



Protein Structure Visualization



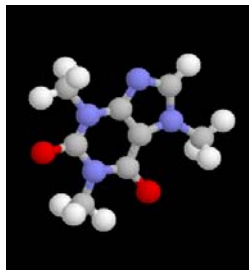
Yi-Chung Liu

2008/07/21

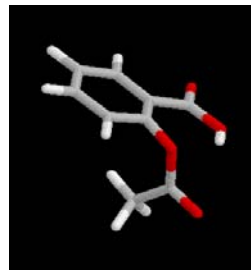


Molecular Structure Visualization

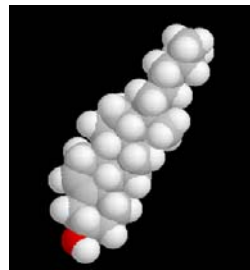
- ◆ 是一種可顯現出**生物巨分子結構**的軟體
 - ✓ 包含蛋白質、DNA、RNA、化學小分子和金屬等。
- ◆ 可以輔助觀察巨分子的**結構、作用力、表面特性**等。
- ◆ 在**藥物設計、分子模擬**上有很大的應用空間。



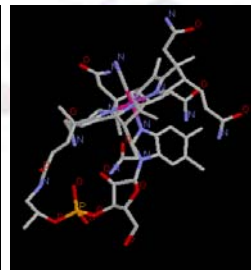
咖啡因



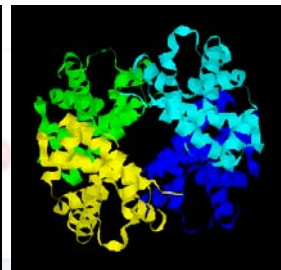
阿斯匹靈



膽固醇



維生素B₁₂



血紅蛋白

Software of Molecular Structure Visualization

RasMol	http://www.umass.edu/microbio/rasmol/
Chime	http://www.mdlchime.com/chime/
MolPOV	http://www.chem.ufl.edu/~der/der_pov2.htm
MolMol	http://www.chem.ufl.edu/~der/der_pov2.htm
Ribbon	http://www.chem.ufl.edu/~der/der_pov2.htm
MolSc	http://www.chem.ufl.edu/~der/der_pov2.htm
WebLab ViewerLite and ViewerPro	http://www.chem.ufl.edu/~der/der_pov2.htm
Swiss-PDB Viewer	http://www.expasy.ch/spdbv/
XtalView	http://www.scripps.edu/pub/dem-web/toc.html
MolView and MolView Lite	http://bilbo.bio.purdue.edu/~tom/

