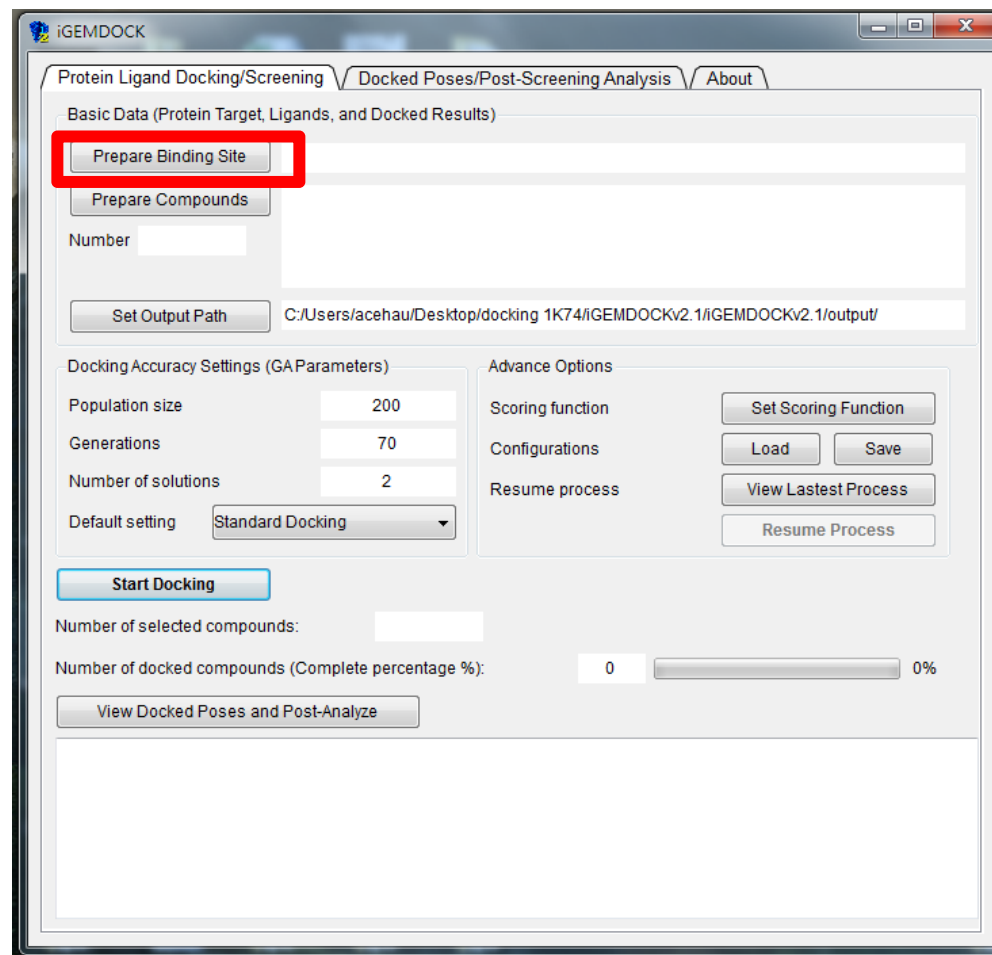
點選iGEMDOCKv2.1資料夾 -> bin -> iGemdock.exe

