Software for Protein Structure Visualization

呂平江

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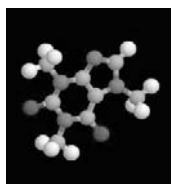
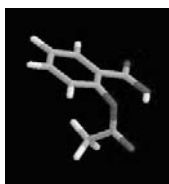2012/06/27
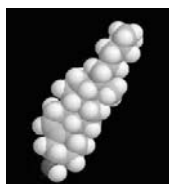

Molecular Structure Visualization

- 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。
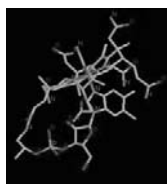
- 可以輔助觀察巨分子的結構、作用力、表面特性等。

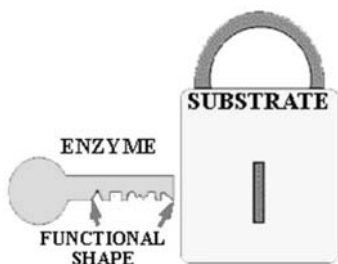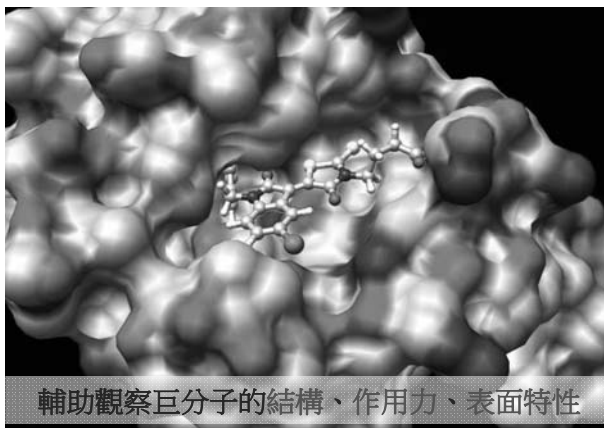- 在藥物設計、分子模擬上有很大的應用空間。

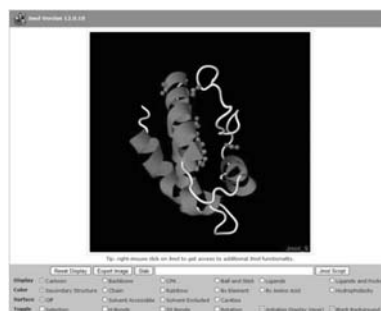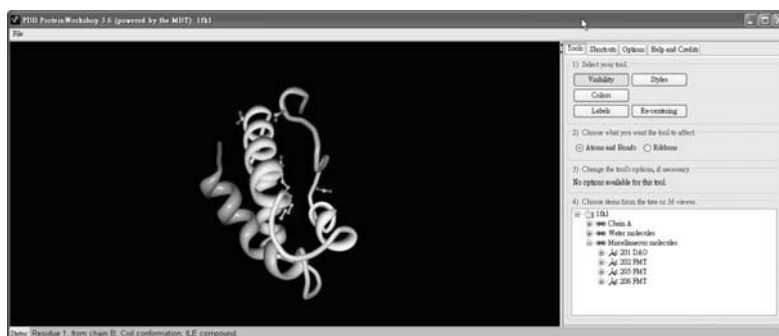| 咖啡因 | 阿斯匹靈 | 膽固醇 | 維生素B$_{12}$ | 血紅蛋白 |

LIGAND/RECEPTOR PAIRS
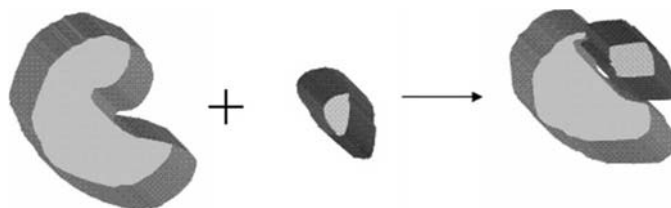
Just as a key has a functional shape that allows it to unlock a unique lock, so does each enzyme have a shape that allows it to act on a unique substrate.