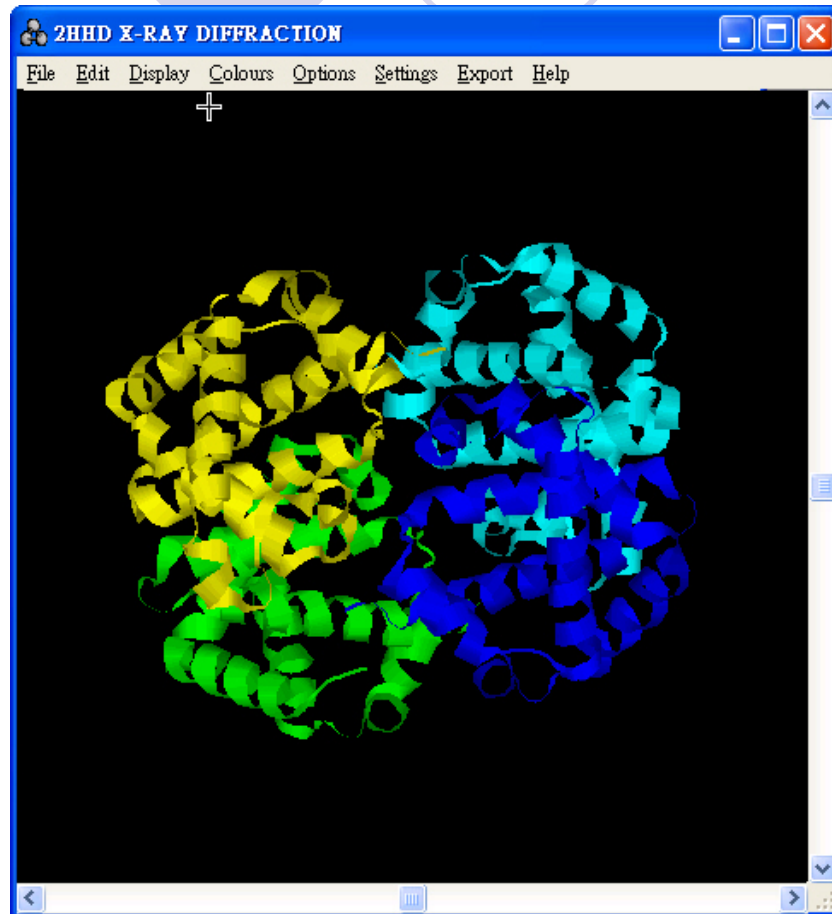
RasMol & Chime

What's RasMol ?

- ❖ RasMol 讀取描述**分子立體結構的原子座標檔**，將分子的立體結構，藉由生動的顏色及模型，以**互動**的形式展現在電腦螢幕上。
- ❖ 利用 RasMol 可將抽象的分子，經由不同的角度來檢視。
- ❖ 尤其對複雜的生化分子，蛋白質、核酸等，經過適當的顏色或模型的標記，有助於瞭解**大型分子的各級結構、分析活性區的作用力**等。

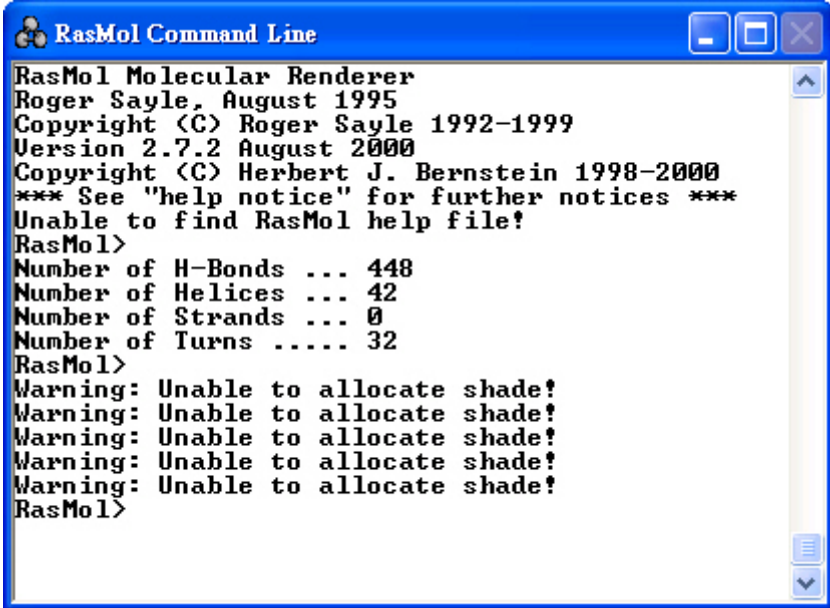


RasMol 程式介面有兩個視窗



圖形視窗:

