

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help Tutorial

PyMOL(TM) Incentive Product - Copyright (C) 2006 DeLano Scientific LLC.

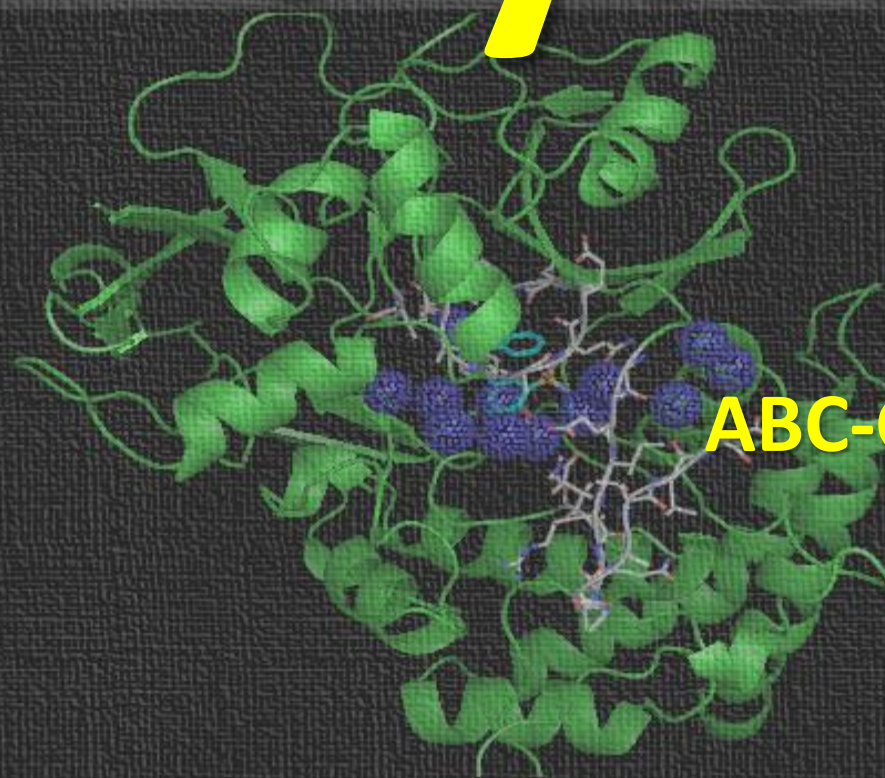
A current PyMOL Maintenance and/or Support Subscription may be required for legal use of this Build beyond a finite honor-system evaluation period. Please visit <http://www.pymol.org/funding.html> for more information.

This PyMOL Executable Build incorporates Open-Source PyMOL 0.99rc6. Executive: Loading version 1.00 session... ScenePNG: wrote 640x382 pixel image to file "E:/pymol-0_99rc6-bin-win32/data/ts/abc.png".

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

PyMOL

```
PyMOL Viewer
/3fbr-for-glide//A 2 11 5 21 26 3 3 41 all A S H L C
PK WH DRVY TK IGE TFK E ASF RPLSLSLRG 3fbr-for-glide A S H L C
/xp-refine-no-protein/** 1 1 1 1 (sele) A S H L C
N339-001 1 -09 L3 52 78-03 F733 20 xp-refine-no-pro A S H L C
/3FBR_pharmacophore_1/// 1 POK pharmacophore A S H L C
```



ABC-G13: 李佟清 杨 成
 王晓琦 吴雨旦

Mode: B B on Viewing
 8 Keys: Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl +/- PkAt Pk1 MvSZ
 CtrlSh Sele Orig Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Menu PkAt
 Selecting Residues
 Frame [47/29641 0/sec

PyMOL 简介

- PyMol是一个开放源码，由使用者赞助的分子三维结构显示软件，由Warren Lyford DeLano编写，并且由DeLano Scientific LLC负责商业发行。
- Pymol被用来创作高品质的分子（特别是生物大分子如蛋白质）三维结构。据软件作者宣称，在所有正式发表的科学论文中的蛋白质结构图像中，有四分之一是使用Pymol来制作的。
- Pymol名字的来源：“Py”表示该软件基于python这个计算机语言，“Mol”则是英文molecule的缩写



21/6/1972–3/11/2009

SCHRÖDINGER.

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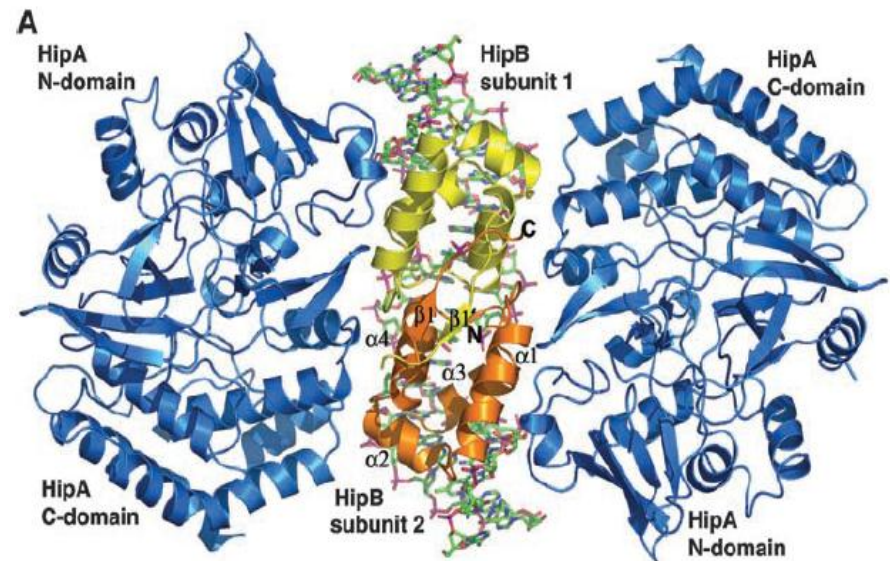
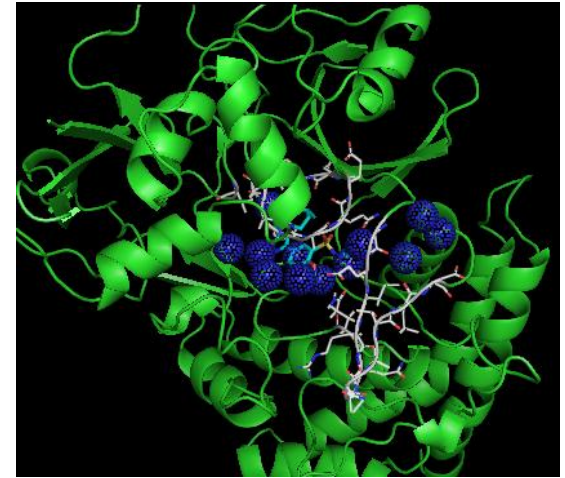
8/1/2010



