



Software for Protein Structure Visualization

劉益忠 博士

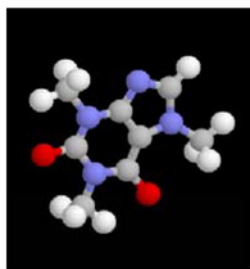
2013/06/26



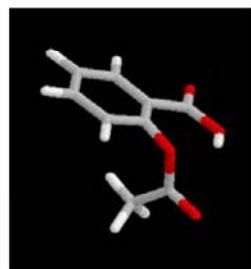
Molecular Structure Visualization



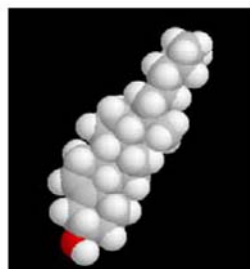
- 是一種可顯現出生物巨分子結構的軟體
 - 包含蛋白質、DNA、RNA、化學小分子和金屬等。
- 可以輔助觀察巨分子的結構、作用力、表面特性等。
- 在藥物設計、分子模擬上有很大的應用空間。



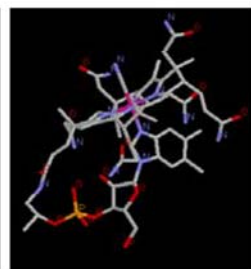
咖啡因



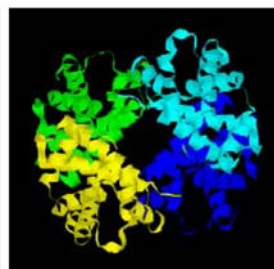
阿斯匹靈



膽固醇



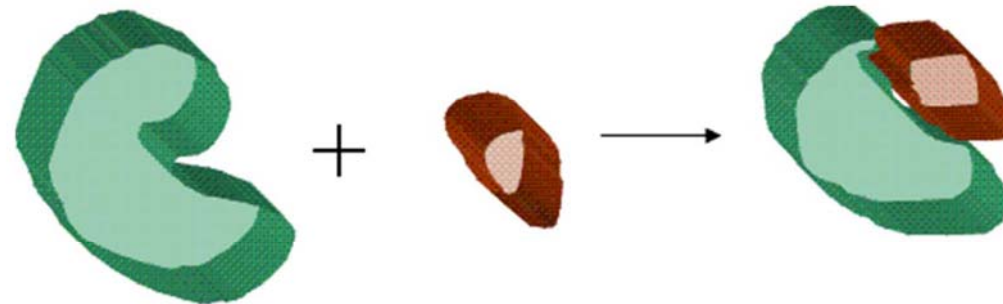
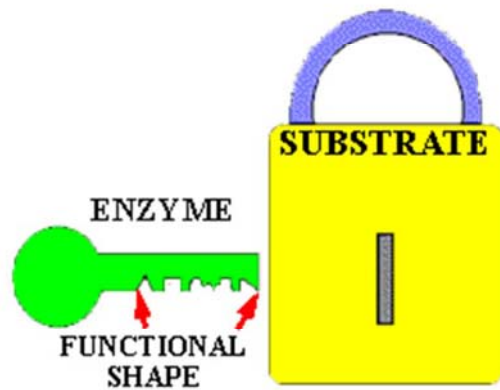
維生素B₁₂