# 操作步驟



此為iGEMDOCK程式介面

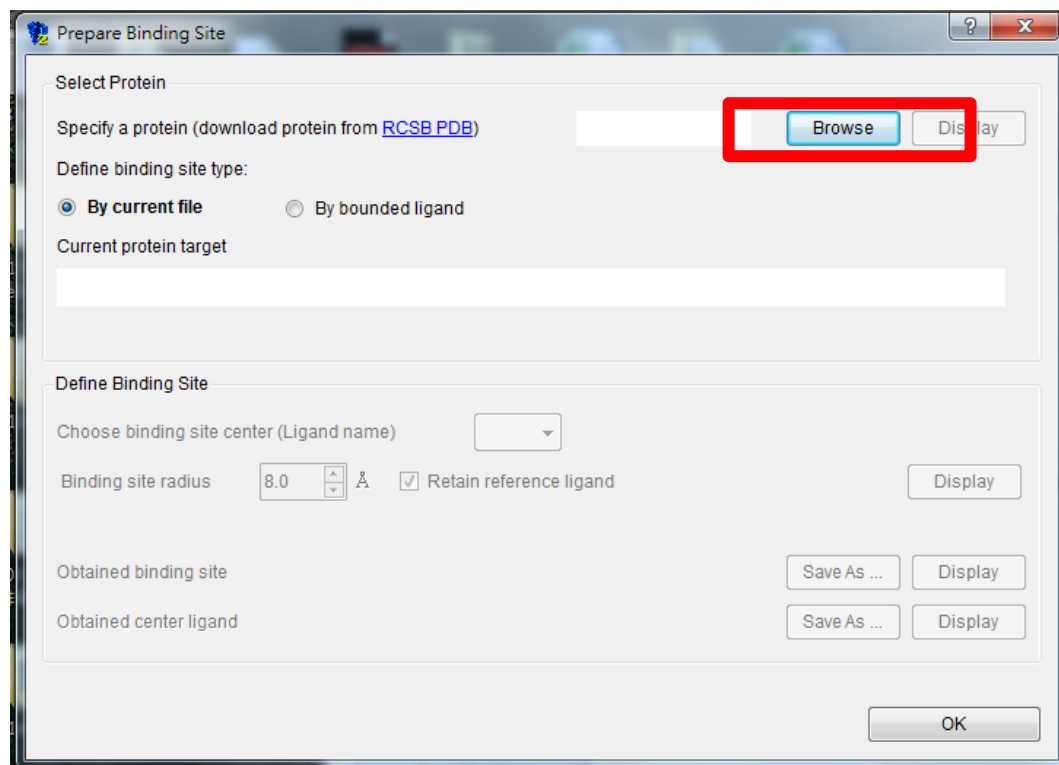
# 操作步驟



步驟四：按下Prepare Binding Site

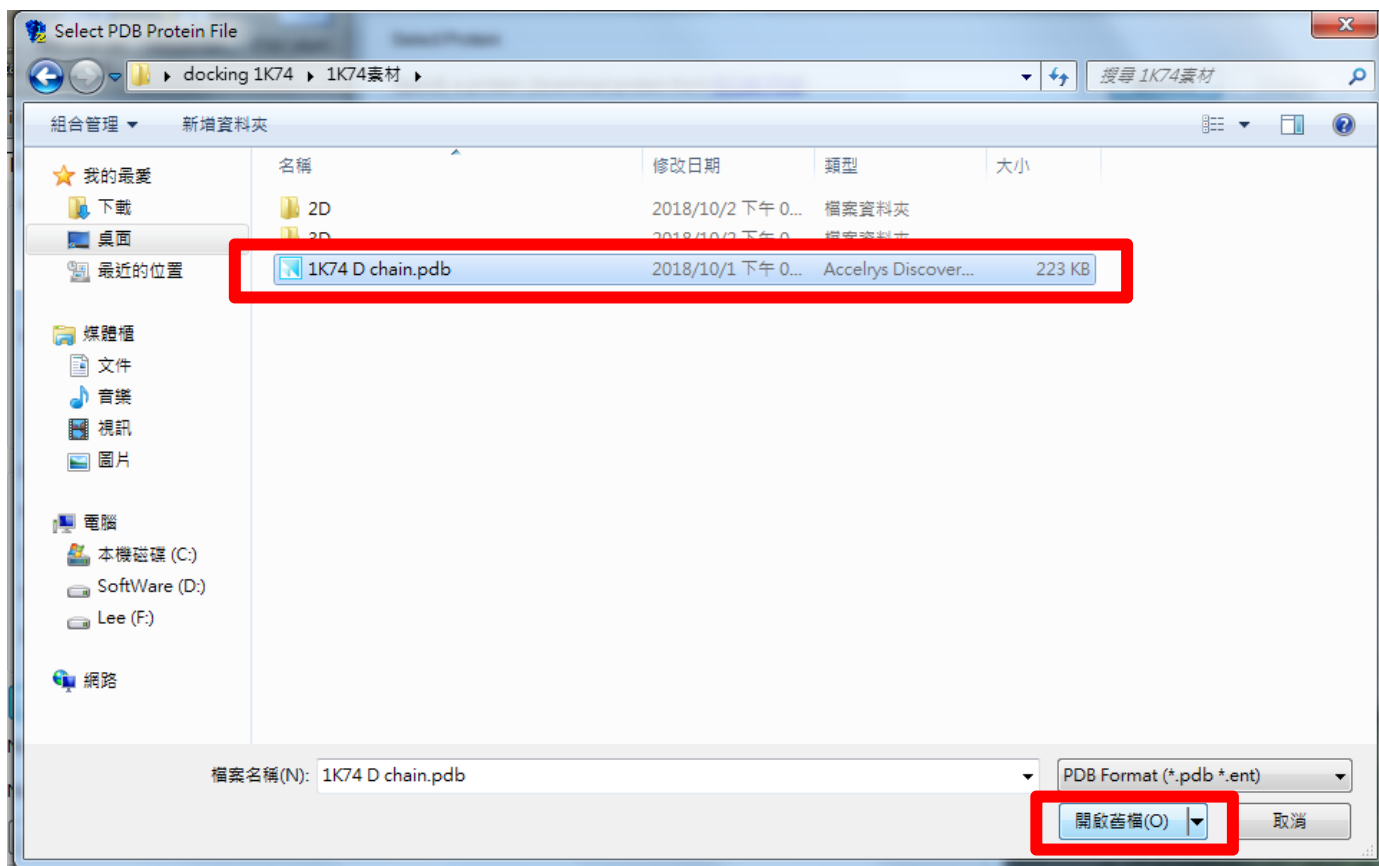


# 操作步驟



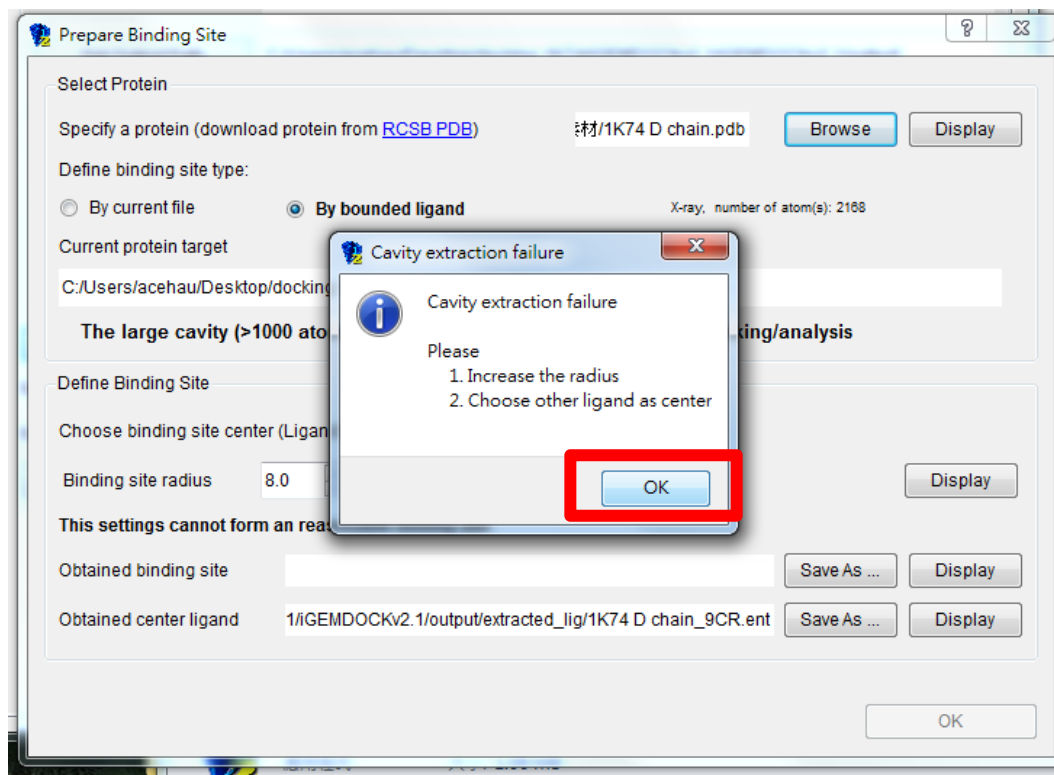
步驟五：按下Browse

# 操作步驟



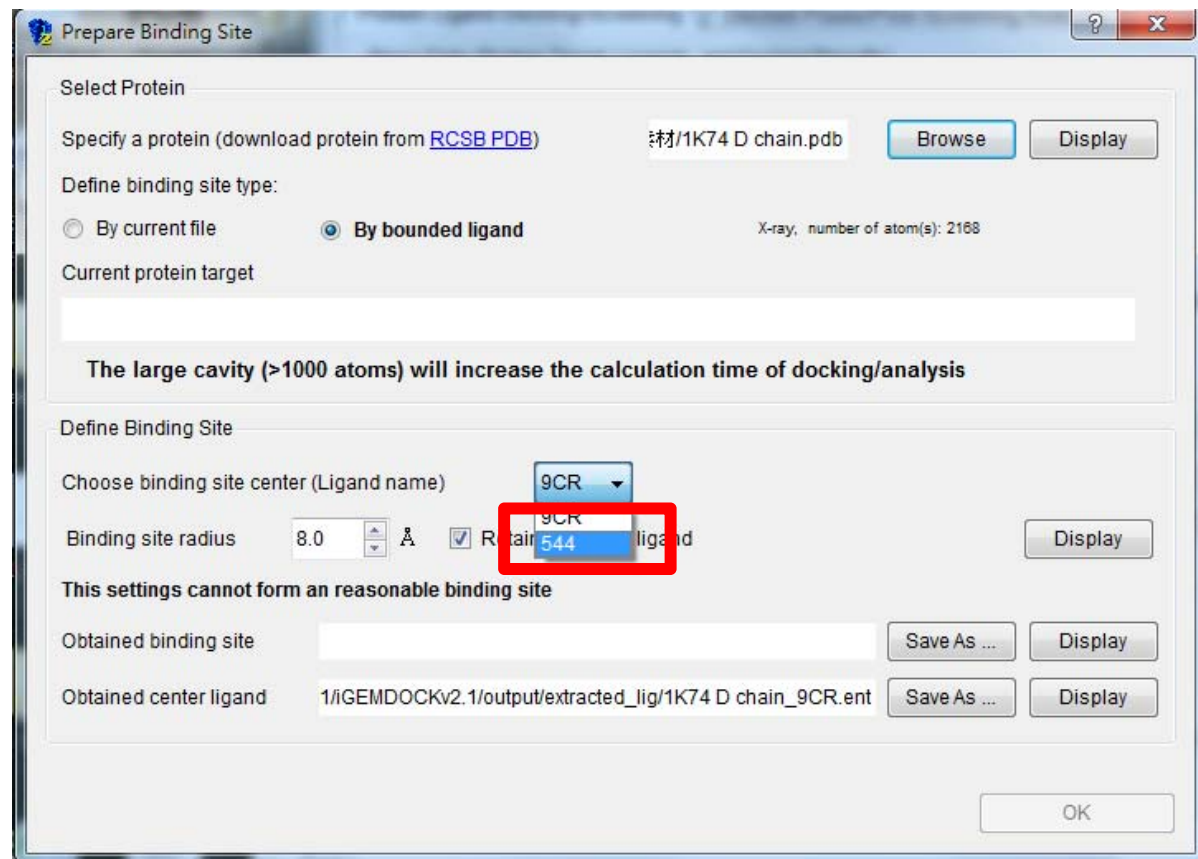
步驟六：找到先前存放好的蛋白質檔案，並開啟

# 操作步驟



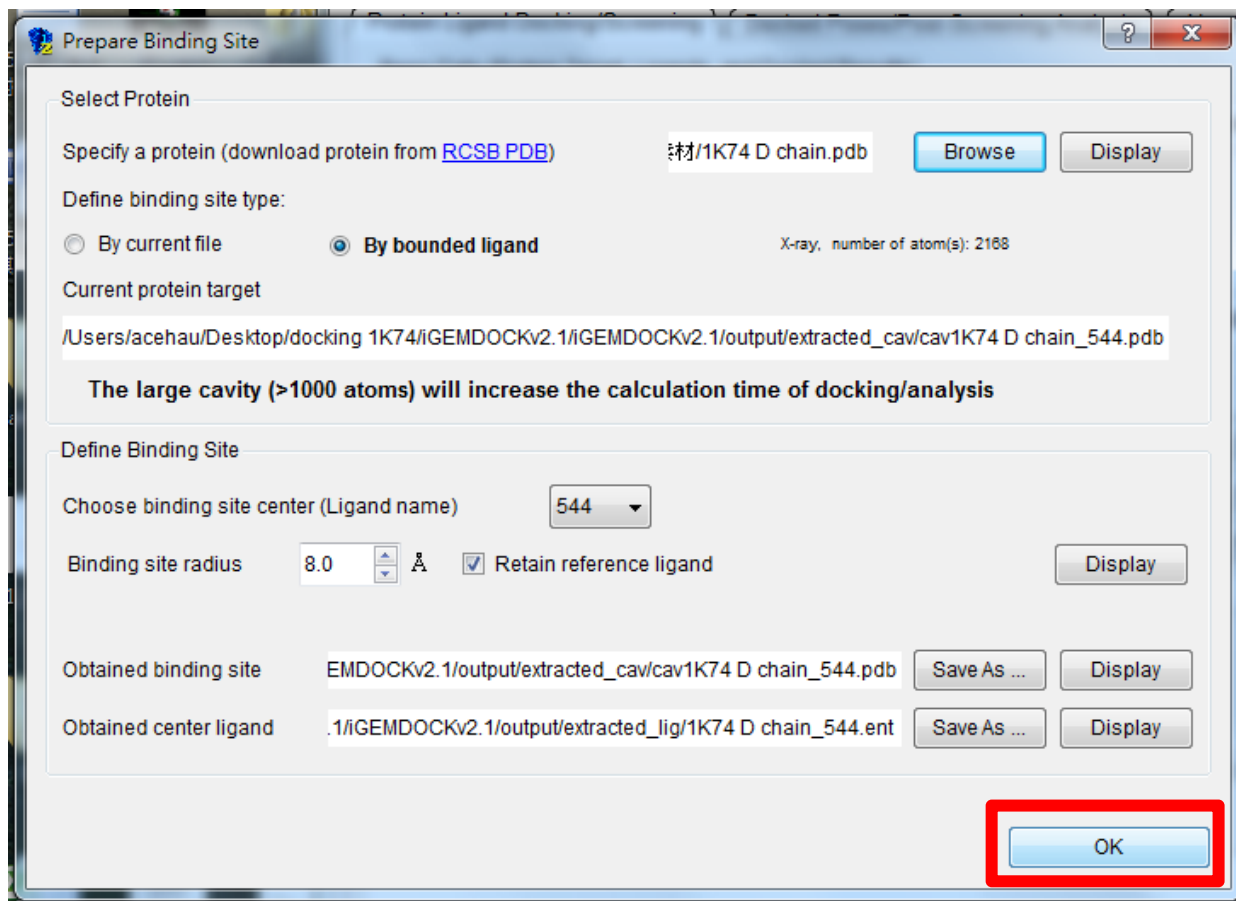
步驟七：程式會出現設定binding site的提醒視窗，按下OK即可

# 操作步驟



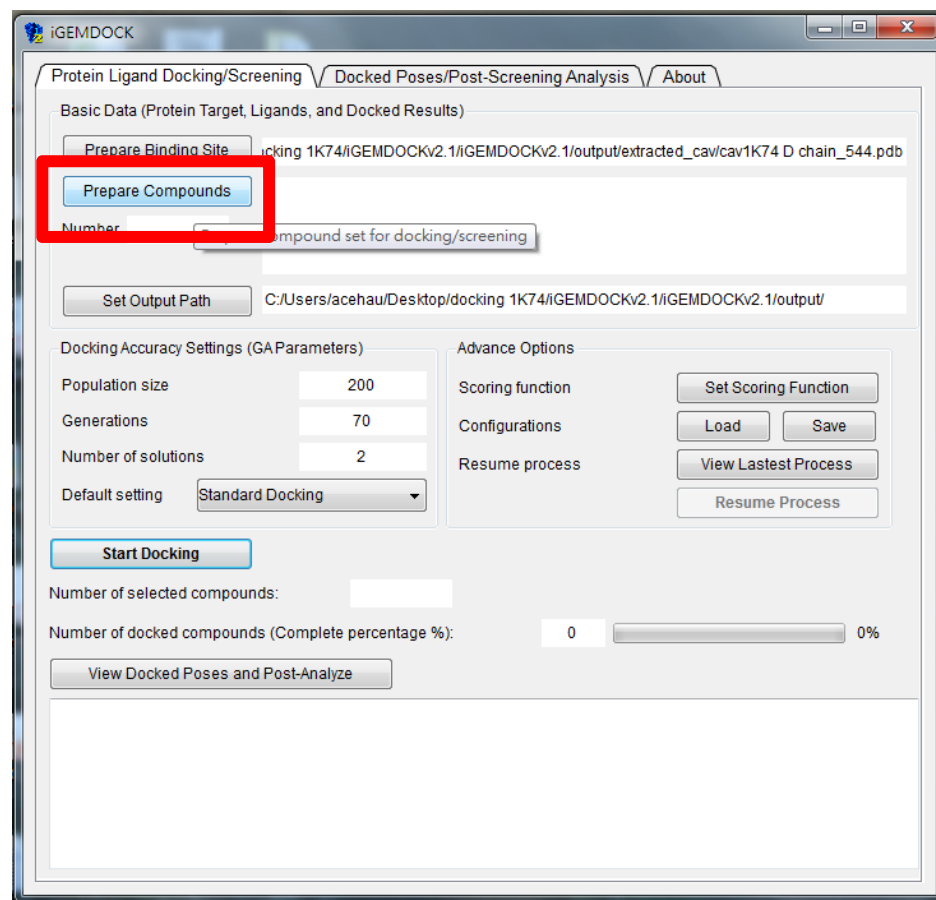
步驟八：選擇ligand 544 8Å範圍作為binding site

# 操作步驟



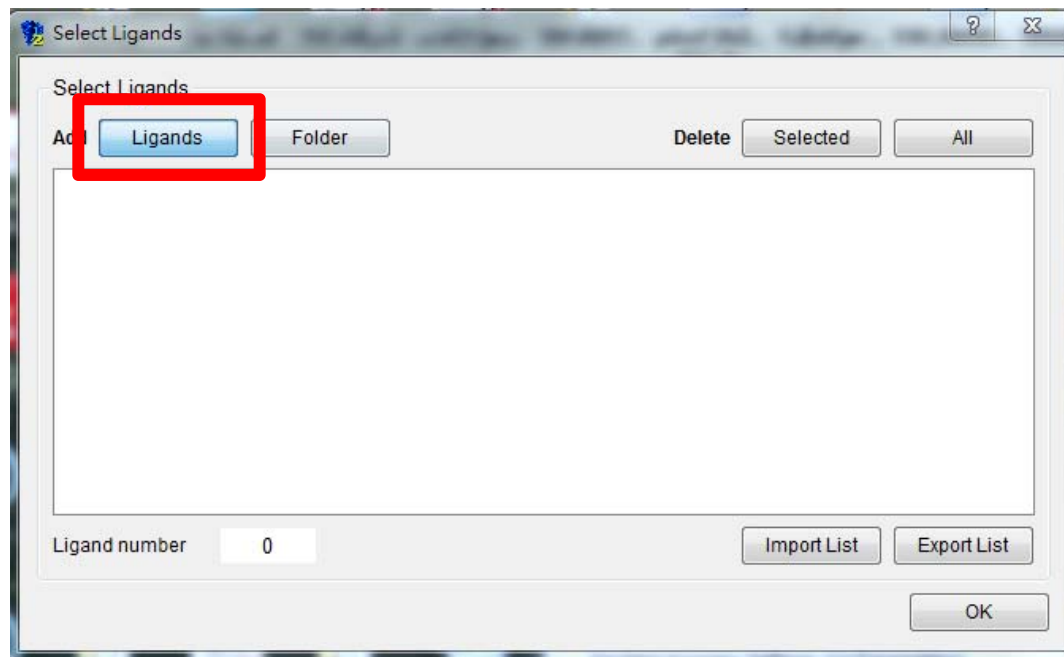
步驟九：設定好後，點選OK

# 操作步驟



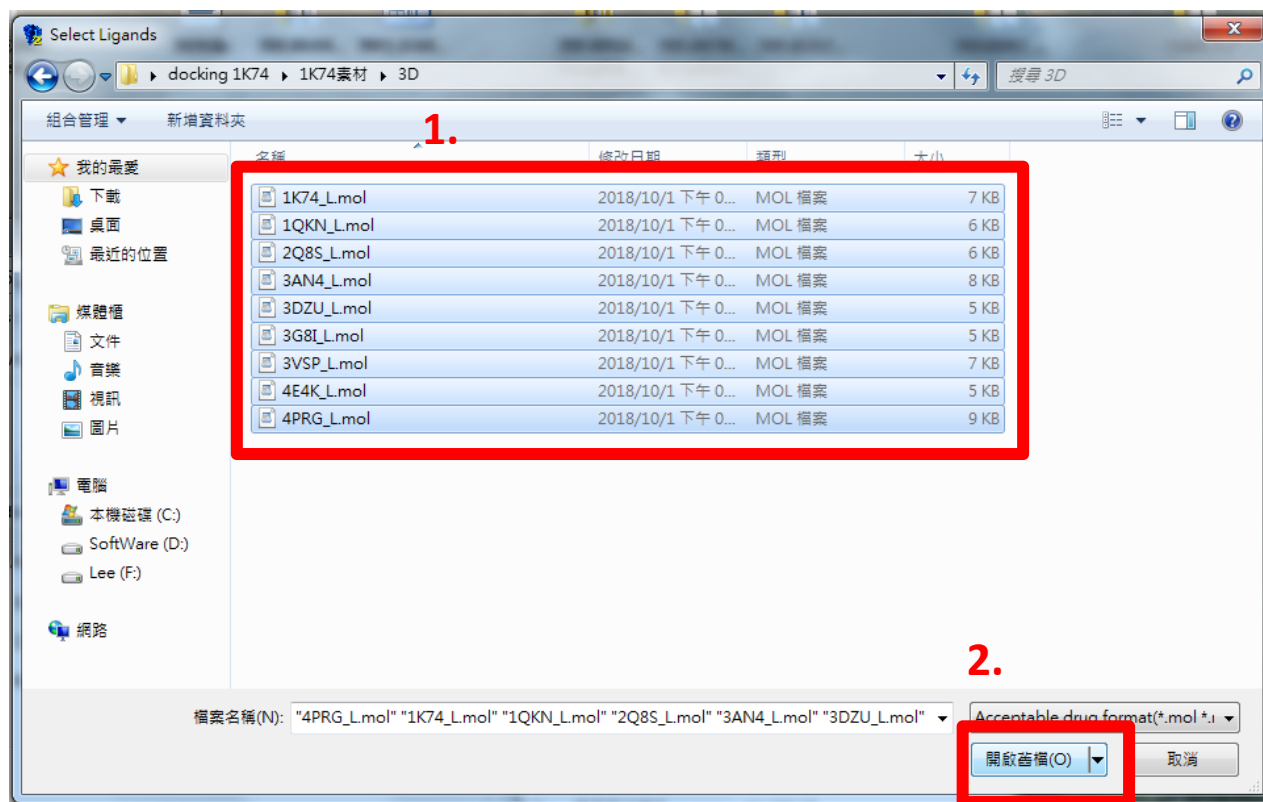
步驟十：按下Prepare Compounds，載入要計算的小分子

# 操作步驟



步驟十一：按下Ligands鈕