<http://www.schrodinger.com>

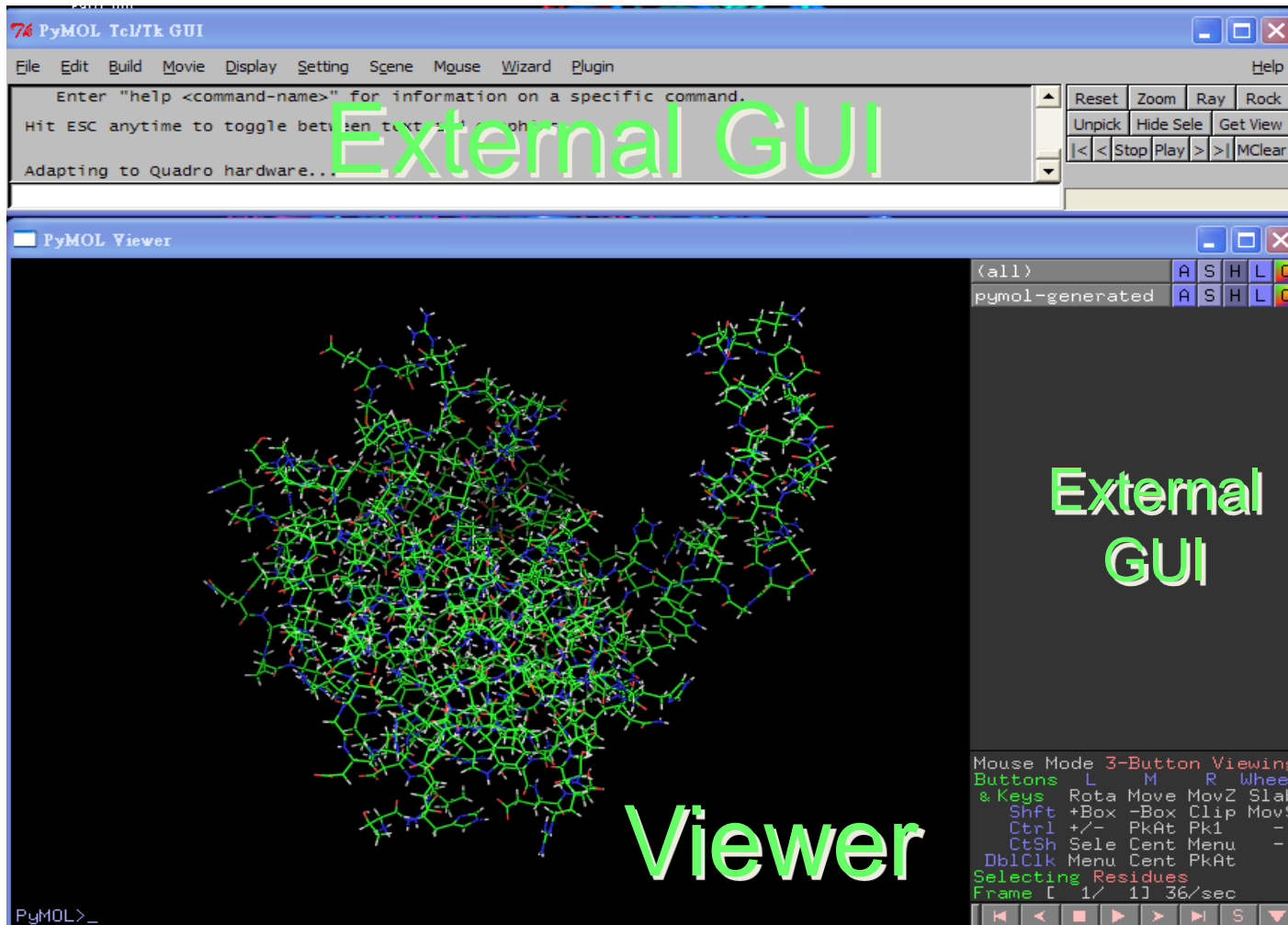
PyMOL 特征

- 实时3D可视化软件
- 高质量科学论文发表图形
- 动画制作能力
- 模块化
- 灵活的应用程序界面
- 免费的开放源码
- C和Python语言编写
- 多种功能插件

