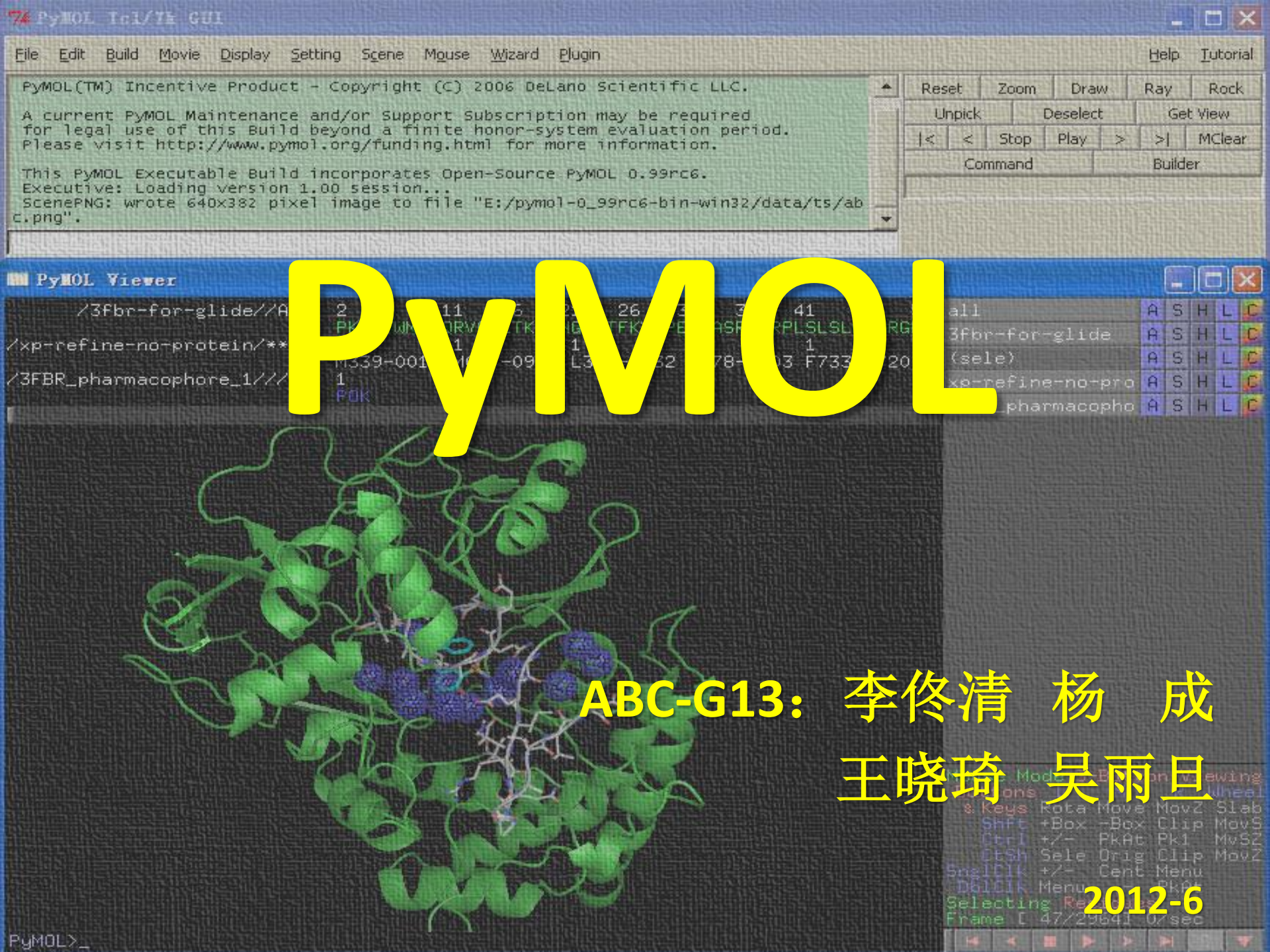

PyMOL
ABC-G13：李佟清 杨 成
王晓琦 吴雨旦
2012-6

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 DeLan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molucule的缩写

