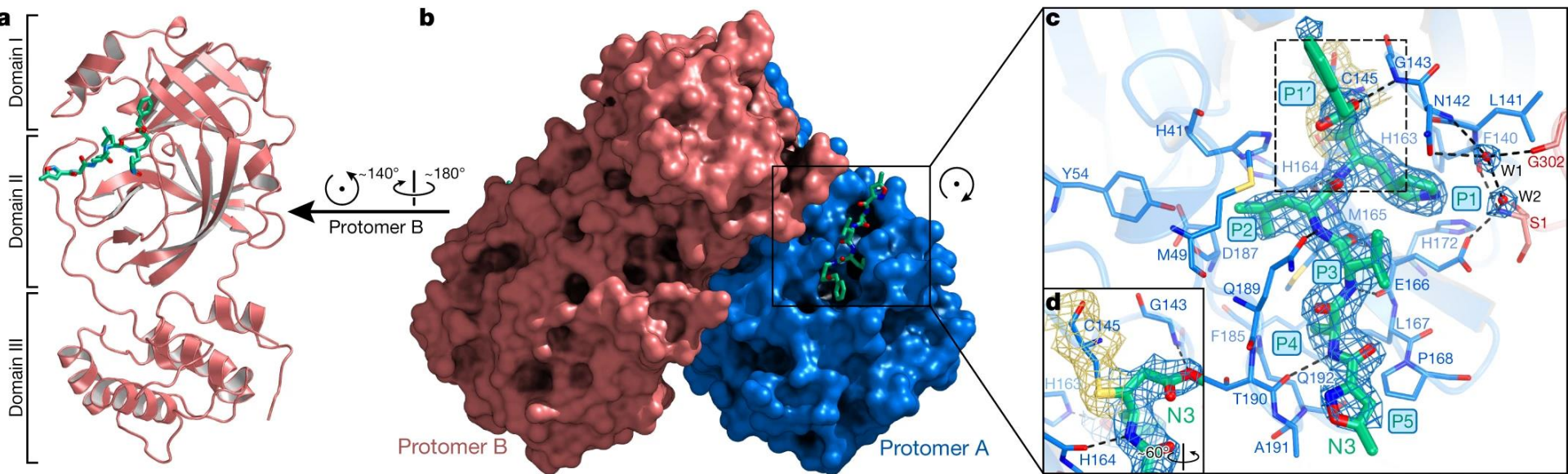


PDB数据库的使用

检索靶点结构



新冠SARS-CoV-2主蛋白酶和抑制剂PF-07321332

检索靶点结构

旧网址: <https://www.uniprot.org/> 新网址: <https://beta.uniprot.org/>



Find your protein

UniProtKB ▾

SARS-CoV-2 main protease

Advanced | List

Search

Examples: Insulin, APP, Human, P05067, organism_id:9606

UniProt is the world's leading high-quality, comprehensive and freely accessible resource of protein sequence and functional information. [Cite UniProt](#)

Accessing UniProt programmatically? Have a look at the new API documentation.

Proteins
UniProt Knowledgebase

Species
Proteomes

Protein Clusters
UniRef

Sequence Archive
UniParc

在不知道靶点其他信息的情况下，可以用靶点名称用此方法检索靶点的所有结构物

检索靶点结构

UniProt BETA BLAST Align Peptide search ID mapping SPARQL UniProtKB SARS-CoV-2 main protease Advanced | List Search Help

Status

- Reviewed (Swiss-Prot) (19)
- Unreviewed (TrEMBL) (4)

Taxonomy

Filter by taxonomy

Proteins with

- 3D structure (8)
- Active site (5)
- Activity regulation (3)
- Alternative products (isoforms) (7)
- Alternative splicing (2)

More items

Protein existence

- Protein level (21)
- Homology (2)

UniProtKB 23 results

BLAST Align Map IDs Download Add View: Table Card Share

P0DTD1 · R1AB_SARS2

Replicase polyprotein 1ab · Severe acute respiratory syndrome coronavirus 2 (2019-nCoV) (SARS-CoV-2) · Gene: rep · 7096 amino acids · Evidence at protein level · **Annotation score: 5/5**

#Endonuclease #Exonuclease #Helicase #Hydrolase #Lyase #Methyltransferase #Nuclease #Nucleotidyltransferase #Protease #RNA-binding #RNA-directed RNA polymerase #Thiol protease #Transferase #Activation of host autophagy by virus #Decay of host mRNAs by virus #Eukaryotic host gene expression shutoff by virus #Eukaryotic host translation shutoff by virus #Host gene expression shutoff by virus #Host mRNA suppression by virus #Host-virus interaction #Inhibition of host innate immune response by virus #Inhibition of host interferon signaling pathway by virus #Inhibition of host IRF3 by virus #Inhibition of host ISG15 by virus #Inhibition of host NF-kappa-B by virus #Inhibition of host RLR pathway by virus #Inhibition of host TBK1 by virus #Inhibition of host TLR pathway by virus #Modulation of host ubiquitin pathway by viral deubiquitinase #Modulation of host ubiquitin pathway by virus #Ubl conjugation pathway #Viral immunoevasion #Viral RNA replication

28 domains · 45 reviewed variants · 19 active sites · 2 isoforms · 120 interactions · 830 3D structures · 22 reviewed publications

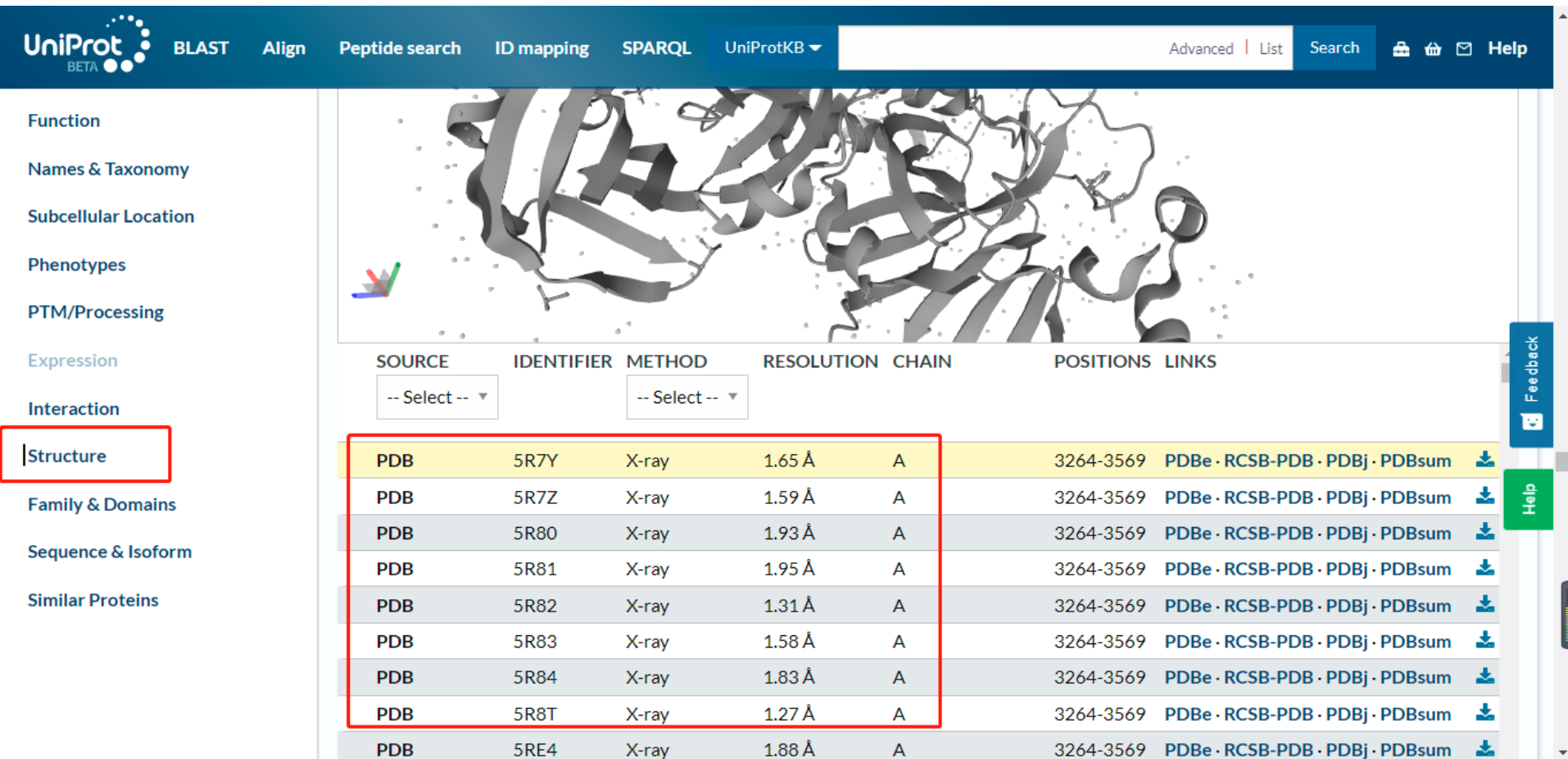
P0DTC1 · R1A_SARS2

Replicase polyprotein 1a · Severe acute respiratory syndrome coronavirus 2 (2019-nCoV) (SARS-CoV-2) · 4405 amino acids · Evidence at protein level · **Annotation score: 5/5**

#Endonuclease #Hydrolase #Nuclease #Protease #RNA-binding #Thiol protease #Activation of host autophagy by virus #Decay of host mRNAs by virus

根据描述，选择第一个即可

检索靶点结构



UniProt BETA BLAST Align Peptide search ID mapping SPARQL UniProtKB Advanced | List Search Help

Function
Names & Taxonomy
Subcellular Location
Phenotypes
PTM/Processing
Expression
Interaction
Structure
Family & Domains
Sequence & Isoform
Similar Proteins

Feedback Help

SOURCE	IDENTIFIER	METHOD	RESOLUTION	CHAIN	POSITIONS	LINKS
-- Select --	-- Select --					
PDB	5R7Y	X-ray	1.65 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R7Z	X-ray	1.59 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R80	X-ray	1.93 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R81	X-ray	1.95 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R82	X-ray	1.31 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R83	X-ray	1.58 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R84	X-ray	1.83 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5R8T	X-ray	1.27 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum
PDB	5RE4	X-ray	1.88 Å	A	3264-3569	PDBe · RCSB-PDB · PDBj · PDBsum

点击左侧“Structure”可以看到所有存在的pdb结构及其信息

检索靶点结构

UniProt BETA BLAST Align Peptide search ID mapping SPARQL UniProtKB Advanced | List Search Help

Function
Names & Taxonomy
Subcellular Location
Phenotypes
PTM/Processing
Expression
Interaction
Structure
Family & Domains
Sequence & Isoform
Similar Proteins

Sequence & Isoformⁱ

[BLAST 2 isoforms](#) [Align 2 isoforms](#)

This entry describes 2 isoformsⁱ produced by **Ribosomal frameshifting**. Normal translation results in Replicase polyprotein 1a. Ribosomal frameshifting at the end of this protein occurs at low frequency and produces Replicase polyprotein 1ab.

P0DTD1-1

This isoform has been chosen as the **canonical** sequence. All positional information in this entry refers to it. This is also the sequence that appears in the downloadable versions of the entry.

Name Replicase polyprotein 1ab **See also** sequence in [UniParc](#) or sequence clusters in [UniRef](#)

Note Produced by -1 ribosomal frameshifting at the 1a-1b genes boundary. [By Similarity](#)

Tools [Download](#) [Add](#) [Highlight](#) [Copy sequence](#)

Length 7,096 **Last updated** 2020-04-22 v1
Mass (Da) 794,058 **Checksumⁱ** A4E62D97150BB8CC

MESLVPGFNE KTHVQLSLPV LQVRDVLVRG FGDSVEEVLS EARQHLKDGT CGLVEVEKGV LPQLEQPYVF IKRSDARTAP HGHVMVELVA

点击左侧“Sequence”可以看到靶点序列

检索靶点结构

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation Careers MyPDB

RCSB PDB PROTEIN DATA BANK

188431 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

PDB-101

WORLDWIDE PDB PROTEIN DATA BANK

EMDataResource Unified Data Resource for XRFM

WORLDWIDE ACID DATABASE

Worldwide Protein Data Bank Foundation

Developers: Join the RCSB

Welcome

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Visualize

Analyze

Download

Learn

A Structural View of Biology

This resource is powered by the Protein Data Bank archive—3D shapes of proteins, nucleic acids, and complex assemblies—so that students and researchers understand all aspects of biomedical research, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and archives

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.



PDB Archive

PF-07321332

in Additional Structure Keywords

SARS-CoV-2, Main protease, PF-07321332, VIRAL PROTEIN

Protease, SARS-CoV-2, covalent complex, inhibitor, HYDROLASE-INHIBITOR complex, Omicron, PF-07321332, HYDROLASE, HYDROLASE-HYDROLASE INHIBITOR complex

, SARS-CoV-2, covalent complex, inhibitor, HYDROLASE-INHIBITOR complex, Omicron, nirmatrelvir, PF-07321332, HYDROLASE, HYDROLASE-HYDROLASE INHIBITOR complex

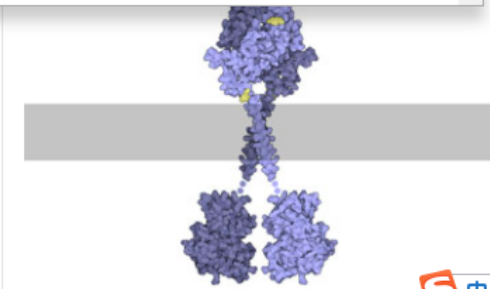
covalent complex, inhibitor, HYDROLASE-INHIBITOR complex, mutant, Omicron, P132H, nirmatrelvir, PF-07321332, HYDROLASE, HYDROLASE-HYDROLASE INHIBITOR complex

in Structure Title

Structure of the SARS-CoV-2 main protease in complex with inhibitor PF-07321332

Room temperature X-ray structure of SARS-CoV-2 main protease (Mpro) in complex with PF-07321332

Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332



可以利用已知的靶点信息在PDB数据库检索 (PDB ID、作者、配体等)

检索靶点结构

SCIENTIFIC NAME OF SOURCE ORGANISM

Severe acute respiratory syndrome coronavirus 2 (11)

TAXONOMY

Riboviria (11)

EXPERIMENTAL METHOD

X-RAY DIFFRACTION (11)
 NEUTRON DIFFRACTION (1)

POLYMER ENTITY TYPE

Protein (11)

REFINEMENT RESOLUTION (Å)

1.5 - 2.0 (8)
 2.0 - 2.5 (4)

RELEASE DATE

2020 - 2024 (11)

ENZYME CLASSIFICATION NAME

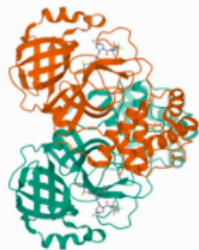
Hydrolases (11)
 Transferases (7)

SYMMETRY TYPE

1 to 11 of 11 Structures

Page 1 of 1 25

Sort by ↓ Score



3D View

7VH8

Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332

Zhao, Y., Zhang, Q., Yang, H., Rao, Z.

(2021) Protein Cell

Released 2021-11-03
Method X-RAY DIFFRACTION 1.59 Å
Organisms Severe acute respiratory syndrome coronavirus 2
Macromolecule 3C-like proteinase (protein)
Unique Ligands 4WI, DMS, H2S

Download File View File



3D View

7SI9

Room temperature X-ray structure of SARS-CoV-2 main protease (Mpro) in complex with PF-07321332

Kovalevsky, A., Kneller, D.W., Coates, L.


(2022) Res Sq

Released 2021-10-20
Method X-RAY DIFFRACTION 2 Å
Organisms Severe acute respiratory syndrome coronavirus 2
Macromolecule 3C-like proteinase (protein)
Unique Ligands 4WI

Download File View File

检索靶点结构

Biological Assembly 1 ?



1 **7VH8**
Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332

2 **PDB DOI: 10.2210/pdb7VH8/pdb**

3 **Classification: VIRAL PROTEIN**
Organism(s): Severe acute respiratory syndrome coronavirus 2
Expression System: Escherichia coli BL21(DE3)

4 **Mutation(s): No**

5 **Deposited: 2021-09-21 Released: 2021-11-03**
Deposition Author(s): Zhao, Y., Zhang, Q., Yang, H., Rao, Z.

6 **Funding Organization(s): National Natural Science Foundation of China (NSFC)**

Experimental Data Snapshot

7 **Method: X-RAY DIFFRACTION**
Resolution: 1.59 Å
R-Value Free: 0.204
R-Value Work: 0.184
R-Value Observed: 0.185

wwPDB Validation **3D Report** **Full Report**

Metric	Percentile Ranks	Value
Rfree		0.195
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		4.9%

8 **3D View: Structure | 1D-3D View | Electron Density | Validation Report | Ligand Interaction**


Global Symmetry: Cyclic - C2 (3D View)
Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

1. PDB ID, 4位: 0-9数字+A-Z字母组合, 每个蛋白序列唯一, 因解析方法、实验条件、实验操作等不同可有不同ID

检索靶点结构

Biological Assembly 1 ?



1 **7VH8**
Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332

2 **PDB DOI: 10.2210/pdb7VH8/pdb**

3 **Classification: VIRAL PROTEIN**
Organism(s): Severe acute respiratory syndrome coronavirus 2
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Global Symmetry: Cyclic - C2 (3D View)
Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

2.关于该结构文献的doi

3.物种来源

4.该结构是否有突变

5.解析日期

检索靶点结构

Biological Assembly 1 ?

1 **7VH8**

Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332

2 **PDB DOI: 10.2210/pdb7VH8/pdb**

Classification: **VIRAL PROTEIN**

3 **Organism(s): Severe acute respiratory syndrome coronavirus 2**

Expression System: Escherichia coli BL21(DE3)

4 **Mutation(s): No**

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Experimental Data Snapshot

7 **Method: X-RAY DIFFRACTION**

Resolution: 1.59 Å

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8 **3D View: Structure | 1D-3D View | Electron Density | Validation Report | Ligand Interaction**

Global Symmetry: Cyclic - C2 (3D View)

Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Display Files Download Files

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.195
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		4.9%

Worse Better

■ Percentile relative to all X-ray structures

□ Percentile relative to X-ray structures of similar resolution

6.解析作者

7.解析方法和分辨率：2.5 Å以下，越小解析结构越精确

8.查看三维结构

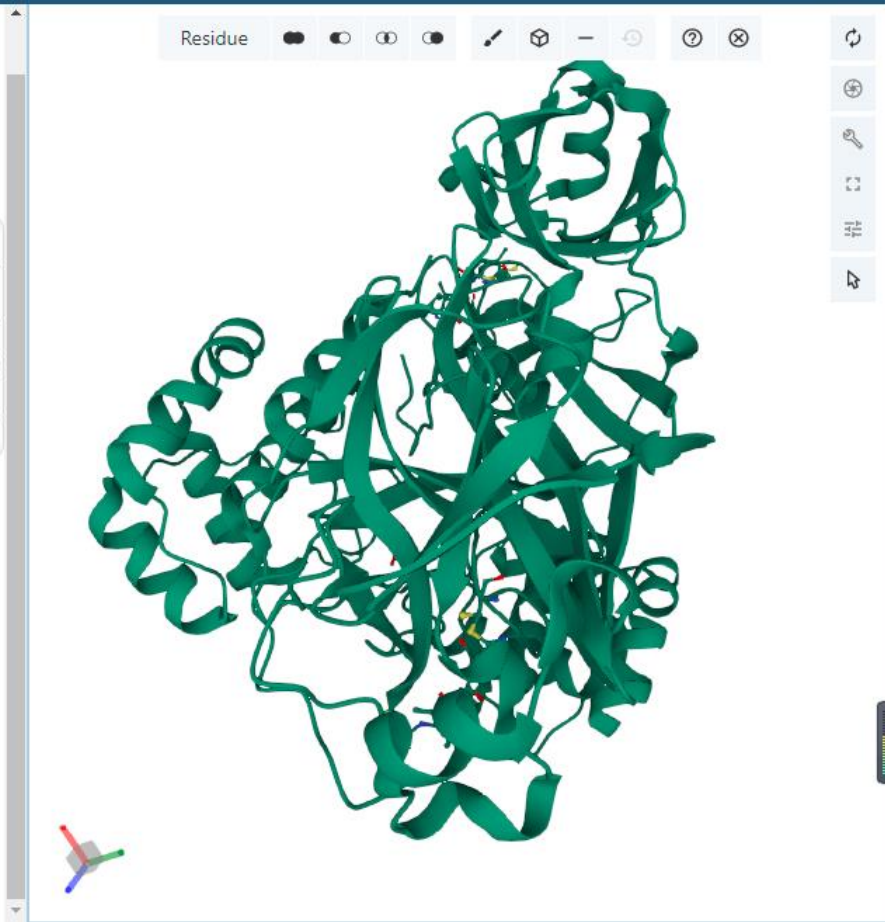
检索靶点结构

Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332

Chain: A Symmetry Partner: 1 (ASM...)

