Software for Protein Structure Visualization

劉益忠　博士
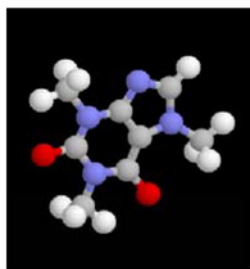
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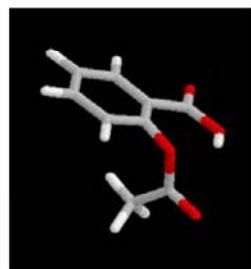
Molecular Structure Visualization
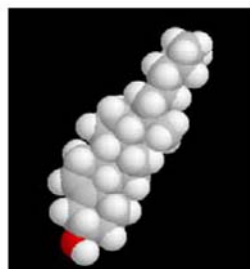
- 是一種可顯現出生物巨分子結構的軟體
  - 包含蛋白質、DNA、RNA、化學小分子和金屬等。
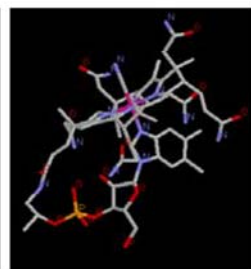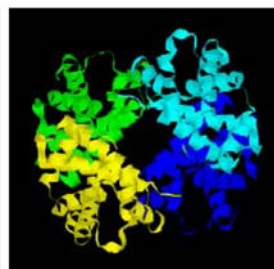
- 可以輔助觀察巨分子的結構、作用力、表面特性等。

- 在藥物設計、分子模擬上有很大的應用空間。

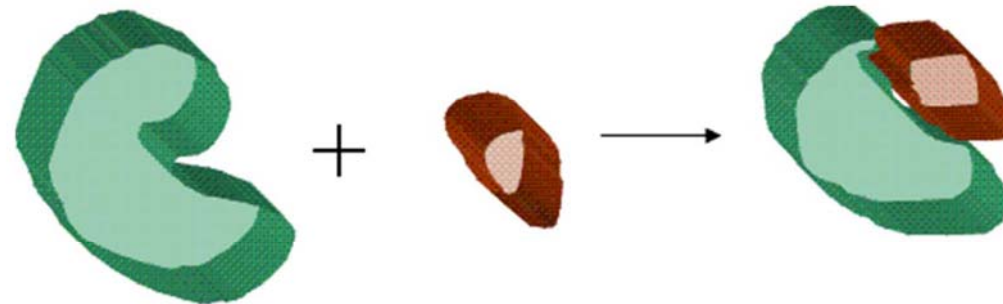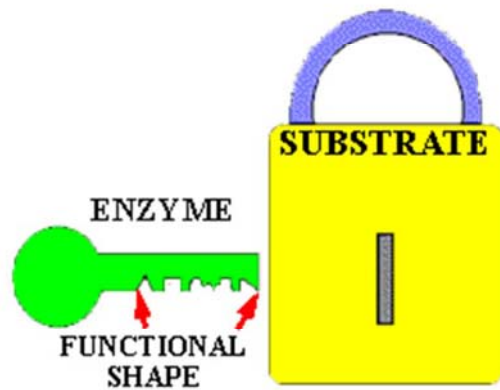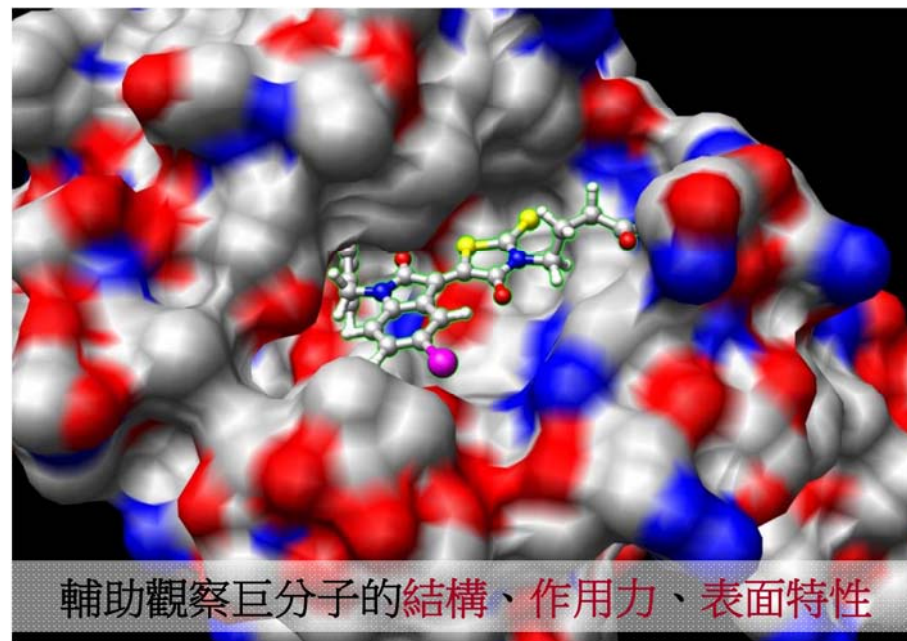| 咖啡因 | 阿斯匹靈 | 膽固醇 | 維生素B$_{12}$ | 血紅蛋白 |