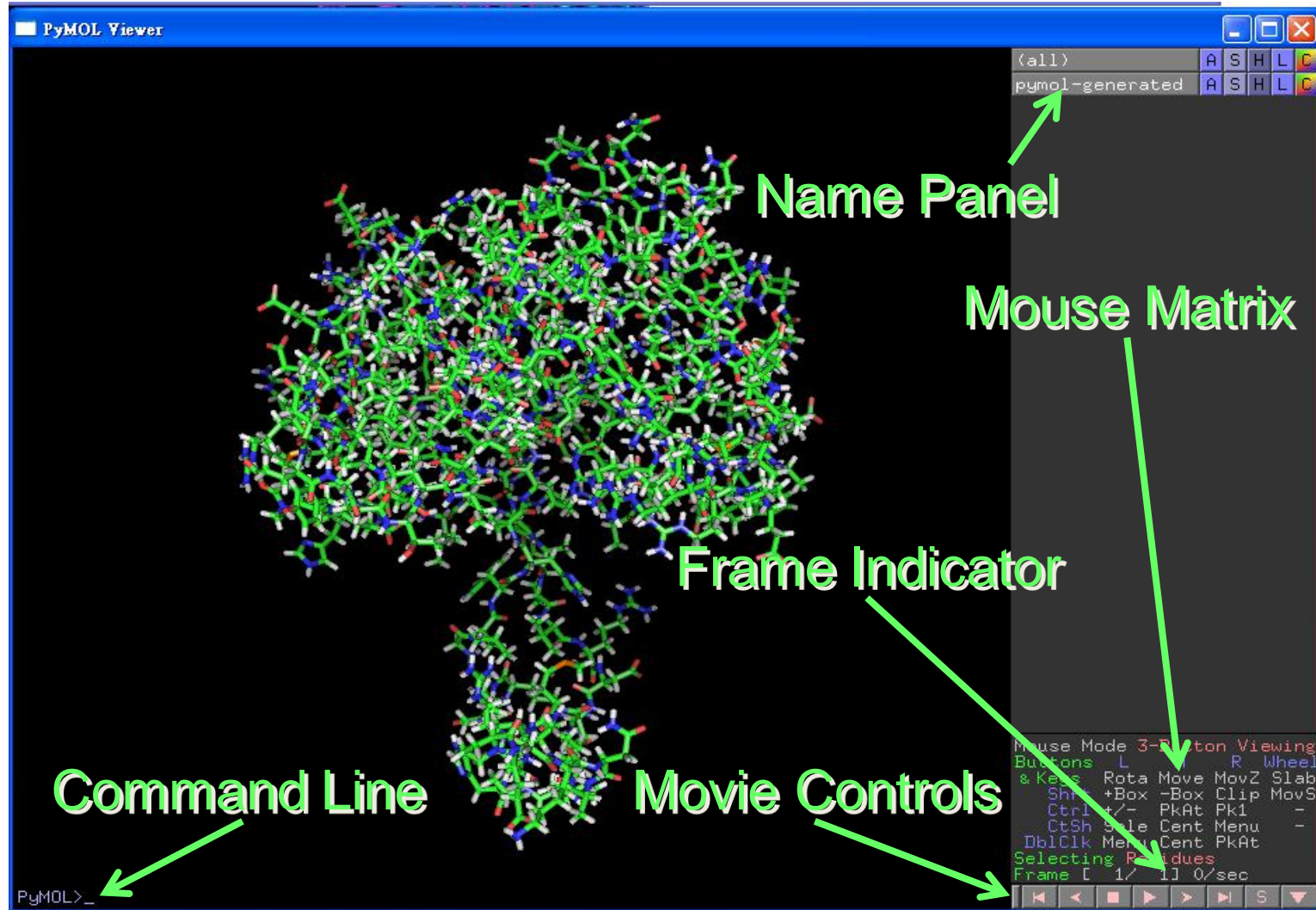


PyMOL的窗口

查看窗口 (viewer window) & 外部(Tcl/Tk)用户图形界面 (external GUI (graphical user interface))



The Viewer Window



The External GUI Window



- 重要优势：标准的“剪切粘贴(Ctrl-X, Ctrl-C, Ctrl-V 分别为剪切，复制和粘贴)”功能，只有External GUI window能用，Viewer window不能用