3C-like proteinase - Severe acute respiratory syndrome coronavirus 2

Help



检索靶点结构

Literature

Download Primary Citation ▾

Crystal structure of SARS-CoV-2 main protease in complex with protease inhibitor PF-07321332.

[Zhao, Y.](#), [Fang, C.](#), [Zhang, Q.](#), [Zhang, R.](#), [Zhao, X.](#), [Duan, Y.](#), [Wang, H.](#), [Zhu, Y.](#), [Feng, L.](#), [Zhao, J.](#), [Shao, M.](#), [Yang, X.](#), [Zhang, L.](#), [Peng, C.](#), [Yang, K.](#), [Ma, D.](#), [Rao, Z.](#), [Yang, H.](#)
(2021) Protein Cell

PubMed: [34687004](#) [Search on PubMed](#)

[Search on PubMed Central](#)

DOI: [10.1007/s13238-021-00883-2](#)

Primary Citation of Related Structures:

[7VH8](#)

关于该结构文献的信息显示

检索靶点结构

Macromolecules

Find similar proteins by: Sequence ▾ (by identity cutoff) | [3D Structure](#)

Entity ID: 1

Molecule	Chains ⓘ	Sequence Length	Organism	Details	Image
3C-like proteinase	A	306	Severe acute respiratory syndrome coronavirus 2	Mutation(s): 0 ⓘ EC: 3.4.22.69 (PDB Primary Data), 3.4.19.12 (UniProt), 3.4.22 (UniProt)	

UniProt

Find proteins for [P0DTC1](#) (*Severe acute respiratory syndrome coronavirus 2*)

Explore [P0DTC1](#) ⓘ

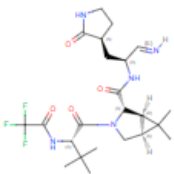

Go to UniProtKB:

[P0DTC1](#)

该蛋白的信息，分子名称，链，序列长度，突变信息等每个蛋白质的氨基酸序列唯一，序列号唯一，可因科学家和实验条件等不同，解析出不同PDB ID的蛋白结构，两个网站可互通访问。

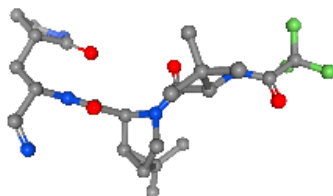
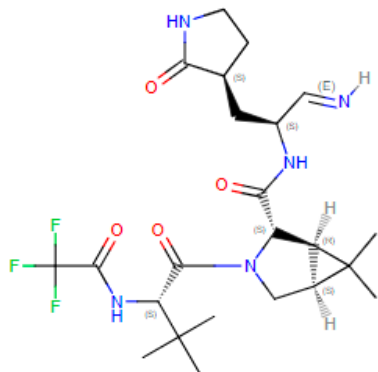
检索靶点结构

Ligands 3 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
4WI (Subject of Investigation/LOI) Query on 4WI Download Ideal Coordinates CCD File Download Instance Coordinates	B [auth A]	(1R,2S,5S)-N-((1E,2S)-1-imino-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl)-6,6-dimethyl-3-[3-methyl-N-(trifluoroacetyl)-L-valyl]-3-azabicyclo[3.1.0]hexane-2-carboxamide C ₂₃ H ₃₄ F ₃ N ₅ O ₄ WDVIRQQKRMIXGS-XIFHJVQQSA-N		Ligand Interaction
DMS Query on DMS Download Ideal Coordinates CCD File Download Instance Coordinates	C [auth A]	DIMETHYL SULFOXIDE C ₂ H ₆ O S IAZDPXIOMUYVGZ-UHFFFAOYSA-N		Ligand Interaction
H2S Query on H2S Download Ideal Coordinates CCD File Download Instance Coordinates	D [auth A]	HYDROSULFURIC ACID H ₂ S RWSOTUBLDIXVET-UHFFFAOYSA-N	H₂S	Ligand Interaction

该结构所含配体分子的信息

检索靶点结构



4WI

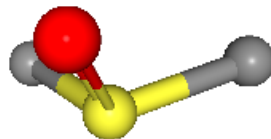
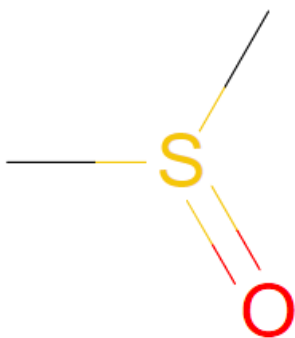
[View / Download Files](#)

(1R,2S,5S)-N-((1E,2S)-1-imino-3-[(3S)-2-oxo pyrrolidin-3-yl]propan-2-yl)-6,6-dimethyl-3-[3-methyl-N-(trifluoroacetyl)-L-valyl]-3-azabicyclo[3.1.0]hexane-2-carboxamide

Find entries where: 4WI

as a non-polymer is covalently linked to polymer or other heterogen groups **8 entries**

Find related ligands:



DMS

[View / Download Files](#)

DIMETHYL SULFOXIDE

Find entries where: DMS

is present as a standalone ligand in **3211 entries**

as a non-polymer is covalently linked to polymer or other heterogen groups **3 entries**

Find related ligands:

[Similar Ligands \(Stereospecific\)](#)

[Similar Ligands \(including Stereoisomers\)](#)

活性残基分析

活性位点关键氨基酸残基分析

<https://www.mrc-lmb.cam.ac.uk/rajini/index.html>

Protein Contacts Atlas

Home

Advanced Features ▾

About ▾

Contact

Protein Contacts Atlas

Structural insights through visualization and analysis of non-covalent contacts

Examine a protein structure

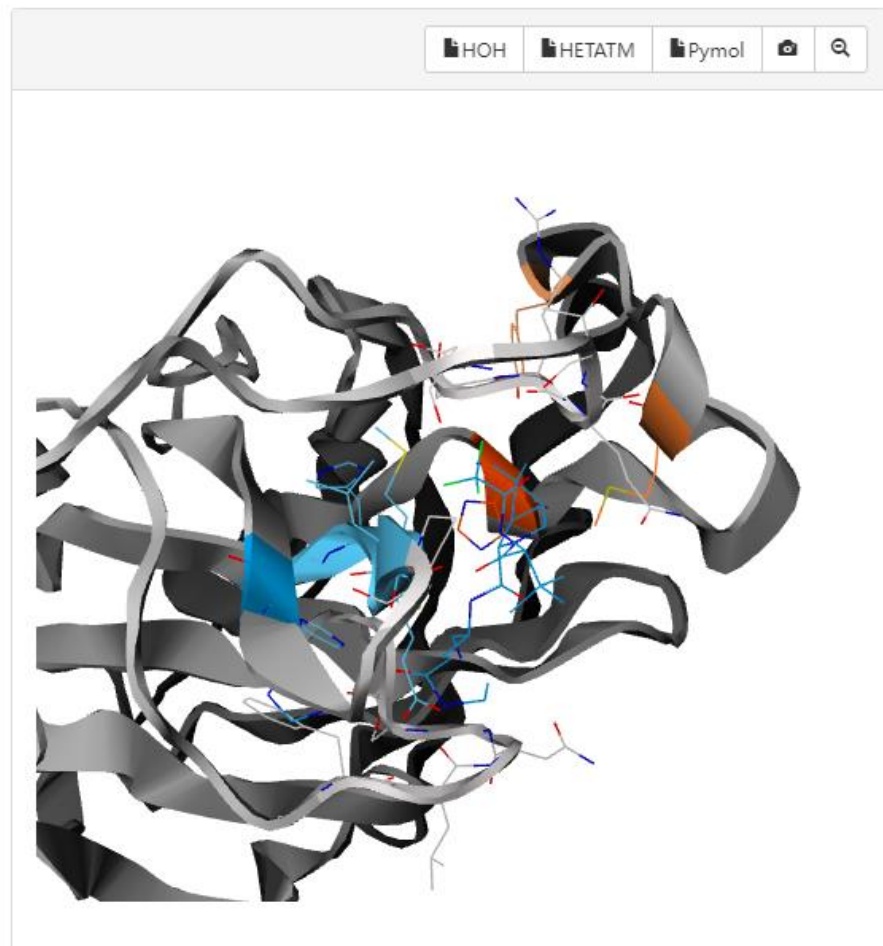
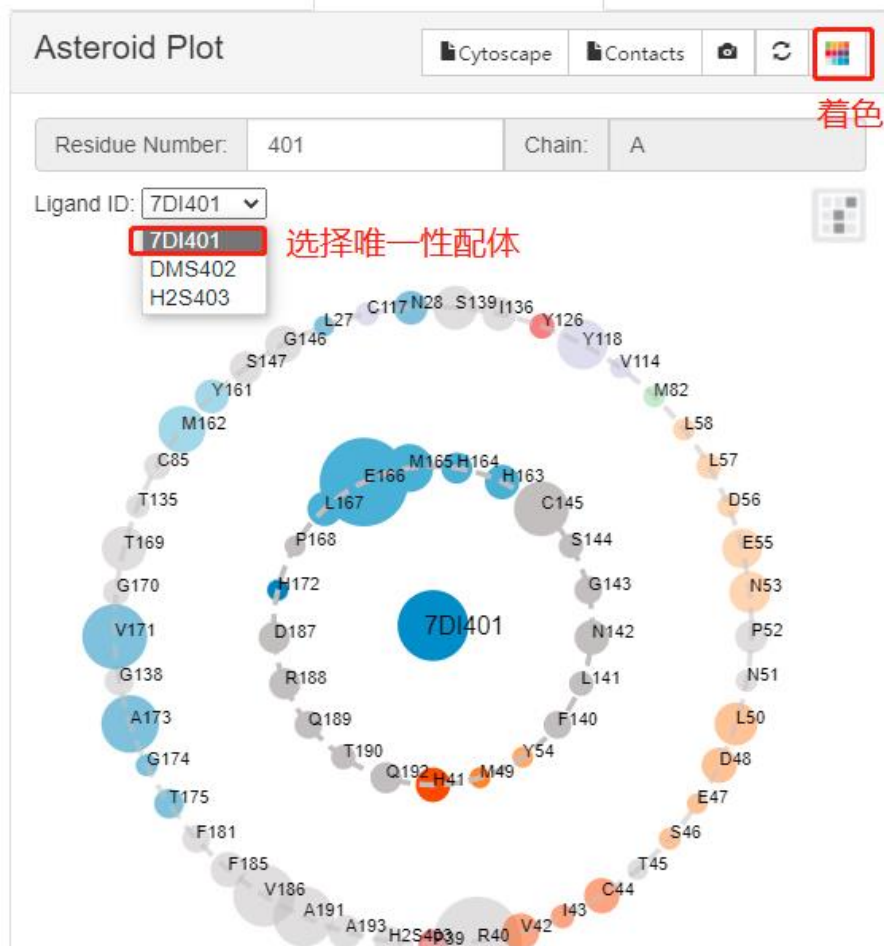
PDB ID (crystal structures only)

Process structure!

(Examples: [3SN6](#), [2HPY](#), [1QNE](#))

以主蛋白酶为例，7VH8、7QBB、5RHC

活性残基分析



7VH8

活性位点检测

靶点蛋白的活性位点预测



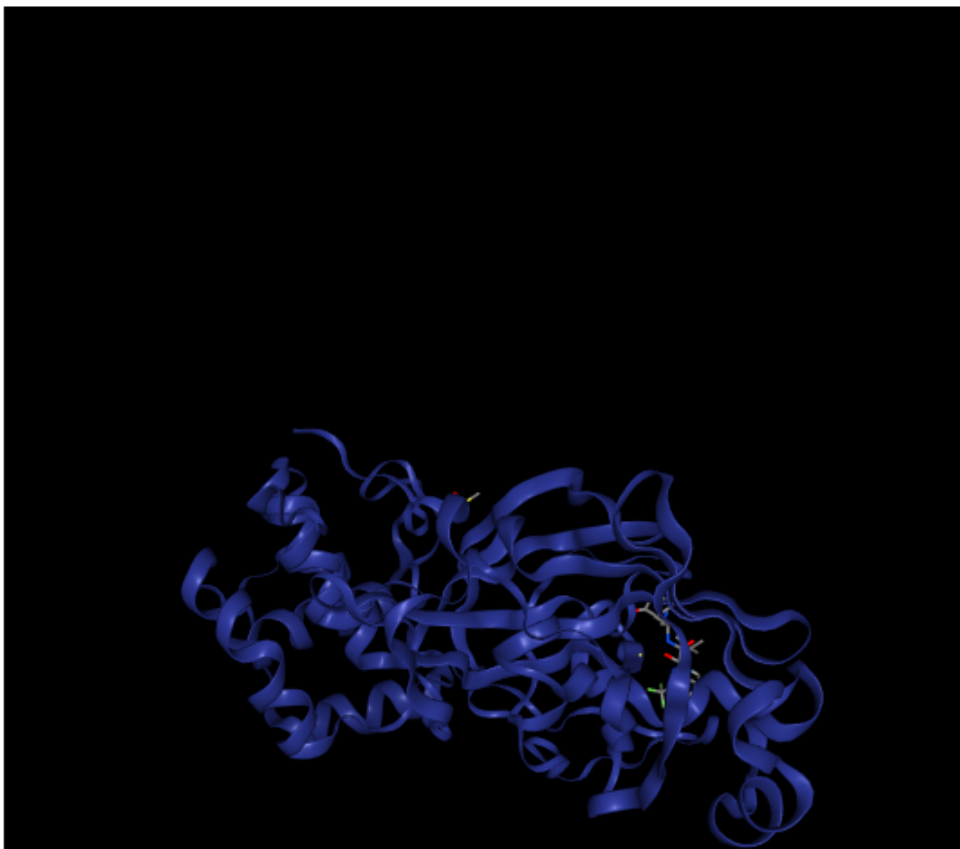
PDB-Code (PDB Database) or UniProt accession number (AlphaFold Database) or search term:

⊕ Upload Protein (PDB format): 未选择文件

⊕ Upload Ligand (SDF format): 未选择文件

[Advanced search](#)

活性位点检测



Ligands Pockets

Ligands

7DI_A_401

[create pocket](#)

DMS_A_402

Protoss Hydrogen prediction

[DoGSiteScorer Binding site detection](#)

DoGSiteScorer is a grid-based method which utilises binding pockets - solely based on the 3D structure. Global properties, describing the size, shape (sub)pockets are calculated. Per default, a simple (sub)pocket, based on a linear combination of accessibility and enclosure. Furthermore, a subset of support vector machine (libsvm) to predict the (score zero and one). The higher the score the more druggable.

1. A. Volkamer, D. Kuhn, T. Grombacher, F. Rippl, *Protein Structure* for structure-based druggability prediction

[DoGSiteScorer](#)

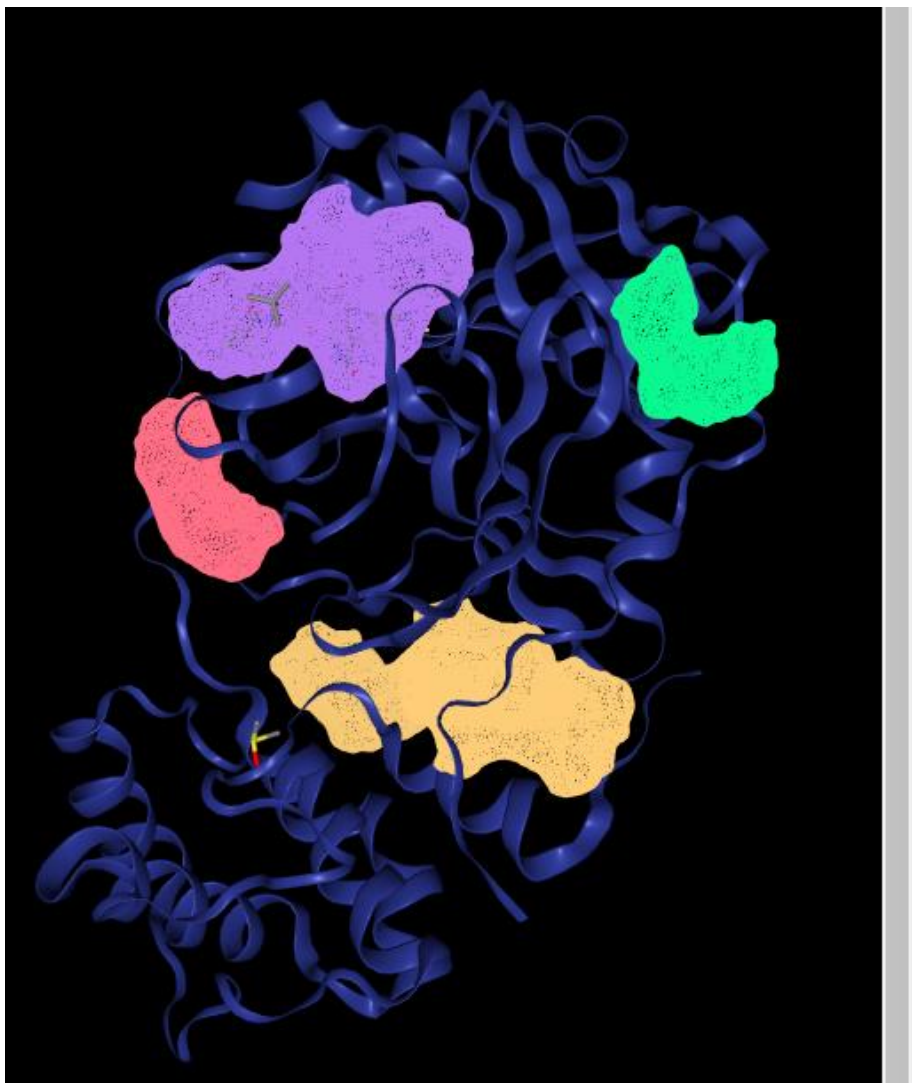
[PoseView 2D interaction diagrams](#)

[SIENA Structure ensemble assembly](#)


[HyPPI Protein-protein interactions classification](#)

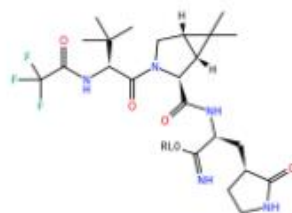
点击 calculate


活性位点检测



Ligands


7DI_A_401 



create pocket 

DMS_A_402 


















create pocket 

DoGSiteScorer is a grid-based method which uses a Difference binding pockets - solely based on the 3D structure of the prote