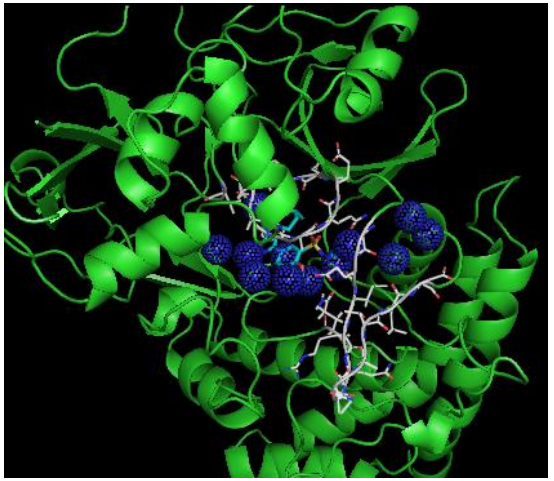
21/6/1972–3/11/2009

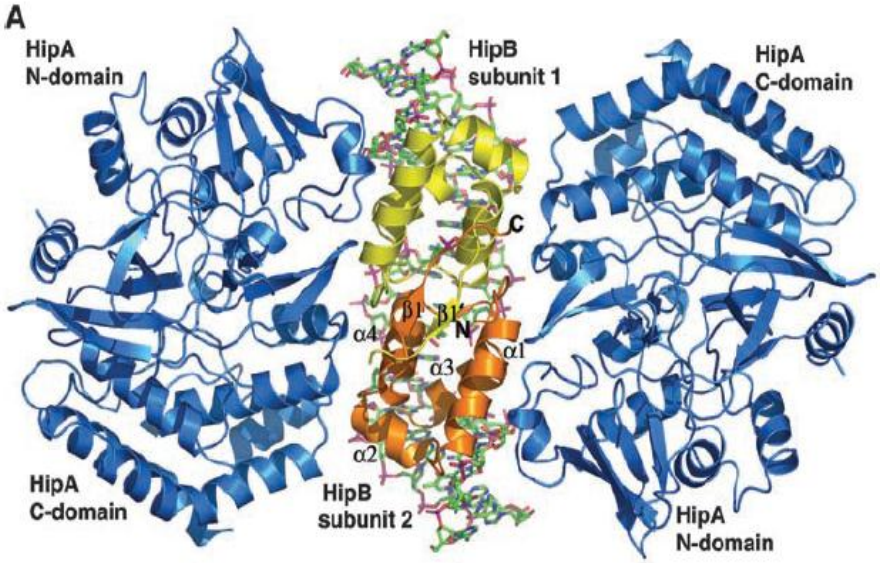
8/1/2010

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

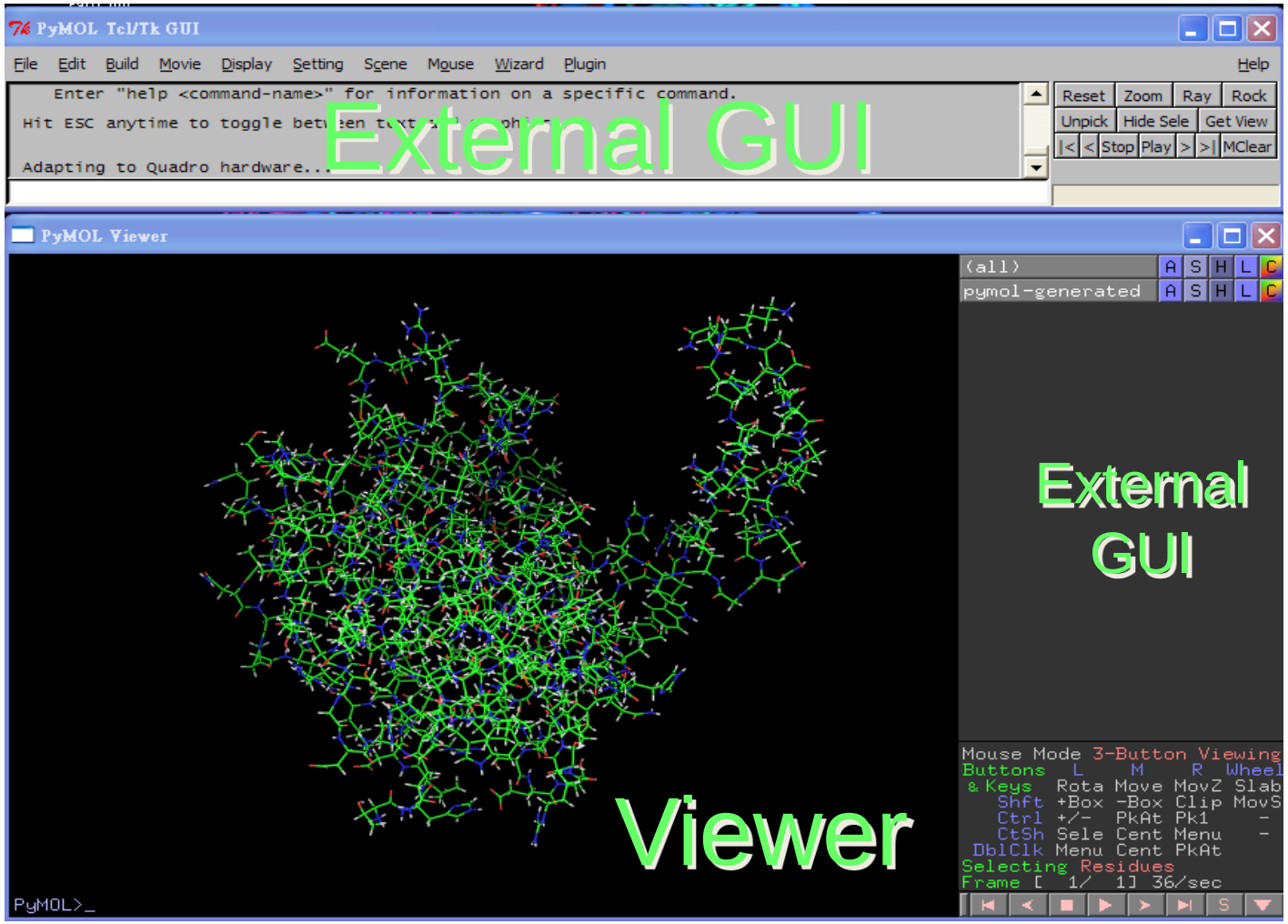




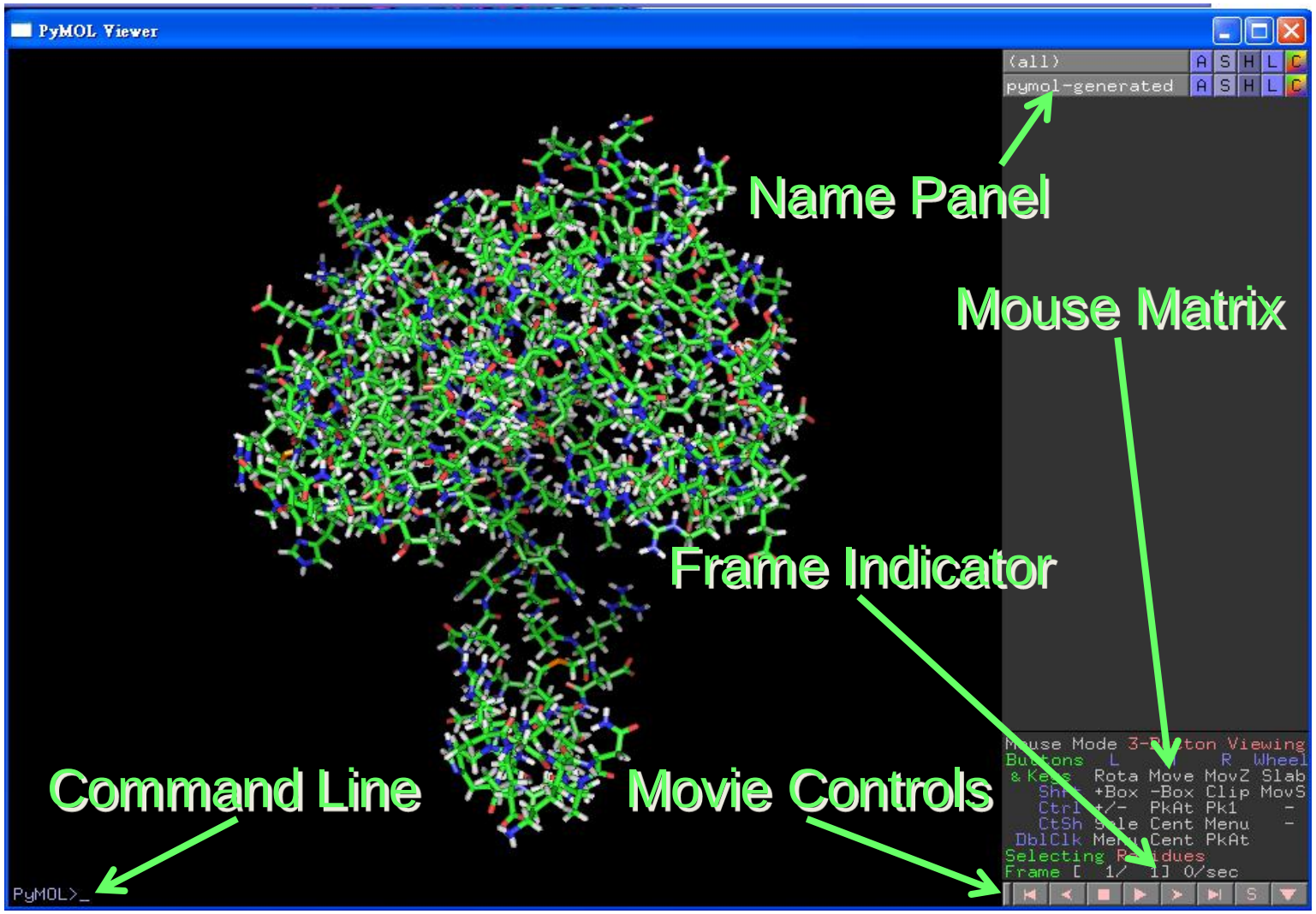
Schumacher *et al*. 2009. Science

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