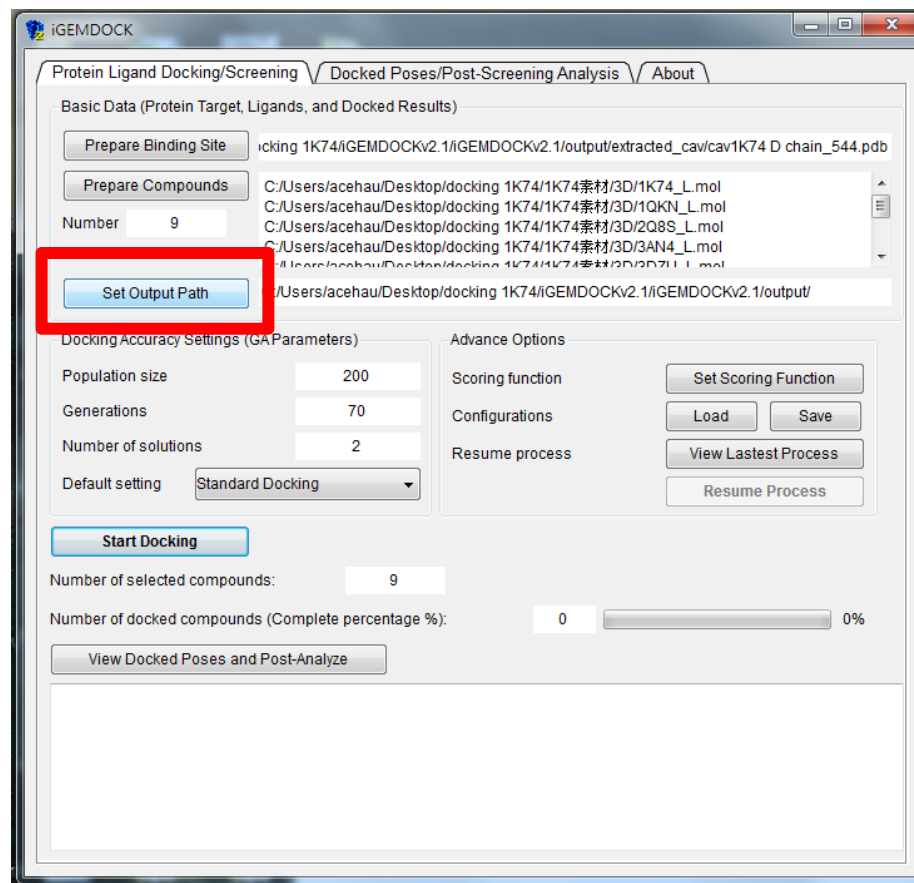
# 操作步驟



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

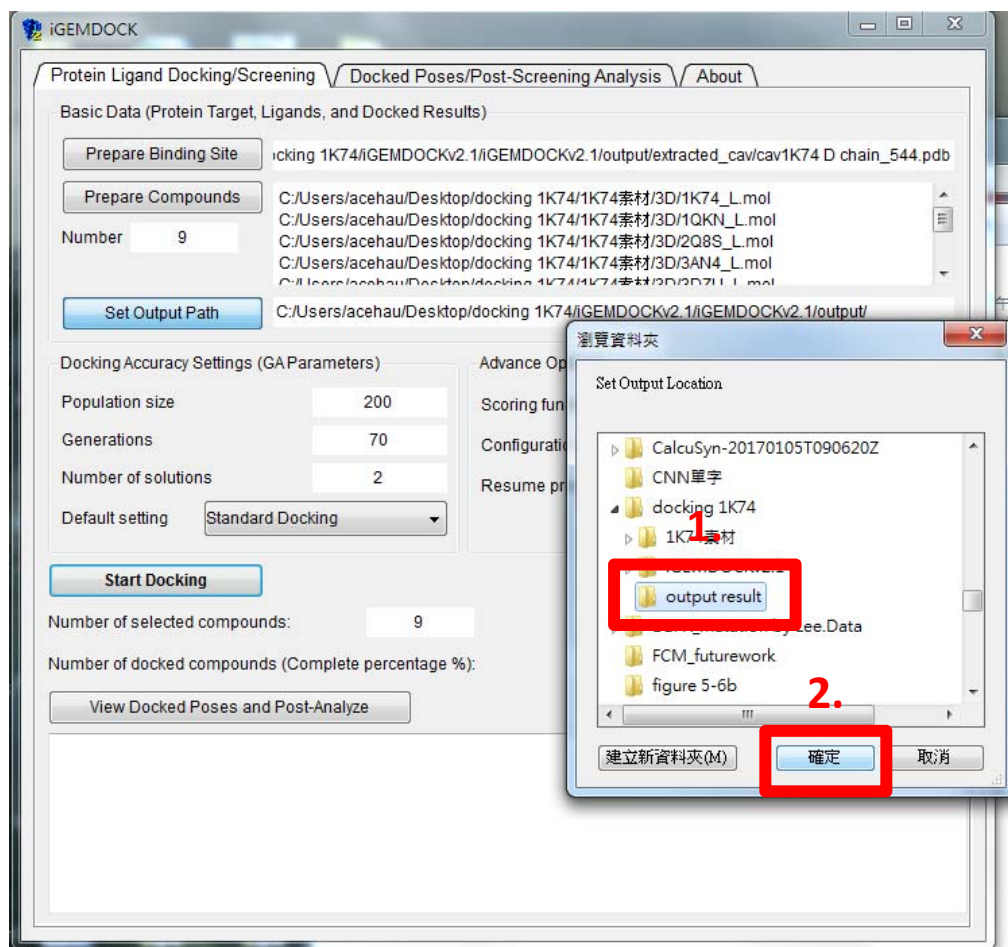


# 操作步驟



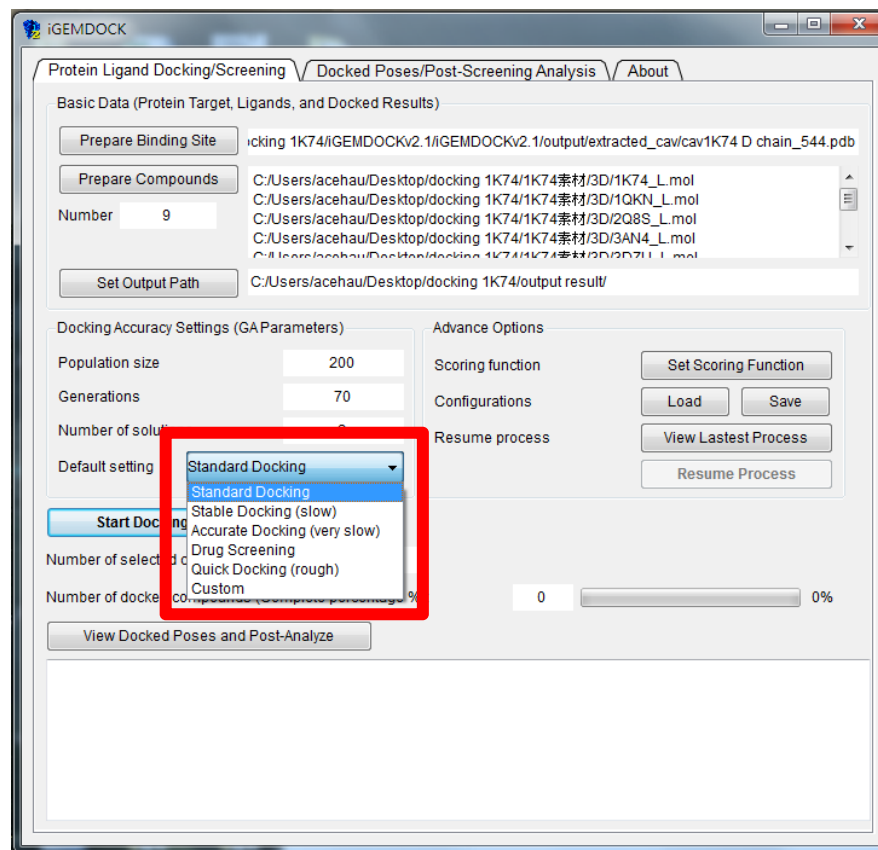
步驟十三：按下Set Output Path

# 操作步驟



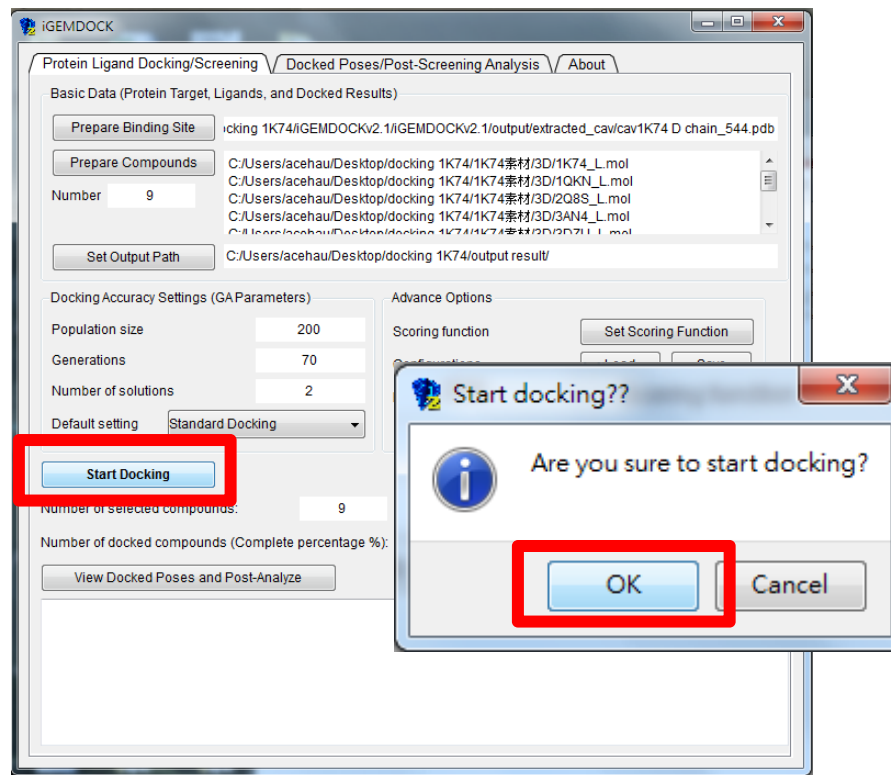
步驟十四：1. 選擇要存放的資料夾 2. 按下「確定」完成設定

# 操作步驟



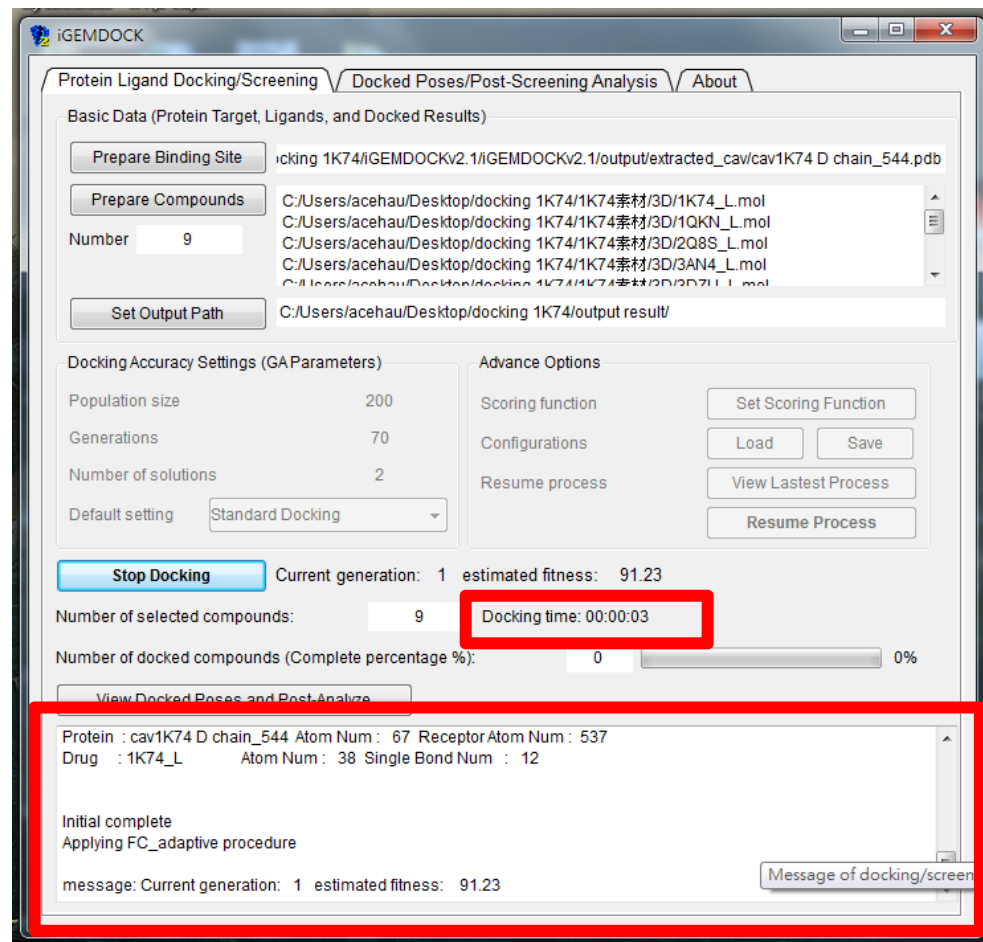
步驟十五：在Default setting的地方，選擇你要的計算模式

# 操作步驟



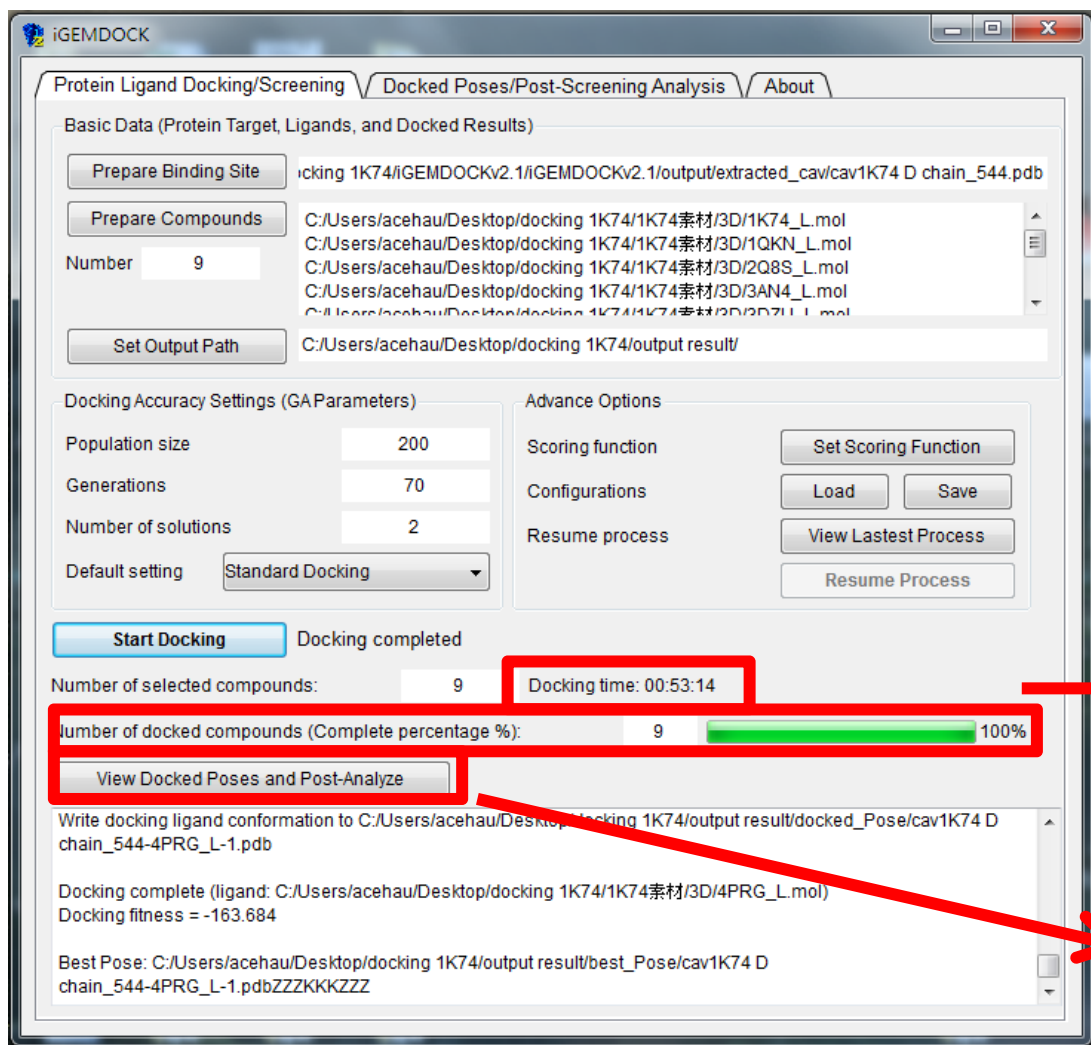
步驟十六：最後按下Start Docking，並在確認視窗中按下OK開始計算。

# 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

The screenshot shows the iGEMDOCK software interface. The main window is titled "iGEMDOCK" and has tabs for "Protein Ligand Docking/Screening", "Docked Poses/Post-Screening Analysis", and "About". The "Docked Poses/Post-Screening Analysis" tab is active, showing a table of docked poses. The table has columns for "Compound", "Energy", "VDW", "HBond", and "Elec". The first row is selected, and its energy value is -188.83. A red box highlights the table columns. A blue box highlights the "Save" button and the "Excel" option in the "Save" dropdown menu.

Compound	Energy	VDW	HBond	Elec
<input checked="" type="checkbox"/> cav1K74 D chain_544-1K74_L...	-188.83	-165.81	-18.85	-4.16
<input type="checkbox"/> cav1K74 D chain_544-1QKN_L...	-134.53	-121.34	-13.19	0
<input type="checkbox"/> cav1K74 D chain_544-2Q8S_L...	-142.84	-121	-17.45	-4.39
<input type="checkbox"/> cav1K74 D chain_544-3AN4_L...	-132.45	-127.63	-4.82	0
<input type="checkbox"/> cav1K74 D chain_544-3DZU_L...	-98.53	-83.64	-12.25	-2.64
<input type="checkbox"/> cav1K74 D chain_544-3G8L_L-0...	-126.39	-114.93	-11.46	0
<input type="checkbox"/> cav1K74 D chain_544-3VSP_L...	-136.91	-125.27	-8.33	-3.31
<input type="checkbox"/> cav1K74 D chain_544-4E4K_L...	-106.19	-105.95	-0.24	0
<input type="checkbox"/> cav1K74 D chain_544-4PRG_L...	-164.07	-144.57	-15.68	-3.82

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