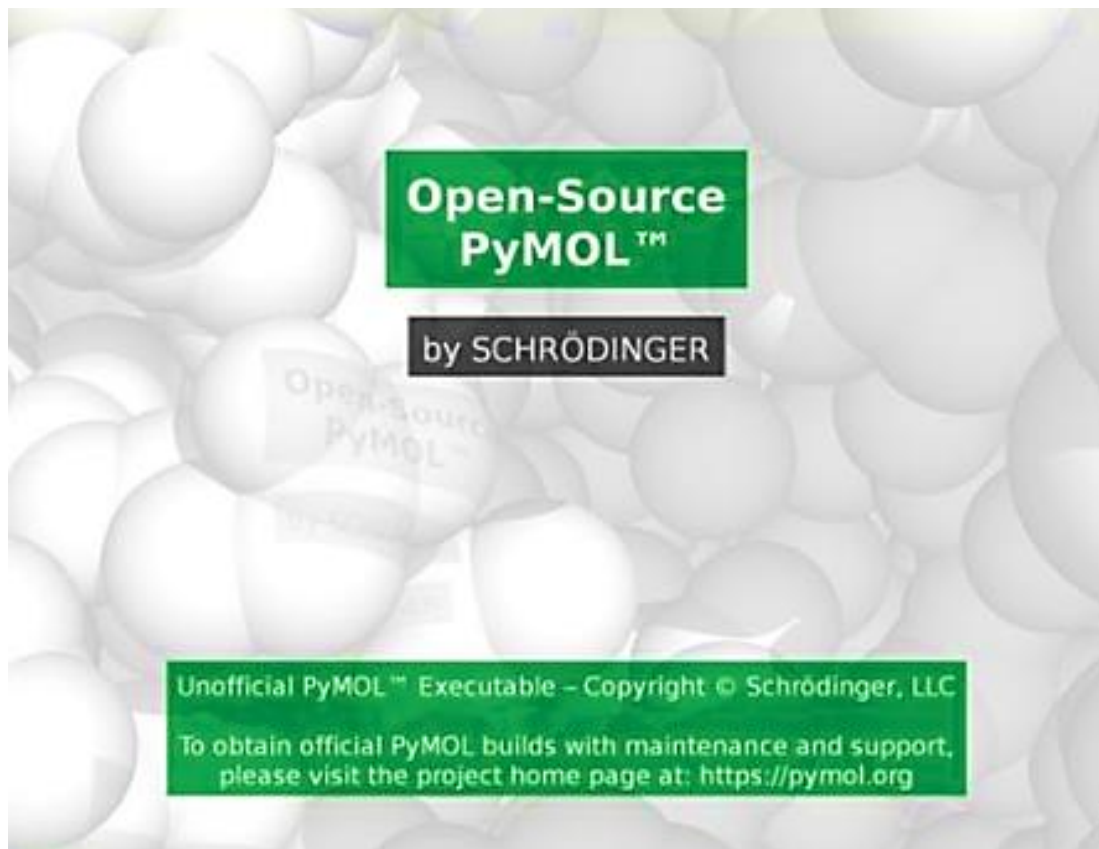
Result

Click on the plus to see your selected parameters: 

Show entries

		Name 	Volume Å ³ 	Sur-face Å ² 	D
		P_0	736.0	1120.98	0
		P_1	630.53	675.28	0
		P_2	240.19	442.82	0
		P_3	160.26	380.18	0
		P_4	143.04	243.73	0

PyMol的介绍与使用



PyMol介绍

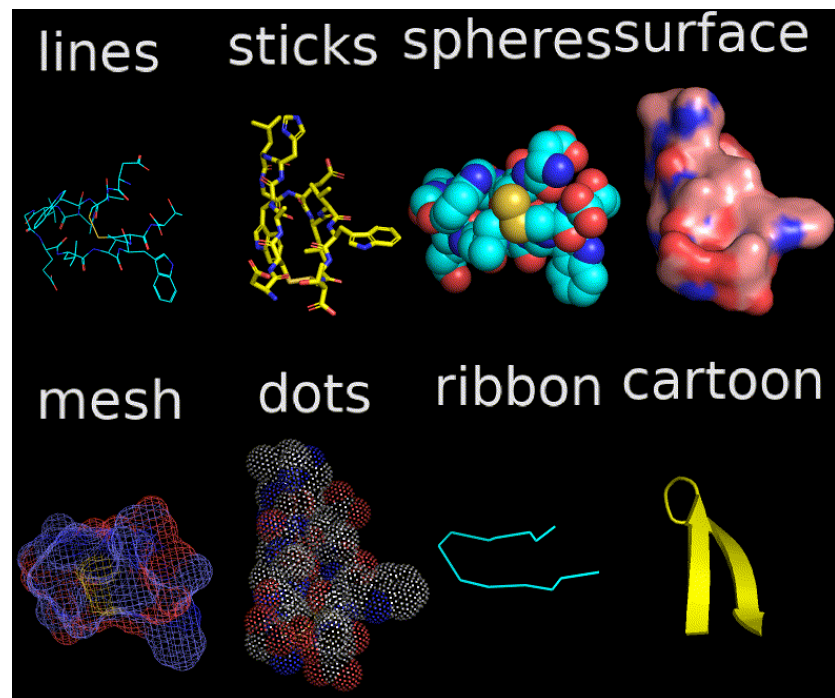
“Py” ----python, 该软件
基于此计算机语言

“Mol” ----molecule, 该
软件是用来显示分子结构

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

比对结构、光线追踪, 探
测静电力学、测距、动画
制作等



PyMol下载

网址: <https://pymol.org/edu/>

Schrödinger为教师、高中生和大学生免费
提供仅供教育使用的PyMOL构建

Registration For Educational-Use-Only PyMOL Builds

Schrödinger offers **Educational-use-only** PyMOL builds available at no cost to **teachers and high school and college students** (including online courses, homeschooling, etc.) for classroom instruction, homework assignments, and to provide a means for creating high quality figures. Please note that it is not provided for the purposes of academic research or publication.

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I am a:

Your First Name:

Your Last Name:

Your Email Address:

Your Telephone Number:

Institution:

Comments (optional):

Degree:

Subject Matter:

Name of Your Advisor or Instructor:

Anticipated Award Year:

Download Educational-Use-Only PyMOL

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PyMOL Executable Builds for Educational Use Only

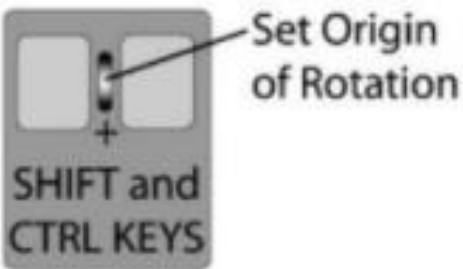
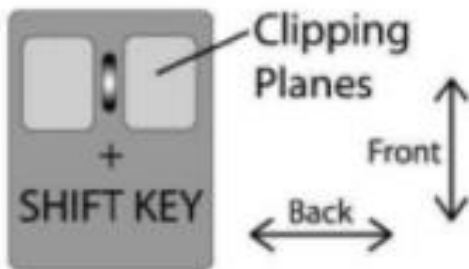
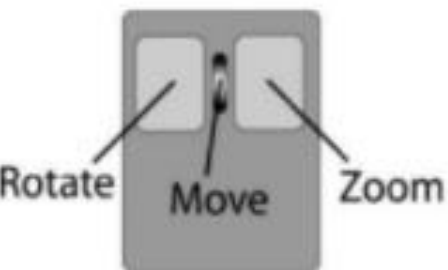
The Educational-use-only PyMOL builds are provided "AS IS" with no obligation to grant download access, fix bugs, furnish updates, provide documentation, or meet any other need related to the educational-use PyMOL builds. Purchased [PyMOL Academic Subscriptions](#) with up to three years of maintenance are available to meet your longer-term educational use needs.

PyMOL 2.0 (September 2017)

License File: [pymol-edu-license.lic](#)

Installers: [PyMOL Download Page](#)

PyMol基本操作



The screenshot displays the PyMOL software interface. The top menu bar includes File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, and Help. The main window is titled "PyMOL" and contains a command line with the following text:

```
Detected GLSL version 4.60.  
OpenGL graphics engine:  
GL_VENDOR: NVIDIA Corporation  
GL_RENDERER: GeForce 6200  
GL_VERSION: 4.1.0 NVIDIA 310.10.06  
License Expiry date: 01-oct-2022  
Detected 4 CPU cores. Enabled multithreaded rendering.
```

The interface is divided into two main sections:

- External GUI:** The top right corner features a toolbar with buttons for Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, Stop, Play, MCLear, Builder, Properties, Rebuild, Undo, and Redo.
- Internal GUI:** The main area displays "Edu PyMOL v2.x" with the URL <http://pymol.org/educational>. Below this is a large "Viewer" label and a molecular structure. The text reads: "Schrödinger offers Educational-use-only PyMOL builds available at no cost to teachers and high school and college students for classroom instruction, homework assignments, and to provide a means for creating high quality figures. It is not provided for the purposes of academic research or publication. There is no technical support from Schrödinger for 'Edu' PyMOL, please use the pymol-users mailing list if you need help. Licenses for academic: <http://pymol.org/academic> Licenses for industry: <http://pymol.org/contact> SCHROEDINGER."

The bottom right corner shows a "Mouse Mode 3-Button Viewing" table:

Buttons	L	M	R	Wheel
& Keys	Rota	Move	MovZ	Slab
Shft	+Box	-Box	Clip	MovS
Ctrl	Move	PkAt	Pk1	MvSZ
CtSh	Sele	Orig	Clip	MovZ
SngrClk	+/-	Cent	Menu	
Db1Clk	Menu	-	PkAt	
Selecting Residues				
State	1/	1		

The bottom status bar shows "PyMOL>_" and navigation icons.

PyMol界面介绍

The screenshot displays the PyMOL interface with several key components:

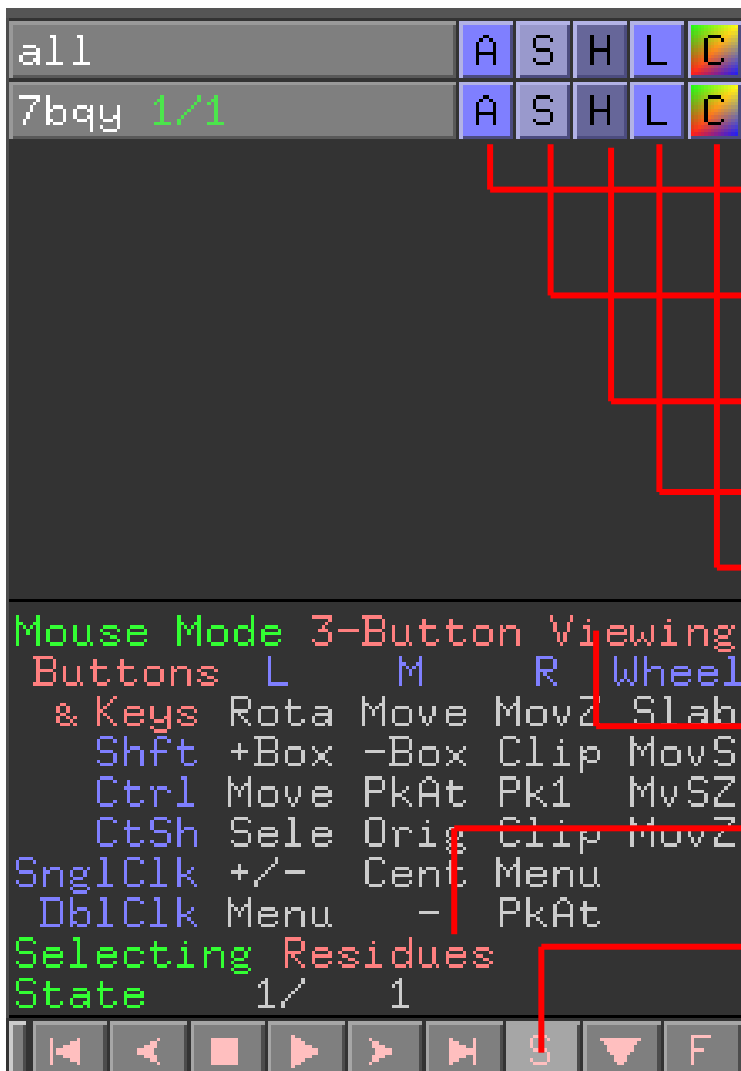
- Command Line:** Located at the top left, it contains a list of compound information. A red box highlights the text: `COMPND 6 EC: 3.4.22.69;`, `COMPND 7 ENGINEERED: YES;`, `COMPND 8 MOL_ID: 2;`, `COMPND 9 MOLECULE: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N~1~-`, `COMPND 10 ((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE;`, `COMPND 11 YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE;`, `COMPND 12 CHAIN: C;`, and `COMPND 13 ENGINEERED: YES`. A red arrow points to this area with the text "命令行或其他控制操作的进程显示屏幕".
- Input Line:** Below the command line, a red box highlights the input field containing the sequence: `/7bqy//A/1 6 11 16 21 26 31 36 41 46 51 all`. A red arrow points to this area with the text "输入pymol命令行".
- Protein Structure:** The main 3D view shows a protein structure rendered in green ribbon representation. A red box highlights the sequence `SGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDVVCPRHVICTSEDMLNP` in the sequence viewer below the input line. A red arrow points to this area with the text "氨基酸残基序列, 以及其他杂分子序列".
- Control Panels:** On the right side, there are several panels including "Reset", "Zoom", "Orient", "Draw/Ray", "Unpick", "Deselect", "Rock", "Get View", "Builder", "Properties", "Rebuild", "Undo", and "Redo". At the bottom right, there is a "Mouse Mode 3-Button Viewing" panel with various keyboard shortcuts and a "Selecting Residues" panel with a red box around the "S" button.