輔助觀察巨分子的結構、作用力、表面特性

Simple Viewer in PDB

Jmol Viewer for 1FK1

RCSB - Simple Viewer
只有簡單結構展示功能
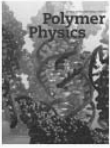
Software of Molecular Structure Visualization

RasMol	http://rasmol.org/
Chime	http://www.symyx.com/downloads/index.jsp
PyMOL	http://www.pymol.org/
MolMol	http://www.mol.biol.ethz.ch/wuthrich/software/molmol/
Ribbons	http://www.cmc.uab.edu/ribbons/
MolScript	http://www.avatar.se/molscript/
WebLab ViewerLite and ViewerPro	http://www.accelrys.com/about/msi.html
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/

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http://www.pymol.org/

PyMoL

PyMOL-created Journal Covers

Image of two short stretches of double-stranded DNA linked by a ruthenium 'light-switch complex', October 25, 2011; 108 (43) [[1]]	Protein Science, Vol. 20, No. 12, Dec 2011	Journal of Polymer Science, Nov 15 2011	Biophysical Journal, Aug 3 2011	Focused Evolution of HIV-1 Neutralizing Antibodies Revealed by Structures and Deep Sequencing, [Science, Sept. 16, 2011].
Deconstructing honeybee vitellogenin J. Exp. Biol., Volume 214, Issue 4, 2011 .	Binding of 14-3-3g to membranes FEBS lett., Volume 585, Issue 8, 2011 .	FLT3 Activation by an Oncogenic Insertion Molecular Cell, Volume 13 Number 2, January 30, 2004.	PI3K Inhibitors C&EN, April 11, 2011.	Microbiology of article entitled "Genetic mapping of the interface between the ArsD metallochaperone and the ArsA ATPase. Volume 79, Feb, 2011, Molecular Microbiology

http://www.pymolwiki.org/index.php/Covers

PyMOL Academic Price List

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Class/Offering	PyMOL		AxPyMOL		PyMOL + AxPyMOL		Description
	One-Year Subscription	Three-Year Subscription	One-Year Subscription	Three-Year Subscription	One-Year Subscription	Three-Year Subscription	
Professional	$99 Select	$249 Select	$49 Select	$125 Select	$148 Select	$374 Select	License for one person
Laboratory & Classroom	$269 Select	$689 Select	$135 Select	$345 Select	$404 Select	$1034 Select	License for one researcher/instructor and his/her students
Department	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	License for one academic department
Other Situations	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	Contact us at sales@schrodinger.com	For example: site licenses, computing centers, multi-site collaborations

http://pymol.org/academic.html

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PyMOL
A *USER-SPONSORED* molecular visualization system on an *OPEN-SOURCE* foundation

DOWNLOAD Version 1.5

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To download, right-click for "Save Target As...", "Save Link As...", or "Download Linked File".

Current Release

- **PyMOL 1.3r1 edu** (Sept 2010)

  Windows: **pymol-v1.3r1-edu-Win32.msi**
  MD5SUM: 265fa652aa4880304f4a59e1af653a1b

  Macintosh: **MacPyMOL-v1.3r1-edu.tar.bz2**
  MD5SUM: 260793a054ef791987af9e6300ed1ce0

  Linux: **pymol-v1.3r1-edu-Linux-x86-TclTk8.5.tar.bz2**
  MD5SUM: 96da619d58ec137bbf05769e9f59ce4b

PRIOR RELEASE

- **PyMOL 1.2edu1** (August 2009)

  Windows: **pymol-1_2edu1-bin-win32.msi**

  Macintosh: **macpymol-1_2edu1.tgz**

  Linux: **pymol-1_2edu1-bin-linux-x86-centos45.tgz**

Download PyMoL (v0.99) from
alpha.life.nthu.edu.tw

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Today	32
Yesterday	87
This week	32
This month	242
All	41331

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週四, 23 十月 2008 11:27 管理者

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1. Rasmol 2.7.5 (新版)
2. Rasmol Help File (rasmol.hlp) (Command mode)
3. Rasmol Help File (raswin.hlp) (Windows HELP file)
4. MDL Chime SP6
5. Swiss-pdb viewer
6. Cn3D
7. Pymol
8. 蛋白質結構下載: 1D66

最近更新 (週二, 31 八月 2010 11:06)

生物資料庫課程相關軟體下載
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網頁製作與影像處理：

1. DreamWeaver MX 中文試用版
2. Flash MX 2004 中文試用版
3. SWiSH Max2 繁體中文試用版

最近更新 (週二, 31 八月 2010 10:43)

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NEXT

Please link to : **PyMOL Tutorial**

http://140.114.98.89/sg/pymol/

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1. Getting started: explore a protein