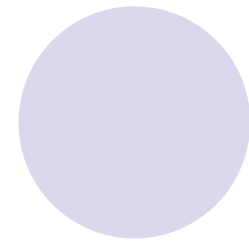
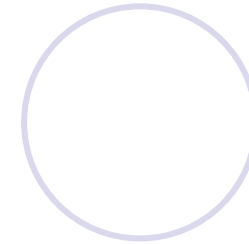
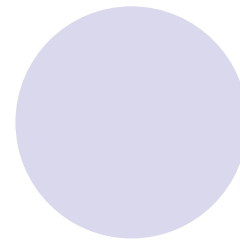
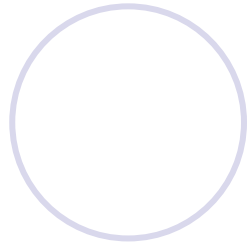
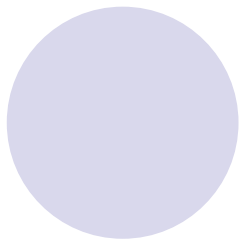
分子模型顯示的視窗, 可利用滑鼠來檢視分子模型 (縮小、放大、轉動、移動等), 並可點選選單中一些預設的常用指令, 以得到所要的分子模型。



```
RasMol Molecular Renderer
Roger Sayle, August 1995
Copyright (C) Roger Sayle 1992-1999
Version 2.7.2 August 2000
Copyright (C) Herbert J. Bernstein 1998-2000
*** See "help notice" for further notices ***
Unable to find RasMol help file!
RasMol>
Number of H-Bonds ... 448
Number of Helices ... 42
Number of Strands ... 0
Number of Turns ..... 32
RasMol>
Warning: Unable to allocate shade!
Warning: Unable to allocate shade!
Warning: Unable to allocate shade!
Warning: Unable to allocate shade!
Warning: Unable to allocate shade!
RasMol>
```

指令視窗:

對於比較複雜進階的分子模型處理, 可由指令視窗輸入指令。結果會顯示在圖形視窗



RasMol- Download

<http://alpha.life.nthu.edu.tw/download.htm>



Download the demo protein:

Protein: [1D66](#)

Download the structure file from **PDB**

RCSB
PDB
PROTEIN DATA BANK



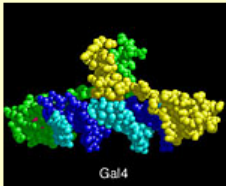


After download the demo protein: **1D66**

Please open the RasMol- **User manual**

1	讀檔
2	看看有多少個鏈
3	protein/DNA之外的物質
4	疏水性胺基酸
5	Cd離子
6	儲存影像
7	Script
8	二級結構
9	兩原子間的距離
10	protein/DNA間的鍵結
11	分子內部圖(Slab)
12	固定DNA軸旋轉
13	原子的展現方法
14	標示原子
15	分子3D圖(stereo)
16	指定特定的原子
17	Tips
18	滑鼠
19	練習

RasMol for Dummies



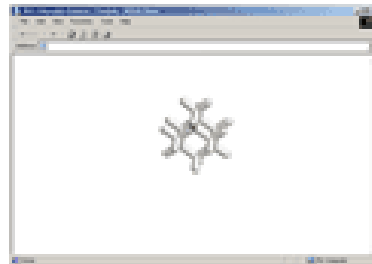
A Tutorial for the Rasmol Basics

<http://mod.life.nthu.edu.tw/bioinfo/rasmol/rasmol.php>



Protein Structure Visualization -

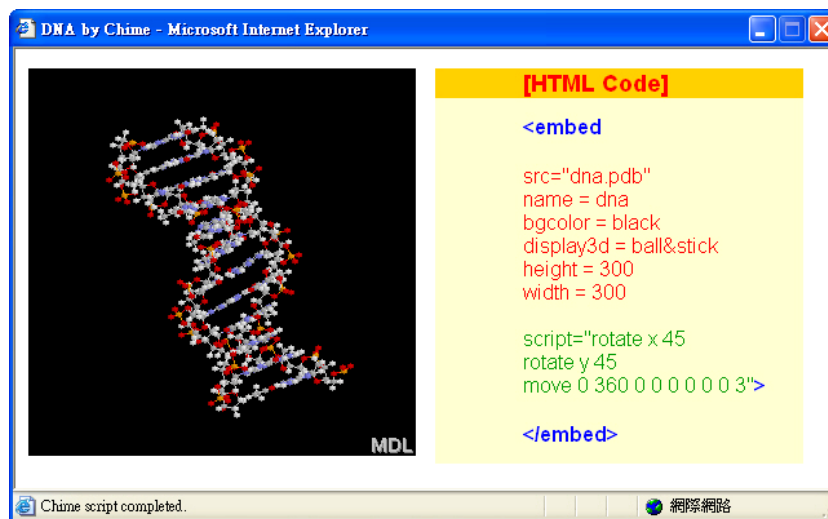
Chime



Chime vs. RasMol-1

Chime is Built upon RasMol

- Chime是一套plug-in的軟體，搭配瀏覽器(IE or Netscape)來觀察化學結構，其是以RasMol語言介面所建立，所以功能大都跟RasMol一樣，可說是RasMol的瀏覽器版。