命令行或其他控制操作的进程显示屏幕

输入pymol命令行

氨基酸残基序列, 以及其他杂分子序列

PyMol界面介绍



Action:对目标对象进行特定操作

Show:显示目标对象的特定样式

Hide:隐藏目标对象的特定样式

Label:调整目标对象的标注

Color:调整目标对象的颜色

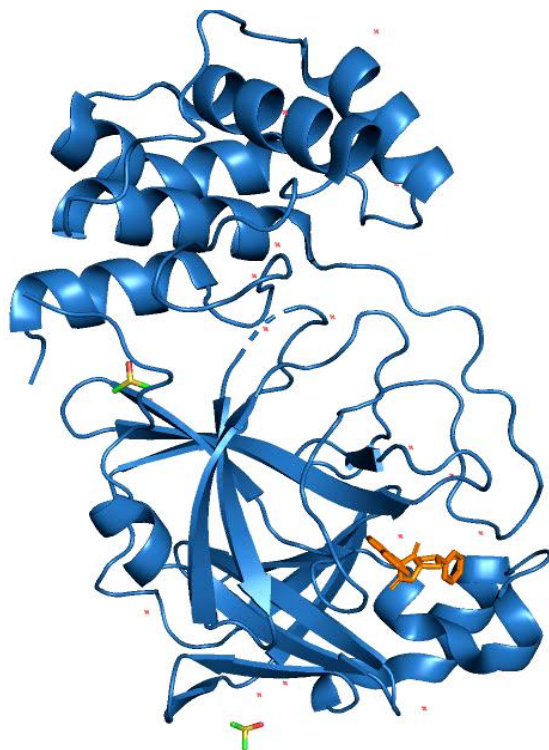
单击可变换鼠标模式: viewing/editing

单击可切换选择模式

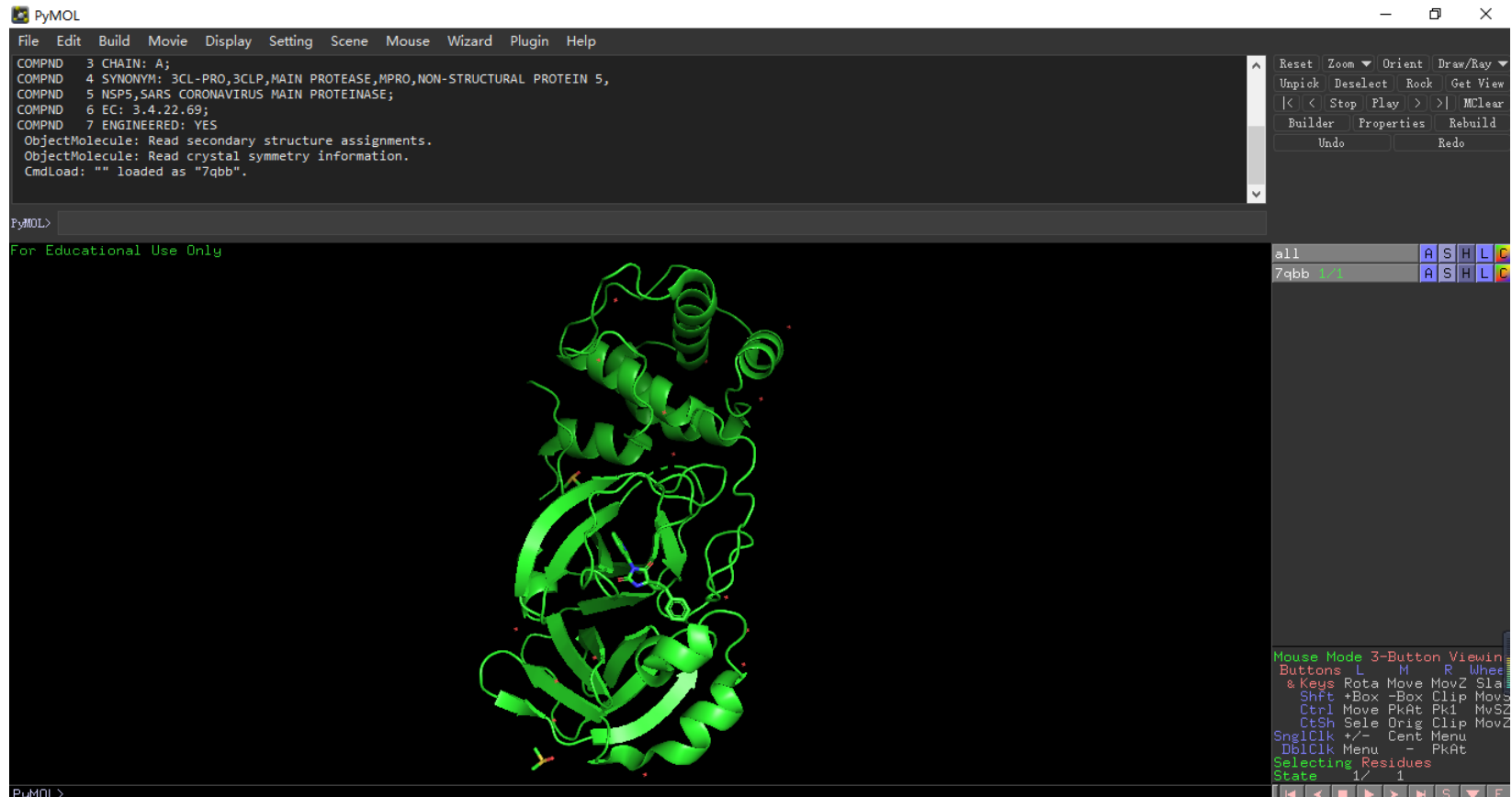
单击显示序列信息

PyMol实践一

简易动画制作

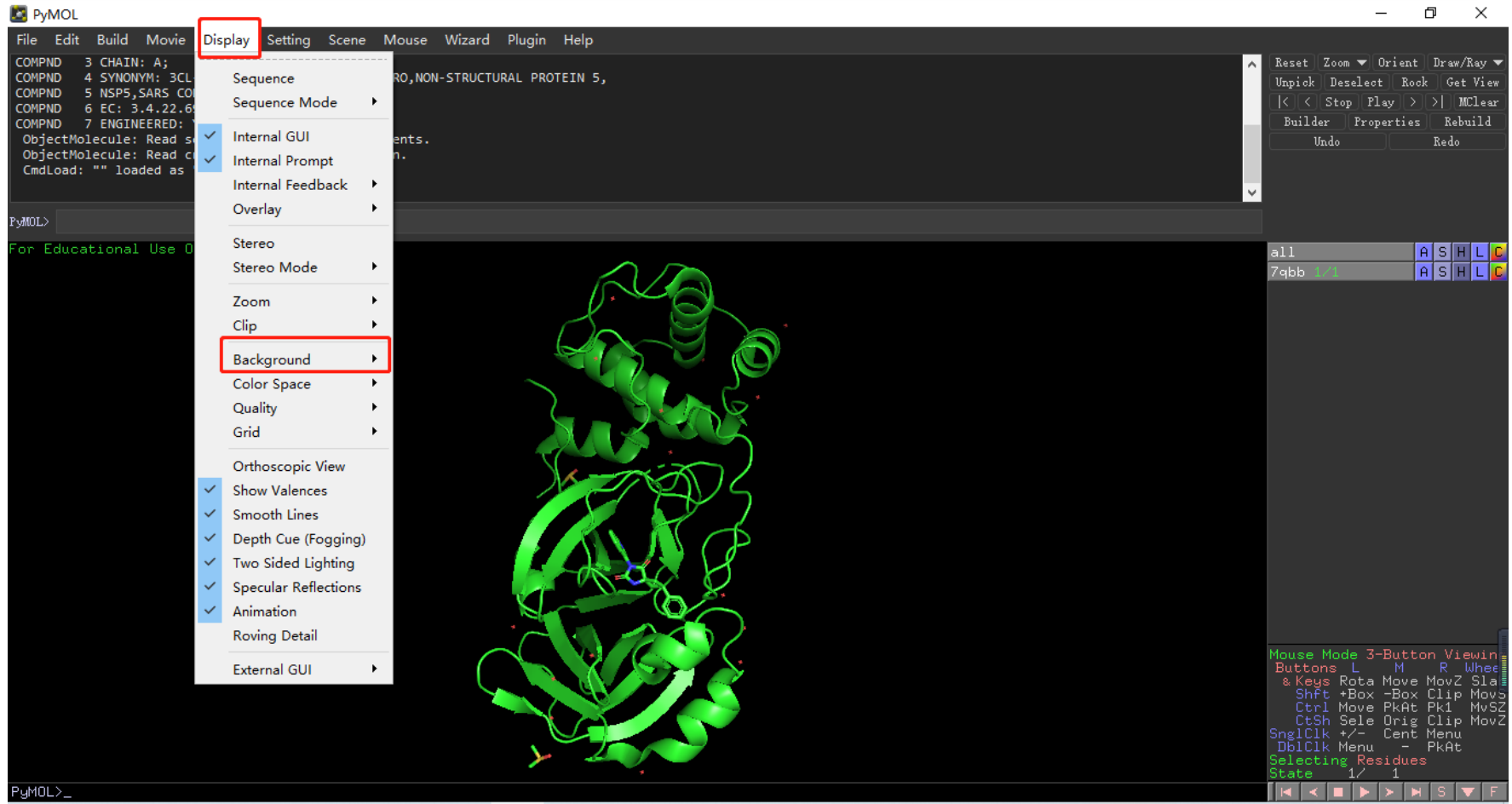


简易动画制作



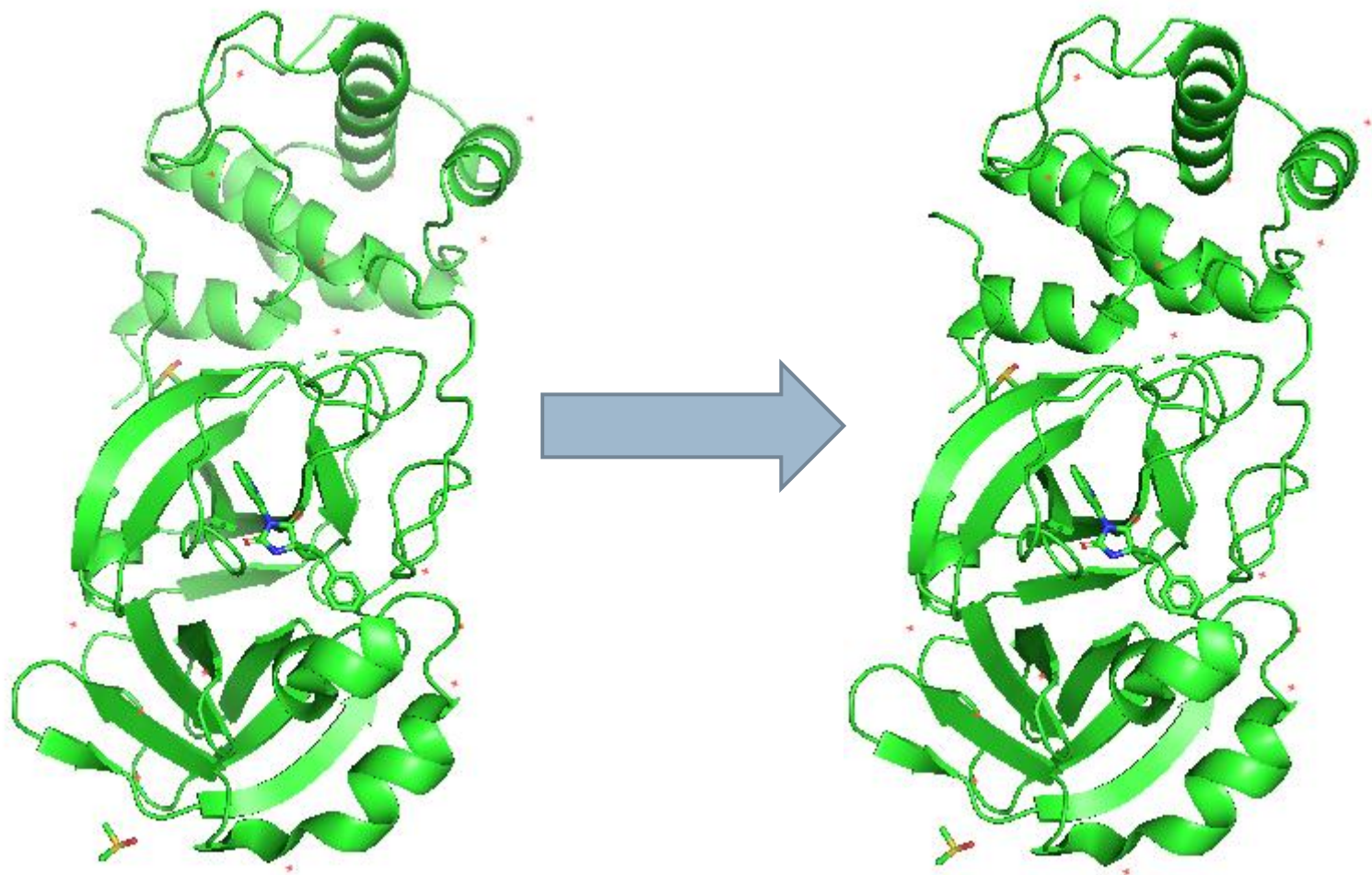
①用pymol打开SARS-CoV-2酶的晶体结构7qbb.pdb
或者直接在pymol的命令框中输入 `fetch 7qbb`

简易动画制作



②将背景设置为白色， Display>Background>white
或者在命令行输入 bg white

简易动画制作



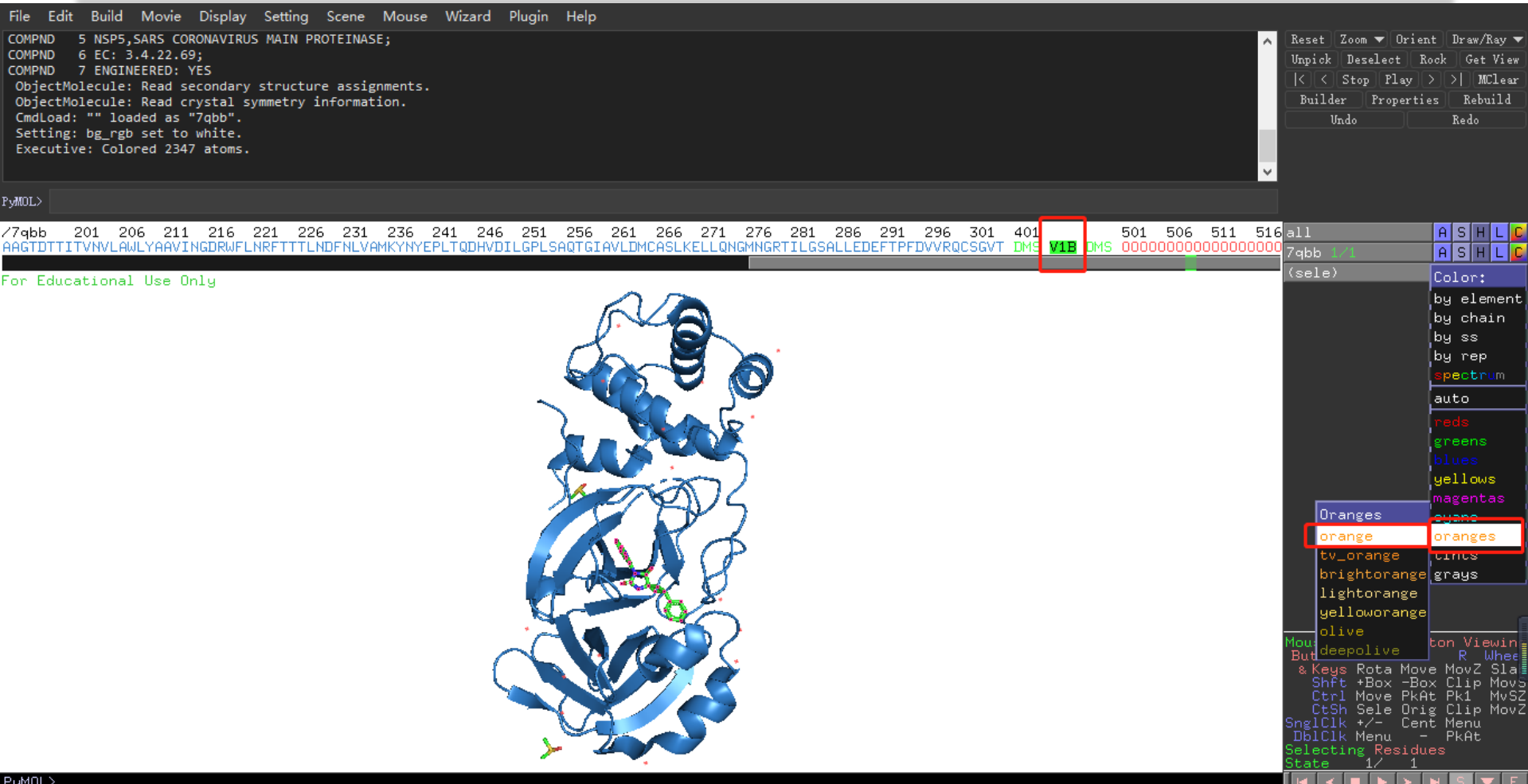
③滚动鼠标滑轮，关闭景深效果，可以看到上图的变化

简易动画制作

The screenshot displays the PyMOL software interface. The top menu bar includes File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, and Help. The main window shows a protein structure rendered in green and pink. The sequence editor at the bottom is open, showing the amino acid sequence: `AGTDTITVNVLAWLYAAVINGDRWFLNRFITLNDNFNVAMKYNVEPLTQDHVDLGLPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALEDEFTPFDFVVRQCSGVI`. A red box highlights this sequence, and a red '2' is placed above it. The right sidebar contains a toolbar with buttons like Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rook, Get View, Stop, Play, MClear, Builder, Properties, Rebuild, Undo, and Redo. Below the toolbar is a color selection menu with a 'Color:' dropdown. The 'skyblue' option is selected and highlighted with a red box, and a red '4' is placed to its left. At the bottom right, the 'Selecting Residues' section shows 'State 1/ 1' with a red box around the '1' and a red '1' next to it. The bottom status bar shows 'PyMOL>_'. The text 'For Educational Use Only' is visible in the bottom left of the main window.

④打开序列 (S) 选中所有氨基酸残基序列 (不包括溶剂和其他小分子), 将颜色设置为skyblue

简易动画制作



The screenshot displays the PyMOL molecular visualization software. The main window shows a blue ribbon representation of a protein structure. The command line at the bottom left shows the sequence editor with the residue 'V118' highlighted in orange. The right-hand panel shows the 'Color' menu with 'orange' selected. The top menu bar includes File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, and Help. The status bar at the bottom indicates 'State 1/ 1'.

⑤ 点击空白处，取消上一步的选择，然后在序列上仅选择抑制剂配体VBI，将颜色设置为orange

简易动画制作

The screenshot displays the PyMOL molecular visualization software interface. The main window shows a blue ribbon representation of a protein structure. The command line at the bottom left contains the text `PyMOL> mplay`, with the `mplay` command highlighted by a red box. The top right corner features a toolbar with buttons for `Reset`, `Zoom`, `Orient`, `Draw/Ray`, `Unpick`, `Deselect`, `Rock`, `Get View`, `Builder`, `Properties`, `Rebuild`, `Undo`, and `Redo`. The bottom right corner shows a mouse control panel with various buttons and a keyboard shortcuts table. The status bar at the bottom indicates `Frame 1 / 240 State 1`.

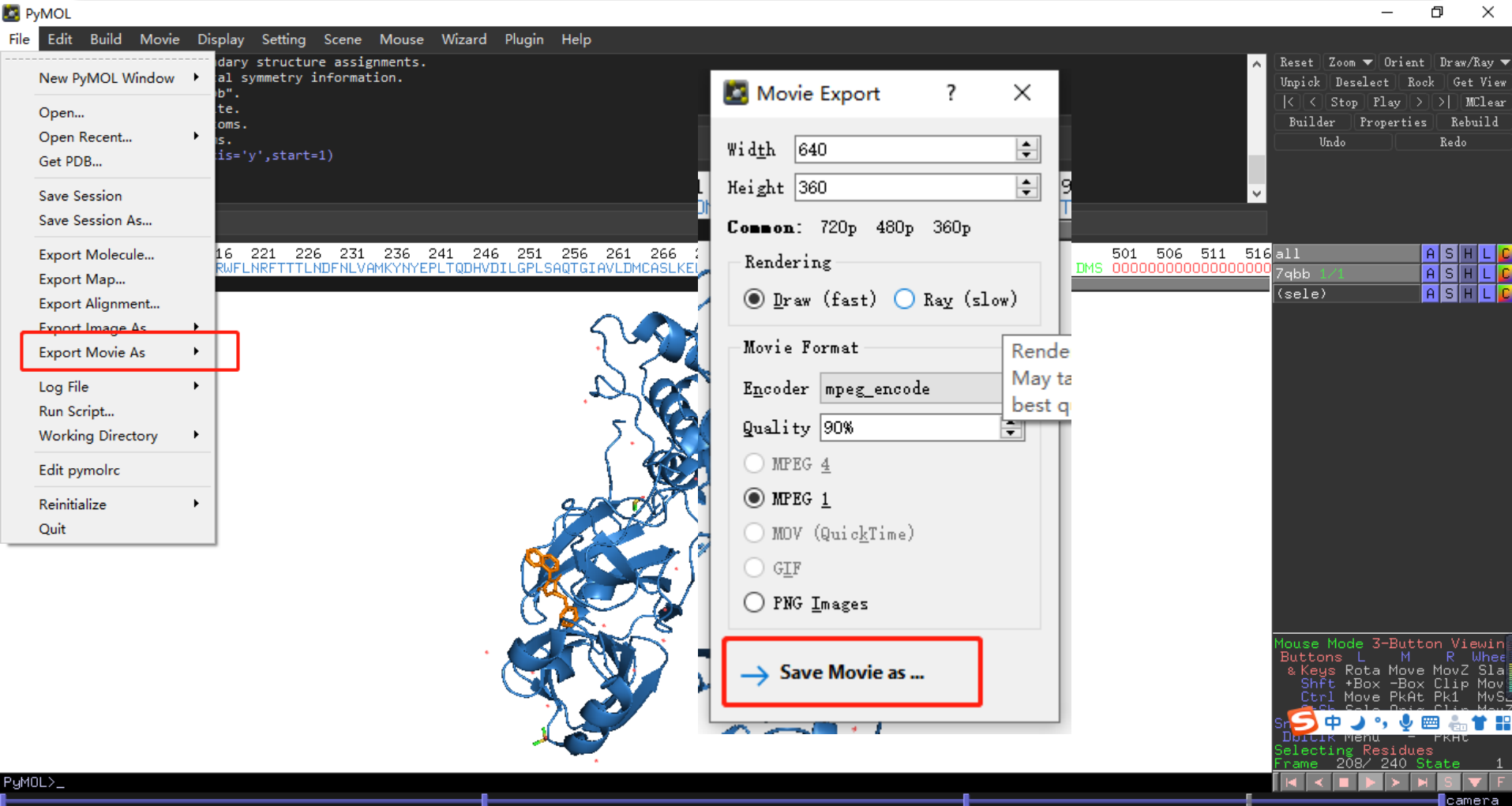
```
COMPND 7 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "7qbb".
Setting: bg_rgb set to white.
Executive: Colored 2347 atoms.
Executive: Colored 26 atoms.
PyMOL>movie.add_roll(8.0,axis='y',start=1)

PyMOL> mplay

/7qbb 201 206 211 216 221 226 231 236 241 246 251 256 261 266 271 276 281 286 291 296 301 401 501 506 511 516
AAGTDTTITVNVLAWLYAAVINGDRWFLNRFTTTLNDFNLVAMKYNNEPLTQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFVDVVRQCSTV DMS V1B DMS 00000000000000000000
For Educational Use Only
```