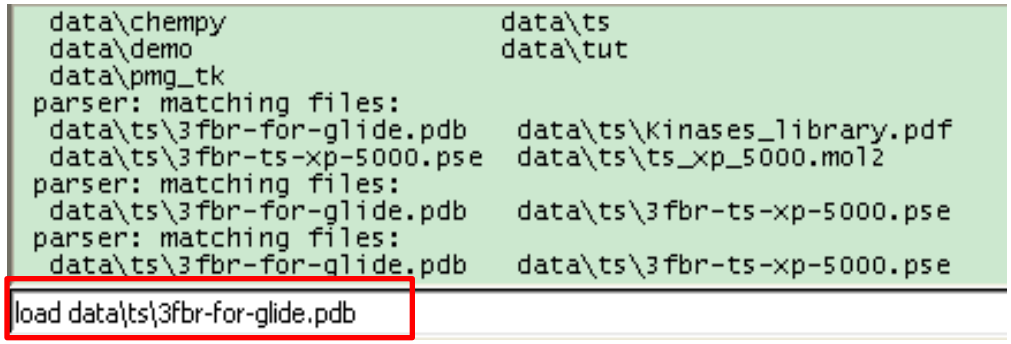
1. 打开文件

***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

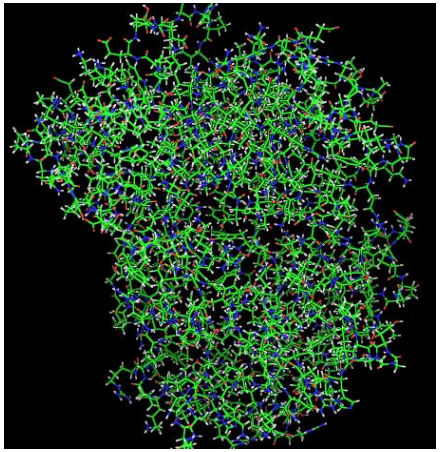
命令

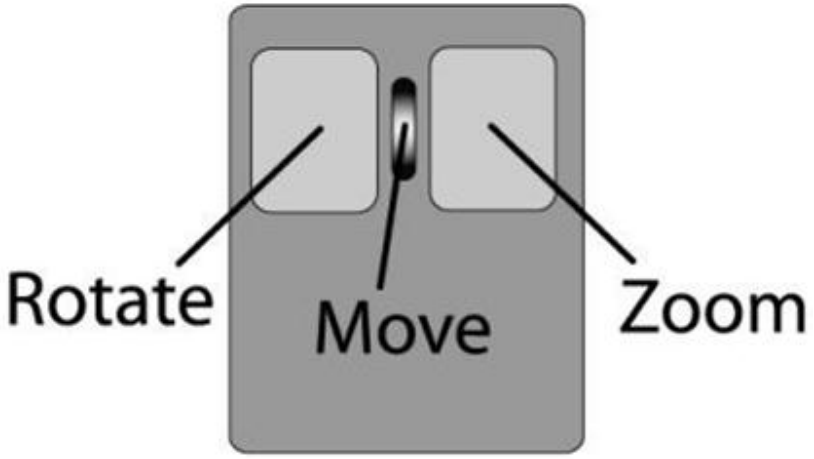
- 语法
  - load <filename>
- 例子
  - load data/ts/3fbr-for-glide.pdb
    - ✓默认路径
    - ✓英文名
    - ✓Tab键



