

Pymol使用简介及实例简析

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主要内容

- Pymol简介
- Pymol功能概述
- 实例
 - ✓ OsSAMS的ligand结合位点
 - ✓ 集胞藻PCC 6803中砷酸还原酶SynArsC还原机理与结构的关系

Pymol简介

- Pymol: Python + Molecule
- 创作高品质小分子或是生物大分子（特别是蛋白质）的三维结构图像。
- 开放源代码视觉化工具
- Warren Lyford DeLano (Jun 21, 1972 - Nov 3, 2009)编写，之后DeLano Scientific LLC将其商业化。
- 版本： Incentive PyMOL / Educational PyMOL / AxPyMOL / Open Source PyMOL / Mobile PyMOL
- <http://pymol.org>

PyMOL Product Comparison Matrix

BUY PyMOL

> Show ALL Products

CLICK TO ADD/ REMOVE PRODUCTS FROM MATRIX

Expand Tabs below by clicking them. Compare fewer products by clicking the "Remove" box above any product on the right.	<input checked="" type="checkbox"/> Incentive PyMOL	<input checked="" type="checkbox"/> Educational PyMOL*	<input checked="" type="checkbox"/> Open Source PyMOL	<input checked="" type="checkbox"/> AxPyMOL	<input checked="" type="checkbox"/> Mobile PyMOL
<input checked="" type="checkbox"/> Price					
<input checked="" type="checkbox"/> Support					
<input checked="" type="checkbox"/> System Integration					
Compiled and Ready to Use (Windows, Mac, Linux)	●	●		●	●
Drag & Drop (Mac)	●	●		N/A	N/A
3D Space Navigator Support (Mac)	●			N/A	N/A
MS PowerPoint Integration (Windows)	N/A	N/A	N/A	N/A	●
<input checked="" type="checkbox"/> Scientific Integration					
MTZ Map Reading	●				N/A
Stereochemical Determination and Labeling	●				N/A
Improved MOL2 and MMD atom typing	●			N/A	N/A
Advanced Molecular Morphing Wizard with RigiMOL	●				N/A
APBS Integration	●				N/A
Direct MPEG/QuickTime export	●				N/A
MMFF94 Forcefield	●				N/A
<input checked="" type="checkbox"/> Graphics					
High Speed Graphics	●	●	●	●	●
High Quality Real-time Graphics	●	●	●	●	●
Real-time Antialiasing	●				●
Volume Visualization	●	●	●		●
Volume Visualization (pre-integrated)	●				●
Ambient Occlusion of Surfaces	●	●	●		●
Arbitrary Background Images	●	●		●	●
Advanced labels and callouts	●	●		●	●
Focal blur	●	●			
Ray Tracing	●		●	●	●
<input checked="" type="checkbox"/> Usability					
Multilevel Undo	●				N/A
Annotated Settings	●	●			N/A
New Plugin/Script Manager	●	●	●		N/A
CTRL-F to find objects/selections	●	●			N/A
Maestro and MOE file reading support	●	●			●

*-- Academic, nonprofit, non-professional research only.

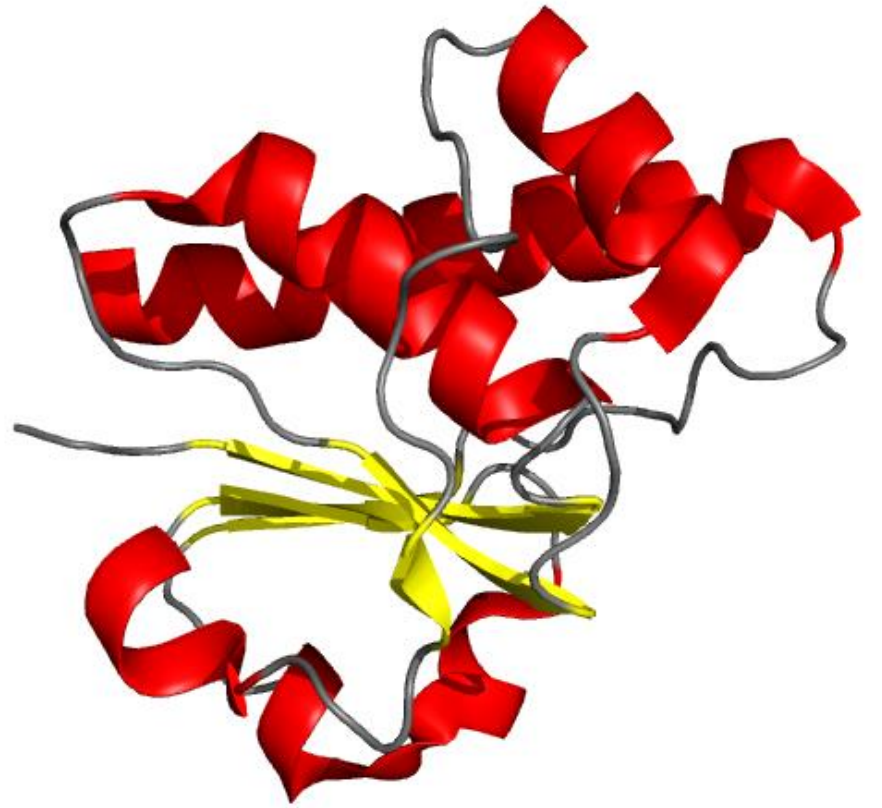
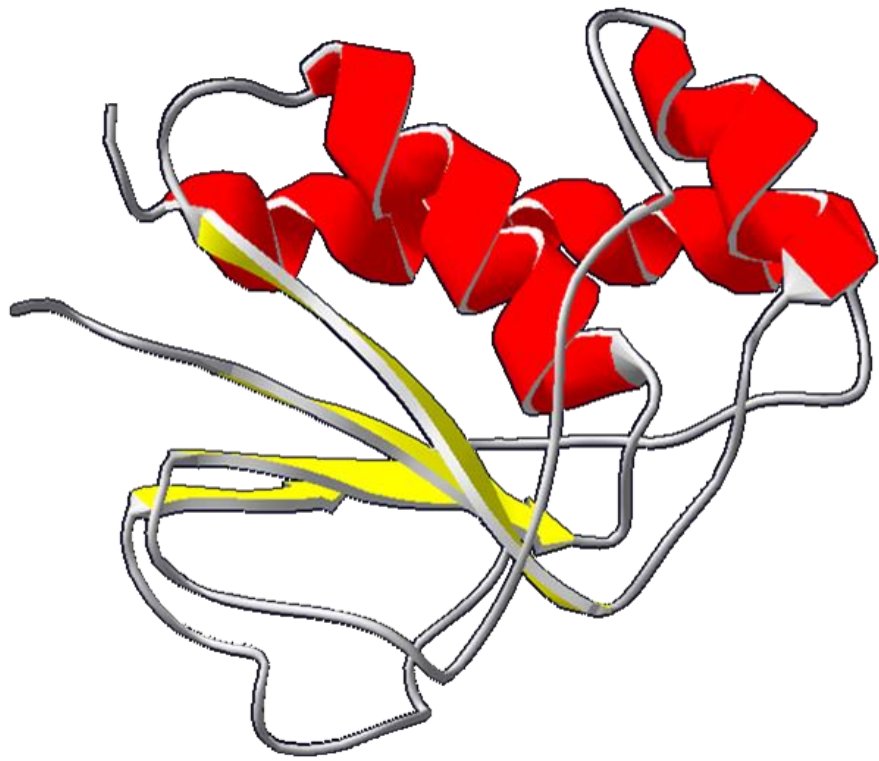
†-- Provided as a professional service.

