

PyMOL 概述及实例简析

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主要内容

一. PyMOL概述

二. PyMOL功能

三. 应用实例

黄素氧还蛋白家族结构分析

一. PyMOL概述

➤ 名字来源:

“Py”-python, 该软件基于此计算机语言;

“Mol”-molecule, 该软件用来显示分子结构。

➤ 主要功能:

创作高品质的小分子或是生物大分子（特别是蛋白质）的三维结构图像。

➤ 网站: <http://PyMOLwiki.org/>

➤ PyMOL优点

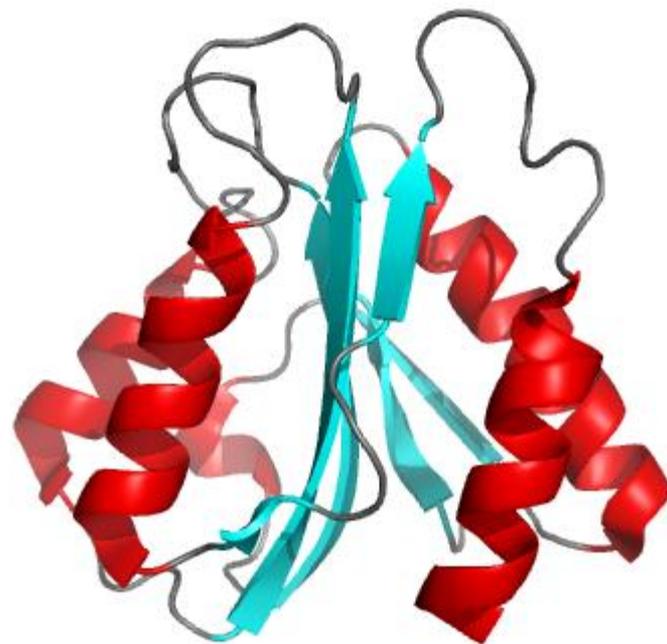
强大的分子可视化软件
高质量科学论文发表图形
动画制作
文档文件和绘画文件并存
鼠标操作与命令行操作
安装插件

➤ PyMOL缺点

缺乏足够的文件资料
没有**UNDO**功能

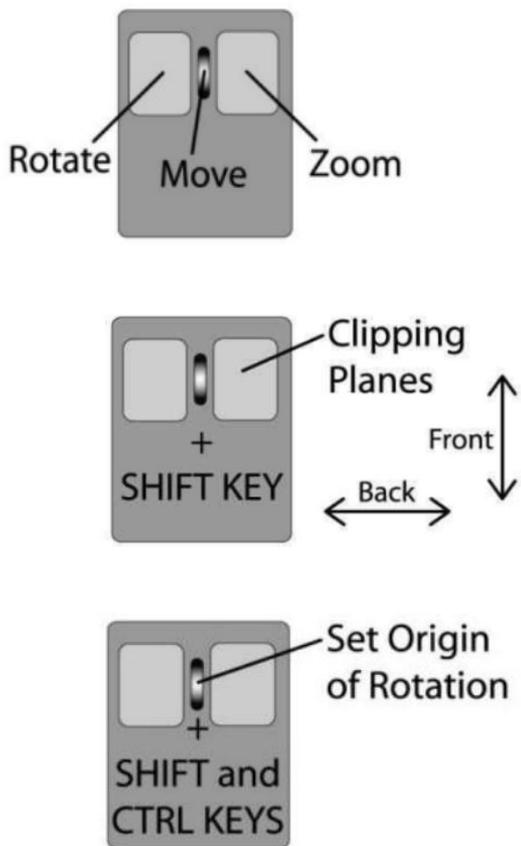
二. PyMOL功能简介

- 操作视图
- 比对
- 光线追踪
- 探测静电力学
- 晶体对称性
- 测量
- 动画
- 绘制晶体密度图



2HNA

➤ 操控视图



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

PYMOL(TM) Incantation Product - Copyright (C) 2006 Delano Scientific, LLC.
A current PyMOL Manual and a Selections script may be required for legal use of this build beyond a personal system. Please visit http://www.pymol.org for more information.
This PyMOL Executable Build Incorporates Open-Source PyMOL 0.99rc6.

External GUI

PyMOL Viewer

lines sticks spheres surface

mesh dots ribbon cartoon

Viewer

all	A	S	H	L	C
rep1	A	S	H	L	C
rep2	A	S	H	L	C
rep3	A	S	H	L	C
rep4	A	S	H	L	C
rep5	A	S	H	L	C

Demonstrations

Representations

Cartoon Ribbons

Transparency

Ray Tracing

Sculpting

Scripting

Electrostatics

CGOs

Molscript/R3D Input

End Demonstration

Mouse Mode 3-Button Viewing

Buttons L M R Wheel

Keys Rota Move MovZ Slab

Shift +Box -Box Clip MovS

Ctrl +/- PkAt Pk1 MvS2

CtSh Sele Drig Clip MovA

SingleClick +/- Cent Menu

DoubleClick Menu - PkAt

Selecting Residues

Frame 1 / 13 11/sec

Internal GUI

➤ 比对

- 基于蛋白序列

->Actions->align->to molecule

PyMOL>align (A and name ca),(B and name ca)