2. 鼠标操作

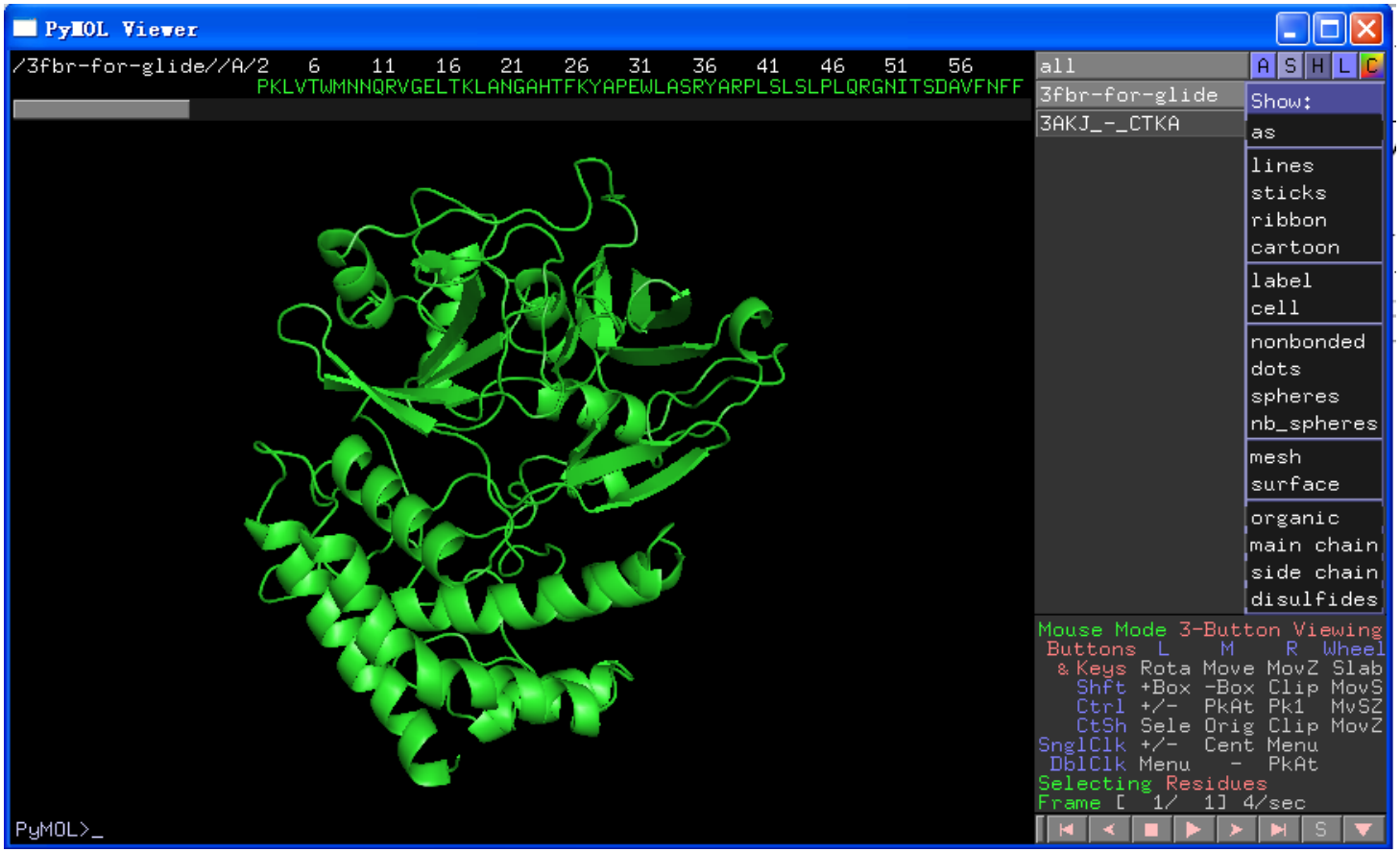
	L	M	R	Wheel
	Rota	Move	MovZ	Slab
Shift	+Box	-Box	Clip	MovS
Ctrl	+/-	PkAt	Pk1	-
CtSh	Sele	Cent	Menu	-
DblClk	Menu	Cent	PkAt	