Swiss PDBviewer

- 在同源建模(homology modeling)方面具有优势
- 与Swiss-Model紧密相连
- 有详细的说明文档

Pymol

- 出色的PDB文件显示软件
- 软件的作者宣称，在所有正式发表的科学文献中的蛋白质结构图像中，有四分之一是使用PyMOL制作
- 缺乏文件资料



Pymol的优点

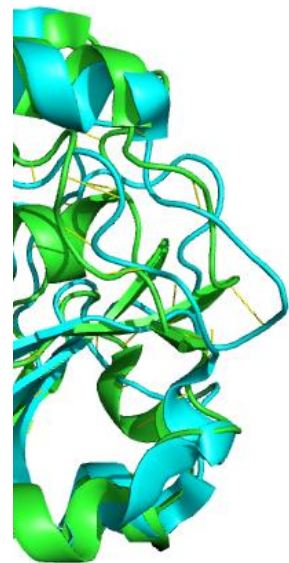
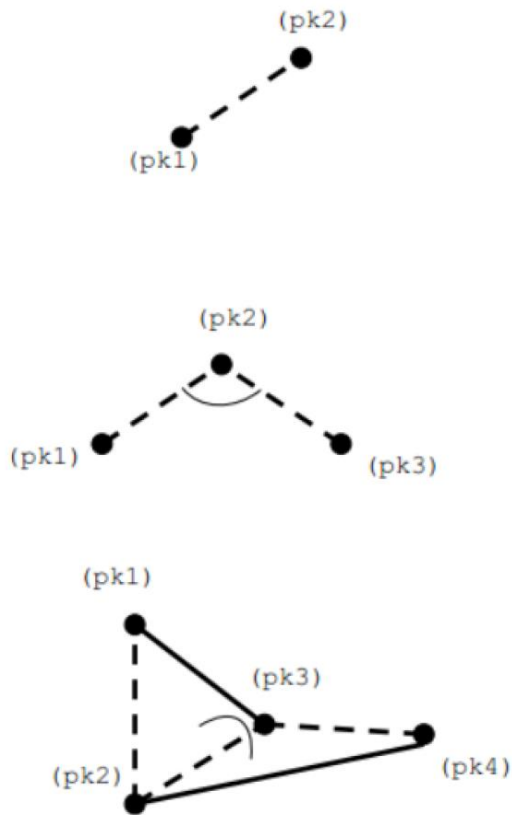
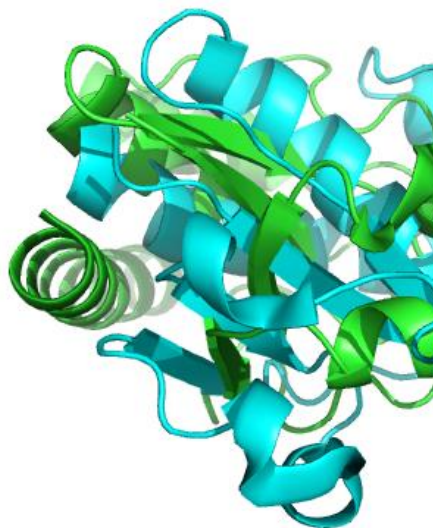
- 强大的分子可视化软件
- 高质量科学论文发表图形
- 文档文件和会话文件并存
- 鼠标操作与命令行操作
- 动画制作
- 免费的开放源码