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/

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] 🔗]
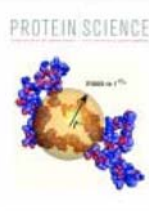
Protein Science, Vol. 20, No. 12, Dec 2011
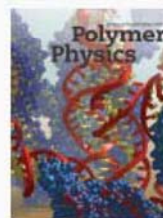
Journal of Polymer Science, Nov 15 2011

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 🔗.
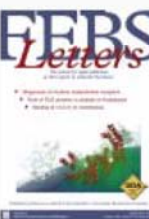
Binding of 14-3-3g to membranes FEBS lett., Volume 585, Issue 8, 2011 🔗.
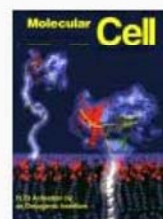
FLT3 Activation by an Oncogenic Insertion Molecular Cell, Volume 13 Number 2, January 30, 2004.

PI3K Inhibitors C&EN, April 11, 2011.
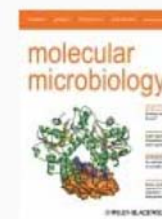
Microbiology of article entitled "Genetic mapping of the interface between the ArsD metallochaperone and the ArsA ATPase. Volume 79, Feb, 2011, *Molecular Microbiology* 🔗

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

PyMOL Academic Price List

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Class/Offering	PyMOL		AxPyMOL		PyMOL + AxPyMOL		Description
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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

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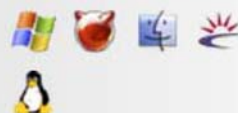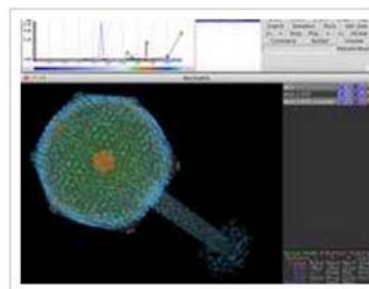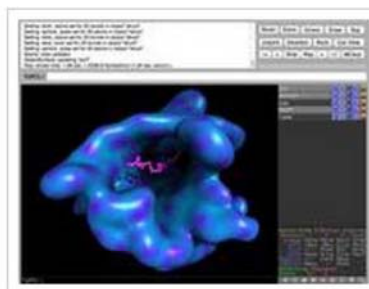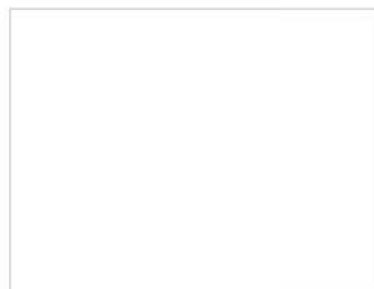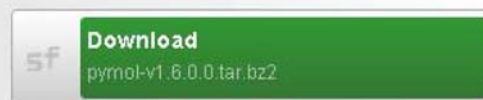
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Version 1.6

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Invoice Password:

Please select "Casual User" below unless you have been designated otherwise.

*User Class:

For multi-user subscriptions, you may provide a comma or space separated list of addresses.

*User Email Address(es):

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A personalized link should arrive shortly via email. *You must follow that emailed link to access our site.*

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

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

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

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

Search
Advanced
Browse

Everything   Author   Macromolecule   Sequence   Ligand

1d66

Search History , Previous Results
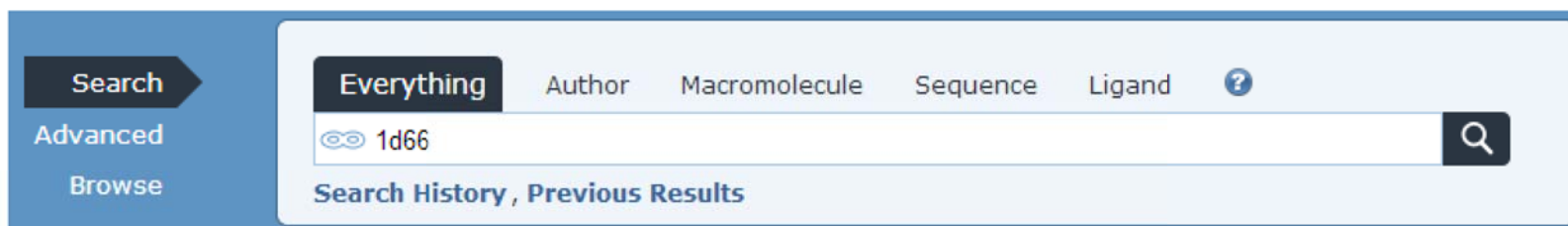
2. Open PyMOL and load 1D66.pdb

PyMOL   1D66.pdb

3. PyMOL Tutorial:
http://140.114.98.75/sg/pymol/

PyMOL for Dummies

PyMOL Tutorial

Edit by Yi-Chung Liu

A Tutorial for the PyMOL Basics

http://140.114.98.75/sg/pymol/

PyMOL Demo:
Wizard > Demo > …

PyMOL Interface

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\>