1. Download a PDB file: 1D66

2. Open PyMOL and load 1D66.pdb

3. PyMOL Tutorial:
http://140.114.98.89/sg/pymol/

結構生物資訊學研習會 @ 2012
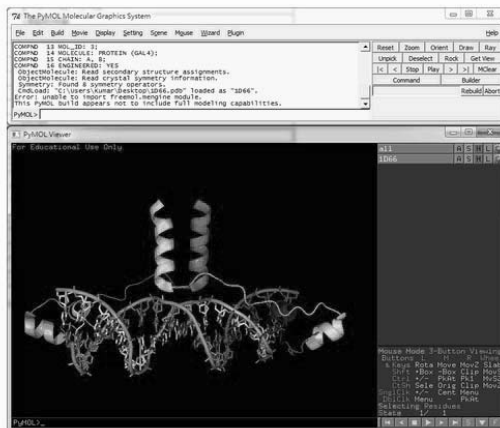
首頁 | 學習目標 | Databases for Protein Structure | PyMoL | Modeling & Prediction | Structural comparison | Exercise

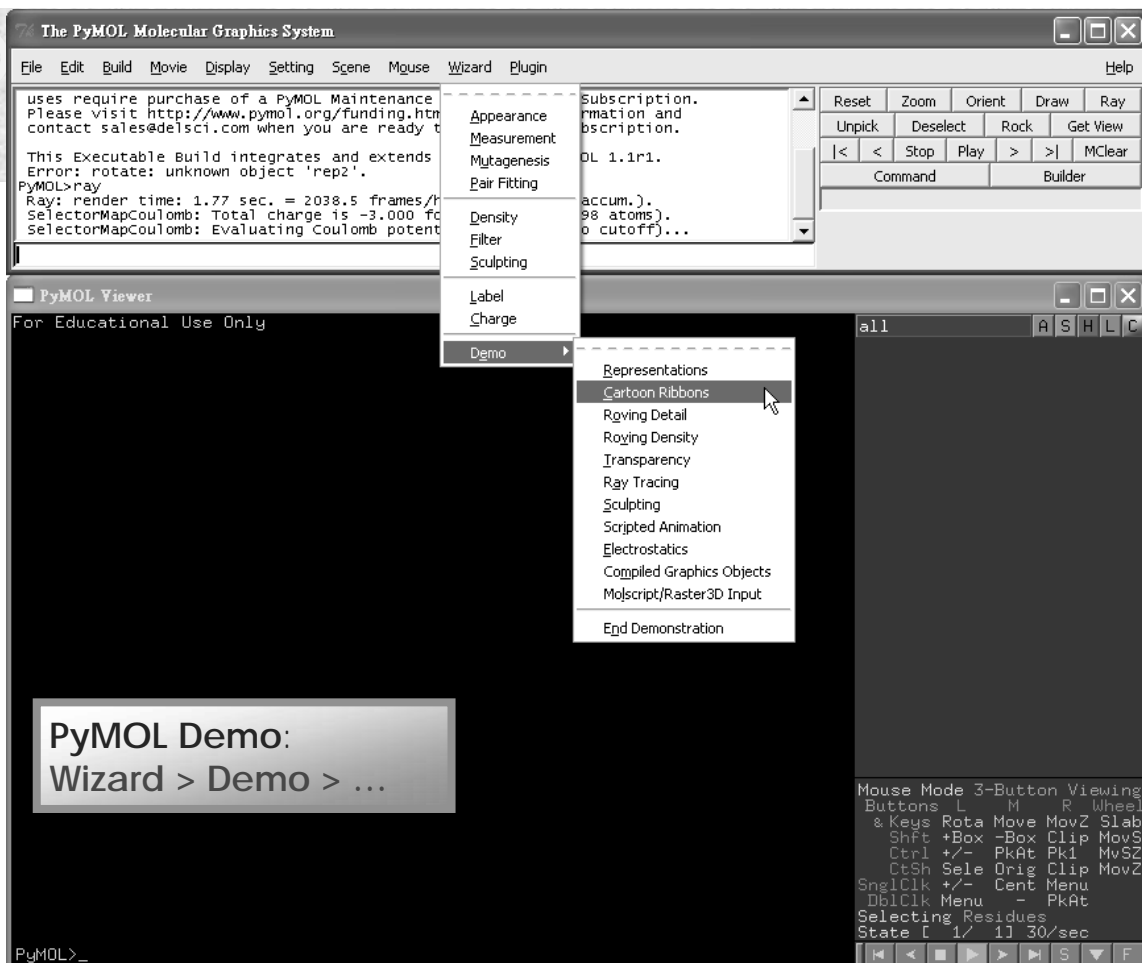**PyMOL Tutorial**

Edit by Yi-Chung Liu

PyMOL for Dummies

A Tutorial for the PyMOL Basics

PC Lyu's Lab TEL:+886-3-5715131-33489 / FAX:+886-3-5715934 / If you have any question, please feel free to e-mail us.
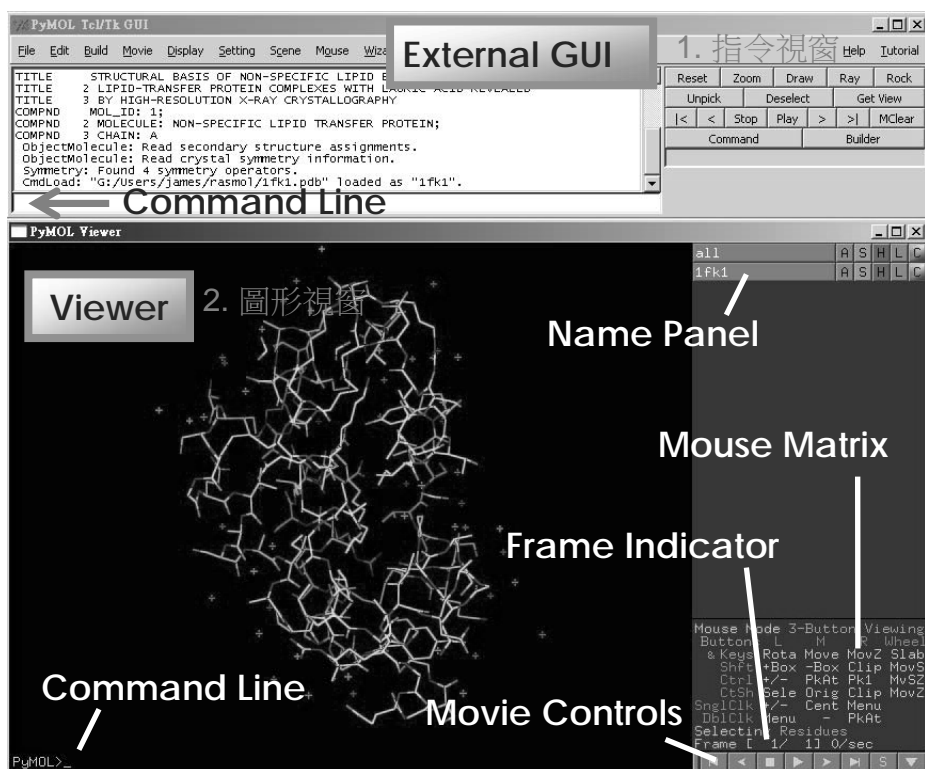
http://140.114.98.89/sg/pymol/

PyMOL Demo:
Wizard > Demo > ...

PyMOL Interface

External GUI

1. 指令視窗

Command Line

Viewer

2. 圖形視窗

Name Panel

Mouse Matrix

Frame Indicator

Command Line

Movie Controls

A: action
S: show
H: hide
L: label
C: color

Table with pre-defined colours

white		black		blue		green		red	
cyan		yellow		magenta		salmon		lime	
slate		hotpink		orange		yellowgreen		bluegreen	
blueviolet		marine		olive		purple		teal	
ruby		forest		deep		grey		carbon	
nitrogen		oxygen		hydrogen		brightorange		pink	
firebrick		chocolate		wheat		violet		density	

指令簡寫參考

name <atom names>	n; <atom names>
resn <residue names>	r; <residue names>
resi <residue identifiers>	i; <residue identifiers>
chain <chain ID>	c; <chain ID>
segi	s;
elem <element symbol>	e; <element symbol>
flag <number>	f; <number>
alt <code>	
numeric_type <numeric type>	nt; <numeric type>
text_type <text type>	tt; <text type>
hydrogen	h;
all	*
visible	v;
id <original-index>	
hetatm	
ss <secondary structure>	
around <distance>	a; <distance>
expand <distance>	e; <distance>
gap <distance>	
in <selection>	
like <selection>	l; <selection>
<selection> and <selection>	<selection> & <selection>
<selection> or <selection>	<selection> | <selection>
<selection> not <selection>	<selection> ! <selection>
<selection> and not <selection>	<selection> & ! <selection>
byres <selection>	br; <selection>
byobject <selection>	bo; <selection>