PyMOL>cealign A, B

Align—基于序列比对

Cealign—基于结构比较

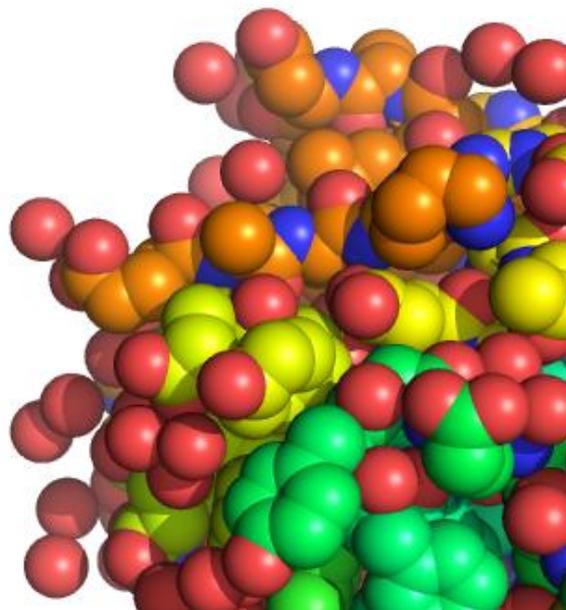
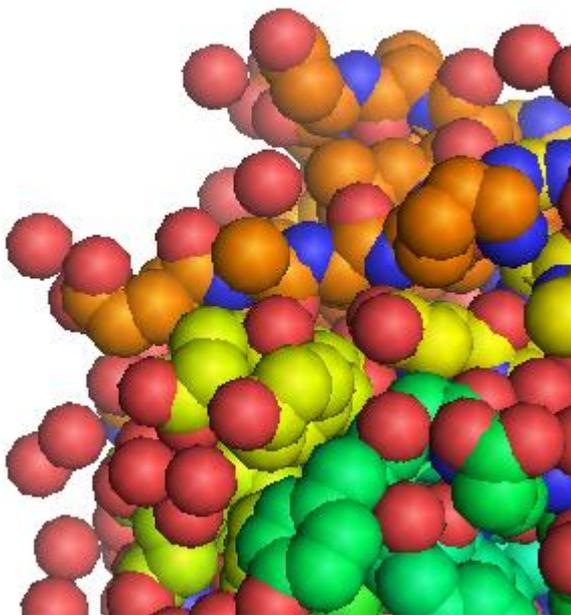
- 基于原子对