⑦播放动画，在命令框中输入mplay 回车，即可以预看动画

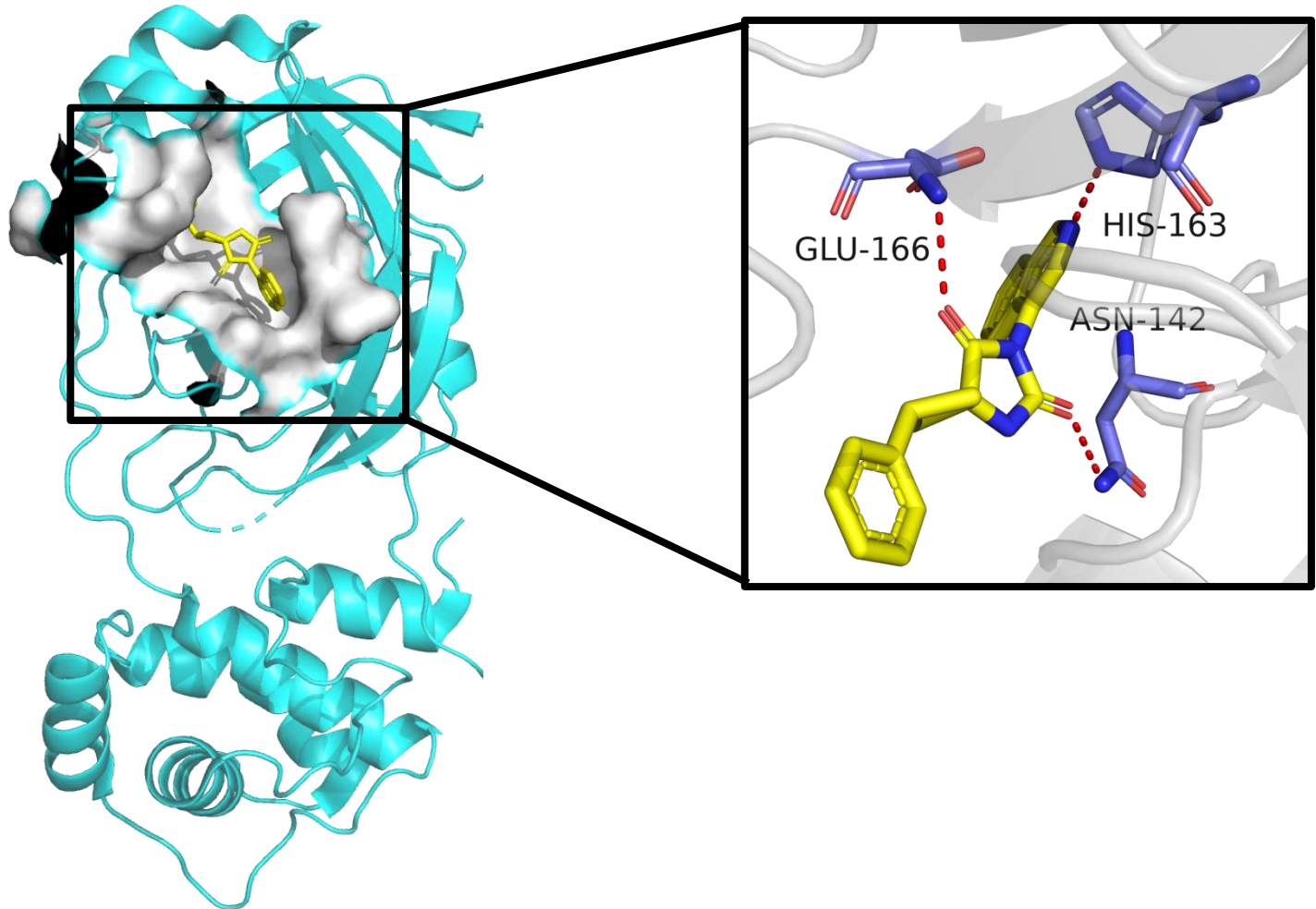
简易动画制作



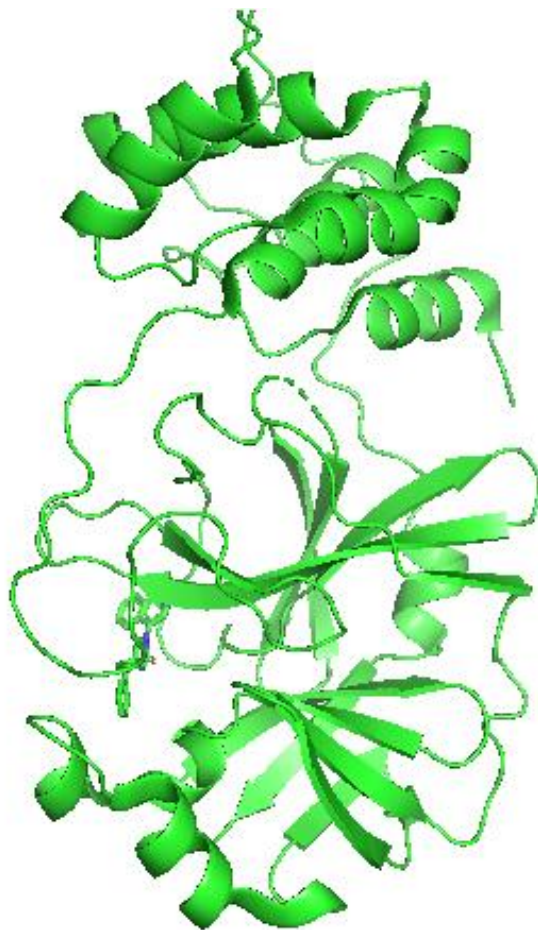
⑧保存动画，File>Export Movie As>MPEG
出现的对话框做简单调整，点击Save Movie as即可

PyMol实践二

精美图片制作

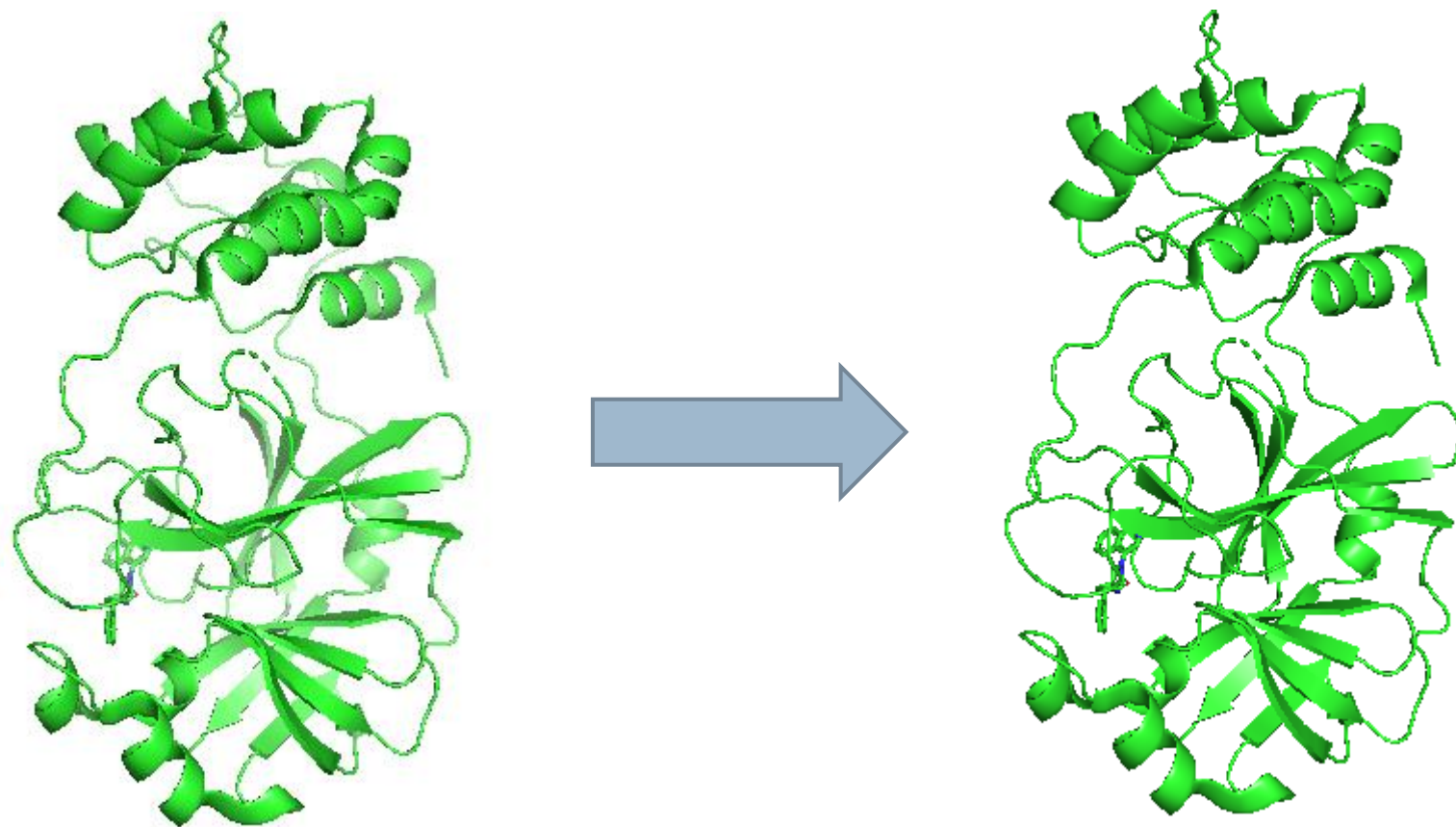


精美图片制作



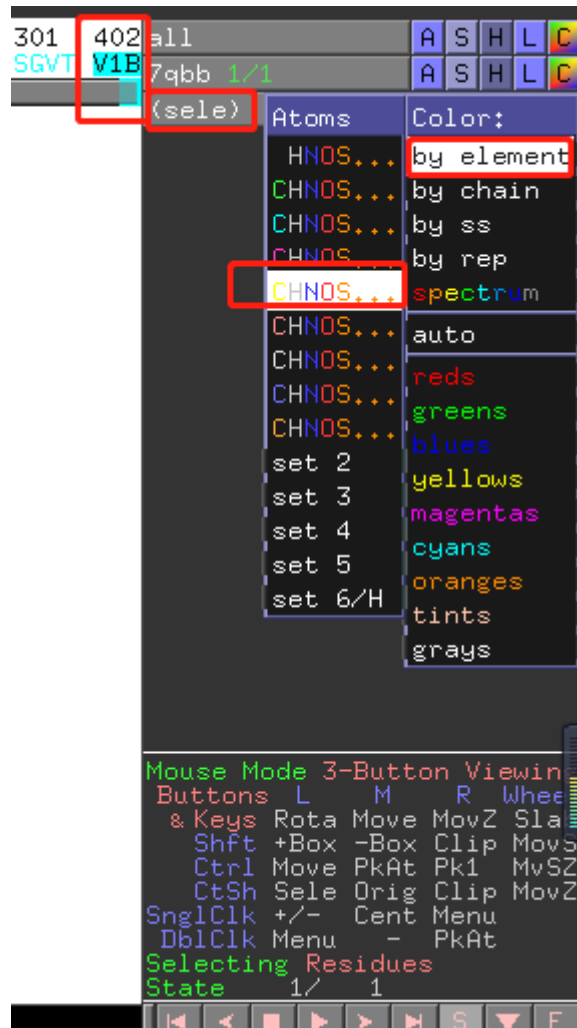
①用pymol打开7qbb文件，将背景调整白色，去除水分子和杂原子（DMS）

精美图片制作



② 去除景深效果，滚动鼠标滚轮，出现上图变化

精美图片制作



③调整颜色

蛋白颜色:

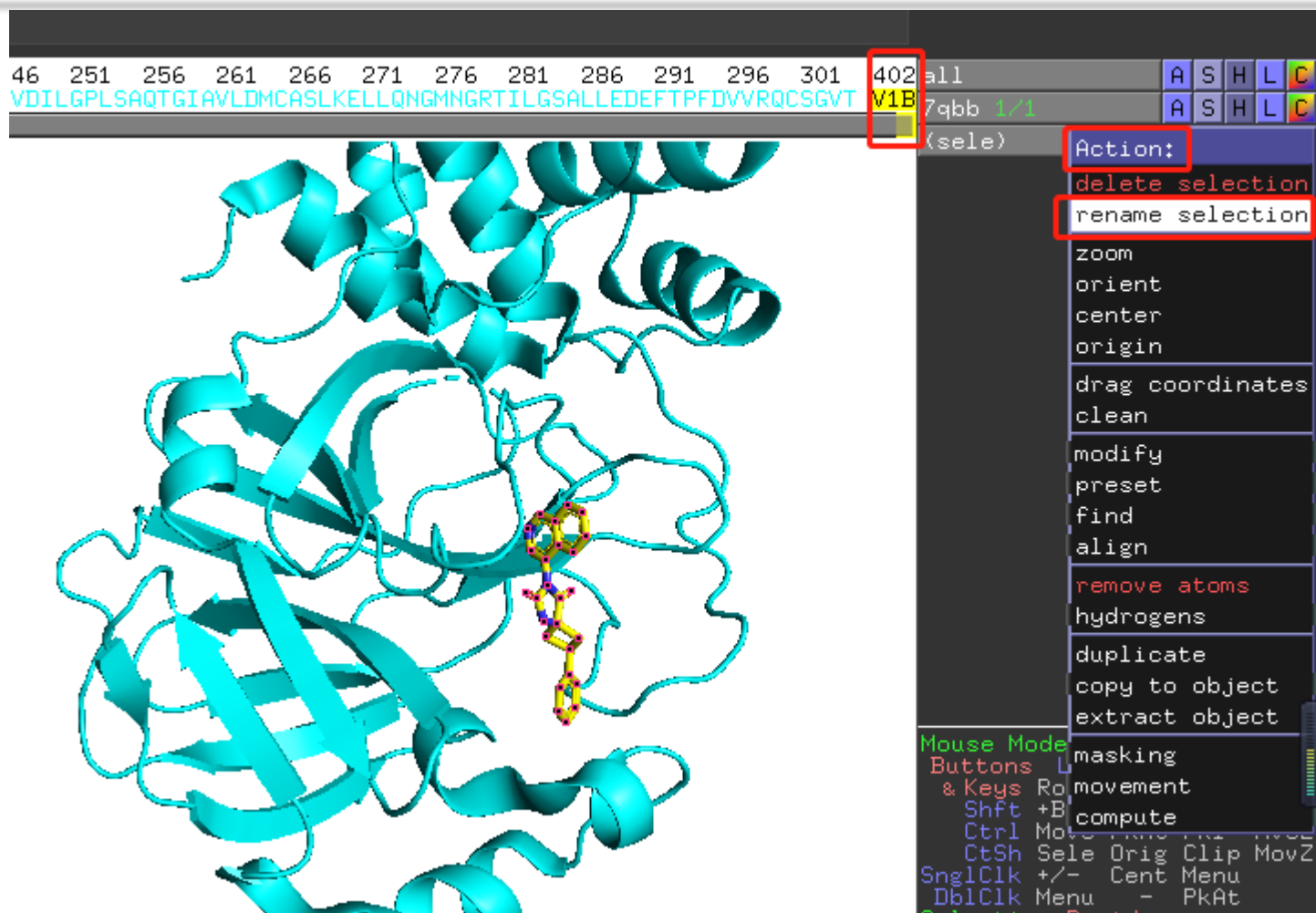
Color>cycans>cyan

配体颜色: 调出序列,
选择配体VIB, (sele)

>C(color)>by element>

黄色

精美图片制作

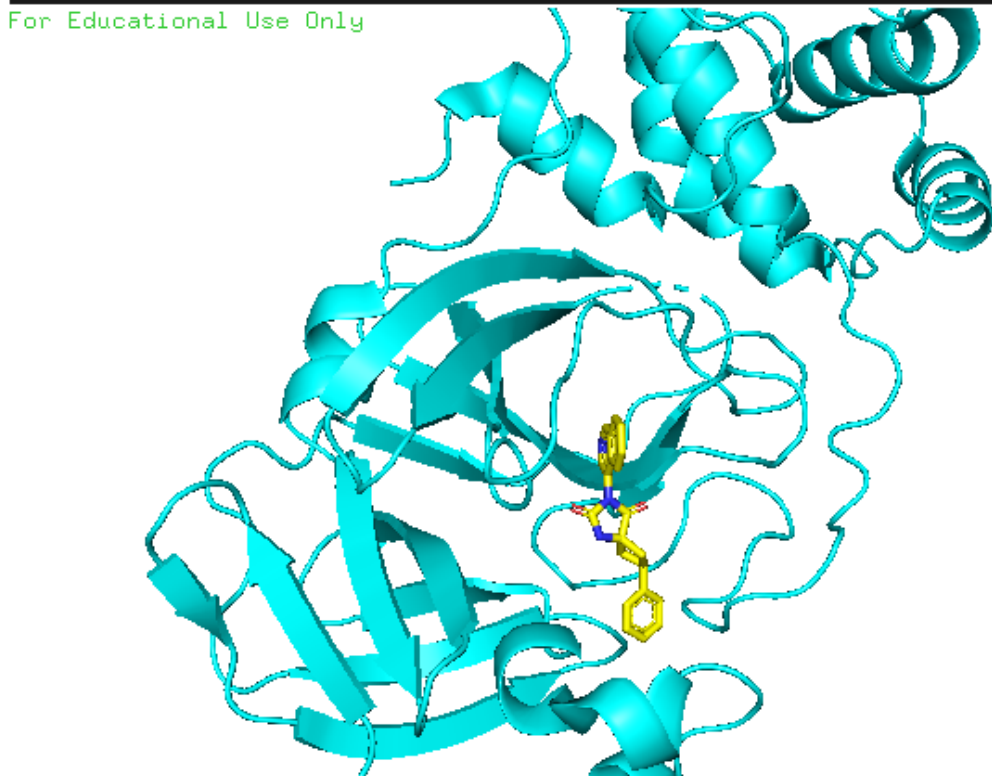


④选中配体后， (sele) >A(Action)>rename selection
将其命名为lig

精美图片制作

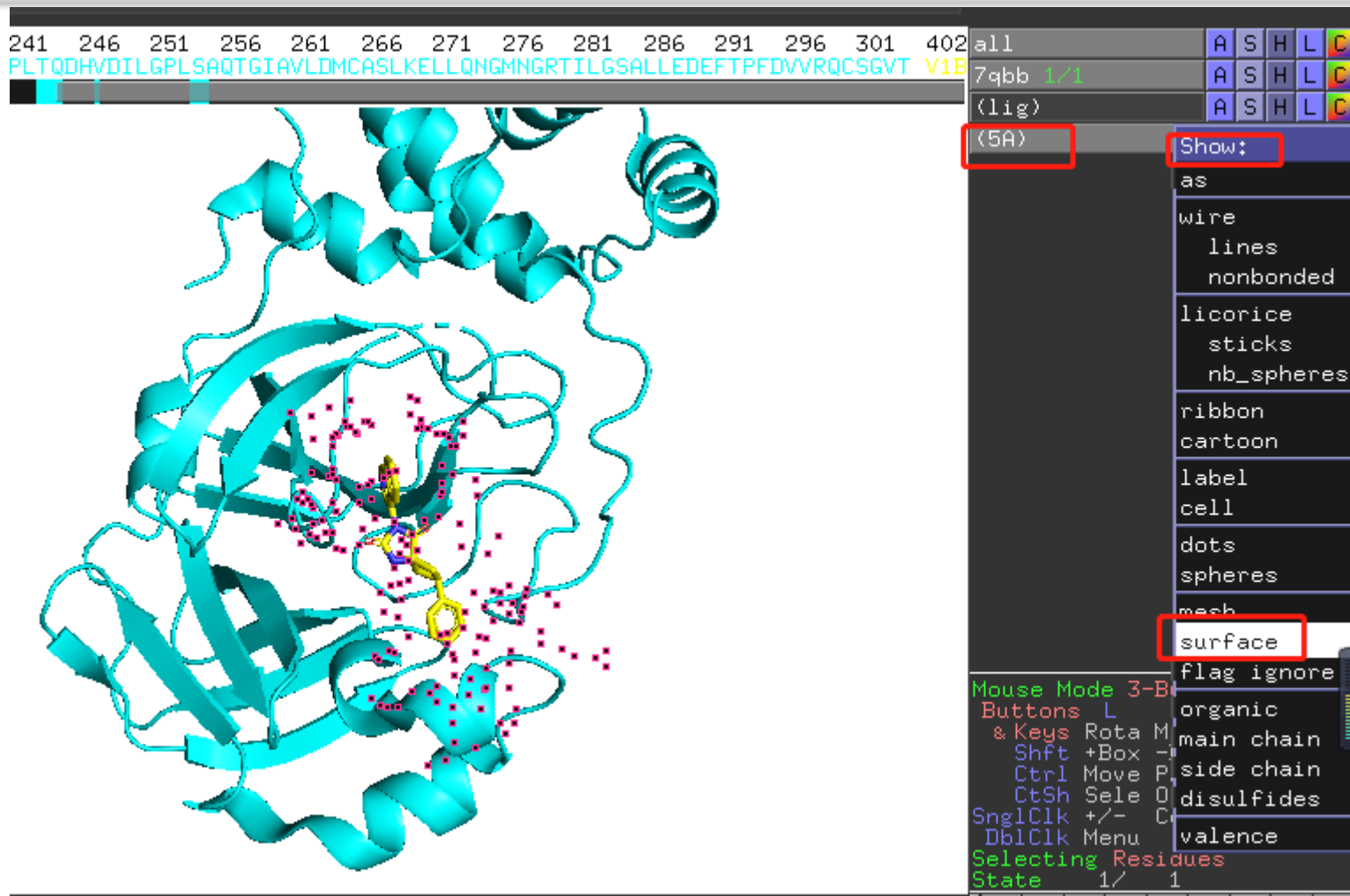
```
PyMOL
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
COMPND 7 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "7qbb".
Setting: bg_rgb set to white.
Executive: Colored 2373 atoms and 1 object.
You clicked /7qbb//A/THR'201/CA
PyMOL>set_name sele,lig
PyMOL> select 5A, byres lig around 5
/7qbb 176 181 186 191 196 201 206 211 216 221 226 231 236 241 246 :
ELPTGVHAGTDLEGNFYGPVFDRQTAQAAGTDTTITVNVLAWLYAAVINGDRWFLNRFTTTLNDFNLYAMKYNYEPLTQDHVDILC
```