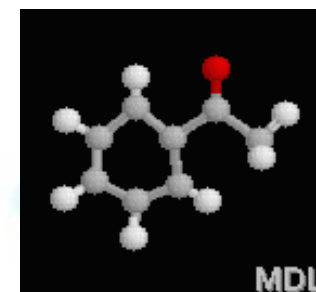


Chime vs. RasMol-2



What Chime Has that RasMol Lacks

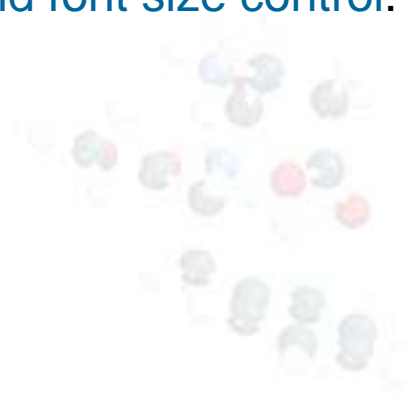
- Chime有新建一些 [script commands](#) , 在educational tutorials上非常有用。 These include clock-timed **move** and **delay**, also **view show, view save, view restore**.
- Hypertext [button-controlled scripting](#).
- 適合發展跨平台的教學工具(with plug-in graphic and HTML/javascript)
- [Molecular animations](#) from XYZ data files.
- Ability to run [multiple plug-ins simultaneously](#).



Chime vs. RasMol-3

Advantages of Chime over RasMol for Educational Tutorials-1

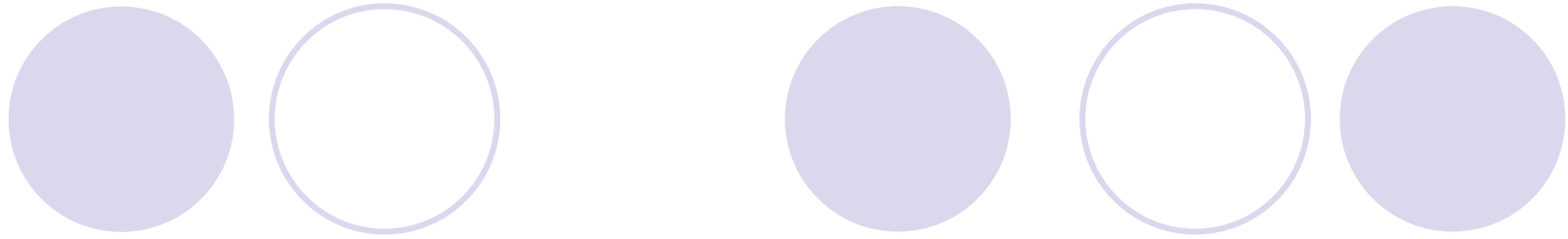
- 內容流程控制項: hypertext, buttons...
- Legends: color-keyed, font control
 - RasMol's legend font is fixed. On high-resolution displays, it becomes too small to read when projected.
 - The HTML control of legends on a Chime web page allows full color and font size control.



[Color]→[CPK]

CPK顏色分類:

- Nitrogen (light blue)
- Carbon (light grey)
- Oxygen (red)
- Hydrogen (white)
- Sulfur (yellow)
- Phosphorus (orange)
- Iron (orange)



Advantages of Chime over RasMol for Educational Tutorials-2

- 結構視窗與動作按鈕解說視窗獨立且可互相配合，提升教學互動效果。
 - For example, [膠原蛋白酵素 \(Collagenase\)](#)
- Hardware-independent timing
 - Chime provides **clocked moves and delays** which occur in specified time intervals, independent (as much as possible) of hardware speed.

Chime vs. RasMol-3

Advantages of RasMol over Chime

○ High-Resolution Printing.

- Chime images 只能以螢幕解析度列印。

○ Source code.