->Wizard->Pair Fitting

➤ 光线追踪

光线追踪能制作出最高质量的分子图像。

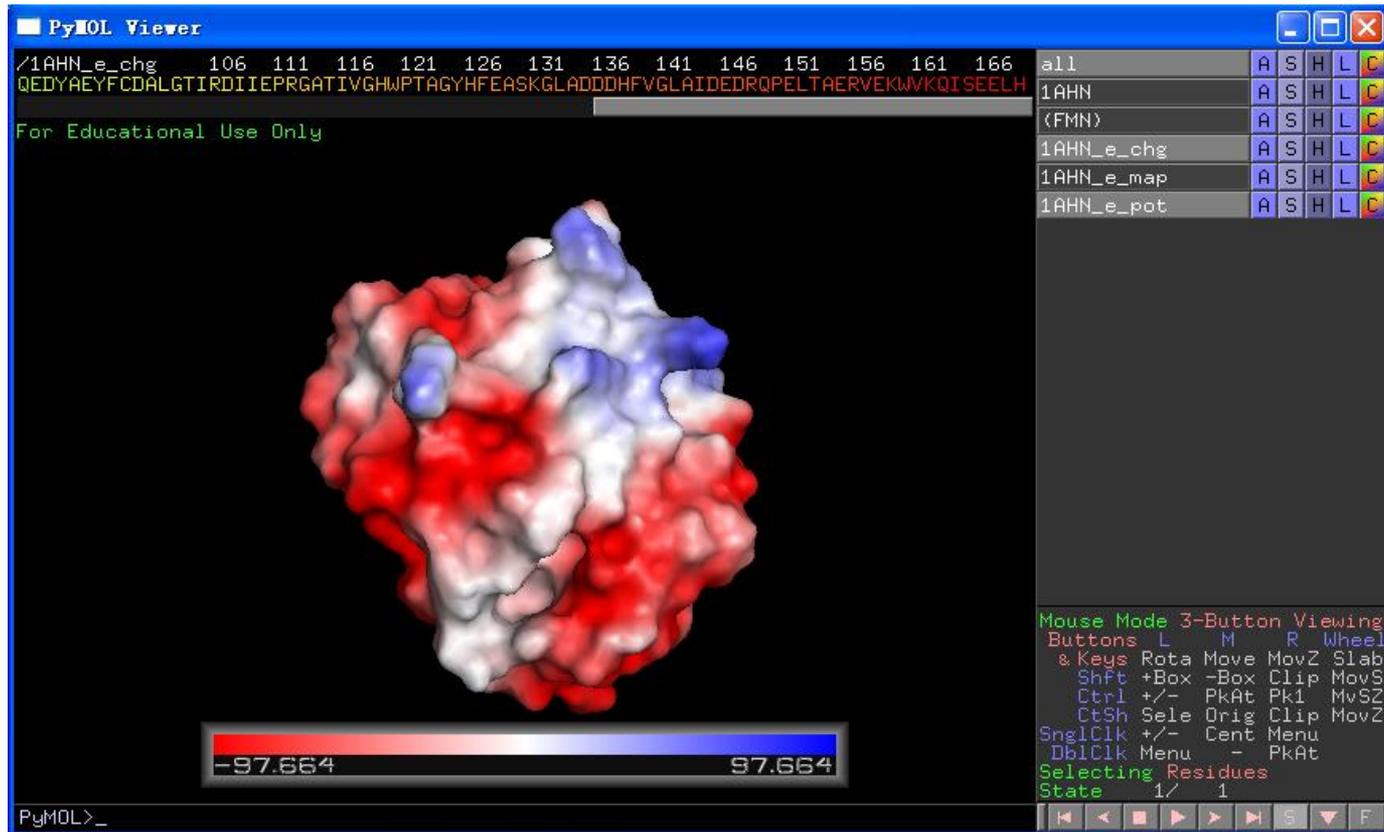
PyMOL是第一个拥有高速光线追踪器的全功能分子图像程序。



➤ 探测静电力学

利用泊松波尔兹曼方程计算水溶液状态下的静电力学。

->Actions->generate->vaccum electrostatics

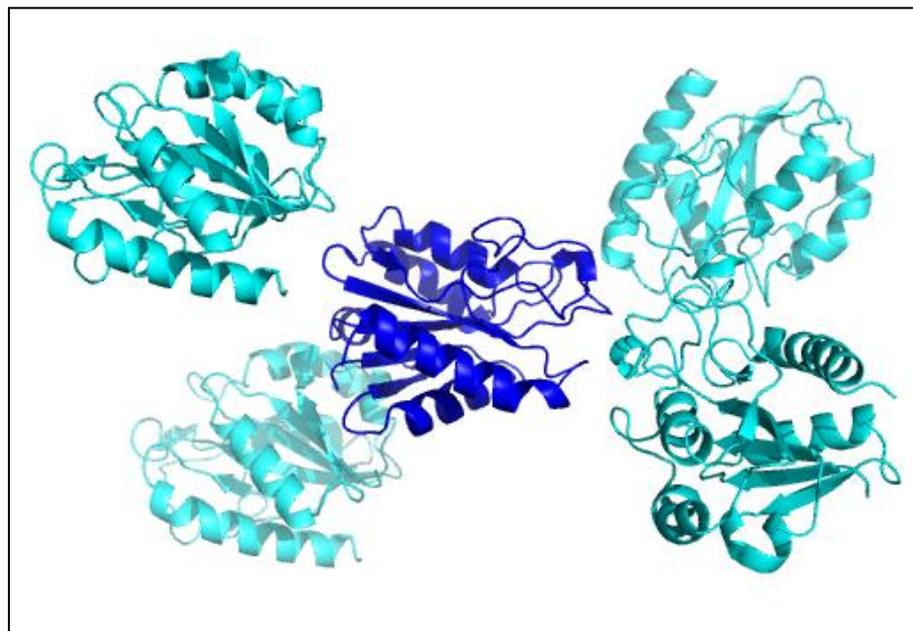


➤ 晶体对称性

读取.pdb文件时，矩阵信息就被输出。

“symexp”命令：

用于显示原子选择中晶胞的对称相关分子。



➤ 测量

- 距离

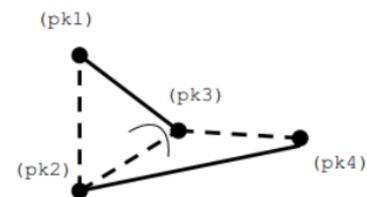
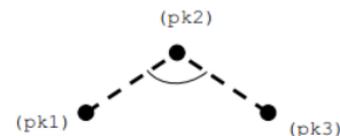
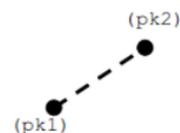
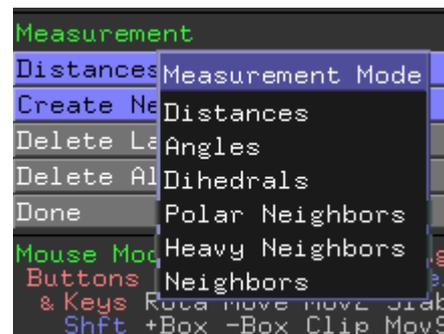
PyMOL> distance A,B

- 角度

PyMOL> angle A, B, C

- 二面角

PyMOL> Dihedral A,B, C, D



➤ 动画

- 创建一个60帧的动画，此动画 ± 45 度摇摆蛋白。
- PyMOL> fetch 1AHN # 载入结构
- PyMOL> mset 1 x30 # 定义60帧动画
- PyMOL> util.mrock 1,30,5,1,1 # mdo命令创建摇摆 ± 45 度的60帧动画
- PyMOL> mplay



Movie.pse

➤ 绘制电子密度图



EDS Electron Density Server



Welcome to the Electron Density Server at Uppsala University

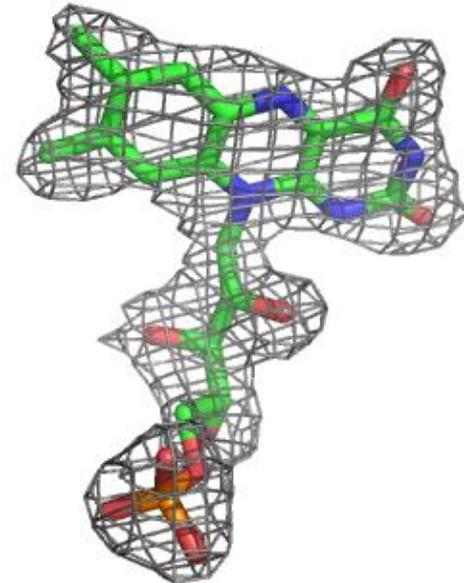
Enter a PDB code (4 characters):

Or enter a search string:

Electron-density map generation for 1ahn

Map format : Type :

(Note: this may take a few seconds to many minutes, depending on the size of your map.)