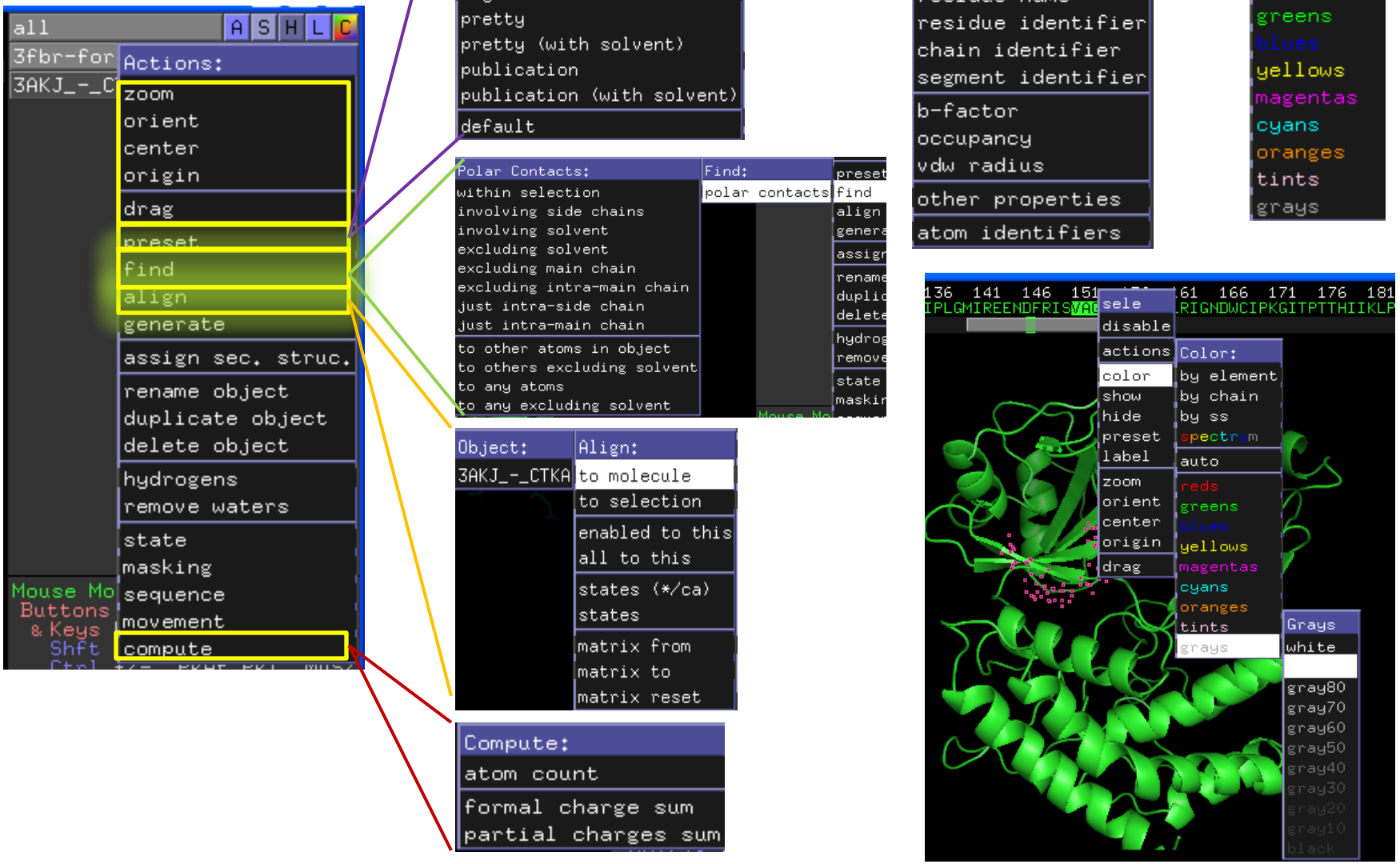




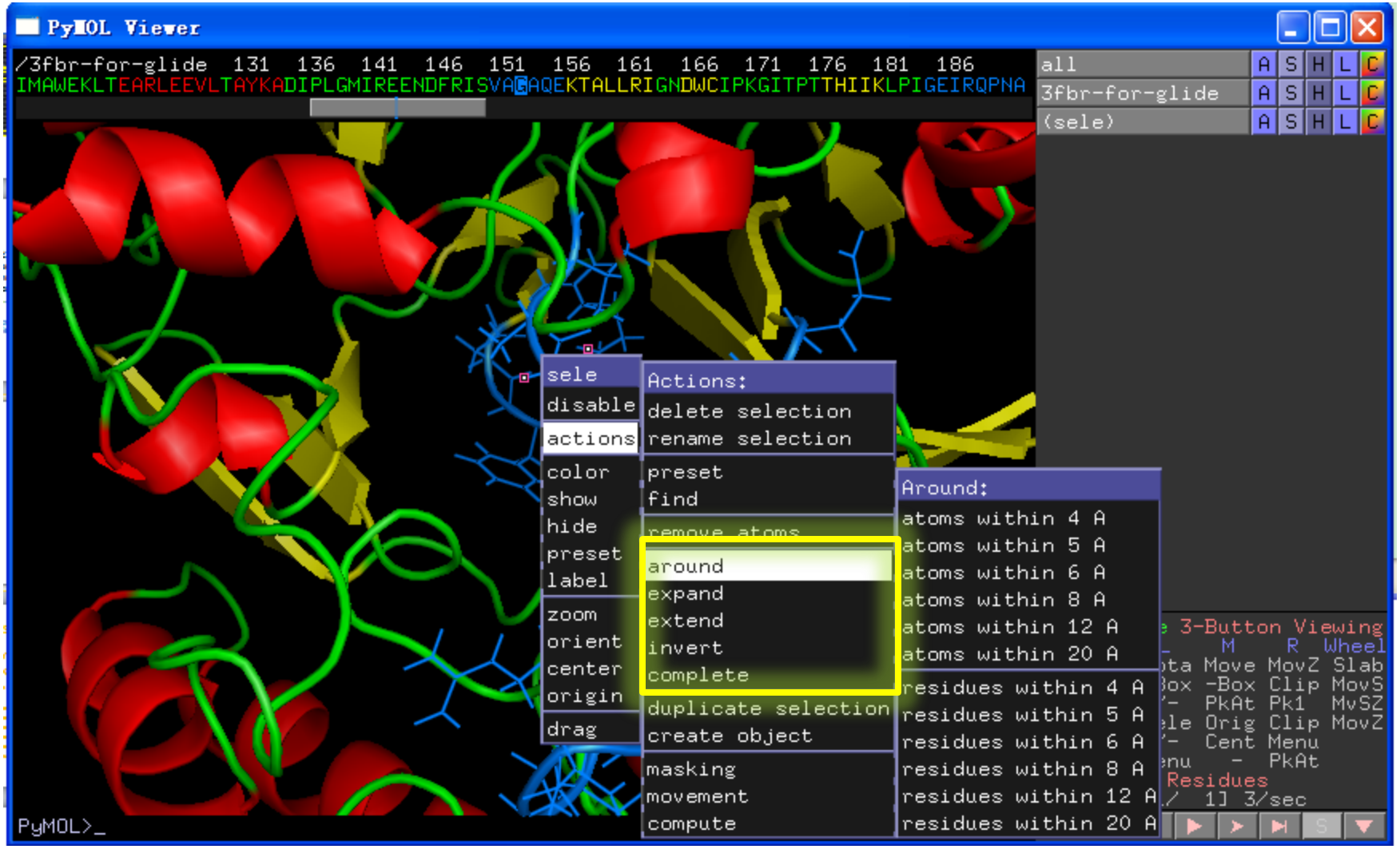
Viewer window的external GUI

- Show & Hide
- Action
- Label
- Colour




all
A S H L 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
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:
polar contacts
preset
find
align
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
sele
disable
actions
color
show
hide
preset
label
zoom
orient
center
origin
drag
Grays
white
gray80
gray70
gray60
gray50
gray40
gray30
gray20
gray10
black