Pymol的缺点

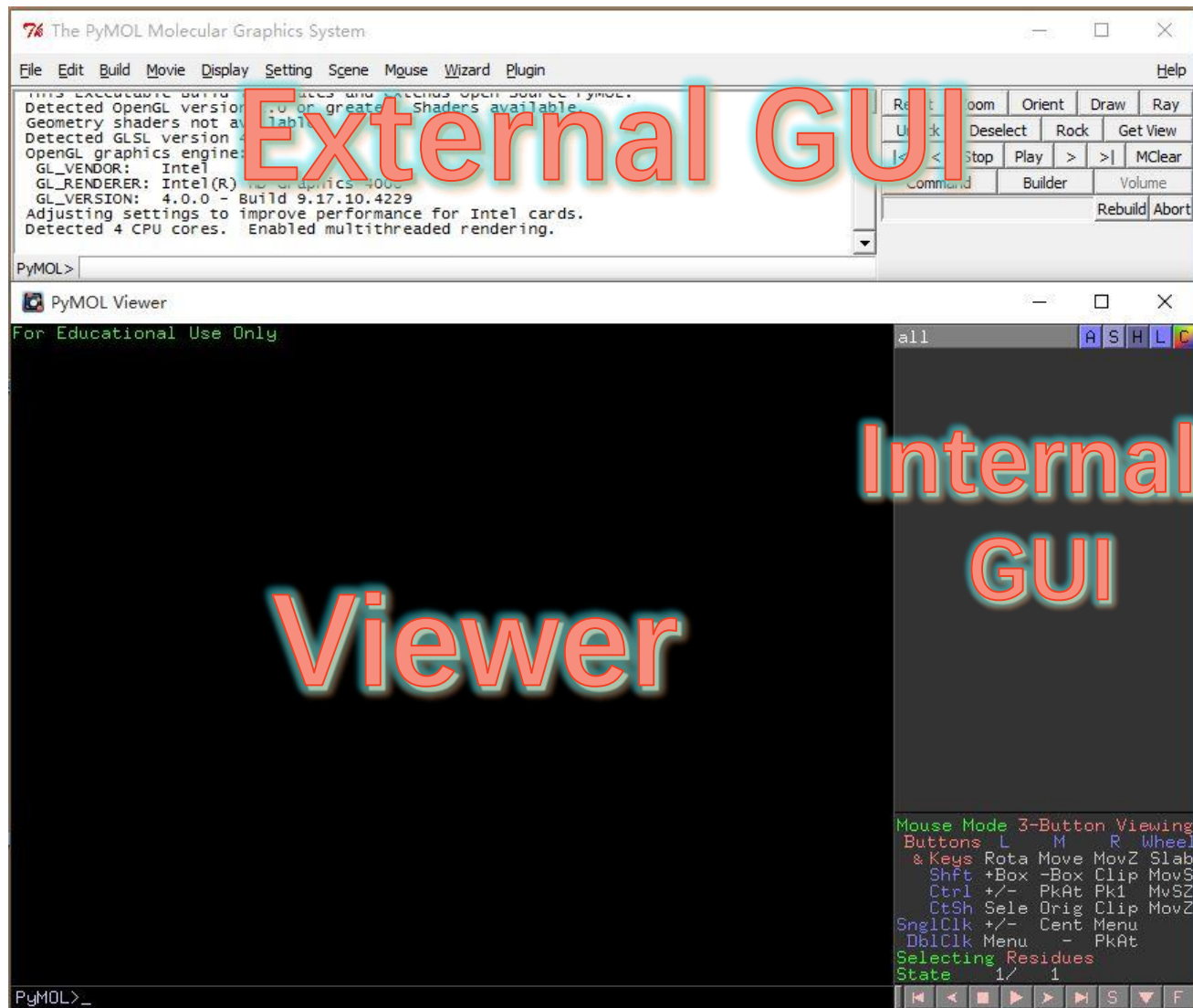
- 没有undo功能
- 缺乏充足的文件资料

功能概述

- 操控视图
- 比对
- 测量
- 光线追踪
- 探测静电力学
- 绘制晶体密度图
- 动画制作
- ...

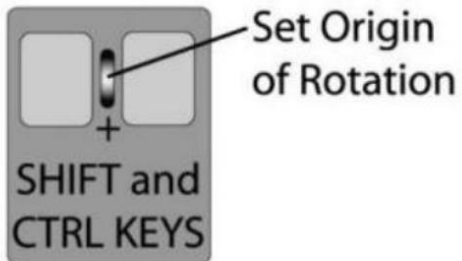
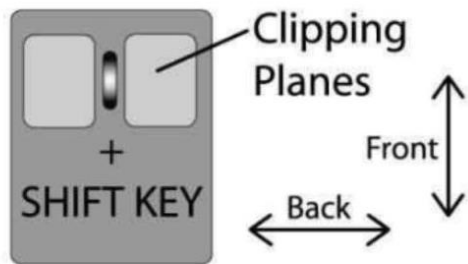
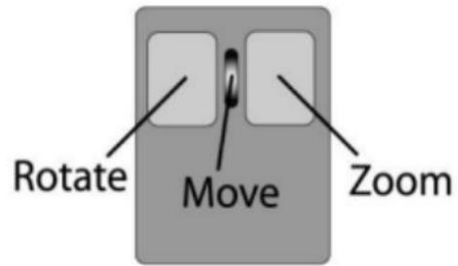