1. Prepare Screening Data

Load: Binding Site D chain\_544.pdb Docked Poses  
Output: /Users/acehau/Desktop/docking\_1K74/output result/ Set Output Path

Generate: Interaction Profile Interaction Analysis  
Save: Summary table Text Excel

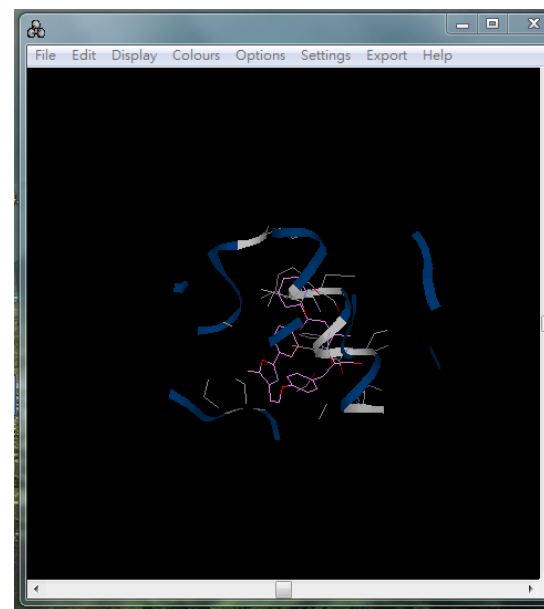
Select: All / None Compound **Display** Sort: Compound Clean Table

	Compound	Energy	VDW	HBond	Elec
1	cav1K74 D chain_544-1K74_L...	-188.83	-165.81	-18.85	-4.18
2	cav1K74 D chain_544-1QKN_L...	-134.53	-121.34	-13.19	0
3	cav1K74 D chain_544-2Q8S_L...	-142.84	-121	-17.45	-4.39
4	cav1K74 D chain_544-3AN4_L...	-132.45	-127.63	-4.82	0
5	cav1K74 D chain_544-3DZU_L...	-98.53	-83.64	-12.25	-2.64