- Viewer panel中选中氨基酸右键的操作



命令

比如：

> zoom

> show cartoon, /3fbr-for-glide

> color blue, /sele

> Show lines, /sele

……

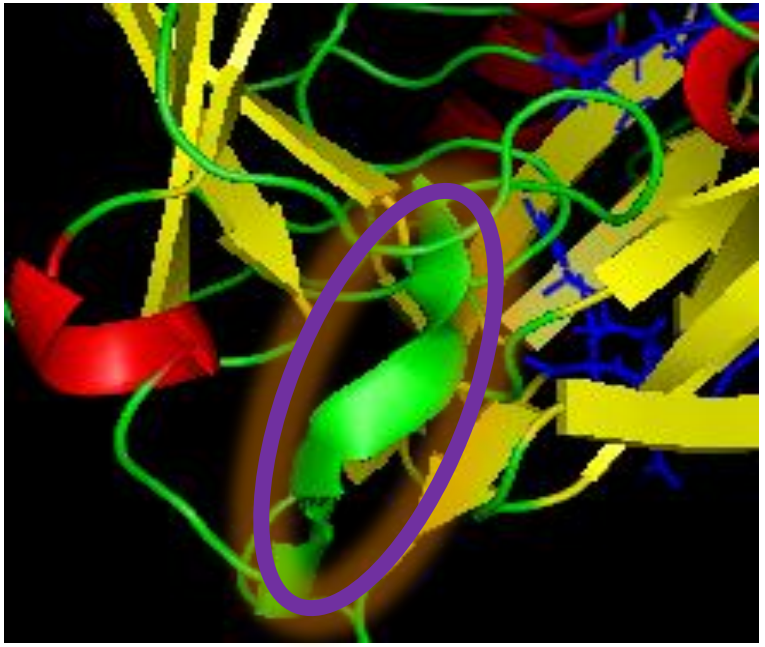
- ***/object-name/segi-identifier/chain-identifier/resi-identifier/name-identifier***