操控视图

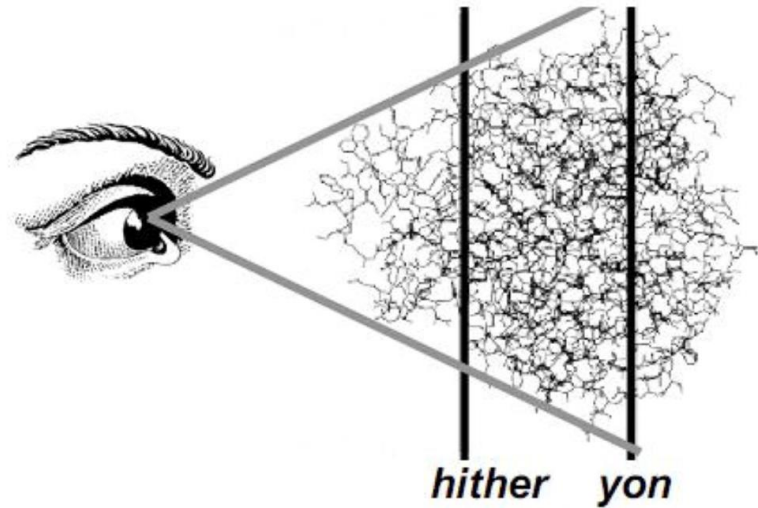


Graphical User Interface

鼠标操作：

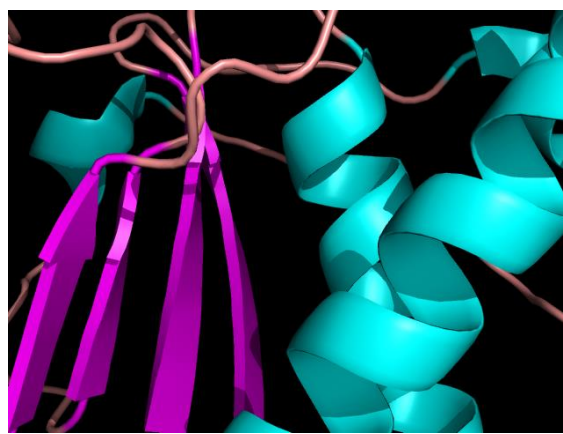
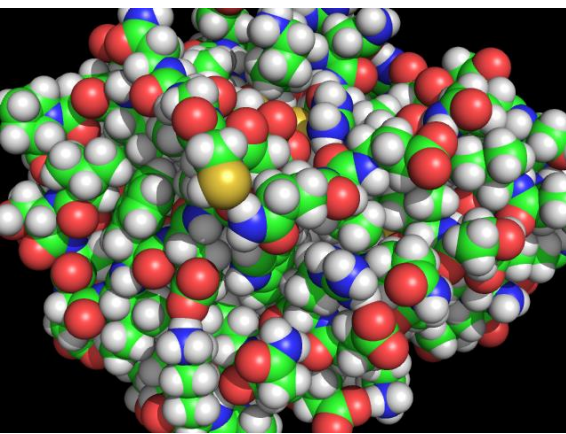
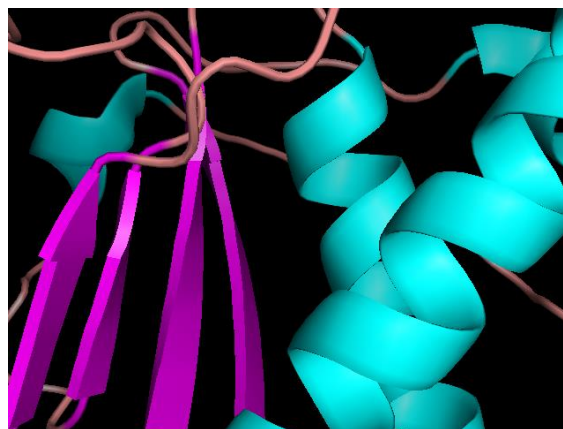
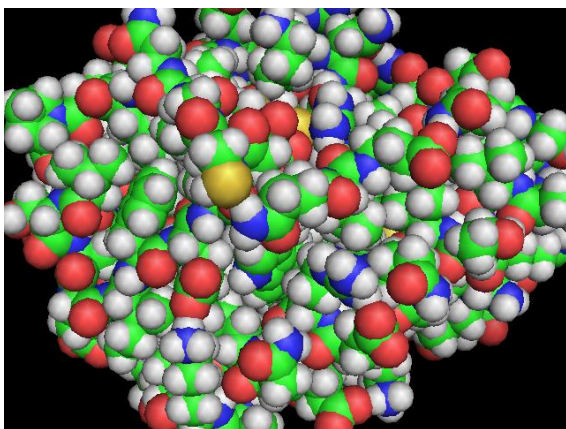


调整剪切面：



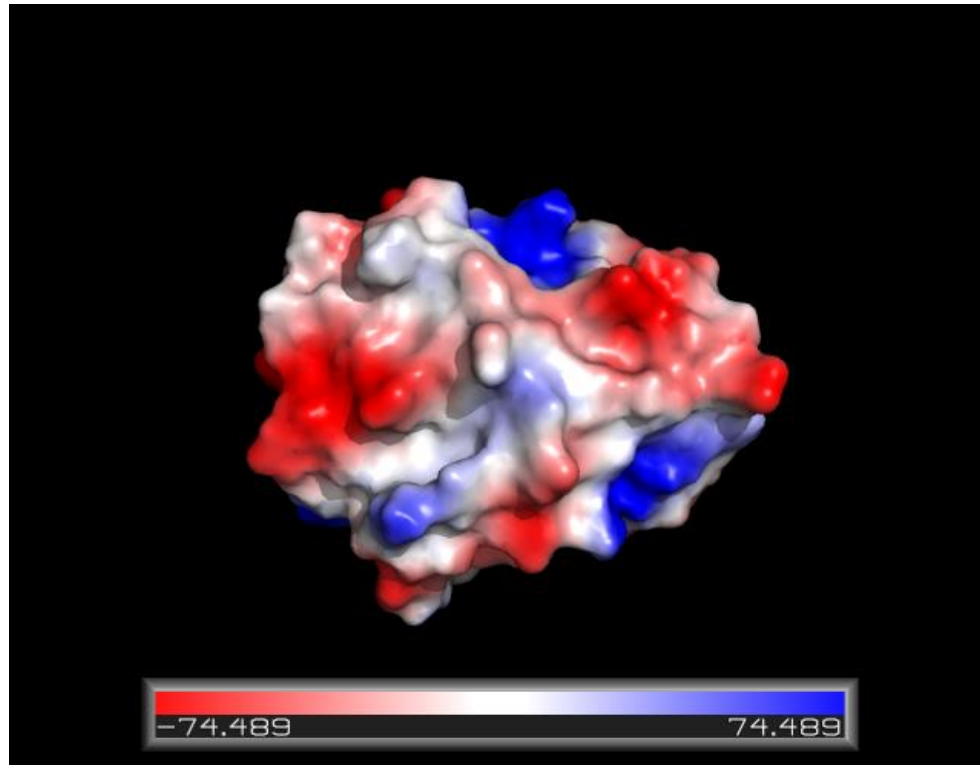
光线追踪

- PyMOL是第一个拥有高速光线追踪器的全功能分子图像程序。
- PyMOL>ray



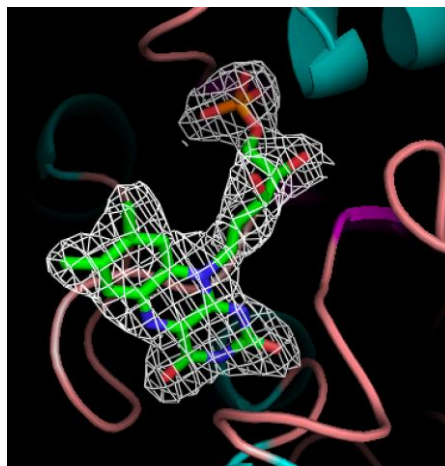
探测静电力学

- 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



绘制电子密度图

- 载入1AHN.pdb
- 载入map.ccp4 #载入结构和电子密度图
- PyMOL> isomesh mesh,map,1 #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