6	cav1K74 D chain_544-3G8L_L-0...	-126.39	-114.93	-11.46	0
7	cav1K74 D chain_544-3VSP_L...	-136.91	-125.27	-8.33	-3.31
8	cav1K74 D chain_544-4E4K_L...	-106.19	-105.95	-0.24	0
9	cav1K74 D chain_544-4PRG_L...	-164.07	-144.57	-15.68	-3.82

2. Cluster Poses  
Features: Interaction & Atom Composition  
Set interaction cluster number: 4  
Set atom composition cluster number: 4  
Cluster

3. Select Cluster  
Select: All / None  
Interaction ClusterID: 0  
Composition ClusterID: 0  
Add Clear

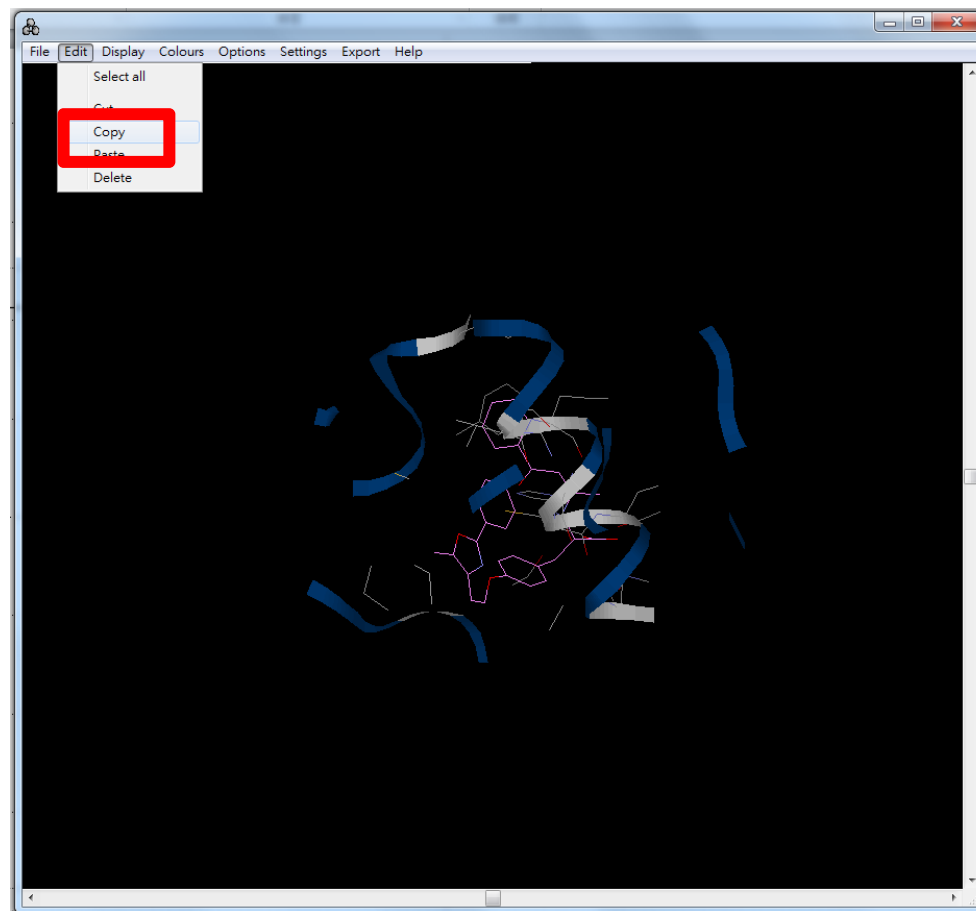
4. Display  
Clustered Interaction Table  
Interaction Profile Clusters  
Atom Composition Clusters