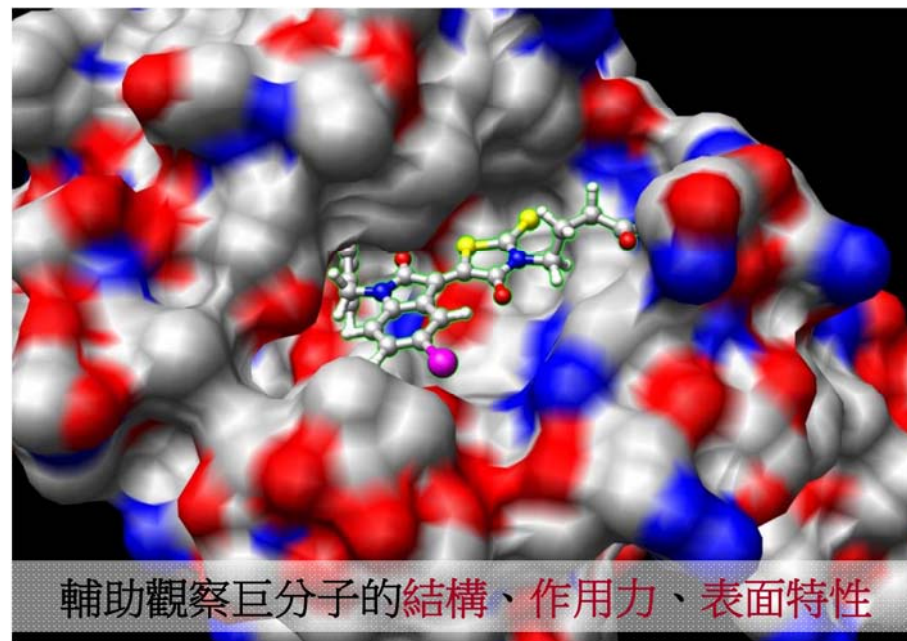
血紅蛋白



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

RCSB PDB
PROTEIN DATA BANK

An Information Portal to Biological Macromolecular Structures
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STRUCTURAL BASIS OF NON-SPECIFIC LIPID BINDING IN MAIZE LIPID-TRANSFER PROTEIN COMPLEXES WITH LAURIC ACID REVEALED BY HIGH-RESOLUTION X-RAY CRYSTALLOGRAPHY

DOI: 10.2210/pdb1fk1/pdb

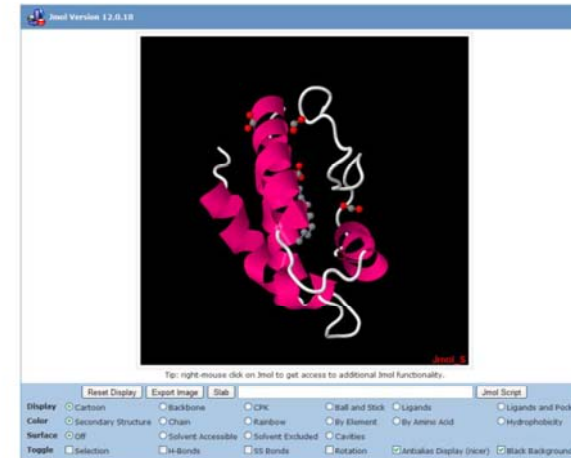
Primary Citation
Structural basis of non-specific lipid binding in maize lipid-transfer protein complexes revealed by high-resolution X-ray crystallography.
Han, G.W., Lee, J.Y., Song, H.K., Chang, C., Min, K., Moon, J., Shin, D.H., Kopka, M.L., Sawaya, M.R., Yuan, H.S., Kim, I.D., Choe, J., Lim, D., Moon, H.J., Suh, S.W.
Journal: (2001) 1 Mol. Biol. 308: 263-278
PubMed: 11327766
DOI: 10.1006/jmb.2001.4559
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PubMed Abstract:
Non-specific lipid transfer proteins (nsLTPs) are involved in the movement of phospholipids, glycolipids, fatty acids, and steroids between membranes. Several structures of plant nsLTPs have been determined both by X-ray crystallography and nuclear magnetic resonance. However, the detailed structural basis of...
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Molecular Description
Classification: Lipid Transport
Structure Weight: 9400.59
Molecule: NON-SPECIFIC LIPID TRANSFER PROTEIN

Biological Assembly
View in Jmol
Other Viewers
Protein Workshop
Biological assembly assigned by authors

Deposition Summary



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/



<http://www.pymol.org/>



PyMOL

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

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PyMOL runs on
  



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3D Molecular Structures

RENDER
Figures Artistically

ANIMATE
Molecules Dynamically

EXPORT
Geometry Data

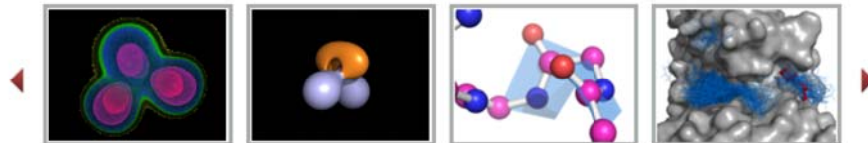
PRESENT
3D Data in PowerPoint

DEVELOP
Customized Visualizations

News

Jan 16, 2012: PyMOL v1.5 is released for licensed users. Review the [list of new features](#), and [download the binaries](#).

Dec 20, 2011: PyMOL v1.5.0 beta 4 is released for licensed users. Review the [list of new features](#), and [download the binaries](#).



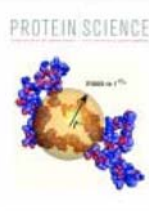
PyMOL is a **user-sponsored** molecular visualization system on an **open-source** foundation. Please support development of this open, effective, and affordable software by purchasing an incentive copy, which is pre-built and comes with maintenance and support.