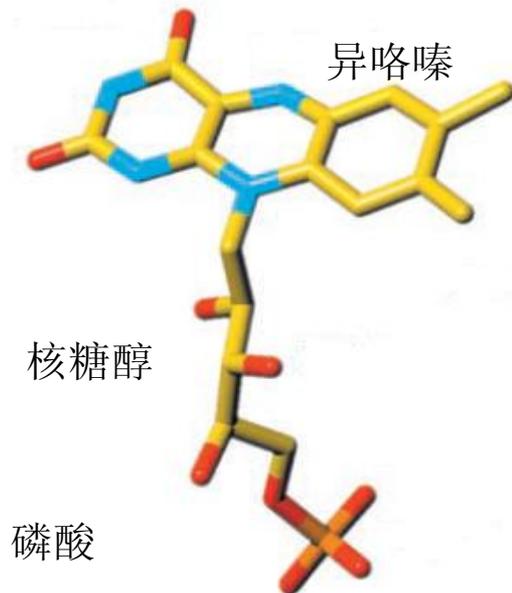


<http://eds.bmc.uu.se/eds/>

三.应用实例-黄素氧还蛋白

黄素氧还蛋白

— 细菌中的常见蛋白，通过结合 **FMN** 参与电子传递。



PS I → Fld → FNR → NADP⁺

Fld → Nitrogenase → N₂

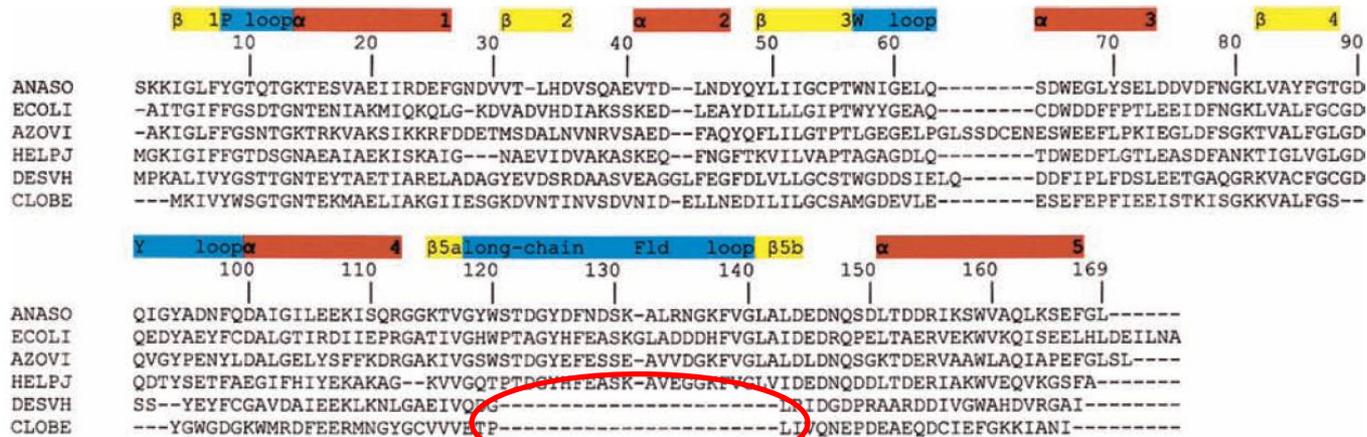
Fld $\xrightarrow{\text{activation}}$ of $\left\{ \begin{array}{l} \text{Methionine synthase} \\ \text{Ribonucleotide reductase} \\ \text{Pyruvate-formate lyase} \\ \text{HMBPP synthase} \end{array} \right.$

FNR → Fld → Biotin synthase → dethiobiotin

Pyruvate → POR → Fld

黄素单核苷酸 (FMN)

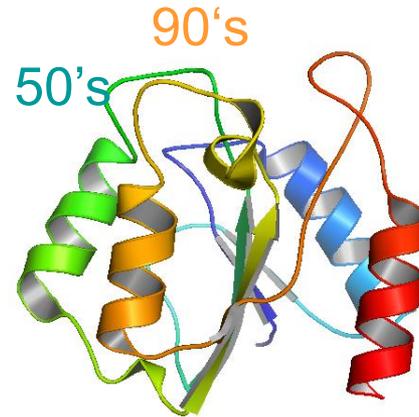
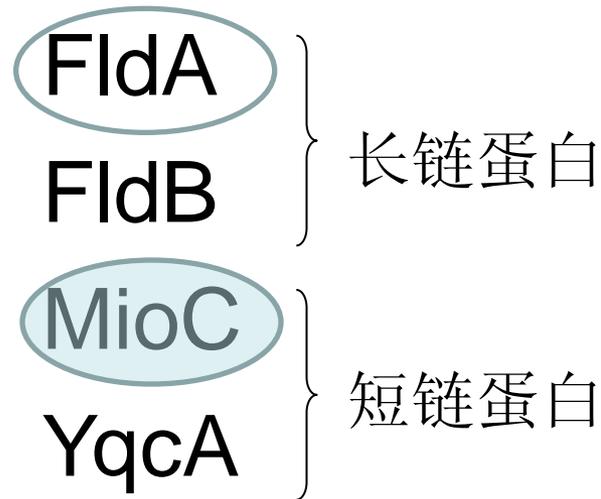
➤ 黄素氧还蛋白家族分类