1. 打开文件

the External GUI 菜单栏

- File > open 然后选择要打开的文件
- 文件可以使pdb, mol2, sdf等多种文件

命令

- 语法
 - load <filename>
- 例子

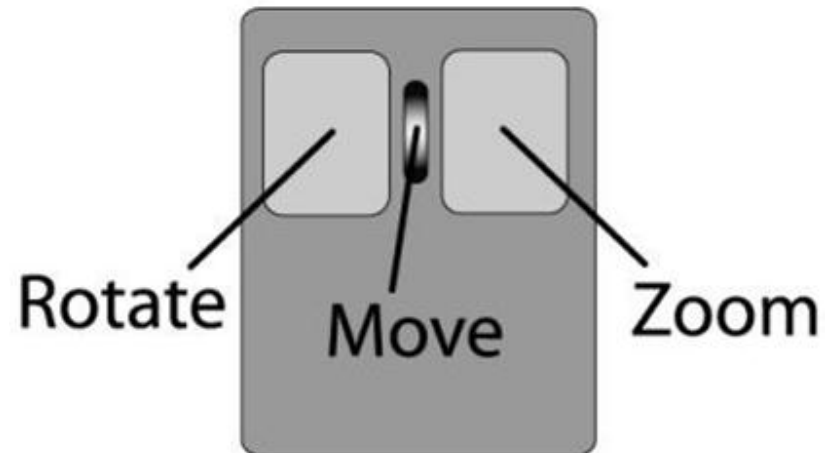
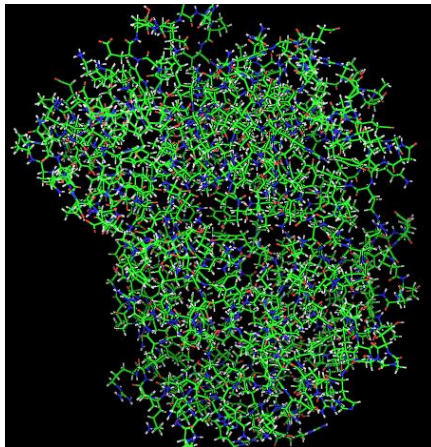
```
data\chempy          data\tt
data\demo            data\tut
data\pmg_tk
parser: matching files:
data\tt\3fbr-for-glide.pdb  data\tt\Kinases_library.pdf
data\tt\3fbr-ts-xp-5000.pse data\tt\tt_xp_5000.mol2
parser: matching files:
data\tt\3fbr-for-glide.pdb  data\tt\3fbr-ts-xp-5000.pse
parser: matching files:
data\tt\3fbr-for-glide.pdb  data\tt\3fbr-ts-xp-5000.pse
load data\tt\3fbr-for-glide.pdb
```

- load data/ts/3fbr-for-glide.pdb
- ✓ 默认路径
- ✓ 英文名
- ✓ Tab键

```
PyMOL>load data/ts/3fbr-for-glide.pdb_
```

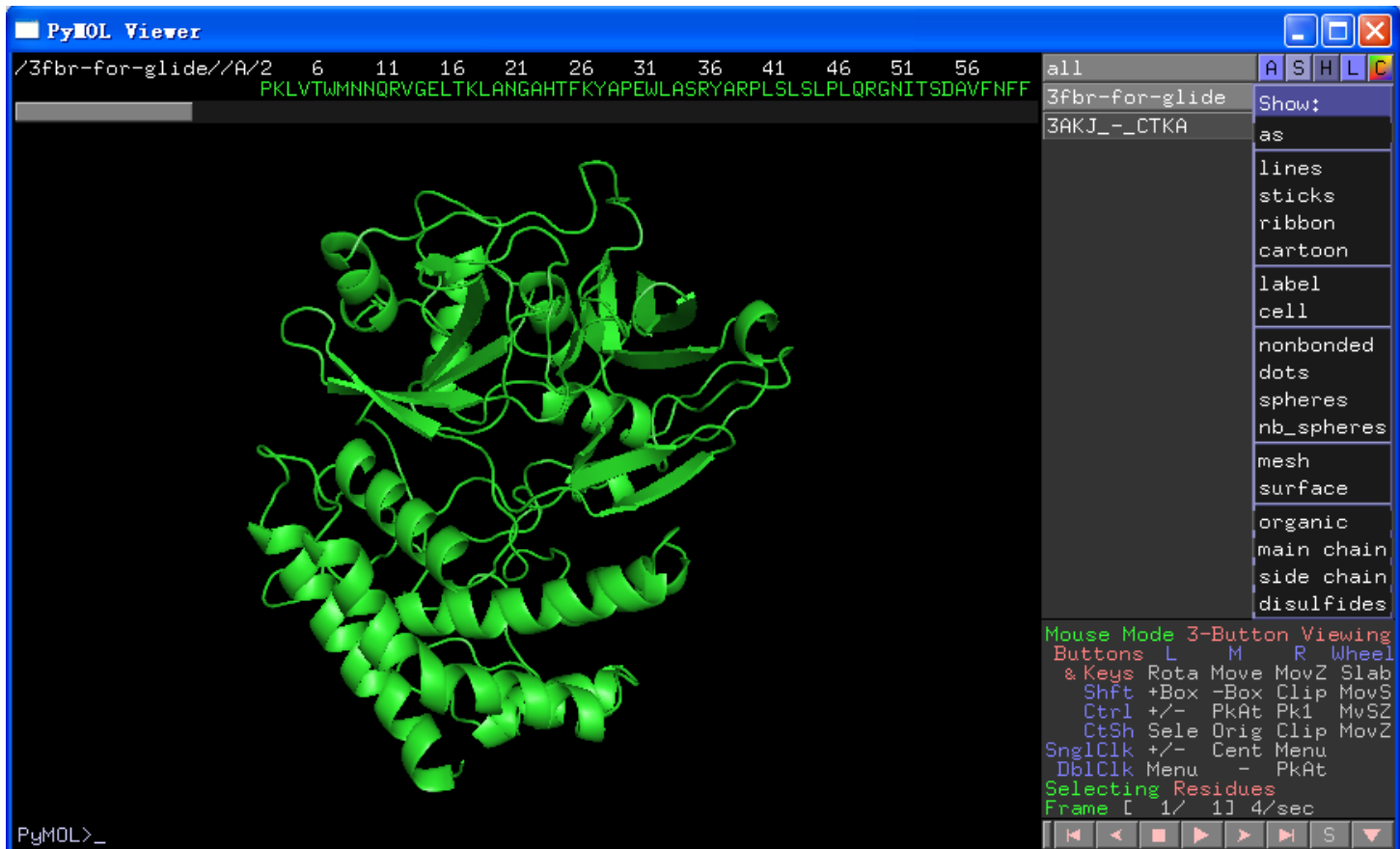
2. 鼠标操作

	L	M	R	Wheel
	Rota	Move	MovZ	Slab
Shift	+Box	-Box	Clip	MovS
Ctrl	+/-	PkAt	Pk1	-
CtSh	Sele	Cent	Menu	-
DblClk	Menu	Cent	PkAt	