- RasMol's source code is in the **public domain**. This allowed individuals to modify RasMol and port it to many operating system platforms.
- Chime source code is **proprietary to MDL**.

○ Rasmol的**script**可進行較細緻的處理，**Chime**有時仍要用到**Rasmol的script**。

*RasMol Version 2.6-beta-2/Chime 0.99 Manual

<http://www.umass.edu/microbio/chime/manual/chimeman.htm>



Let's play Chime now!



Install

- Test your PC...
- Install Chime in [Alpha download page](#)



View and Control

- <http://mod.life.nthu.edu.tw/bioinfo2/Chime/>



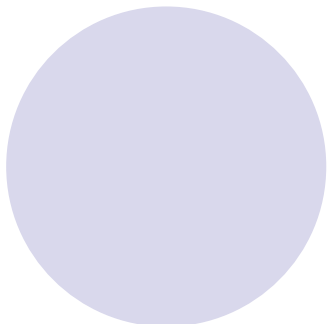
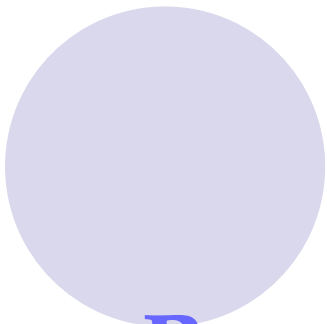
Mouse Controls

Chime rule in **RED** if different than RasMol.

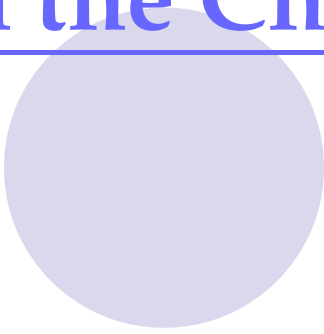
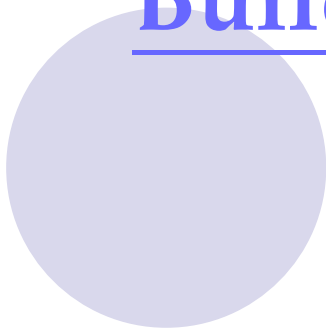
Action	Windows	Macintosh
Rotate X,Y	Left	Unmodified
Translate X,Y	Right Ctrl-Right	Command*
Rotate Z	Shift-Right	Shift-Command*
Zoom	Shift-Left	Shift
Slab Plane	Ctrl-Left	Ctrl
Chime's Menu	Right	Hold Down



Part II



Build the Chime Page




製作一個Chime網頁，主要分成兩個部分，一個是結構視窗 (Display Part)，另一個是動作按鈕(Button Part)。

Protein Story

The Catalytic Domain of the Collagenase

Display Part



MDL

☒ Spin off ☒ Reset ☒ Zoom 200 ☒ Stereo

Display Part

- * active cleft的氨基酸標示 ☒
- * 與此鋅離子作用的氨基酸 ☒

膠原蛋白酶是zinc protease的一員，這個super family特色是它們與鋅的結合有關的序列有很大的共通性—[GSTALIVN]-x(2)-H-E-[LIVMFYW]-{DEHRKP}-H-x-[LIVMFYW6SPQ] (H為 zinc ligands, E為active site residue)，於膠原蛋白酶中此段序列 位在215~224的地方 ☒，序列為VAANELGHSL。

- * 1CGE的二級結構 ☒
- * 三個alpha helices ☒
- * 五個beta strands ☒
- * 306個水分子 ☒
- * 疏水位置 ☒
- * 以groups顯示 ☒

結構視窗

動作按鈕視窗

How to use Chime Plug in

[建立結構視窗]

```
<html>
<head>
<title>Untitled Document</title>
<meta http-equiv="Content-Type" content="text/html; charset=big5">
</head>
<body>
<embed .....(在此處加入Chime的指令)>

</embed>
</body>
</html>
```

於<body>
之後插入

```
<embed src="file name" name= file name
width=300 height=300 bgcolor= black
display3d= ball&stick script="____">
```