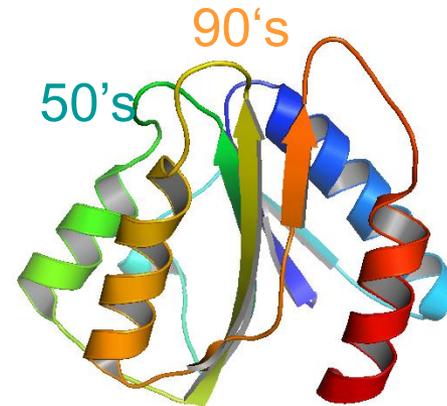
长链蛋白
短链蛋白

- ANASO (*Anabaena* PCC7119) 项圈藻
- ECOLI (*Escherichia coli*) 大肠杆菌
- AZOVI (*Azotobacter vinelandii*) 固氮菌
- HELPHJ (*Helicobacter pylori*) 幽门螺旋杆菌
- DESVH (*Desulfovibrio vulgaris*) 脱硫弧菌
- CLOBE (*Clostridium beijerinckii*) 梭菌

➤ 大肠杆菌中的黄素氧还蛋白



Apo-MioC



Holo-MioC

FldA: flavodoxin A

FldB: flavodoxin B

MioC: locates next to the chromosomal replication initiation origin (oriC)

YqcA:??

➤ 研究目标

—— 阐明黄素氧还蛋白与辅基**FMN**的结合方式。

通过诱导契合 (induced fit) 还是构象选择 (conformational selection)?

实例1. 基本显示及比对

Apo-MioC/Holo-MioC

- 载入结构
- 上色

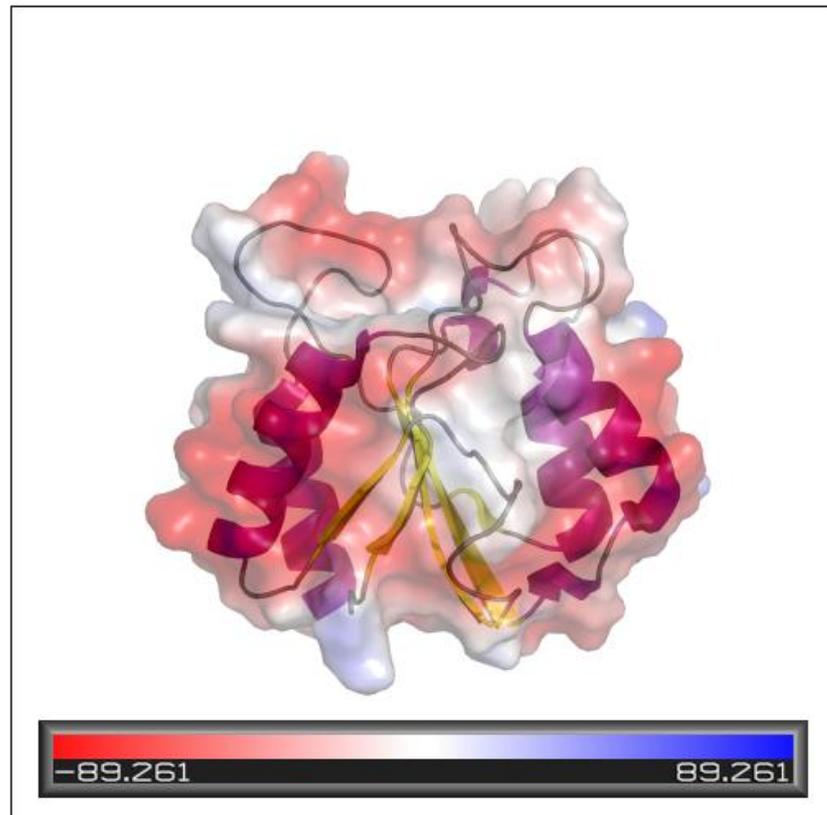
PyMOL> color purple, ss h

PyMOL> color yellow, ss s

PyMOL> color green, ss ""

- 静电力学

->Action ->generate ->vaccum electrostatics



- 比对

->action->align->to molecule->2HNA

整体比对

PyMOL>align(2HNA and name ca+c+n),(2HNB and name
ca+c+n)

自主选择性比对

PyMOL>color yellow,(resi 55-65,88-102)