Viewer window的external GUI

- Show & Hide
- Action
- Label
- Colour



all ASHL C

3fbr-for

3AKJ_--C

Actions:

- zoom
- orient
- center
- origin
- drag
- preset
- find
- align
- generate
- assign sec. struc.
- rename object
- duplicate object
- delete object
- hydrogens
- remove waters
- state
- masking
- sequence
- movement
- compute

Mouse Mo
Buttons
& Keys
Shft
Ctrl

Preset:

- simple
- simple (no solvent)
- ball and stick
- b factor putty
- technical
- ligands
- ligand sites
- pretty
- pretty (with solvent)
- publication
- publication (with solvent)
- default

Polar Contacts:

- within selection
- involving side chains
- involving solvent
- excluding solvent
- excluding main chain
- excluding intra-main chain
- just intra-side chain
- just intra-main chain
- to other atoms in object
- to others excluding solvent
- to any atoms
- to any excluding solvent

Find:

- presat
- polar contacts
- find
- align
- genera
- assign
- rename
- duplic
- delete
- hydrog
- remove
- state
- maskin

Object:

3AKJ_--CTKA

Align:

- to molecule
- to selection
- enabled to this
- all to this
- states (* /ca)
- states
- matrix from
- matrix to
- matrix reset

Compute:

- atom count
- formal charge sum
- partial charges sum

Label:

- clear
- residues
- chains
- segments
- atom name
- element symbol
- residue name
- residue identifier
- chain identifier
- segment identifier
- b-factor
- occupancy
- vdw radius
- other properties
- atom identifiers

Color:

- by element
- by chain
- by ss
- spectrum
- auto
- reds
- greens
- blues
- yellows
- magentas
- cyans
- oranges
- tints
- grays

136 141 146 151 156 161 166 171 176 181

IPLGMIREENDFRISVAG

TRIGNDWCIPKGITPTTHIKLP

sele

- disable
- actions
- color
- show
- hide
- preset
- label
- zoom
- orient
- center
- origin
- drag

Color:

- by element
- by chain
- by ss
- spectrum
- auto
- reds
- greens
- blues
- yellows
- magentas
- cyans
- oranges
- tints
- grays

Grays

- white
- gray80
- gray70
- gray60
- gray50
- gray40
- gray30
- gray20
- gray10
- black

- Viewer panel中选中氨基酸右键的操作

The image shows a PyMOL Viewer window displaying a protein structure. The protein is rendered with red ribbons and green sticks. A context menu is open over a selected amino acid, listing various actions. The 'around' option is highlighted in yellow. The menu items are:

- sele
- disable
- actions
- color
- show
- hide
- preset
- label
- zoom
- orient
- center
- origin
- drag
- masking
- movement
- compute

The 'Actions:' sub-menu contains:

- delete selection
- rename selection

The 'Around:' sub-menu contains:

- atoms within 4 A
- atoms within 5 A
- atoms within 6 A
- atoms within 8 A
- atoms within 12 A
- atoms within 20 A
- residues within 4 A
- residues within 5 A
- residues within 6 A
- residues within 8 A
- residues within 12 A
- residues within 20 A

The PyMOL command line at the bottom shows the command `PyMOL>_`. The top of the window displays the file path `/3fbr-for-glide` and the sequence `131 136 141 146 151 156 161 166 171 176 181 186`. The sequence is `IMAWEKLTARLEEVLTAYKADIPGLMIREENDFRISVAGAQEKTALLRIGNDWICIPKGITPTTHIIKLPIGEIRQPNA`. The right panel shows the selection list with `all`, `3fbr-for-glide`, and `(sele)` entries, each with buttons for `A`, `S`, `H`, `L`, and `C`.

命令

比如：

> zoom

> show cartoon, /3fbr-for-glide

> color blue, /sele

> Show lines, /sele

.....

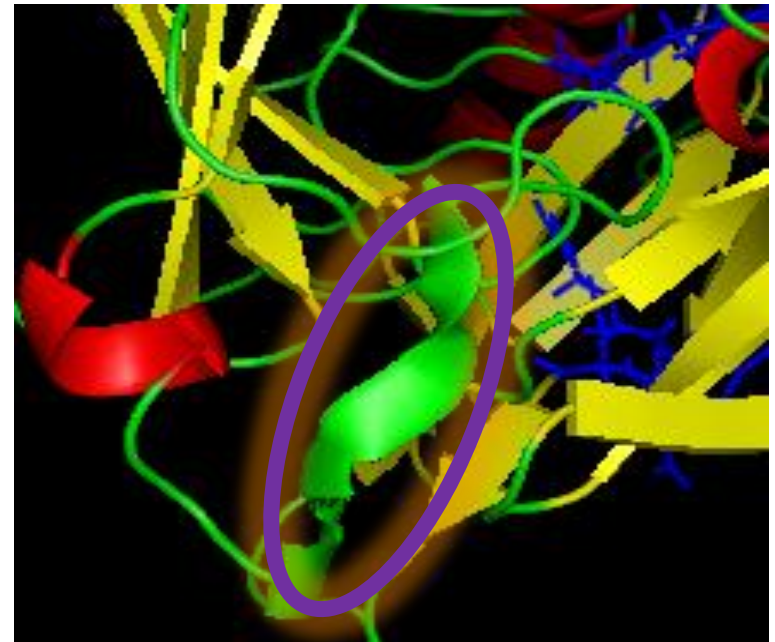
- */object-name/segi-identifiser/chain-identifiser/resi-identifiser/name-identifiser*