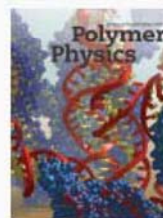
PyMOL-created Journal Covers



Image of two short stretches of double-stranded DNA linked by a ruthenium 'light-switch complex', October 25, 2011; 108 (43) [\[1\]](#) [\[2\]](#)



Protein Science, Vol. 20, No. 12, Dec 2011



Journal of Polymer Science, Nov 15 2011



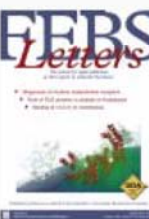
Biophysical Journal, Aug 3 2011



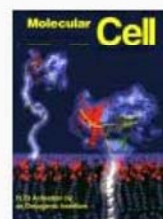
Focused Evolution of HIV-1 Neutralizing Antibodies Revealed by Structures and Deep Sequencing, [Science, Sept. 16, 2011] [\[3\]](#)



Deconstructing honeybee vitellogenin *J. Exp. Biol.*, Volume 214, Issue 4, 2011 [\[4\]](#)



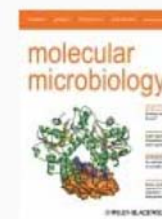
Binding of 14-3-3g to membranes *FEBS Lett.*, Volume 585, Issue 8, 2011 [\[5\]](#)



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* [\[6\]](#)

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



PyMOL Academic Price List

Prices for academic research or other non-profit use.

Class/Offering	PyMOL		AxCyMOL		PyMOL + AxCyMOL		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

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PyMOL

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If you do not receive your link within one hour of completing this form, and you have checked your junk email or spam folder, then please contact licensing@schrodinger.com for assistance.

Open-Source and Educational Users: Please consult & participate in the [PyMOL Community Wiki](#) instead, which has tons of FREE usage information. *The Official PyMOL Downloads and Documentation site is for PyMOL Sponsors only.*

Students and Instructors

Please visit <http://pymol.org/educational> for educational versions of PyMOL.

Open Source Project and Code

PyMOL on SourceForge: <http://sourceforge.net/projects/pymol/>.

PyMOL Source Code on SourceForge: <http://sourceforge.net/projects/pymol/develop>.

* denotes required field



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PyMOL Molecular Graphics System

PyMOL is an OpenGL based molecular visualization system

Brought to you by: [blainebell1](#), [herc111](#), [inchoate](#), [speleo3](#)

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♥ 126 Recommendations

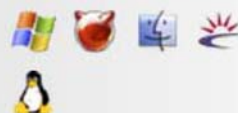
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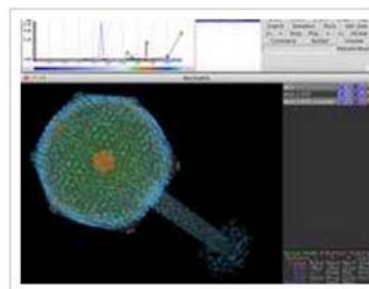
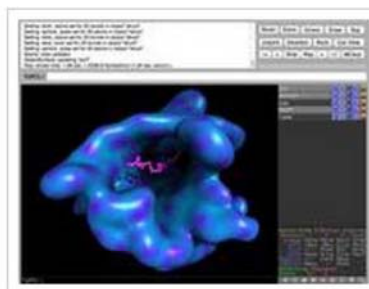
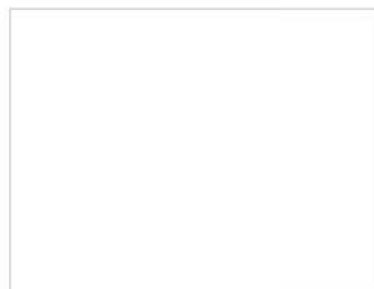
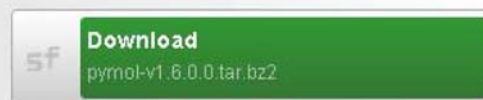
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<http://sourceforge.net/projects/pymol/>

Download PyMoL (v1.6) from alpha.life.nthu.edu.tw



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週四, 23 十月 2008 11:27 管理者

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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](#)

Educational-use-only PyMOL

If you intend to use PyMOL products for professional research, please purchase an Academic PyMOL subscription including access to technical support, screencasts, and additional resources.
<http://alpha.life.nthu.edu.tw/download/pymol.zip>

- 蛋白質結構下載 (按滑鼠右鍵, 另存新檔): [1D66](#)
- Sequence download:
>test001
TTSEAAISCGQVSSAIALCLSYARGQGFAPSAGCCSGVRSLSAARTTADRRAACNCLK
NAARGISGLNAGNAASIPSKCGVSVPTISTSTDCSRVS
- pymol 顯示雙箭鍵
show sticks, (cys/ca+cb+sg) and byres (cys/sg and bound_to cys/sg)
color yellow, (cys/ca+cb+sg) and byres (cys/sg and bound_to cys/sg)