动画制作

□ 举例：蛋白质在120帧中旋转360°

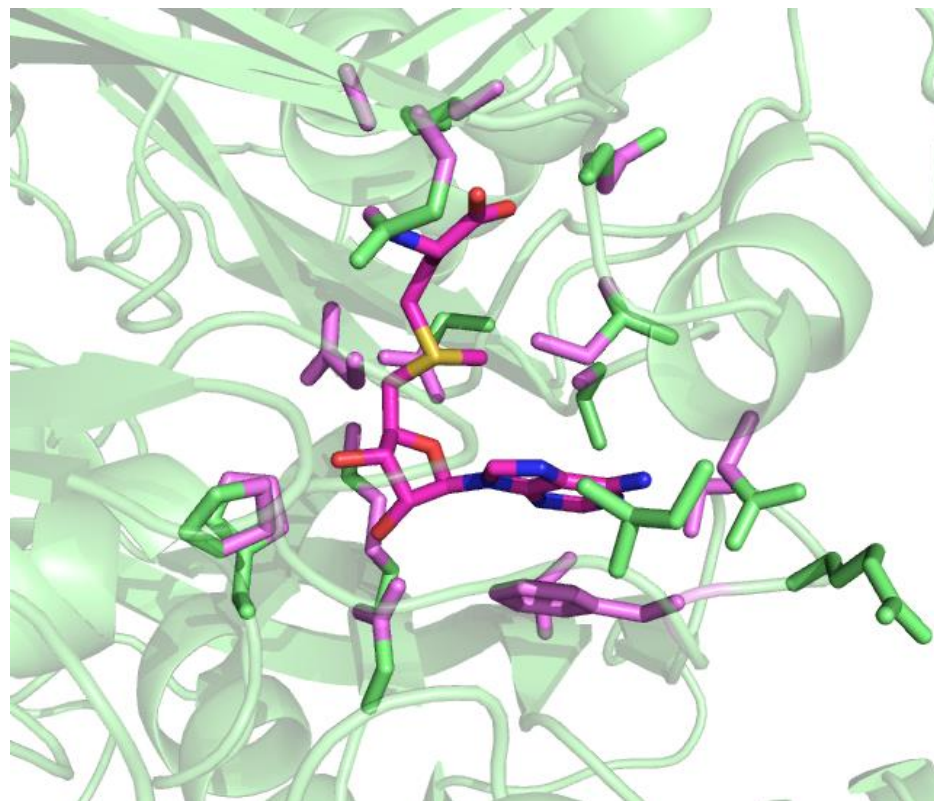
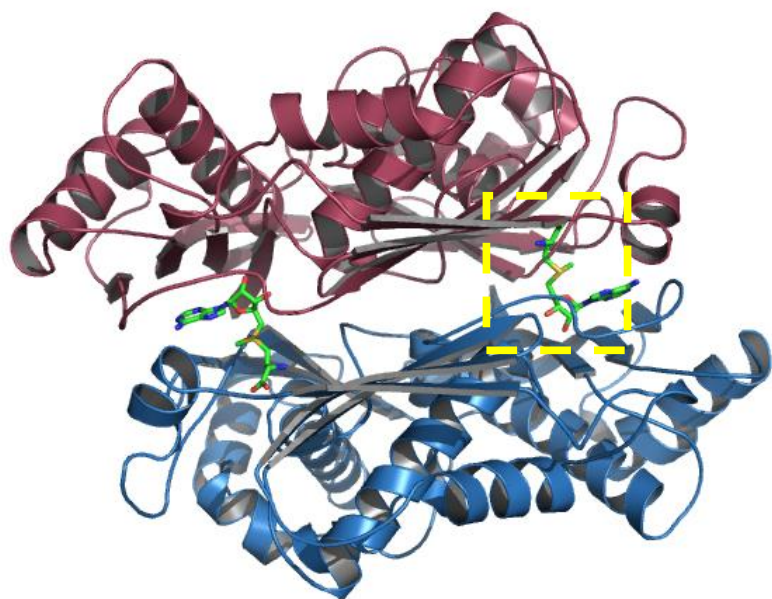
- PyMOL> load 2myu #载入结构
- PyMOL> mset 1 x120 #定义120帧动画
- PyMOL> util.mroll 1,120,1 #mro命令创建绕y轴旋转360°的120帧动画
- PyMOL> mplay

□ Ray-traced动画

- Pymol> set ray_trace_frames,1 #打开光线追踪
- Pymol> set cache_frames,0
- Pymol> Mpng mov #自动创建png图片



OsSAMS的ligand结合位点



基本显示

□载入结构

- ->File->open
- PyMOL>load humanm.pdb #fetch

□调整显示方式

- PyMOL> as cartoon

□上色

- PyMOL>color red, 2myu and ss h
- PyMOL>color yellow, 2myu and ss s
- PyMOL>color blue, 2myu and ss l+"

Pymol> keyword *argument*

Pymol> select *selection-name, selection-expression*

□ 定义ligand

- ->action->rename selection

□ 选择距离sam 4Å 以内的原子

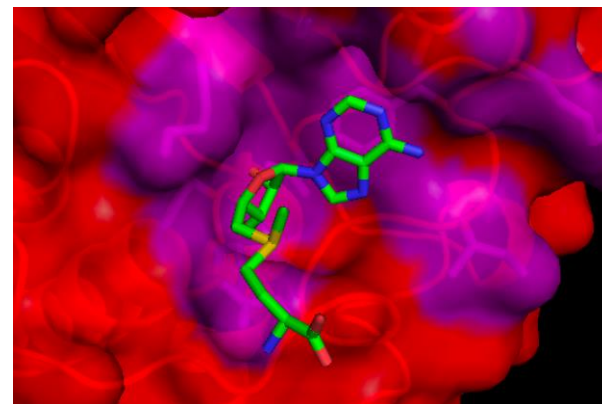
- PYMOL>select sam4, sam around 4
- ->show side chain
- PyMOL>color purple,sam4 #主链ca也被更改颜色
- PyMOL>color red, chaina and name ca
- PyMOL>color marine, chainb and name ca #主链ca颜色修正

□ 生成图片

- PyMOL>set cartoon_transparency, 0.4
- PyMOL>bg_color white
- PyMOL>ray #ray 1000,1000
- PyMOL>png 001

□ 表面显示

PyMOL>show surface, chaina



□ 测量

- 距离

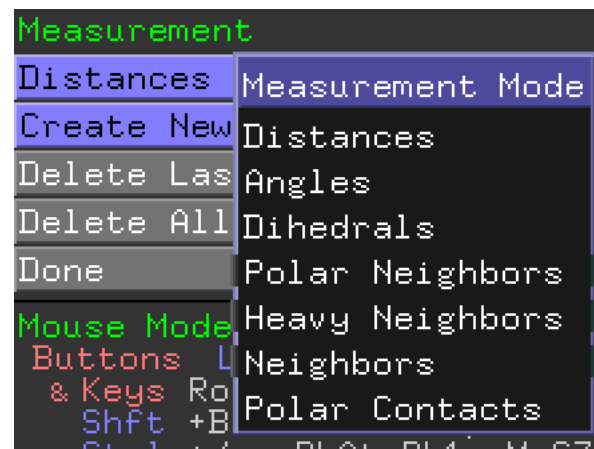
PyMOL> distance (sele1), (sele2)

- 角度

PyMOL> angle (sele1), (sele2), (sele3)

- 二面角

PyMOL> Dihedral (sele1), (sele2), (sele3), (sele4)



□ 标记

- PyMOL>label sam, name #resn, resi, chain...