- 修改背景

->display->background->white

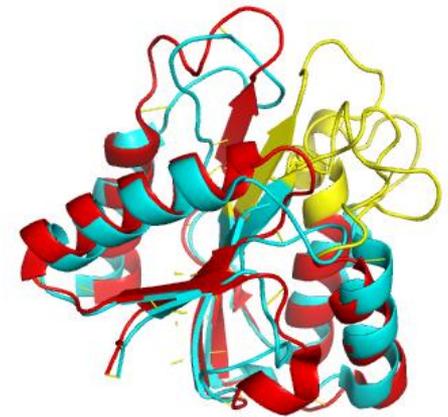
或PyMOL>bg_color white

- 修改投影

->setting->rendering->shadows

- 光线追踪

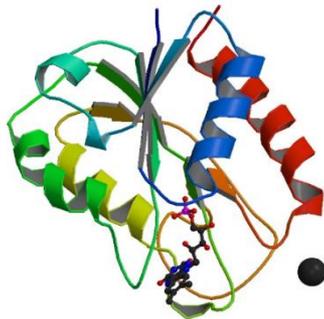
PyMOL>ray



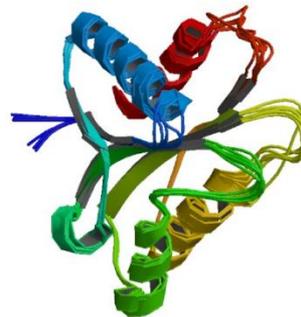
练习：

- 长链蛋白Holo-FldA（1AHN）与短链蛋白holo-MioC（2HNB）的比较。
- 关注点：
长链蛋白与短链蛋白的区别之处。

E.Coli
1.8Å
X-ray structure
Hoover DM. (1997) *Protein Science*



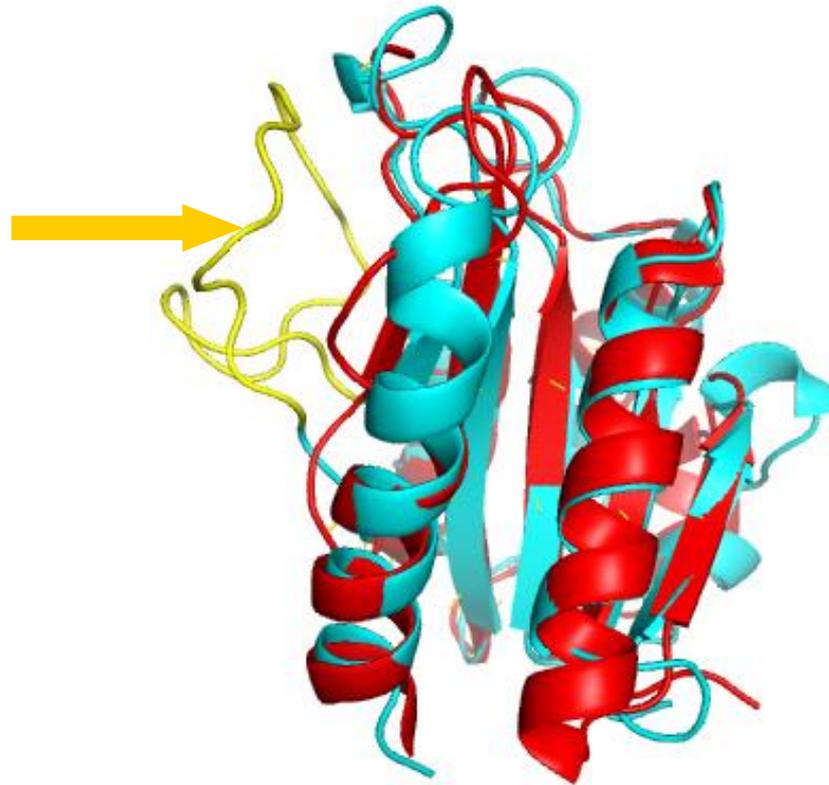
Holo-FldA



Holo-MioC

E.Coli
NMR solution structures
Yunfei Hu. (2006) *JBC*

FldA
120-140



MioC/FldA

实例2. 活性位点侧链、表面显示及距离测量

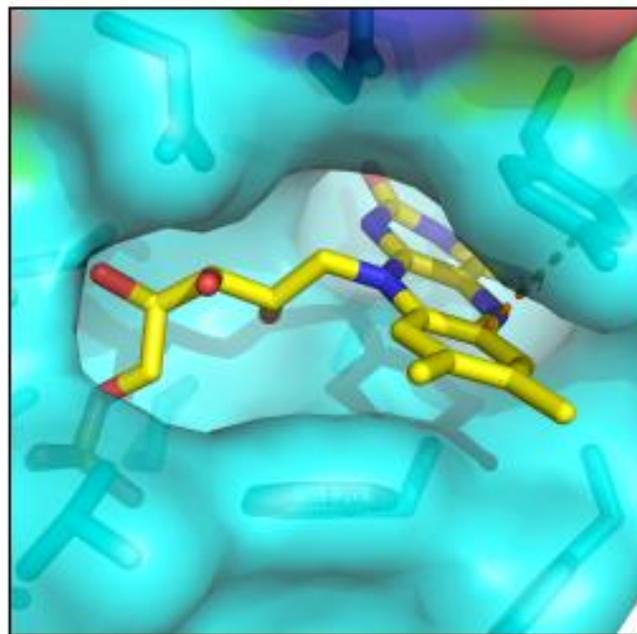
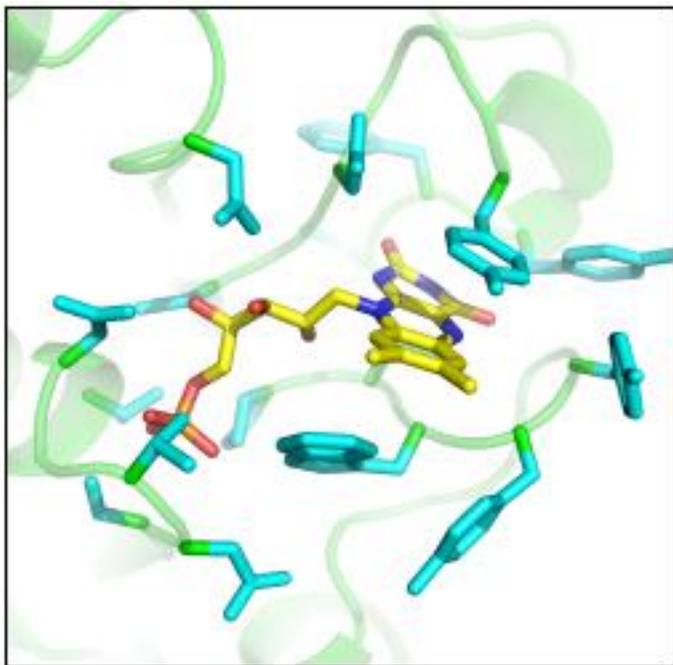