最近更新 (週五, 21 六月 2013 01:25)

網路連線工具

週四, 23 十月 2008 11:25 管理者

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043466

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週四, 23 十月 2008 11:06 管理者

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最近更新 (週二, 31 八月 2010 10:43)



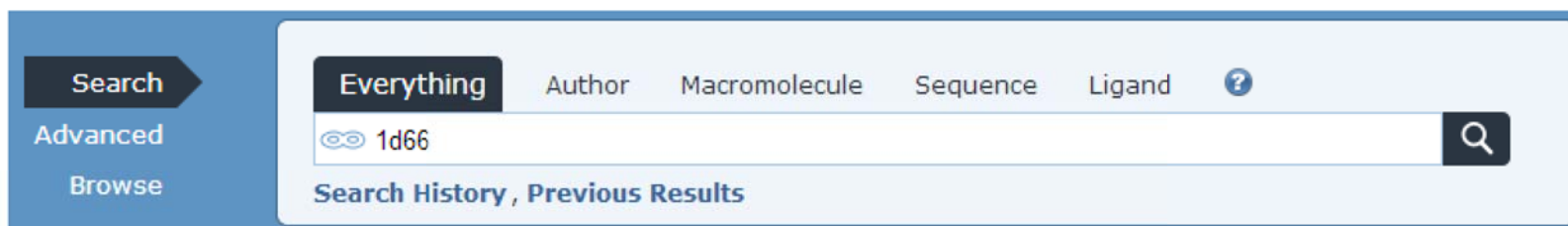
NEXT

Please link to : **PyMOL Tutorial**
<http://140.114.98.75/sg/pymol/>



1. Getting started: explore a protein

1. Download a PDB file: 1D66



2. Open PyMOL and load 1D66.pdb



3. PyMOL Tutorial:

<http://140.114.98.75/sg/pymol/>

結構生物資訊學研習會 @ 2013

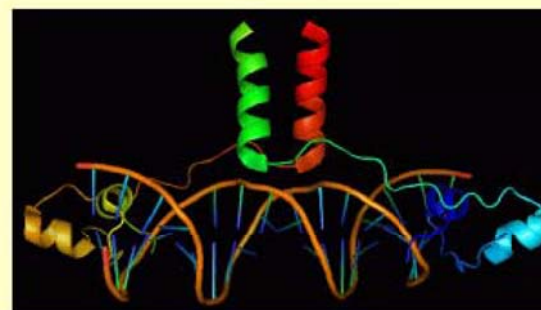
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PyMOL Tutorial

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1	讀檔
2	看看有多少個鍵
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	設定透明surface
18	滑鼠
19	Tips

Edit by Yi-Chung Liu

PyMOL for Dummies



A Tutorial for the PyMOL Basics

74 The PyMOL Molecular Graphics System

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

uses require purchase of a PyMOL Maintenance
Please visit <http://www.pymol.org/funding.htm>
contact sales@delsci.com when you are ready to

This Executable Build integrates and extends
Error: rotate: unknown object 'rep2'.

PyMOL>ray
Ray: render time: 1.77 sec. = 2038.5 frames/hr
SelectorMapCoulomb: Total charge is -3.000 for
SelectorMapCoulomb: Evaluating Coulomb potent

Appearance
Measurement
Mutagenesis
Pair Fitting

Density
Filter
Sculpting

Label
Charge

Demo

Subscription.
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bscription.

OL 1.1r1.

accum.).
98 atoms).
o cutoff)...

Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder

PyMOL Viewer

For Educational Use Only

all

A S H L C

PyMOL Demo:
Wizard > Demo > ...