再比如二级结构重置:

> alter 36-41/, ss='H'

> Rebuild

Ss,二级结构: H, S, L

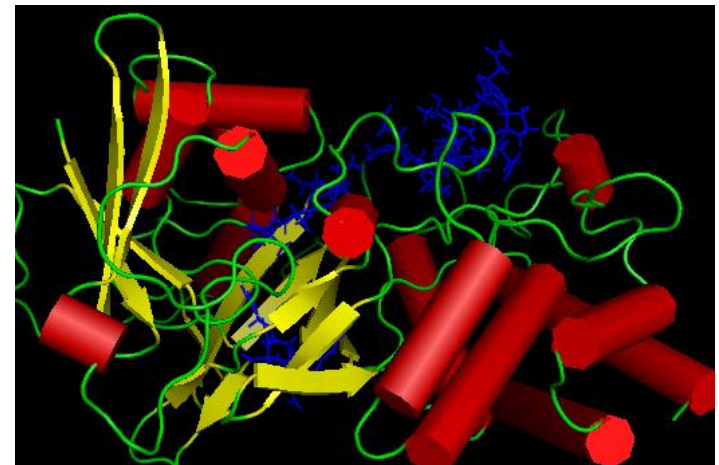
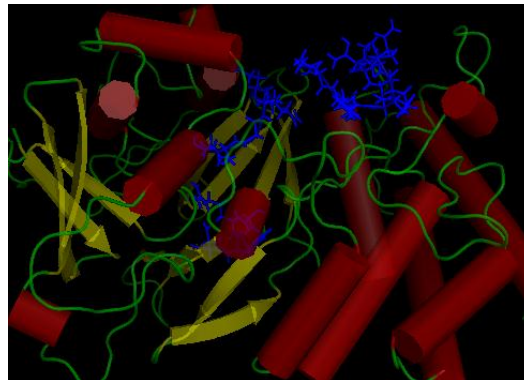


Cartoon的类型:

> set cartoon_cylindrical_helices,1

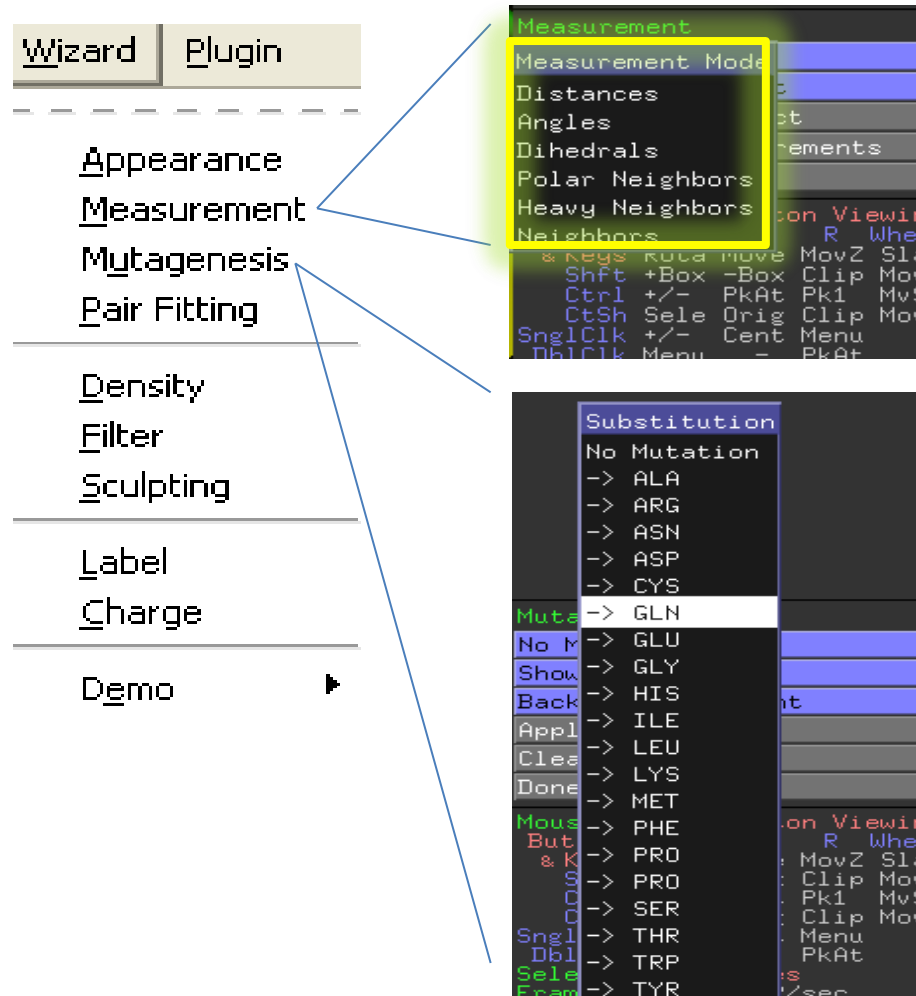
> set cartoon_transparency, 0.5

.....