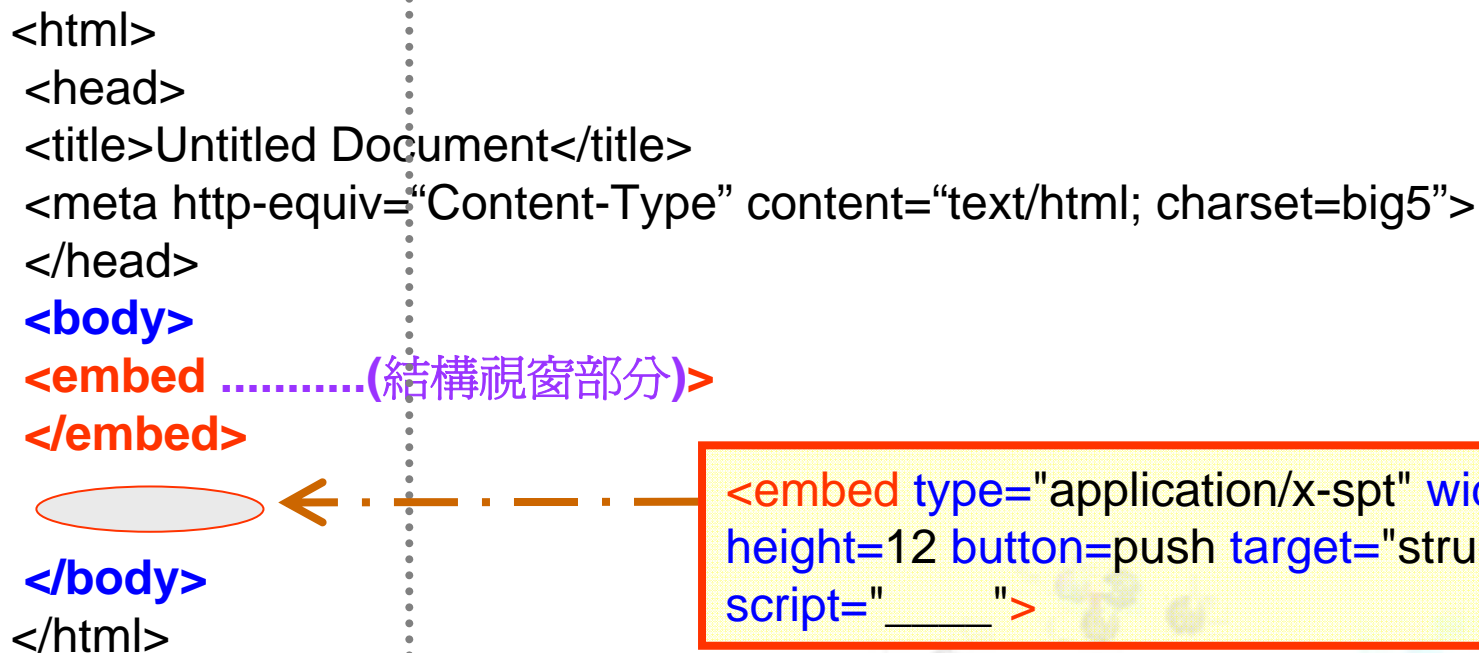
可用的檔案格式有:

```
*.mol, *.pdb, *.xyz and *.skc
```

How to use Chime Plug in

[建立動作按鈕視窗]

```
<html>
<head>
<title>Untitled Document</title>
<meta http-equiv="Content-Type" content="text/html; charset=big5">
</head>
<body>
<embed .....(結構視窗部分)>
</embed>
</body>
</html>
```



```
<embed type="application/x-spt" width=12
height=12 button=push target="struct"
script="____">
```

可用的script格式可參照:

[\[Chime RasMol Tutorial\]](#)