Image size = 1000 x 1000

► 活性位点侧链显示

->action->rename selection

定义配基

PyMOL>select FMN4,FMN around 4
->show side chain

选择距离FMN4Å 内的原子

PyMOL>select FMN4r,byres FMN around 4

选择距离FMN4Å 内的氨基酸

PyMOL>color cyan,FMN4r

主链ca也被更改颜色

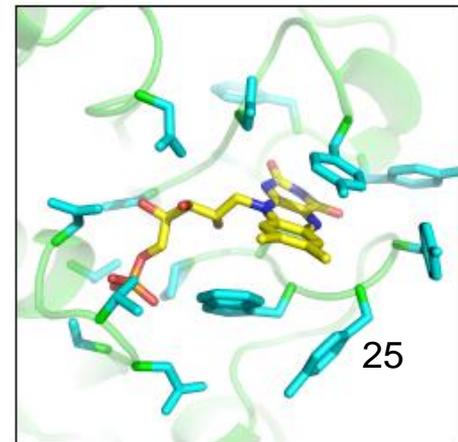
PyMOL>color green,1AHN and name ca

主链ca颜色修正

->setting->transparency->cartoon->50%

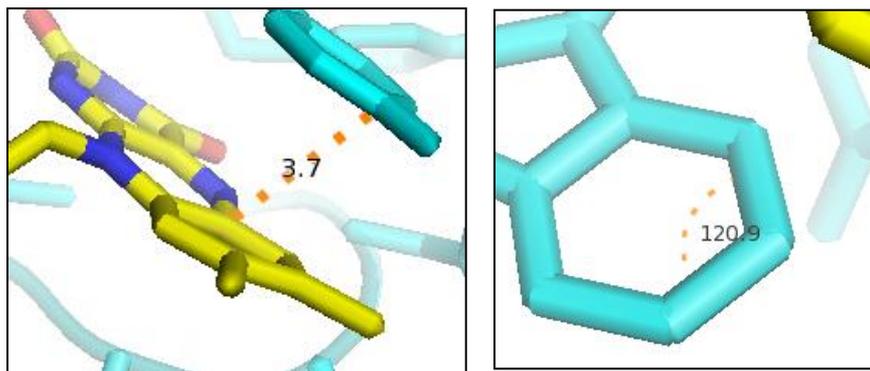
调整卡通透明度

->action->preset->ligand sites->cartoon



➤ 距离测量及表面显示

->wizard->measurement



显示表面

->show->surface

更改透明度

PyMOL>set transparency=0.25

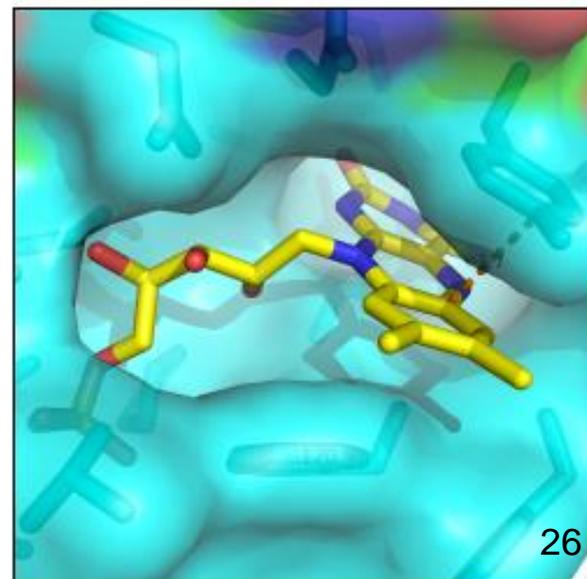
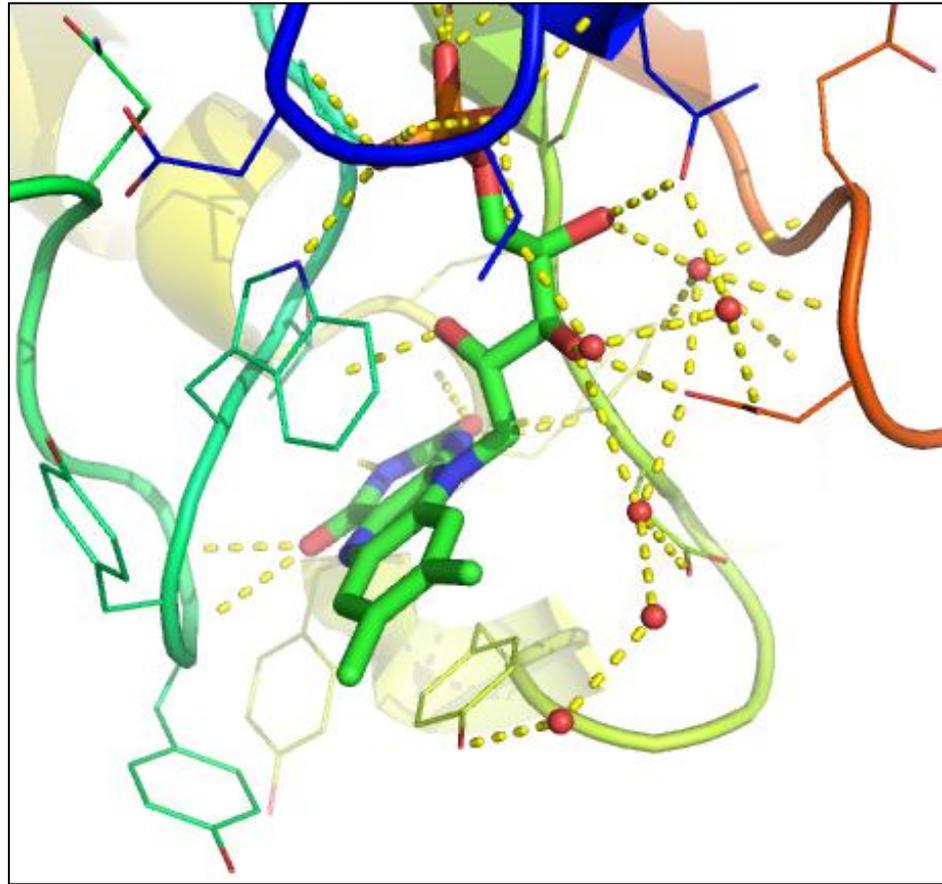