再比如二级结构重置：

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

> Rebuild

Ss,二级结构: H, S, L

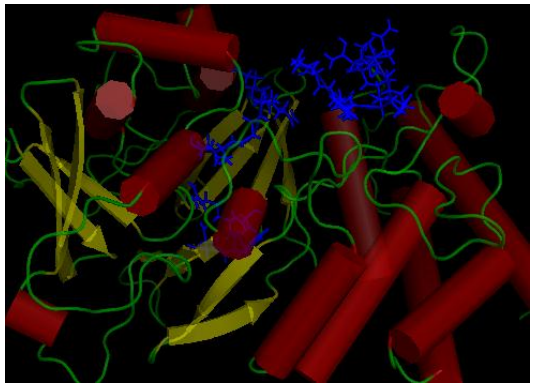


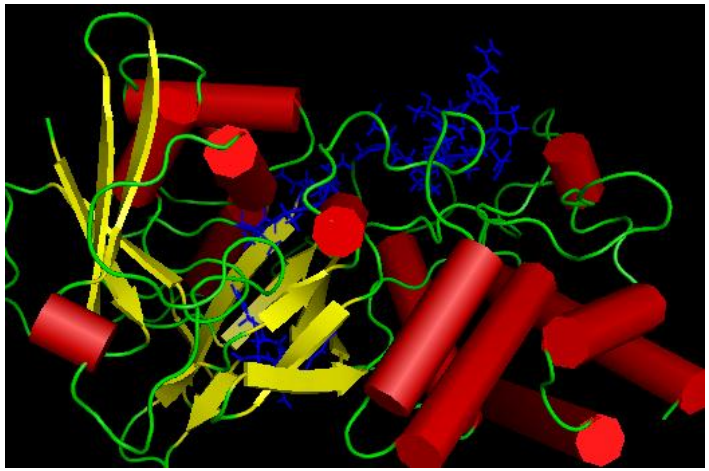
Cartoon的类型：

> set cartoon_cylindrical_helices,1

> set cartoon_transparency, 0.5

……

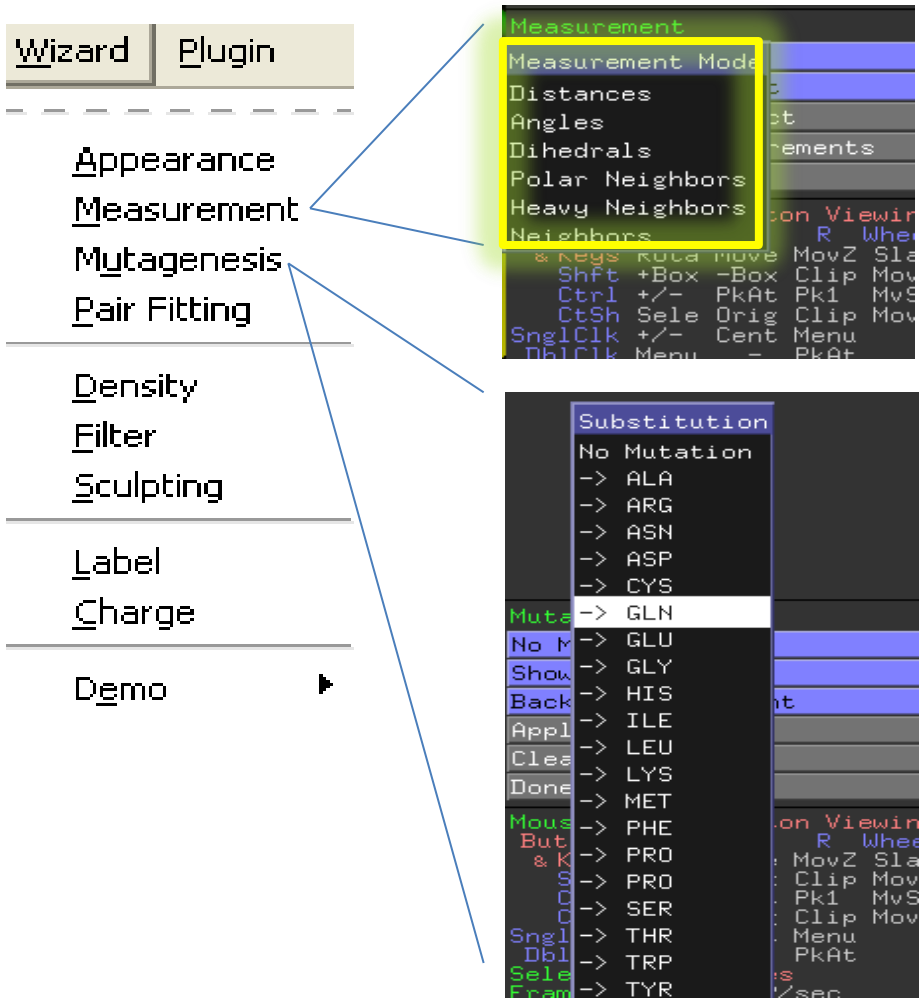




External (Tcl/Tk) GUI

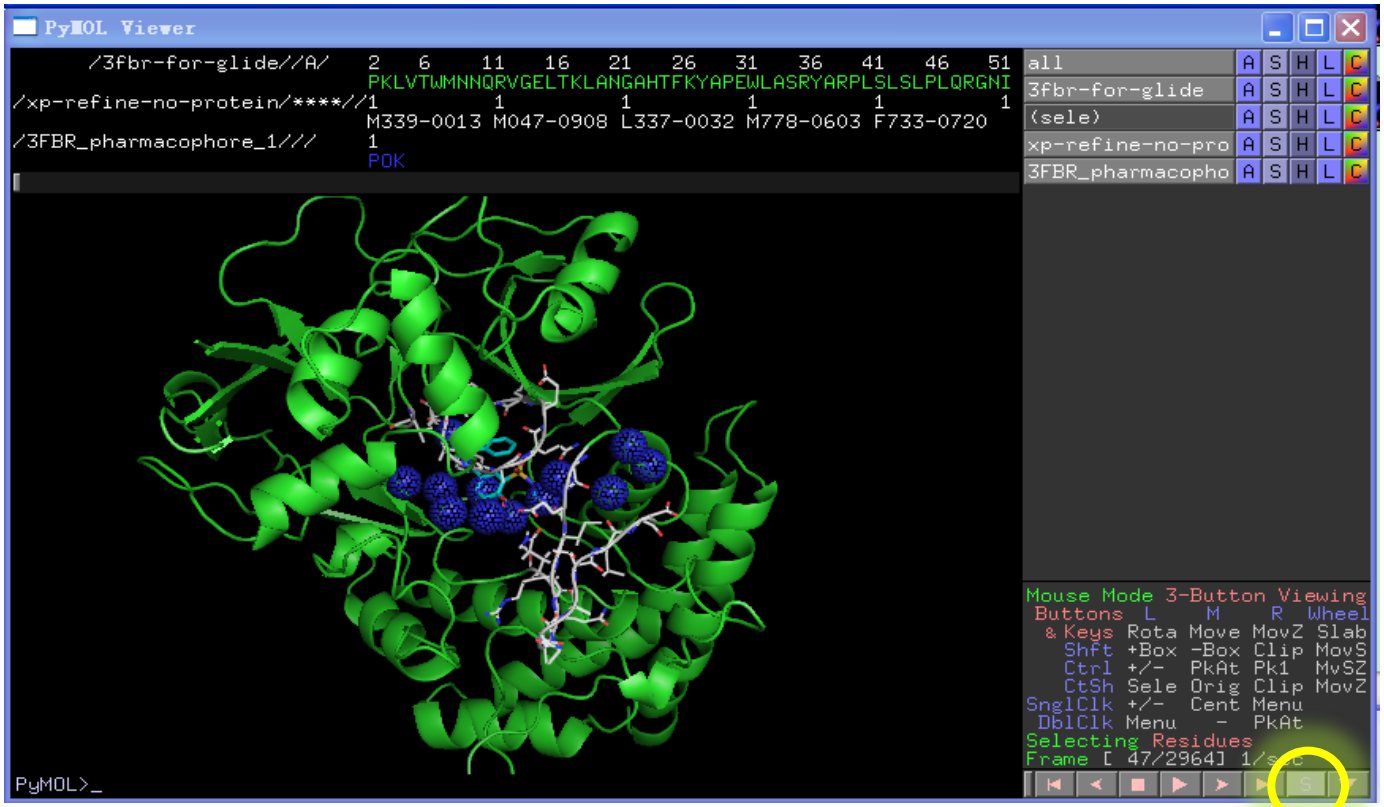
一般根据菜单的名字都能知道是什么操作，重点

wizard:



3. 保存

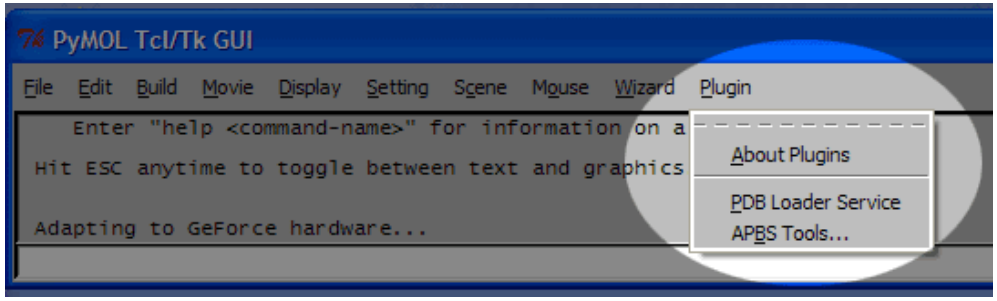
- Save session as将本次所有操作都保存在一个.pse文件
- 右下角显示序列sequence，然后可以将蛋白质的亚基或者蛋白质和小分子单独保存 >> save molecule
- save image会把viewer panel的都存成图片，menu下display > backgroud可以将背底改成白色的