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。

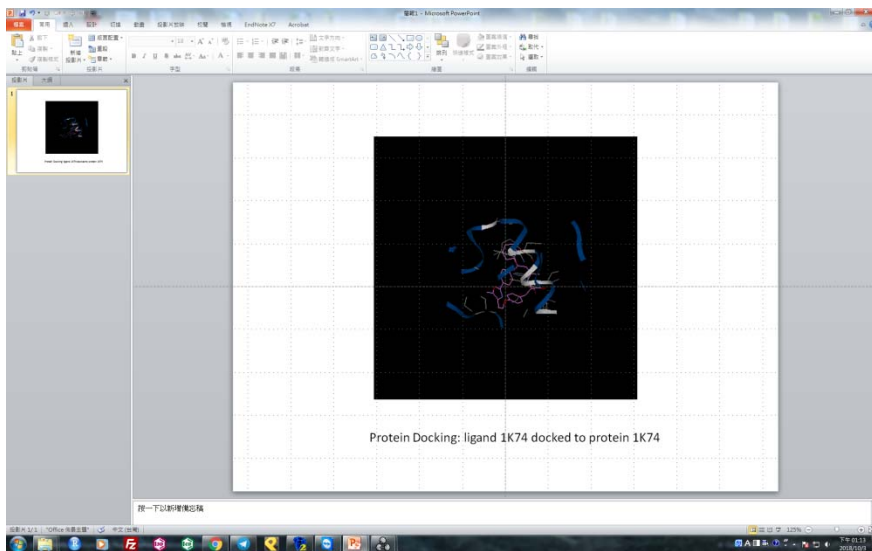


# 操作步驟



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



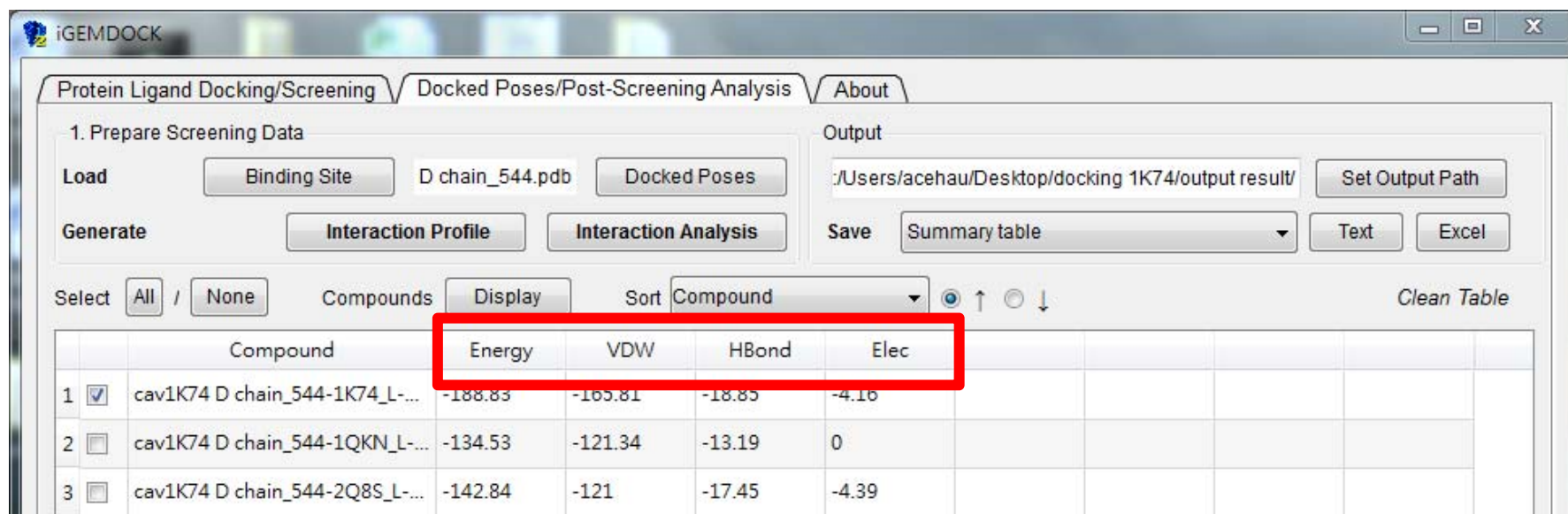
1K74 docking.xls - Microsoft

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	#C:/Users/acehau/Desktop/docking_1K74/iGEMDOCKv2.1/output/extracted_cav/1K74 D													
2	#Ligand	TotalEnerg	VDW	HBond	Elec	AverConFair								
3	cav1K74 D	-188.826	-165.814	-18.8494	-4.16329	27.5789								
4	cav1K74 E	-134.532	-121.34	-13.1917	0	27.6765								
5	cav1K74 E	-142.844	-120.995	-17.4549	-4.39476	25.3548								
6	cav1K74 E	-132.451	-127.634	-4.81702	0	18.9762								
7	cav1K74 E	-98.5328	-83.636	-12.2527	-2.64404	25.2727								
8	cav1K74 E	-126.386	-114.929	-11.4569	0	26.0968								
9	cav1K74 E	-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								
12														
13														
14														
15														
16														
17														
18														
19														
20														
21														

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)？



The screenshot shows the iGEMDOCK software interface. The main window is titled "iGEMDOCK" and has three tabs: "Protein Ligand Docking/Screening", "Docked Poses/Post-Screening Analysis", and "About". The "Docked Poses/Post-Screening Analysis" tab is active. The interface includes a "1. Prepare Screening Data" section with buttons for "Load", "Binding Site", "D chain\_544.pdb", "Docked Poses", "Generate", "Interaction Profile", and "Interaction Analysis". There is also an "Output" section with a text field for the output path and buttons for "Set Output Path", "Save", "Summary table", "Text", and "Excel". Below these sections is a table with columns for "Compound", "Energy", "VDW", "HBond", and "Elec". The table contains three rows of data. The first row is highlighted with a red box.

Compound	Energy	VDW	HBond	Elec
1 <input checked="" type="checkbox"/> cav1K74 D chain_544-1K74_L-...	-188.83	-165.81	-18.85	-4.16
2 <input type="checkbox"/> cav1K74 D chain_544-1QKN_L-...	-134.53	-121.34	-13.19	0
3 <input type="checkbox"/> cav1K74 D chain_544-2Q8S_L-...	-142.84	-121	-17.45	-4.39

# 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.*