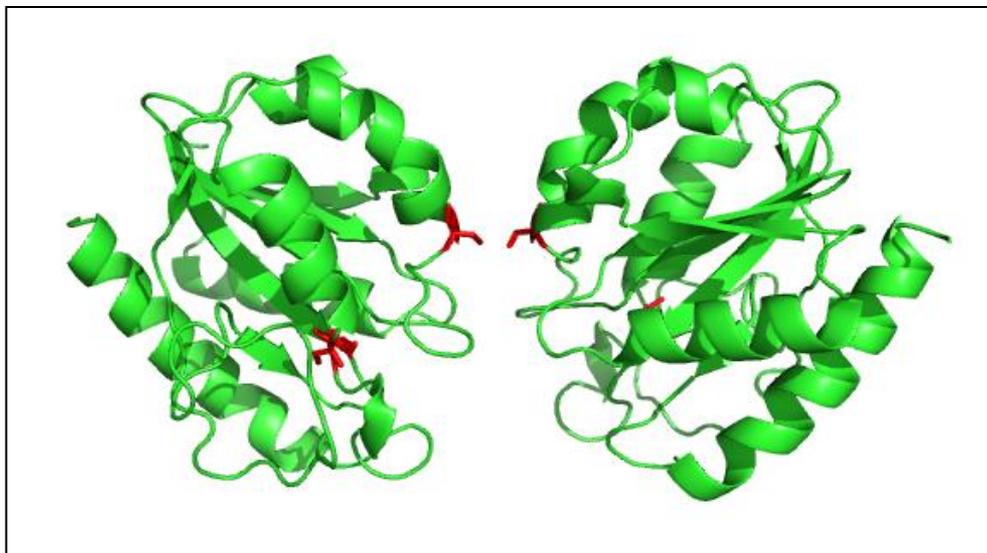
Image size = 1000 x 1000

->action->preset->ligand sites->cartoon



实例3.晶体对称性

```
PyMOL>symexp sym, 1AHN,1AHN,5 #创建对称相关的对象  
PyMOL>hide(not(1AHN expand 5)) #隐藏距离1AHN大于5Å  
                                   的原子  
PyMOL>sel cys, resn cys #选择Cys  
PyMOL>delete sym* #删除所有对称图像
```



实例4.电子密度图的绘制

载入1AHN.pdb

载入map.ccp4

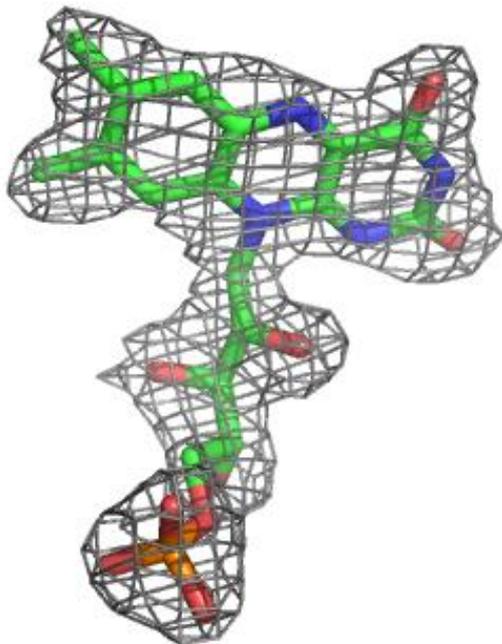
PyMOL> isomesh mesh,map,1

#载入结构和电子密度图

#绘制电子密度图，等势值=1

PyMOL> isomesh mesh2, map,1.0, FMN, carve=1.5

#绘制FMN电子密度图





Thank you!