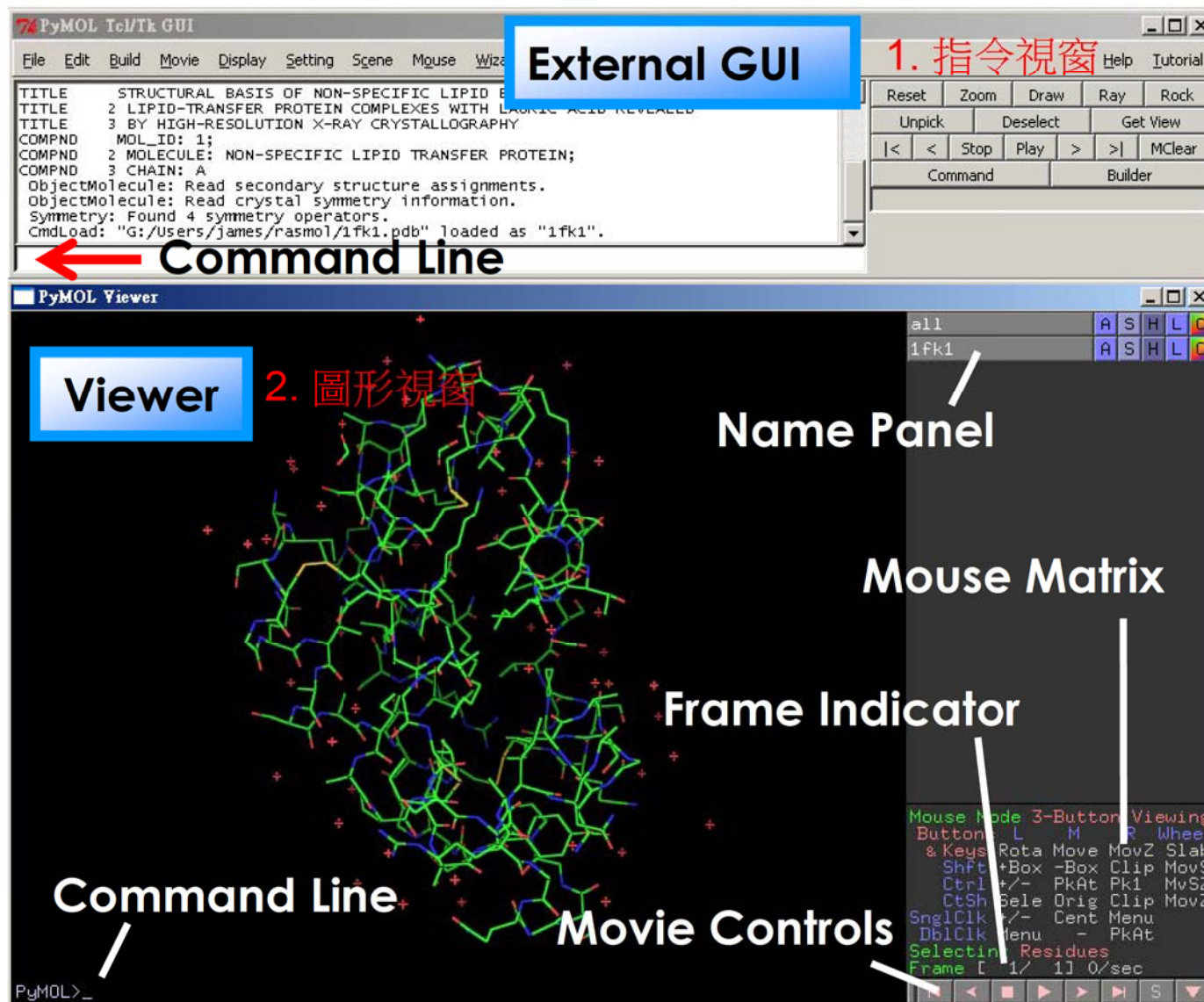
Representations
Cartoon Ribbons
Roving Detail
Roving Density
Transparency
Ray Tracing
Sculpting
Scripted Animation
Electrostatics
Compiled Graphics Objects
Molscript/Raster3D Input

End Demonstration

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rotate Move MoveZ Slab
Shift +Box -Box Clip MoveS
Ctrl +/- PkAt Pk1 MoveS2
CtSh Sele Orig Clip MoveZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State [1/ 1] 30/sec

PyMOL>_

PyMOL Interface



← 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>
resn <residue names>
resi <residue identifiers>
chain <chain ID>
segi <segment identifier>
elem <element symbol>
flag <number>
alt <code>
numeric_type <numeric type>
text_type <text type>
hydrogen
all
visible
id <original-index>
hetatm
ss <secondary structure>
around <distance>
expand <distance>
gap <distance>
in <selection>
like <selection>
<selection> and <selection>
<selection> or <selection>
<selection> not <selection>
<selection> and not <selection>
byres <selection>
byobject <selection>

n; <atom names>
r; <residue names>
i; <residue identifiers>
c; <chain ID>
s; <segment identifier>
e; <element symbol>
f; <number>

nt; <numeric type>
tt; <text type>
h;
*
v;

a; <distance>
e; <distance>

l; <selection>
<selection> & <selection>
<selection> | <selection>
<selection> ! <selection>
<selection> & ! <selection>
br; <selection>
bo; <selection>