高级的操作

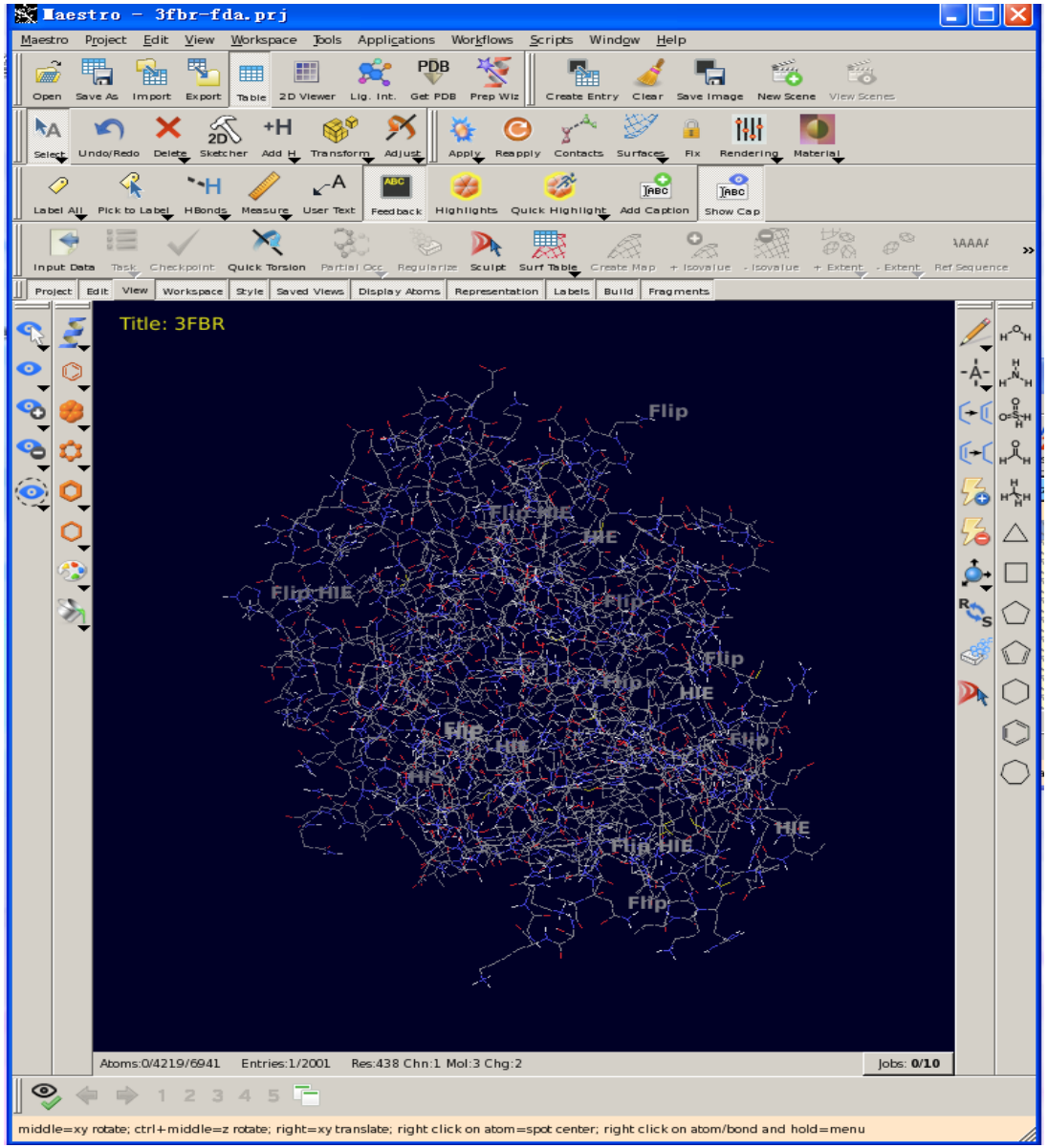
- Movie
  - 看分子动力学模拟MD的轨迹
  - 看核磁共振NMR解的几十个结构氨基酸的运动轨迹
  - 演示相互作用的过程
- Plugin
  - APBS (Adaptive Poisson-Boltzmann Solver)

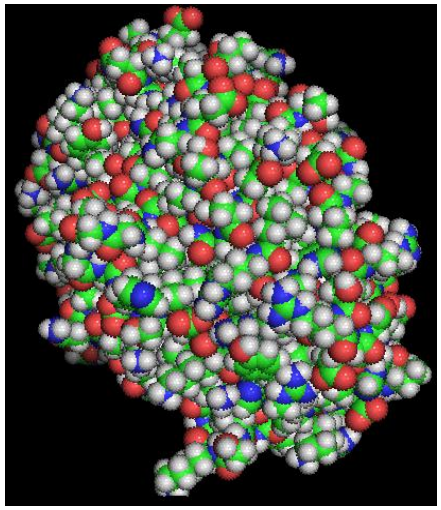
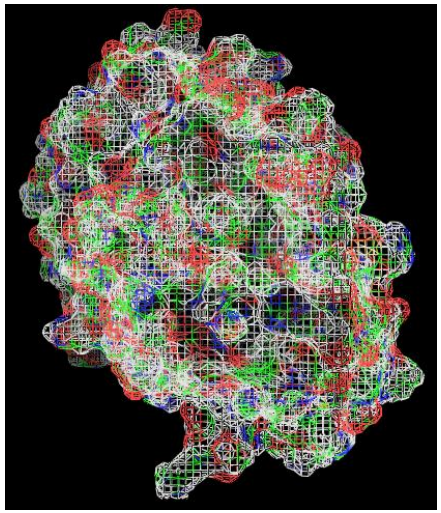
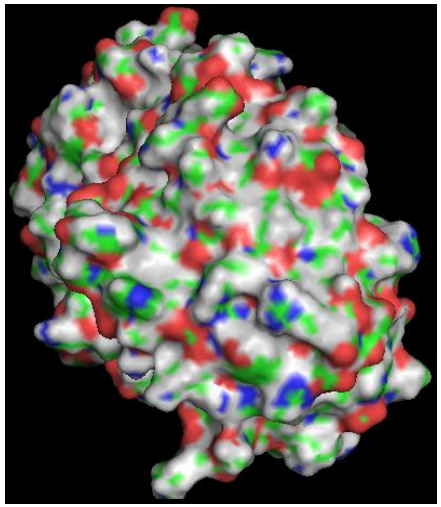
    利用泊松波尔兹曼方程解水溶液中分子间的静电作用



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!