⑤输入命令选中距离配体5Å的残基，并命名为5A



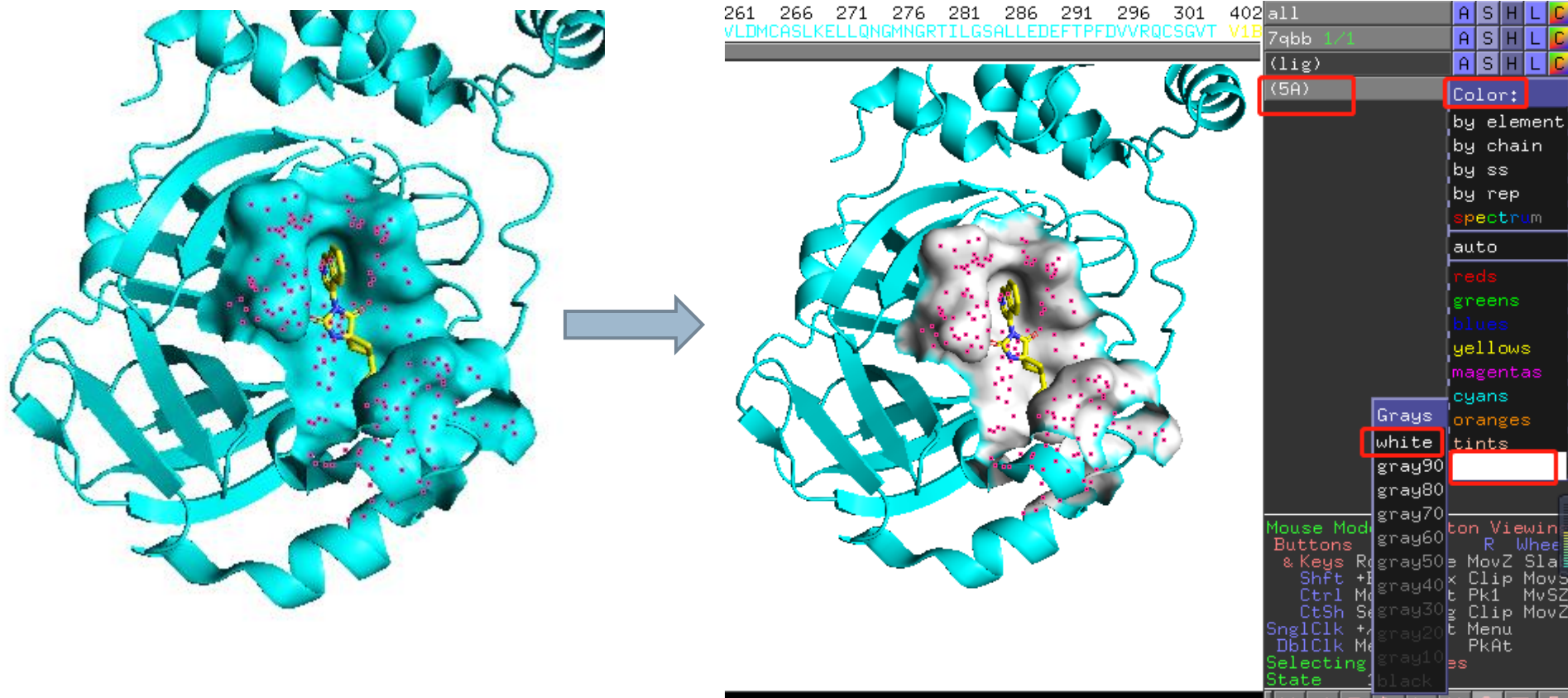
select 5A, byres lig around 5

精美图片制作



⑥将配体5Å范围内的残基，显示为surface
(5A) >S(show)>surface

精美图片制作

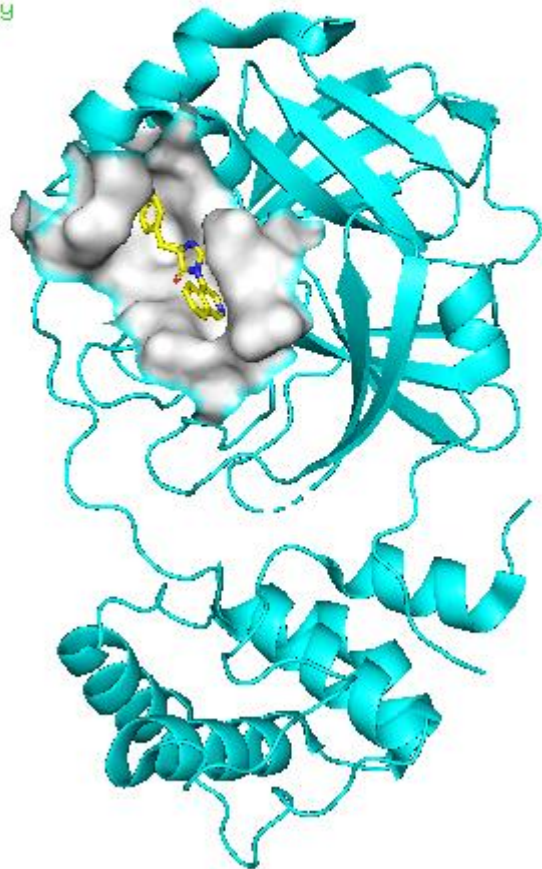


⑦变化表面的颜色为白色

(5A) >C(Color)>grays>white

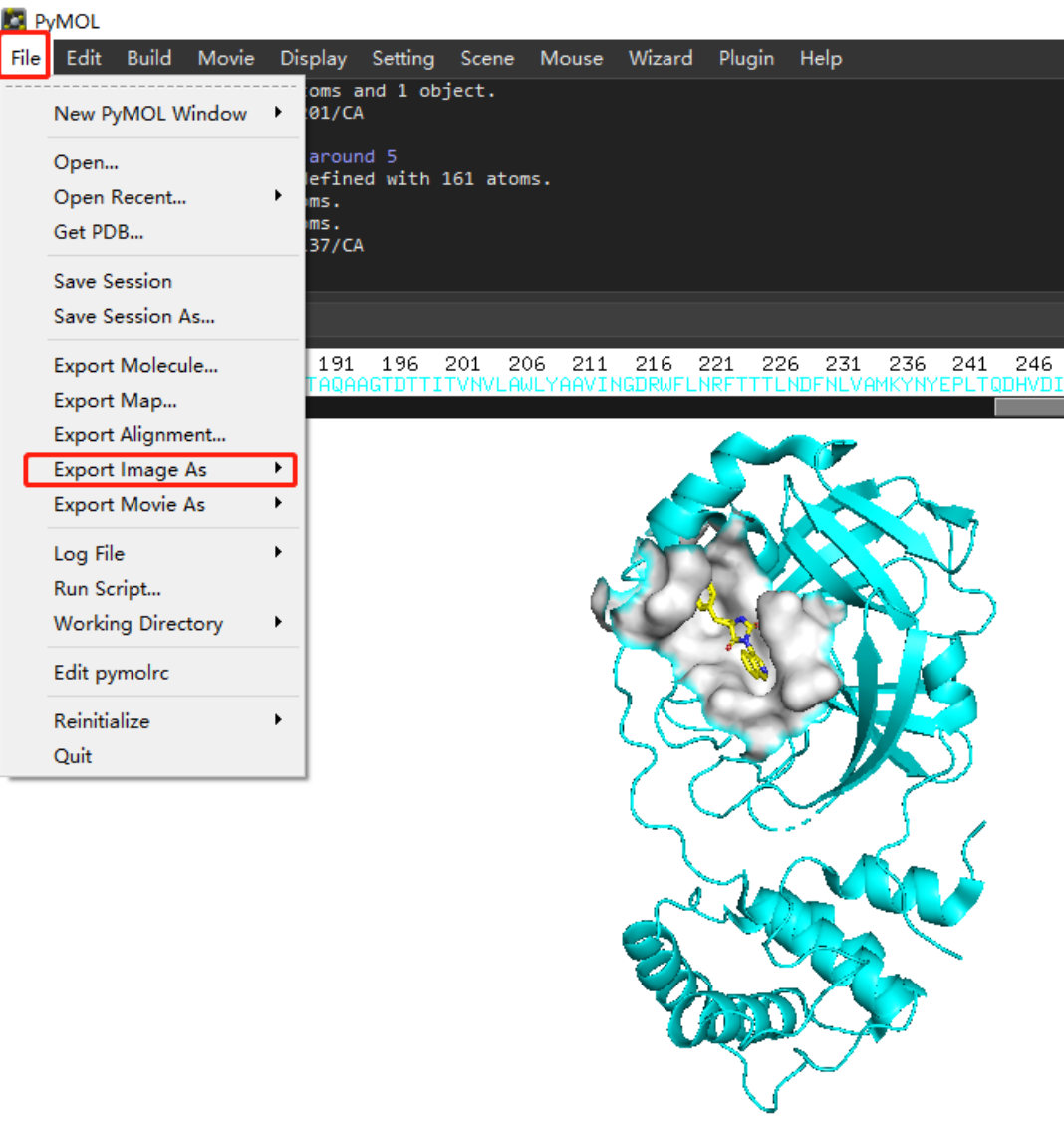
精美图片制作

```
Executive: Colored 161 atoms.  
Executive: Colored 161 atoms.  
  
PyMOL> ray 1000, 1000  
  
/7qbb      176 181 186 191 196 201 206 211 216 221  
_LPTGV AGTDLGNFYGPFV TAQAAGTDTTITVNVLAWLAAVINGDRWFLNRF  
  
For Educational Use Only
```



- ⑧调整合适角度，渲染图像，增加图片质量
- 在命令框输入ray 1000, 1000

精美图片制作

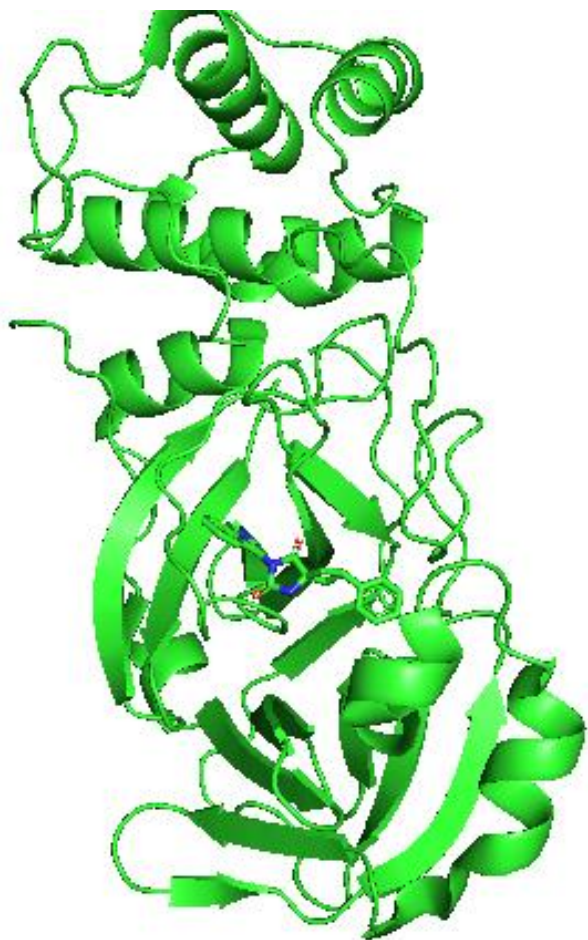


⑧保存图片

File>Export Image As>PNG

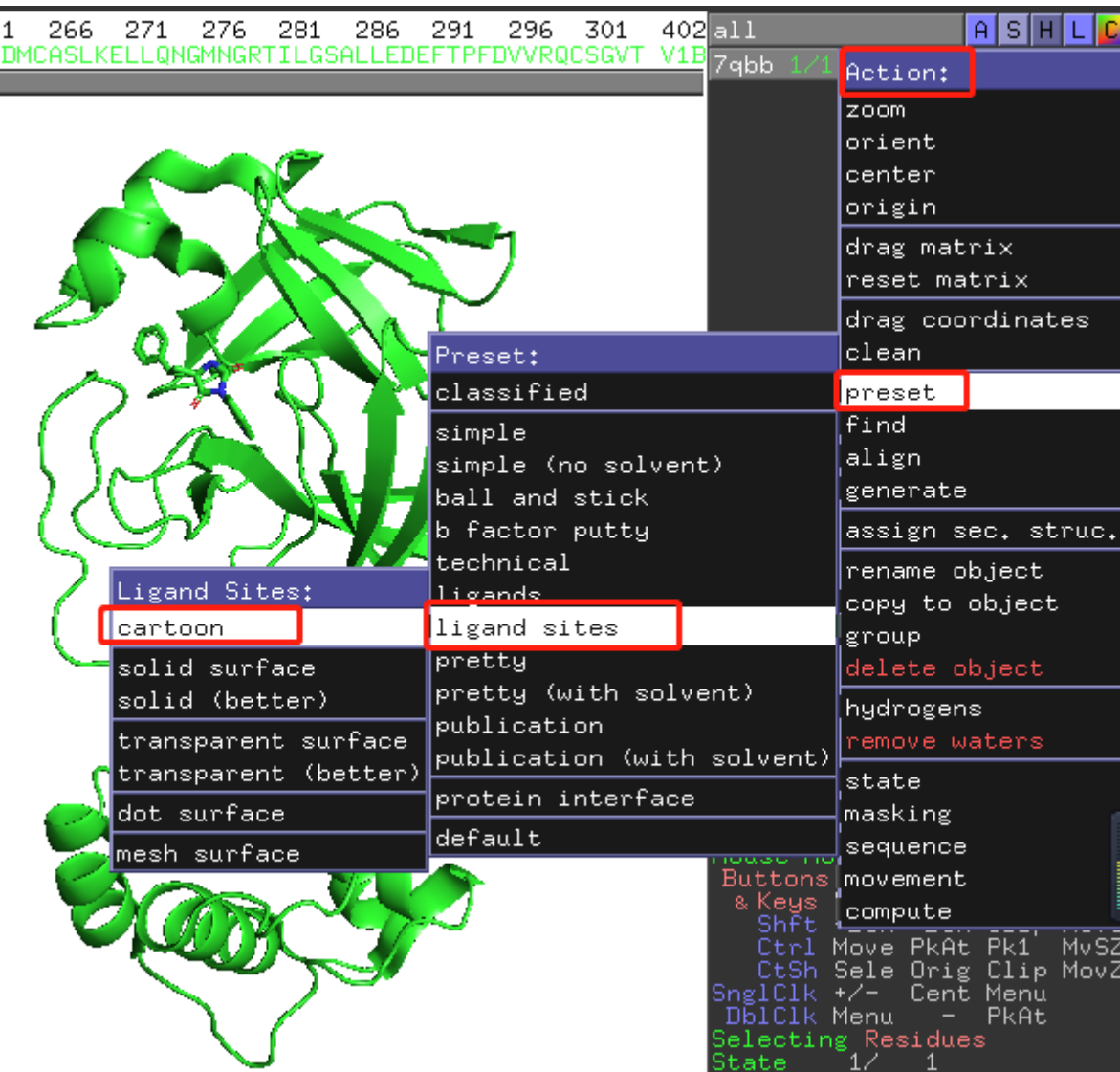
精美图片制作

开始第二部分



⑨重新打开pdb文件，进行预处理：除去水分子和杂原子、背景调成白色、去除景深效果

精美图片制作

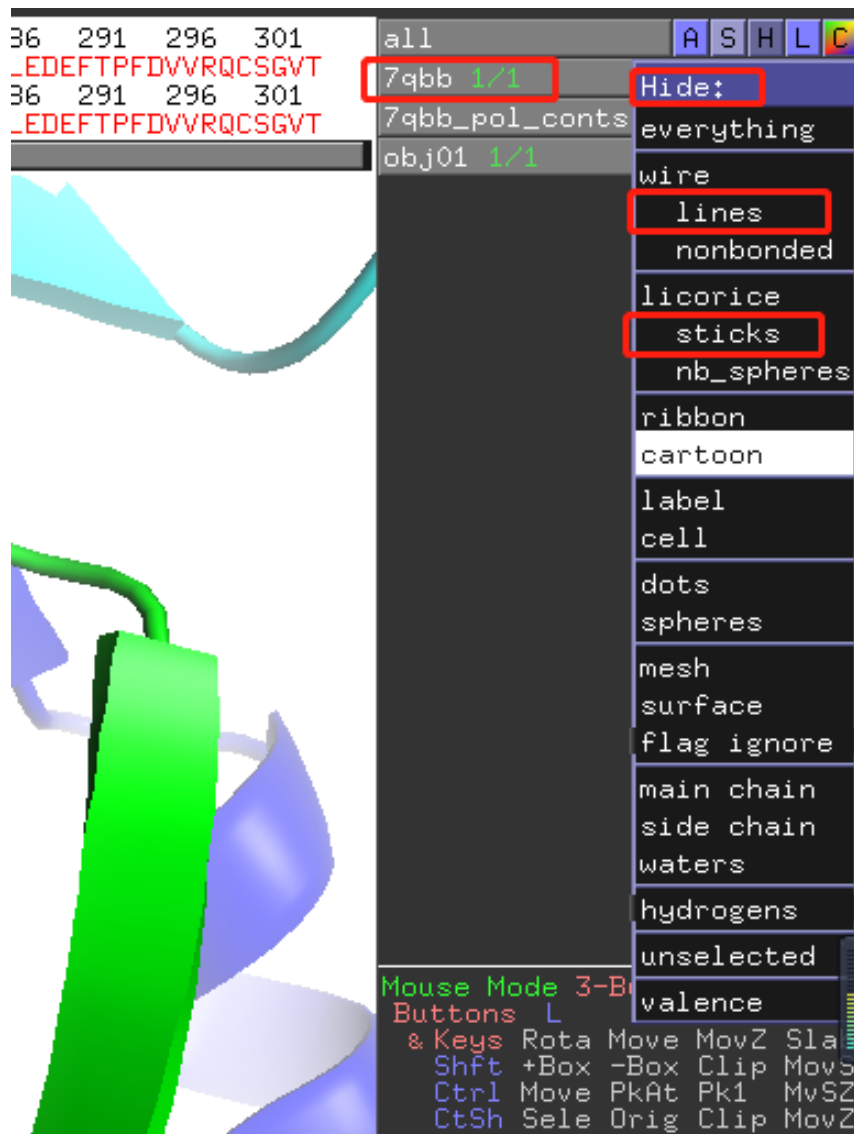


⑩调出活性位点

A (Action) > preset

>ligand site>cartoon

精美图片制作

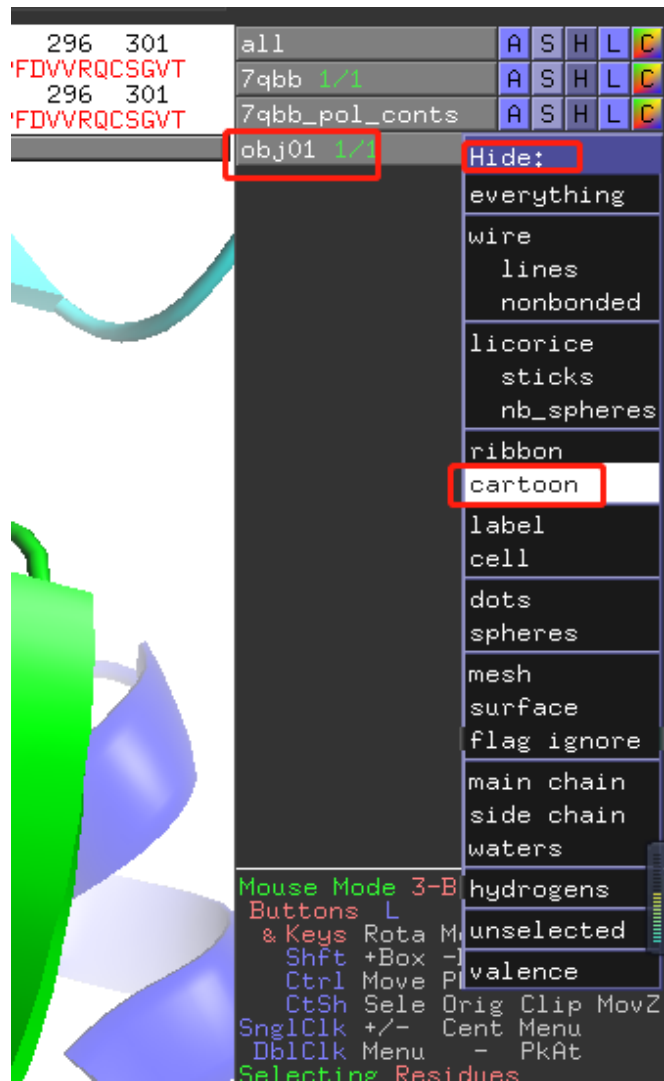


⑫ 隐藏7qbb的stick和line,

只显示cartoon

7qbb>Hide>lines(sticks)

精美图片制作



⑬ 隐藏obj01的cartoon，只
显示lines

obj01>H(Hide)>cartoon

精美图片制作

The image shows a molecular visualization software interface. At the top, a sequence of amino acids is displayed: 26 231 236 241 246 251 256 261 266 271 276 281 286 291 296 301 .NDFNLVAMKYNYEPLTQDHVDILGPLSAQTGIAVLDMCASLKE LLQNGMNGRTILGSALLEDEFTPFDVVRQCSGVT. A red box highlights the entry '7qbb 1/1' in the object list on the right. In the center, a 'Main Pop-Up' menu is open, with 'zoom (vis)' selected and highlighted by a red box. A red arrow points upwards from the menu. The bottom right corner shows a 'Mouse Mode 3-Button Viewin' control panel with various buttons and keyboard shortcuts.