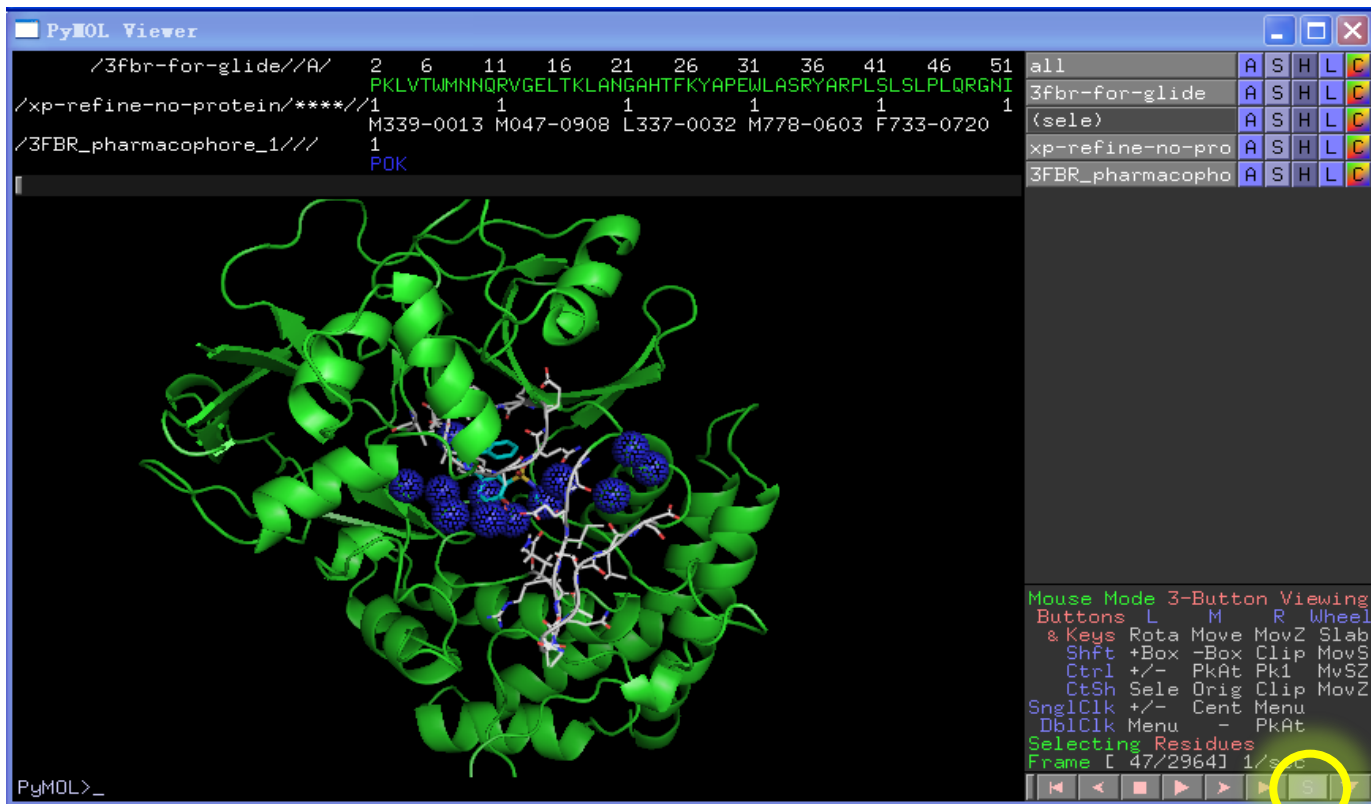
External (Tcl/Tk) GUI

一般根据菜单的名字都能知道是什么操作，重点 wizard:



3. 保存

- Save session as 将本次所有操作都保存在一个.pse文件
- 右下角显示序列sequence，然后将蛋白质的亚基或者蛋白质和小分子单独保存 >> save molecule
- save image 会把viewer panel的都存成图片，menu下 display > background 可以将背底改成白色的