Part III

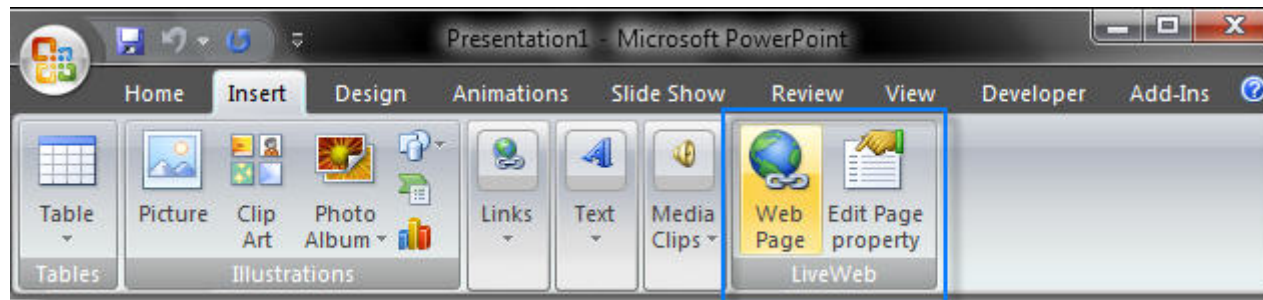
**Embedding Chime Structures
in PowerPoint Presentation**

*PC MAGAZINE - 5 STAR RATING

LiveWeb

- insert and view web pages real-time.

- Use **LiveWeb** to insert web pages into a **PowerPoint** slide and refresh the pages real-time during slide show.



Download the LiveWeb PowerPoint plug-in file from:
<http://skp.mvps.org/liveweb.htm>

How To **Install** the LiveWeb PowerPoint Plug-In in a PowerPoint Slide

1. **Extract** the contents of the zip to a folder.
2. Launch PowerPoint.
3. Click on **Tools | Add-ins** to bring up the add-ins window.
4. Click on Add to bring up the 'Add New PowerPoint Add-in' dialog box.
5. Navigate to the folder where the contents of the zip file was extracted and select '**LiveWeb.ppa**' and click on OK.
6. You might be prompted with the macro virus warning. Enable the macros. When the Add-in is properly loaded, it will display a 'X' against the add-in name.
7. That's it. You have successfully loaded the add-in.

Before you insert a chime page to a PowerPoint Slide

1. To show a rotatable molecule on a PowerPoint slide, you must first **create a web page with a working Chime script**.
2. Make sure that you have the "**chime.htm**" file and the subject molecular structure file ("**something.pdb**"), preferably stored in the **same folder** as your .ppt file.



Protein Story

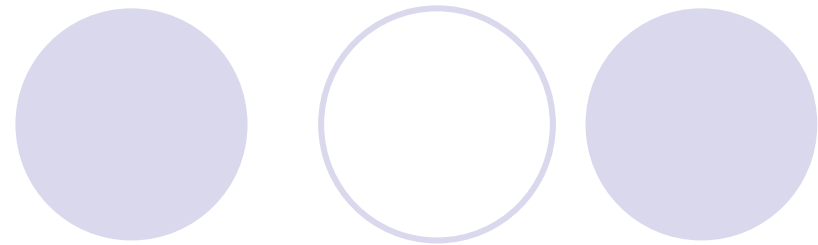
The Catalytic Domain of the Collagenase

- * active cleft的氨基酸標示
- * 與此鋅離子作用的氨基酸
- 膠原蛋白酶是zinc protease的一員，這個superfamily特色是它們與鋅的結合有關的序列有很大的共通性—[GSTALIVN]-x(2)-H-E-[LIVMFYW]-[DEHRKP]-H-x-[LIVMFYW6SPQ] (H為 zinc ligands, E為active site residue)，於膠原蛋白酶中此段序列 位在215~224的地方 ，序列為 VAAHEL6HSL。
- * 1CGE的二級結構
- * 三個alpha helices
- * 五個beta strands
- * 306個水分子
- * 疏水位置
- * 以groups顯示

MDL

Spin off Reset Zoom 200 Stereo

Usage



1. Launch PowerPoint.
2. Click on **Insert | Web Pages...**
3. Enter the list of web page address that you wish to create.
4. Provide the additional info required.
5. LiveWeb will create slides with web browser controls embedded on the slides
6. Run the slide show.
7. The web pages will be displayed during the slide show and refreshed at real-time.