Object	A	S	H	L	C
all					
7qbb 1/1					
/7qbb_pol_conts					
obj01 1/1					

Main Pop-Up
new
zoom (vis)
orient (vis)
center (vis)
reset
movie
scene
enable
disable
(all)
(visible)
ray
delete all
reinitialize
quit

Mouse Mode 3-Button Viewin
Buttons L M R Wheel
& Keys Rota Move MovZ Sla
Shft +Box -Box Clip Mov5
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu

⑭ 点击一下7qbb，即可取消显示，然后右击屏幕空白处，再出现的选项中，选择 zoom (vis)，让其居中

精美图片制作

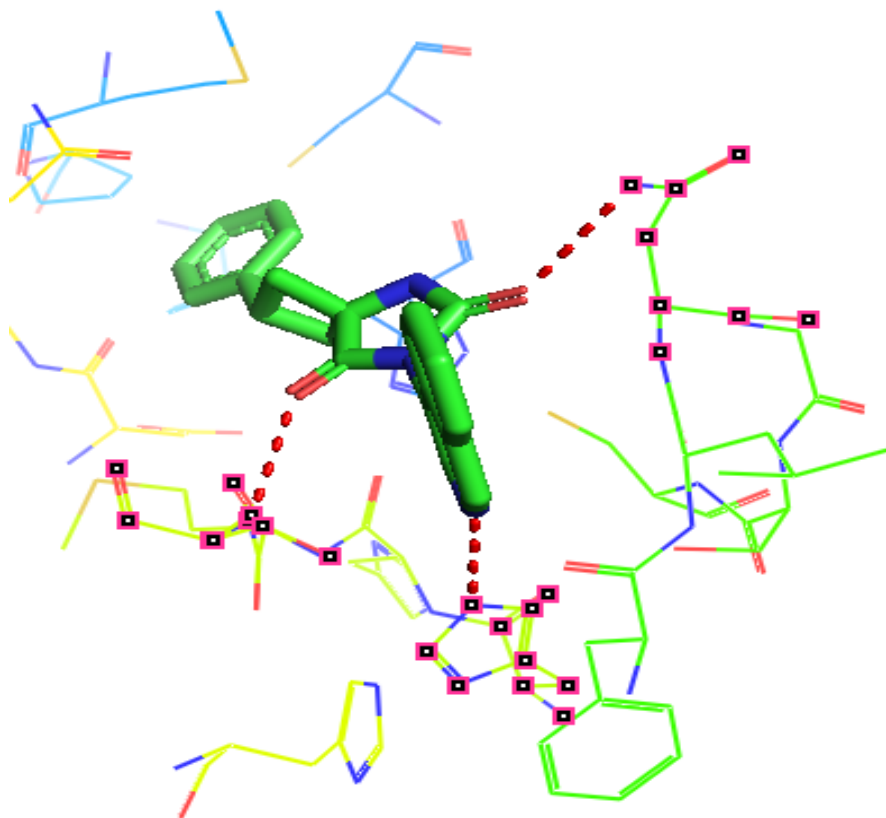


⑮ 改变氢键的颜色

```
7qbb_pol_conts>C(color)>reds>red
```

精美图片制作

```
246 251 256 261 266 271 276 281 286 291 296 301  
HVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFQDVRQCSGVT
```



all	A	S	H	L	C
7qbb 1/1	A	S	H	L	C
7qbb_pol_conts	A	S	H	L	C
obj01 1/1	A	S	H	L	C
(sele)					

Show:

- as
- wire
 - lines
 - nonbonded
- licorice
 - sticks
 - nb_spheres
- ribbon
- cartoon
- label
- cell
- dots
- spheres
- mesh
- surface
- flag ignore
- organic
- main chain
- side chain
- disulfides

Mouse Mode 3-B
Buttons L
& Keys Rota M
Shft +Box -
Ctrl Move PKRC PKI MWSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - RkOt

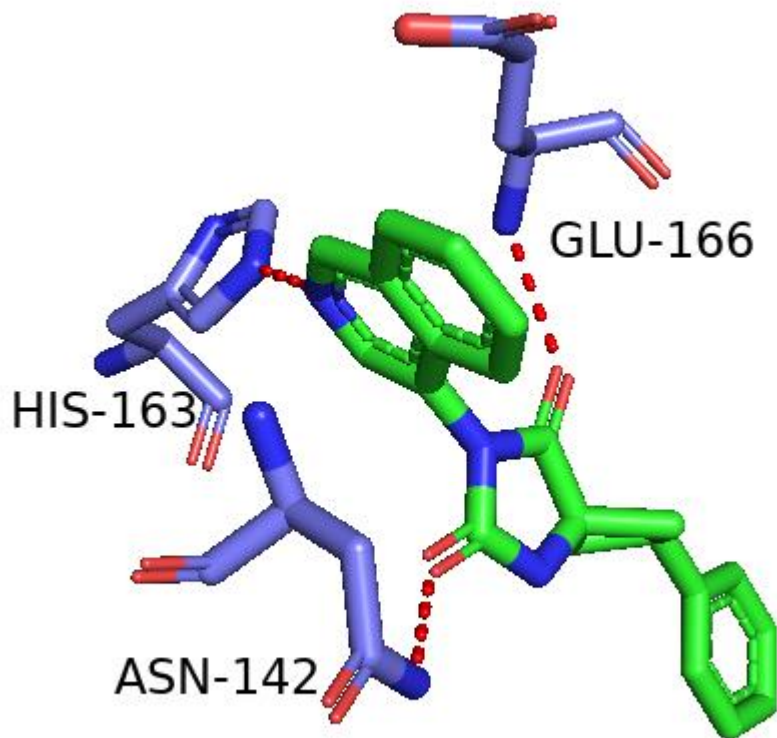
- ⑩在面板上选中参与氢键的残基，然后展示为stick
(sele) >S(show)>sticks
然后obj01>H(Hide)>lines

精美图片制作

The screenshot displays the PyMOL software interface. On the left, the command console shows the selection of a specific residue with the command `(sele)`. The `Color:` menu is open, listing various color options such as `reds`, `greens`, `blues`, `yellow`, `magentas`, `cyans`, `oranges`, `tints`, and `grays`. The `Label:` menu is also open, with `residues` selected. On the right, the `Setting` menu is open, with `Label` selected, and its sub-menu is visible, showing `Size` selected. The background shows a 3D molecular model of a protein structure with a specific residue highlighted in green and blue, and a dashed red line indicating a bond or interaction.

⑰调整关键残基的颜色，显示标记（label），并调整标记的大小（24 sizes）

精美图片制作



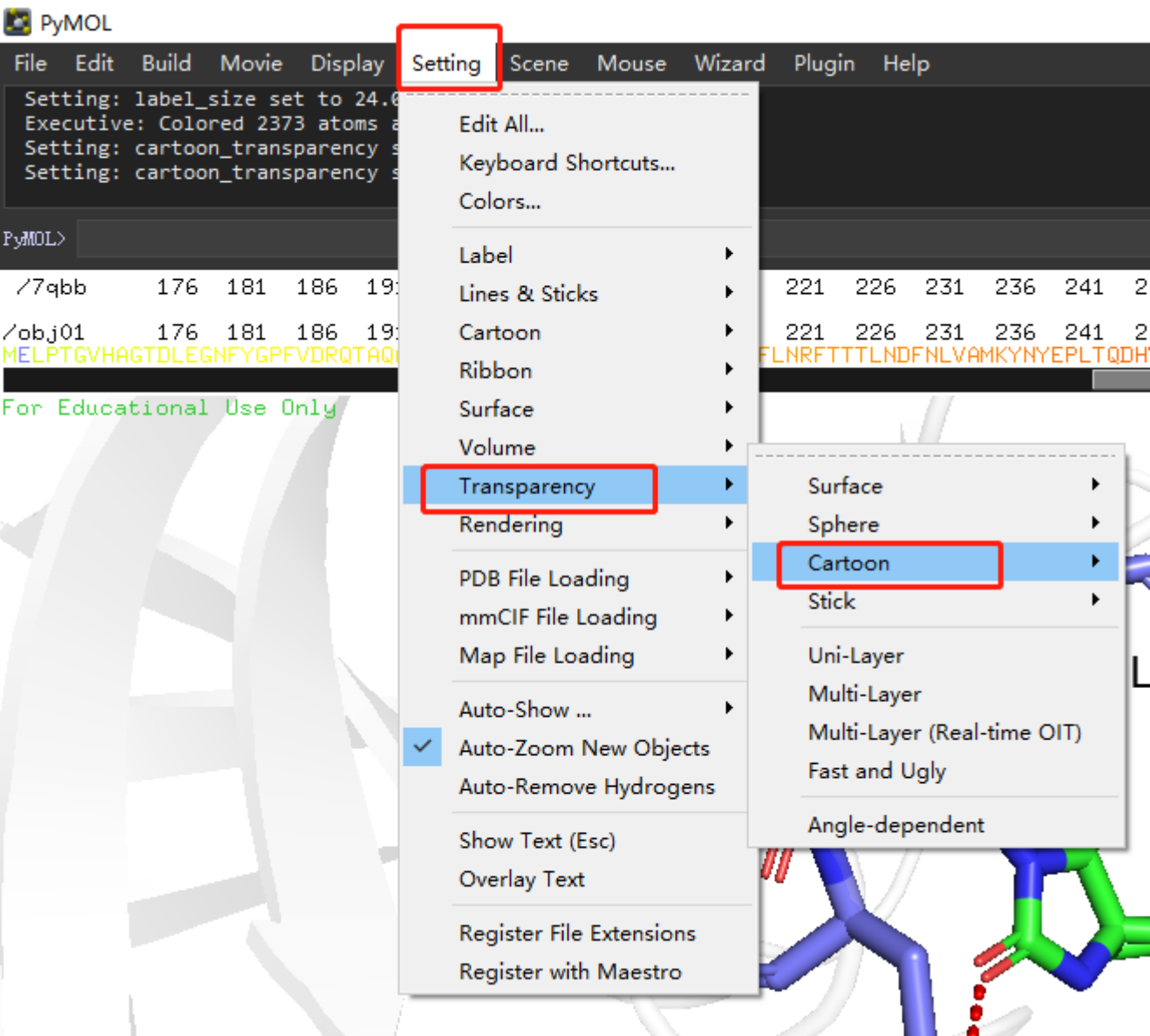
⑱调整合适位置，
让标签和氢键以及
残基都能很好的展
示，并让其居中

精美图片制作



⑲ 点击7qbb让其显示，并把颜色更改为白色

精美图片制作



②0 设置cartoon的
显示透明度为80%

Setting>

Transparency>

Cartoon>80%

精美图片制作

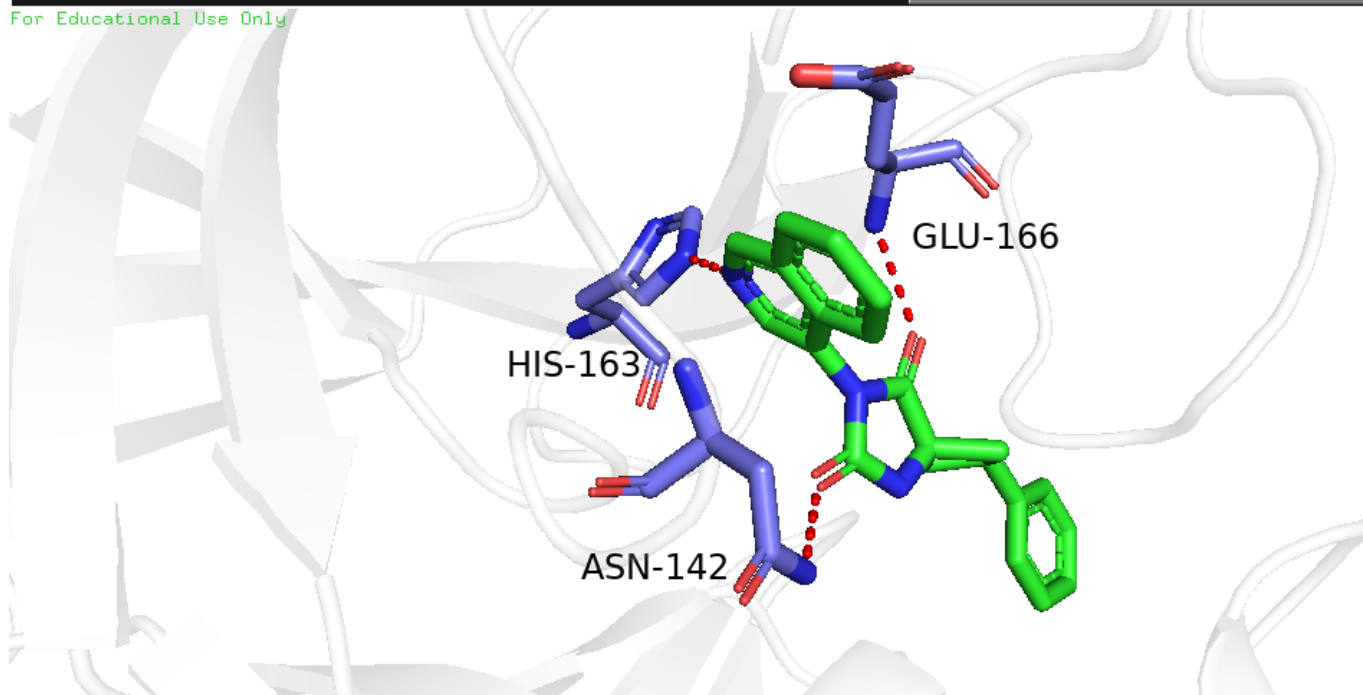
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
Setting: label_size set to 24.00000.  
Executive: Colored 2373 atoms and 1 object.  
Setting: cartoon_transparency set to 0.50000.  
Setting: cartoon_transparency set to 0.80000.
```