高级的操作

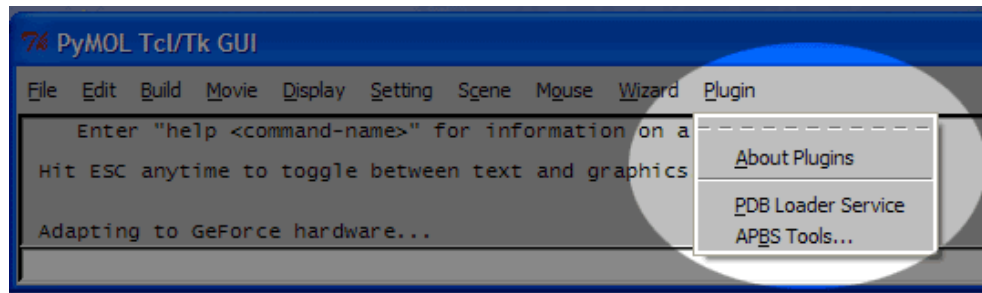
- **Movie**

- 看分子动力学模拟MD的轨迹
- 看核磁共振NMR解的几十个结构氨基酸的运动轨迹
- 演示相互作用的过程

- **Plugin**

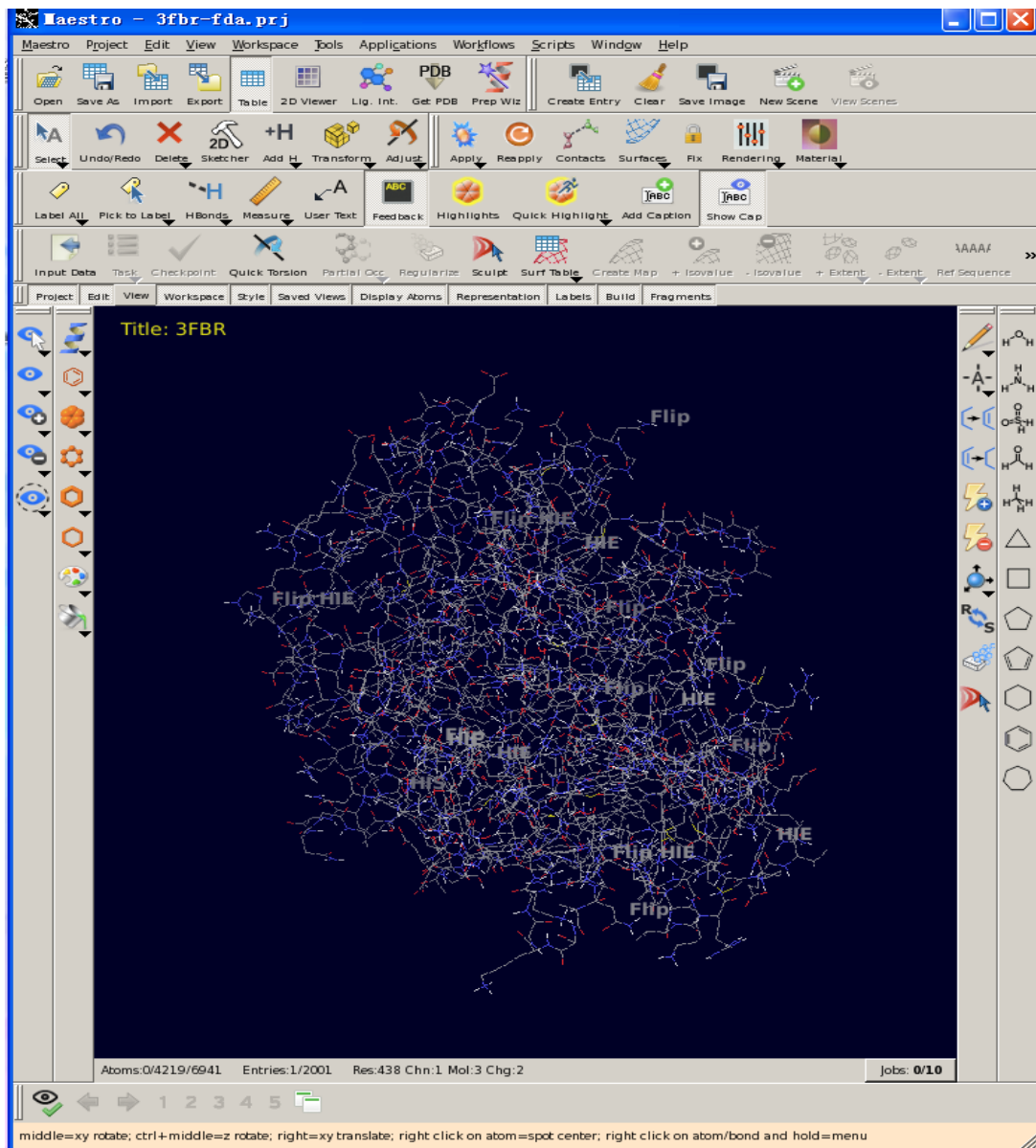
- APBS (Adaptive Poisson-Boltzmann Solver)

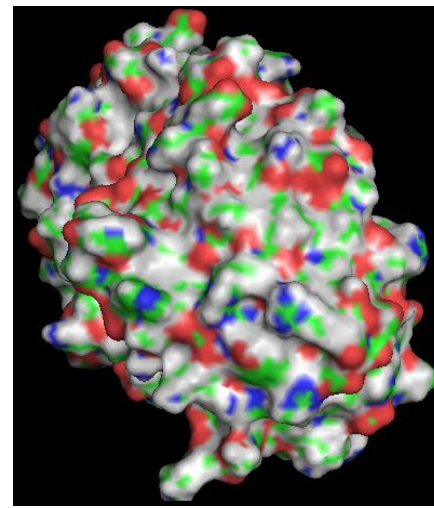
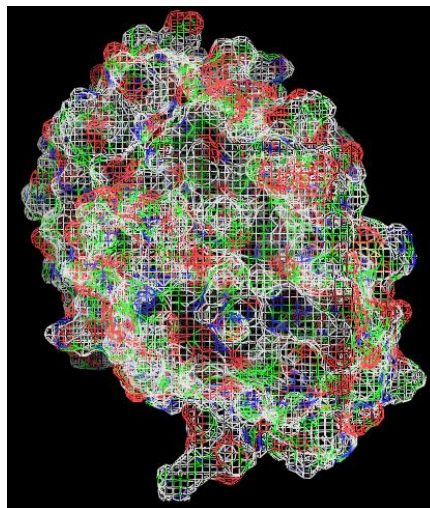
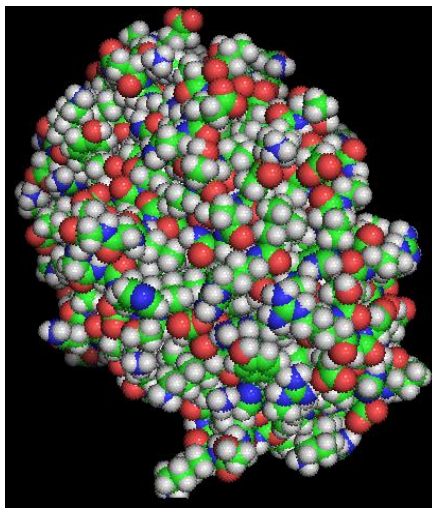
利用泊松波尔兹曼方程解水溶液中分子间的静电作用



缺点

- 很多操作不能做，比如结构优化等，swiss-pdbv可以
- 薛定谔公司的其他软件，如maestro，图形界面非常友好，图像质量也很高，更重要的是能进行上述操作，还能连接glide进行分子对接





Thank you!