集胞藻PCC 6803中砷酸还原酶SynArsC 还原机理与结构的关系

砷酸还原酶: $\text{red-ArsC} + \text{As(V)} \rightarrow \text{oxi-ArsC} + \text{As(III)}$

Arsenate reductase families

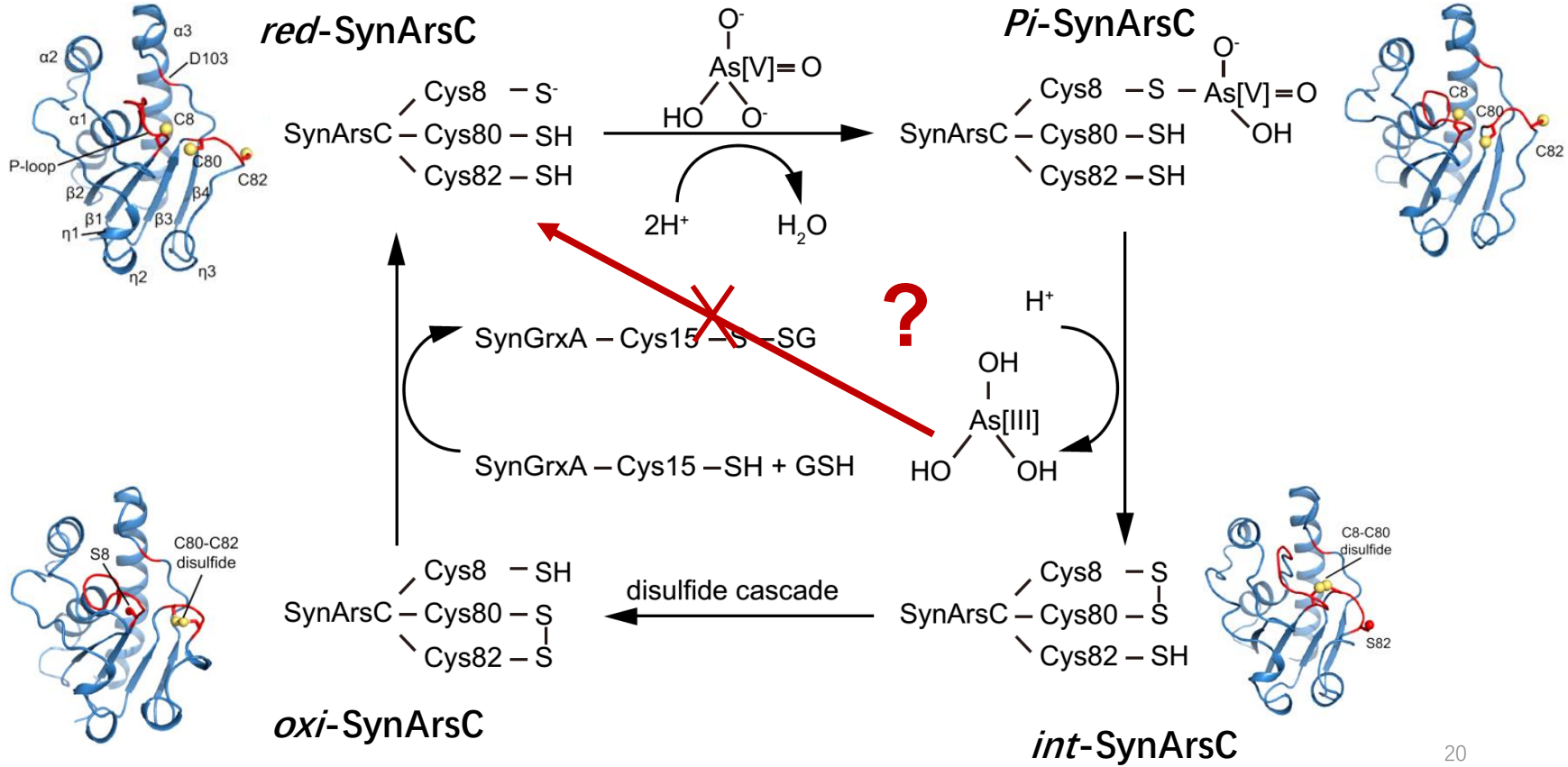
- The glutaredoxin (Grx)-coupled family *E. coli* R773 ArsC *S. cerevisiae* Acr2p
- The thioredoxin (Trx)-coupled family *S. aureus* pl258 ArsC *B. subtilis* BsArsC
- The Trx/Grx hybrid family SynArsC from *Synechocystis* sp. strain PCC 6803
- Other families

SynArsC (the Trx/Grx hybrid family)

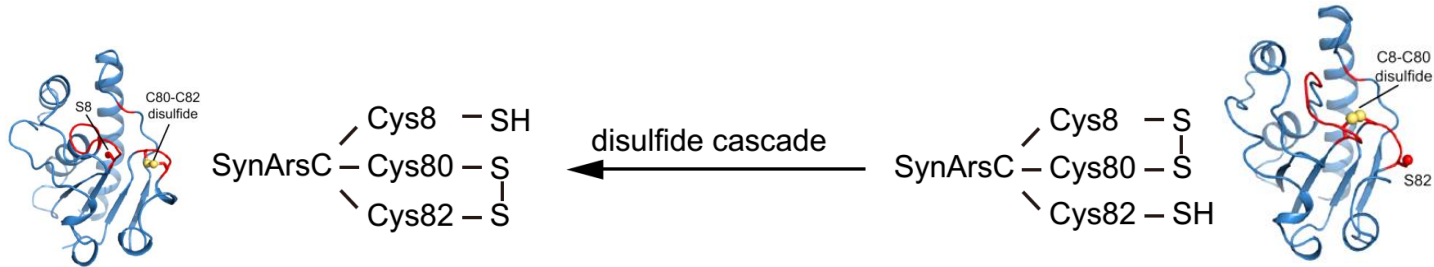
- Structurally similar to the Trx-coupled family
- Contains three essential cysteines
- Requires the Grx system to be regenerated

} Trx-coupled ?

