



分子視覺化軟體

Protein Structure Visualization

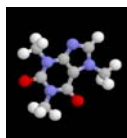
2008/07/15



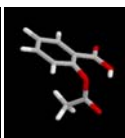
劉益忠

Molecular Structure Visualization

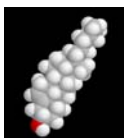
- ◆ 是一種可顯現出**生物巨分子結構**的軟體
 - ✓ 包含蛋白質、DNA、RNA、化學小分子和金屬等。
- ◆ 可以輔助觀察巨分子的**結構、作用力、表面特性**等。
- ◆ 在**藥物設計、分子模擬**上有很大的應用空間。



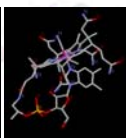
咖啡因



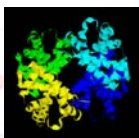
阿斯匹靈



膽固醇



維生素B₁₂



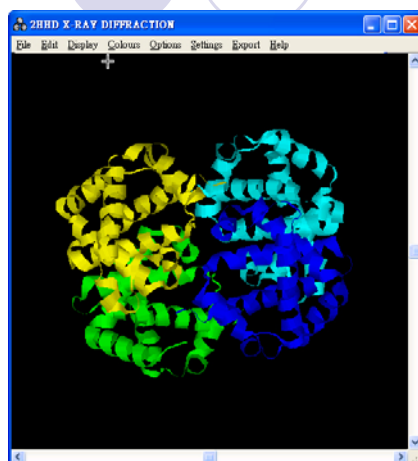
血紅蛋白

什麼是 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，藉由生動的颜色及模型，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，經過適當的颜色或模型的標記，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!
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。

 **RasMol** 之安裝 

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

 **RasMol** 之使用說明

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

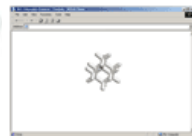
 下載蛋白質結構資料

Structure Explorer - [1D66](#)

Download the Structure File: - [1D66](#)



 Protein Structure Visualization –

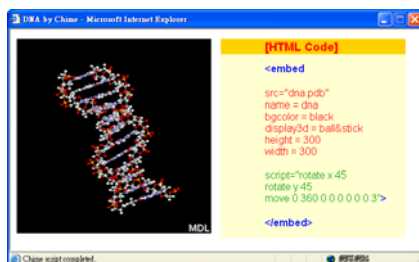


Chime 

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。

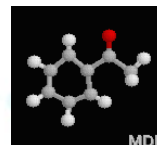


Demo

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]

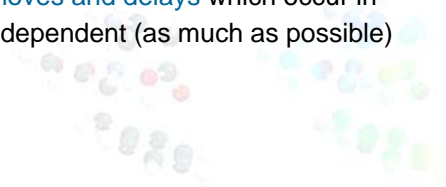
CPK顏色分類:

- 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)。

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:

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

參考網站

- [Tutorial Using RasMol Scripts with Chime](#)
- [Chime: How to use it](#)
- [Chime: Simplest Web Page](#)
- [WWW Home Page Design \(WWW Home Page 的製作與應用\)](#)
- [CuteFTP 使用教學](#) [來源：[高中電腦學習加油站](#)]



除非經過授權，請勿在網頁上放置有版權之圖片或是軟體，以免觸法。