→ Grx-coupled



二硫键级联反应前后的结构变化



□载入结构

- PyMOL> load 2myt #int-SynArsC
- PyMOL> load 2myu #oxi-SynArsC

->File->open

□调整显示方式

- PyMOL> as cartoon

->show->as->cartoon

□上色

- PyMOL>color violet, 2myu
- PyMOL>color greencyan, 2myt

->color

□选择与标记

- PyMOL>select c8c80, 2myt and ((resi 8) or (resi 80))
- PyMOL>select c80c82, 2myu and ((resi 80) or (resi 82))
- PyMOL>select c8sc80s, 2myt and ((resi 8 and name sg) or (resi 80 and name sg))
- PyMOL>select c80sc82s, 2myu and ((resi 80 and name sg) or (resi 82 and name sg))
- PyMOL>show sticks, c8c80 or c80c82
- PyMOL>as spheres, c8sc80s or c80sc82s
- PyMOL>color red, c8sc80s
- PyMOL>color orange, c80sc82s

□ 比对

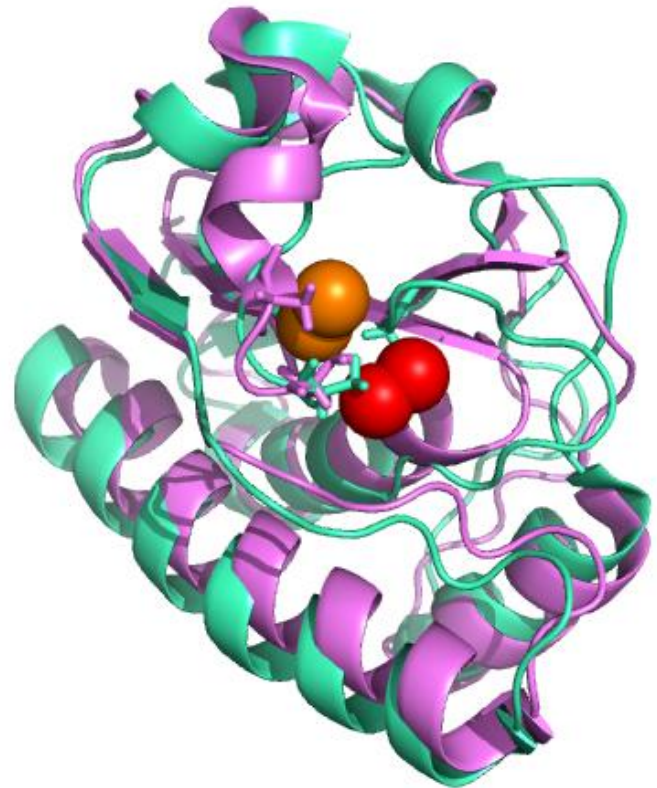
- PyMOL>cealign 2myt, 2myu

□ 调整

- PyMOL>bg_color white
- PyMOL>ray

□ 导出图片

- PyMOL>png 001



比对

□基于蛋白序列

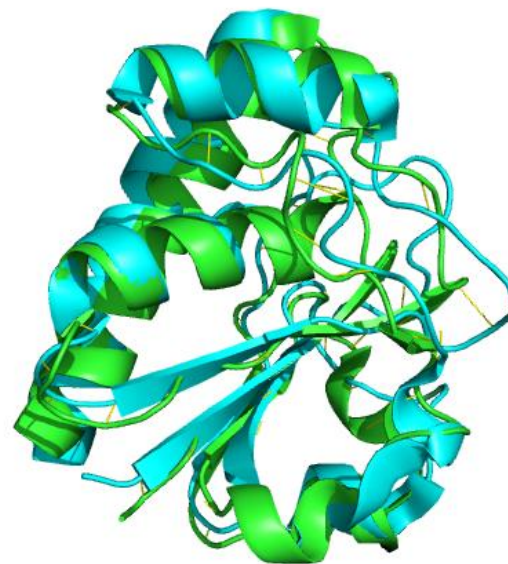
- ->Actions->align->to molecule
- PyMOL>align (A and name ca),(B and name ca)

□基于蛋白结构

- PyMOL>cealign A, B

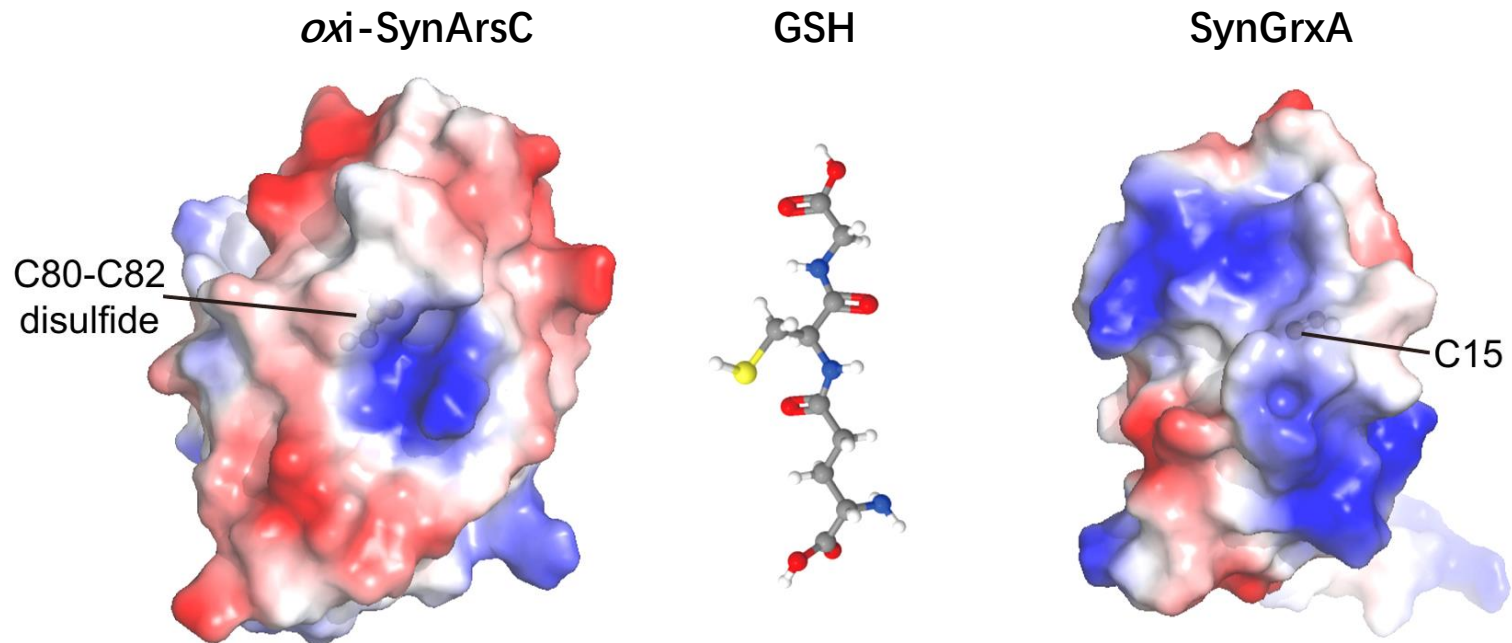
□基于原子对

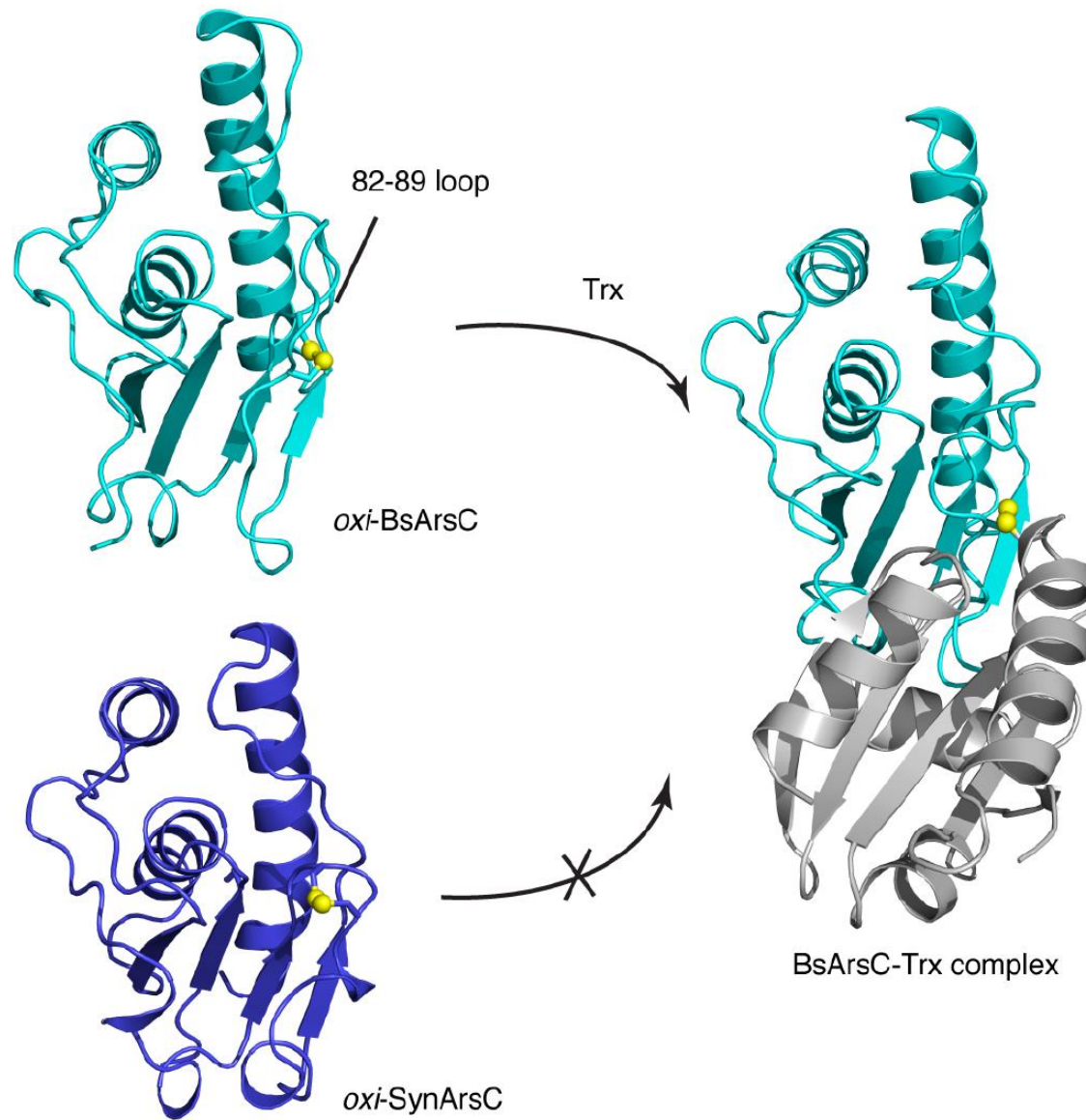
- ->Wizard->Pair Fitting

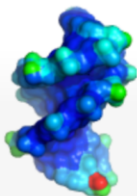


Structural basis for interactions with GSH and SynGrxA

- Electrostatic interactions may play a critical role in the reactivation of SynArsC





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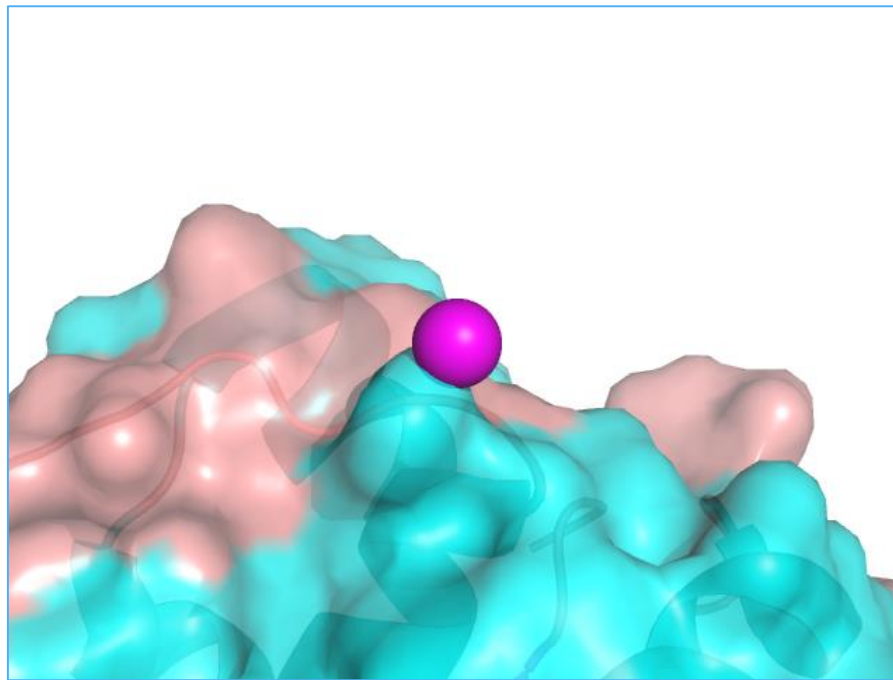
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□练习：胰岛素(4INS)的锌结合位点



谢谢！