```
PyMOL> ray 1000, 1000
```

```
/7qbb 176 181 186 191 196 201 206 211 216 221 226 231 236 241 246 251 256 261 266 271 276 281 286 2'  
/obj01 176 181 186 191 196 201 206 211 216 221 226 231 236 241 246 251 256 261 266 271 276 281 286 2'  
MELPTGVHAGTDLEGNFYGPVDRQTAQAAGTDTTITVHVLAWLYAAVINGDRWFLNRFITTLNDNFNLVAMKYHYEPLTQDHVDILGPLSAQTGI AVLDMCASLKELLQNGMNGRTILGSALLEDEF'  
For Educational Use Only
```



在命令框中输入ray 1000, 1000

渲染完毕后，保存图片即可

蛋白 - 配体相互作用分析

蛋白配体相互作用分析

<https://plip-tool.biotec.tu-dresden.de/plip-web/plip/index>



Protein-Ligand Interaction Profiler



Welcome to the PLIP web tool!

Easy and fast identification of non-covalent interactions between biological macromolecules and their ligands.

enter PDB ID (e.g. 1xdn)

Find PDB ID using our search tool

or

Drop PDB file here (max. 10 MB)

Choose file...

> Advanced Options

ANALYZE

PLIP (Protein-Ligand Interaction Profiler) 是一个蛋白配体非共价相互作用的分析工具；可以分析蛋白配体复合物在原子水平的非共价相互作用，包括氢键，水桥，盐桥，卤键，疏水相互作用， π -堆叠， π -离子相互作用和金属复合物；检测机制主要是基于原子间的空间位置和几何关系。

蛋白 - 配体相互作用分析

Binding Sites in 7VH8

SMALLMOLECULE

4WI

4WI-A-401

配体分子

DMS (Dimethyl Sulfoxide)

DMS-A-402

No Interactions

H2S (Hydrogen Sulfide)

H2S-A-403

↓ Results in XML format

↓ Results in RST format

📄 Your results will be available for 30 days using the current URL.

🔗 7VH8 in the PDB

📄 How to Cite Us

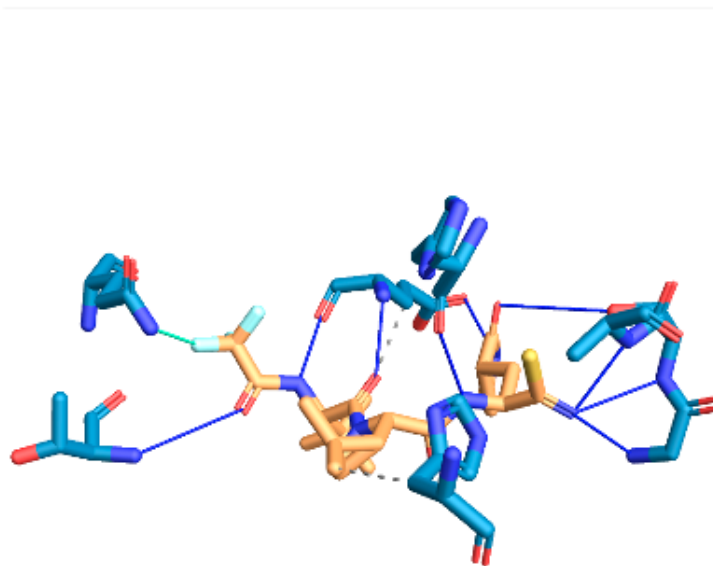
🔄 Run another analysis

SMALLMOLECULE

4WI

4WI-A-401

Interacting chains: A



3D开关

Click for 3D-View

可以分析的相互作用

- Protein
- Ligand
- Water
- Charge Center
- Aromatic Ring Center
- Metal Ion
- Hydrophobic Interaction
- Hydrogen Bond
- Water Bridge
- π -Stacking (parallel)
- π -Stacking (perpendicular)
- π -Cation Interaction
- Halogen Bond
- Salt Bridge
- Metal Complexation

蛋白 - 配体相互作用分析

Download visualization in **PyMol format (.pse)**

pymol作图

Download visualization as image (.png)

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

OpenGL graphics engine:
GL_VENDOR: Intel
GL_RENDERER: Intel(R) HD Graphics 520
GL_VERSION: 4.6.0 - Build 30.0.100.9865
License Expiry date: 01-oct-2022
Detected 4 CPU cores. Enabled multithreaded rendering.
Executive: Loading version 2.001000 session...
Session was saved with: viewport 0, 0

PyMOL>
For Educational Use Only

Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
< < Stop Play > > | MClear
Builder Properties Rebuild
Undo Redo

all	A	S	H	L	C
+ Atoms	A	S <td>H</td> <td>L</td> <td>C</td>	H	L	C
+ Interactions	A	S	H	L	C
+ Structures	A	S	H	L	C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt PK1 MvS2
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
Db1Clk Menu - PkAt
Selecting Residues

蛋白质 - 配体相互作用分析

Hydrophobic Interactions ****

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	41A	HIS	3.61	2397	310
2	166A	GLU	3.69	2400	1284

Halogen Bonds —

Index	Residue	AA	Distance	Donor Angle	Acceptor Angle	Donor Atom	Acceptor Atom
1	192A	GLN	3.15	142.55	96.82	2417 [F]	1485 [Nam]



蛋白质 - 配体相互作用分析

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	143A	GLY	2.38	3.15	134.16	✓	✗	1111 [Nam]	2406 [N2]
2	144A	SER	3.12	3.44	100.59	✓	✗	1115 [Nam]	2406 [N2]
3	144A	SER	3.66	4.07	108.36	✓	✓	1120 [O3]	2411 [O2]
4	145A	CYS	2.10	3.01	153.08	✓	✗	1121 [Nam]	2406 [N2]
5	164A	HIS	2.05	3.02	167.36	✗	✗	2409 [Nam]	1265 [O2]
6	166A	GLU	1.79	2.77	170.61	✗	✗	2410 [Nam]	1283 [O2]
7	166A	GLU	1.88	2.85	166.18	✓	✗	1280 [Nam]	2413 [O2]
8	166A	GLU	2.27	3.02	131.79	✗	✓	2407 [Nam]	1287 [O2]
9	190A	THR	3.39	3.96	119.08	✓	✗	1465 [Nam]	2414 [O2]

ChemDraw

ChemDraw 软件是目前国内外最流行、最受欢迎的化学绘图软件。它是美国CambridgeSoft 公司开发的 ChemOffice 系列软件中最重要的一员。Chemdraw 软件功能十分强大。可编辑、绘制与化学有关的一切图形，例如，建立和编辑各类分子式、方程式、结构式、立体图形、对称图形、轨道等，并能对图形进行编辑、翻转、旋转、缩放、存储、复制、粘贴等等多种操作。用它绘制的图形可以直接复制粘贴到word 软件中使用。最新版本软件还可以生成分子模型、建立和管理化学信息库、增加了光谱化学工具等功能。



ChemDraw

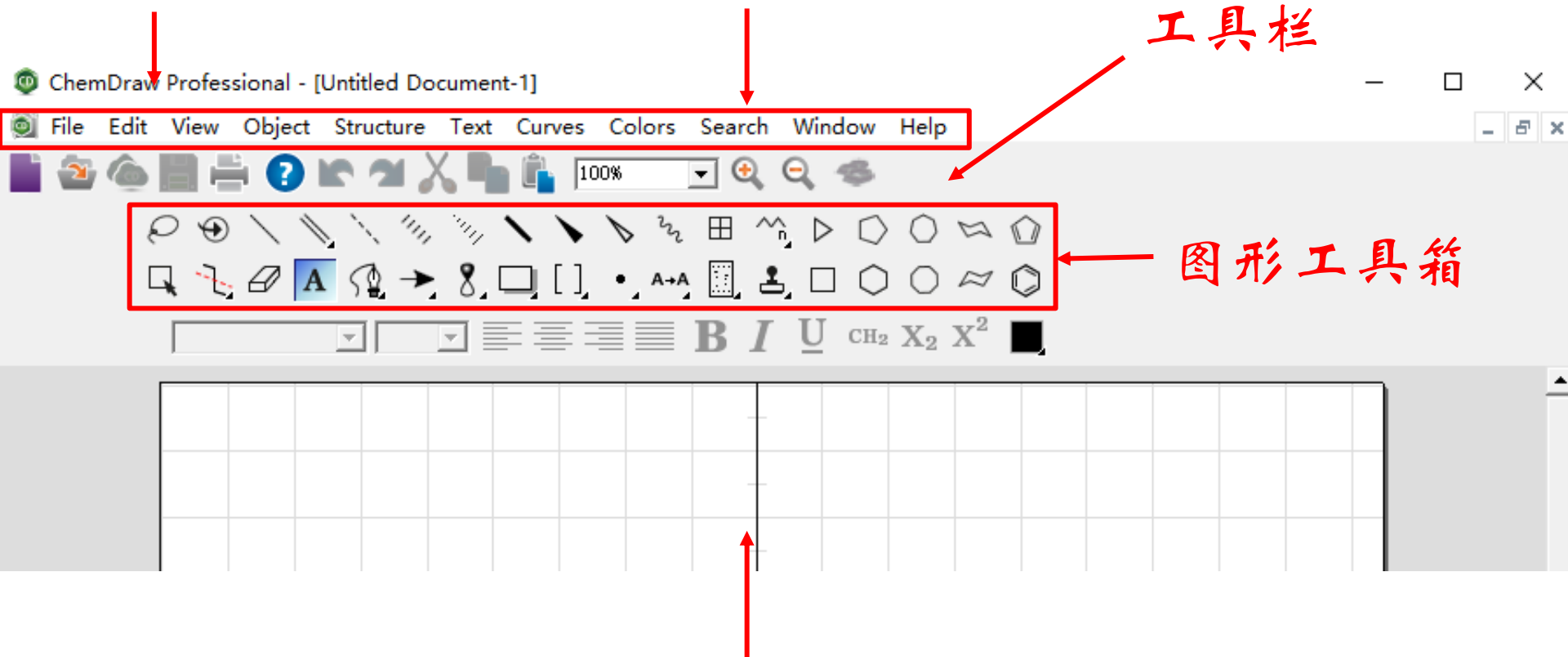
标题栏

菜单栏

工具栏

图形工具箱

绘图区



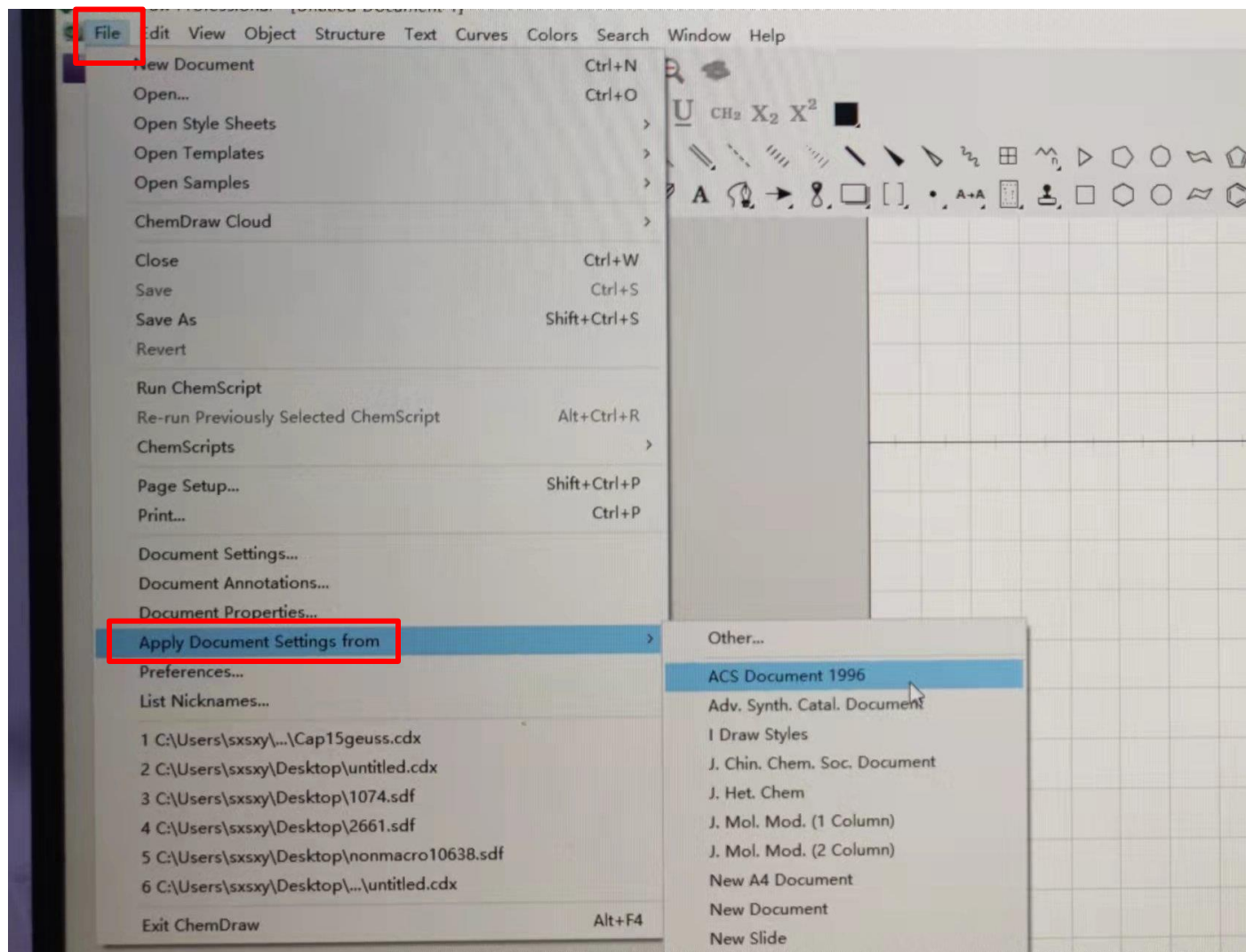
ChemDraw

The image shows the ChemDraw software interface with several toolbars and a template palette. Red boxes and arrows highlight specific tools, with Chinese text labels pointing to them:

- 选择工具结构透视** (Select tool structure perspective): A red box highlights the selection tools (arrow and lasso) at the top of the Tools toolbar.
- 橡皮擦** (Eraser): A red arrow points to the eraser tool in the Tools toolbar.
- 文本编辑** (Text editing): A red arrow points to the text tool (labeled 'A') in the Tools toolbar.
- 轨道** (Orbitals): A red arrow points to the orbital tool in the Tools toolbar, with a corresponding palette of orbital shapes shown to the right.
- 电子** (Electrons): A red arrow points to the electron tool in the Tools toolbar, with a corresponding palette of electron symbols shown to the right.
- 模板** (Templates): A red arrow points to the template palette on the left side of the interface.
- 基本环系** (Basic ring systems): A red arrow points to the basic ring systems tool in the Tools toolbar, which includes shapes for triangles, squares, pentagons, hexagons, heptagons, octagons, and various ring conformations.

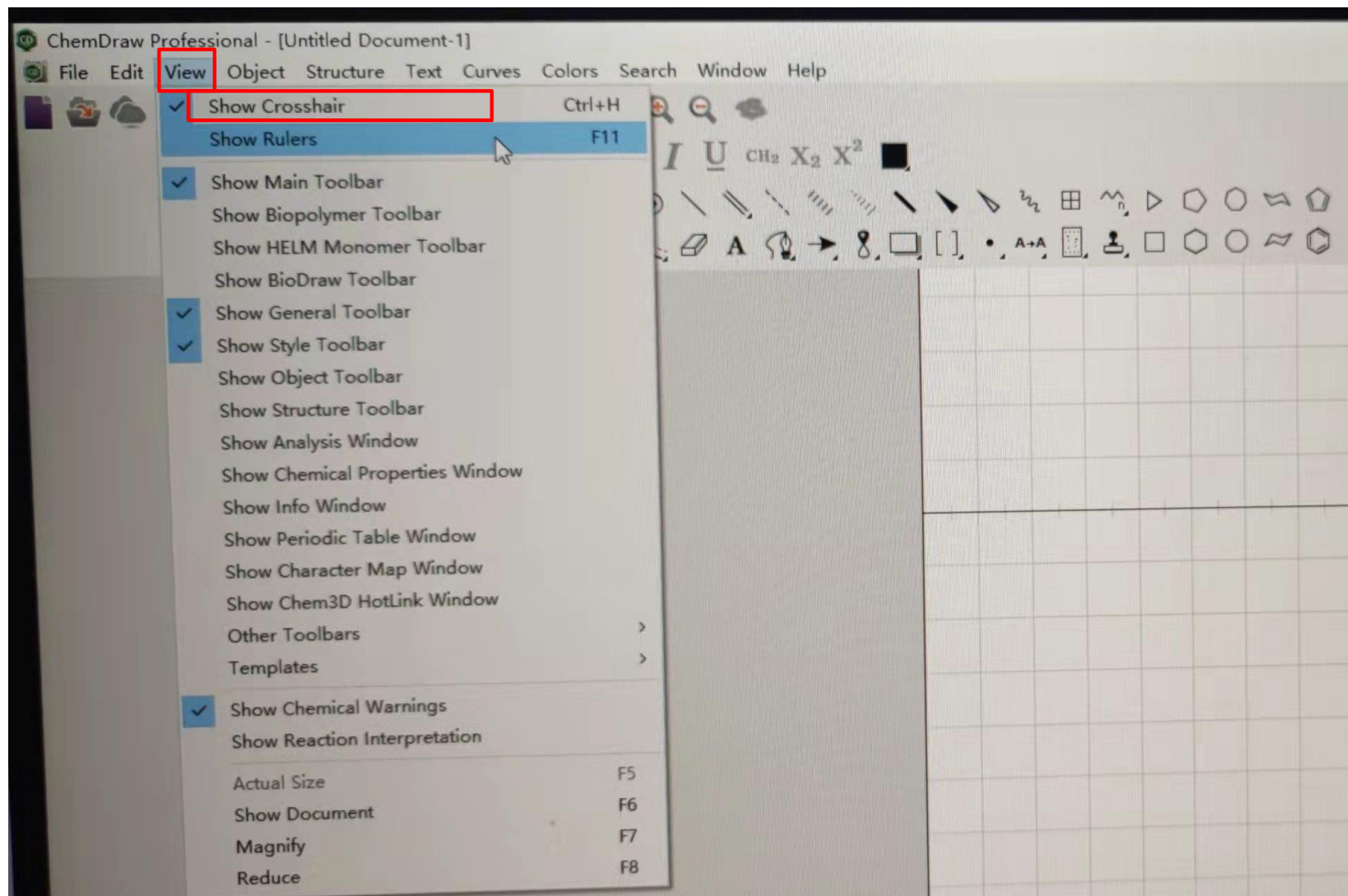
Other visible elements include a secondary toolbar with drawing tools like lines, curves, and arrows, and a template palette on the left with categories such as Amino Acid Side Chains, Amino Acids, Anatomy, Animals, Aromatics, Bicyclics, Bio Instruments, Bio Art, Bugs, Clipware, Conformers, Cp Rings, Cycloalkanes, DNA Templates, Functional Groups, Hexoses, Metalloenes, Microorganisms, Nanotubes, Organelles, Ph Rings, Polyhedra, Polypeptides, RNA Templates, Shapes, Stereocenters, and Supramolecules.

ChemDraw



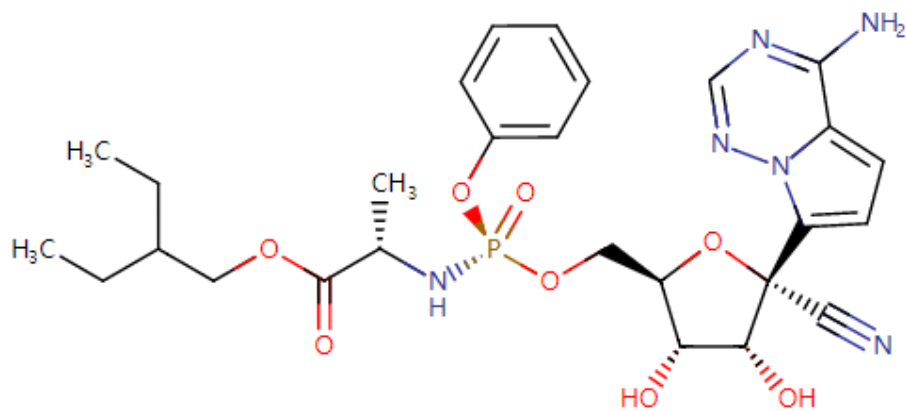
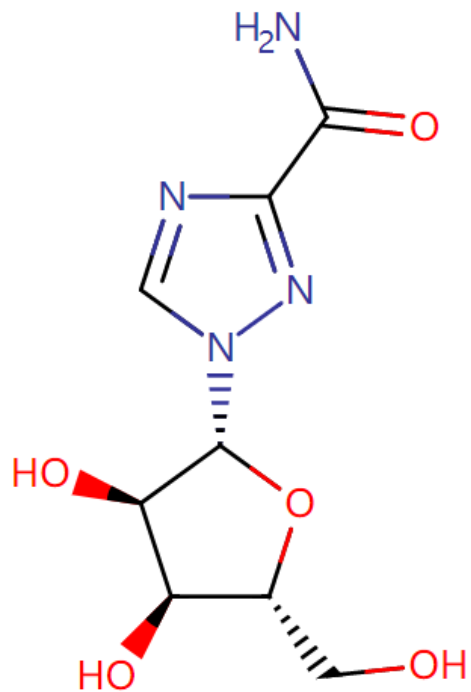
ChemDraw

调出网格状



ChemDraw

小练习



ChemDraw

根据结构转化为化学命名法
根据化学命名法转化为结构

The screenshot displays the ChemDraw Professional software interface. The 'Structure' menu is open, showing various options. The 'Convert Structure to Name' option is highlighted with a red box and a red arrow pointing to the chemical structure below. The chemical structure is a complex molecule consisting of a 1,2,4-triazole ring connected to a tetrahydrofuran ring, which has two hydroxyl groups and a hydroxymethyl group. The triazole ring has a carboxamide group attached to it.

ChemDraw Professional - [new.mol]
File Edit View Object **Structure** Text Curves Colors Search Window Help

Atom Properties...
Bond Properties...
Bracket Properties...
Check Structure
Clean Up Structure Shift+Ctrl+K
Clean Up Reaction Shift+Ctrl+X
Clean Up Biopolymer
Expand Label
Contract Label
Expand Generic Structure
Add Multi-Center Attachment
Add Variable Attachment
R-Logic Query...
Add 3D Property >
Enhanced Stereochemistry >
Map Reaction Atoms
Clear Reaction Map
Analyze Stoichiometry
Autonumber Reaction
Clear Reaction Numbers
Predict ¹H-NMR Shifts
Predict ¹³C-NMR Shifts
Make Spectrum-Structure Assignment
Add Structure to Dictionary...
Define Nickname...
Convert Name to Structure Shift+Ctrl+N
Convert Structure to Name Alt+Ctrl+N

1-((2*R*,3*R*,4*S*,5*R*)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-1*H*-1,2,4-triazole-3-carboxamide

ChemDraw

ChemDraw Professional - [new.mol *]

File Edit View Object Structure Text Curves Colors Search Window Help

Show Crosshair Ctrl+H
Show Rulers F11

Show Main Toolbar
Show Biopolymer Toolbar
Show HELM Monomer Toolbar
Show BioDraw Toolbar
 Show General Toolbar
 Show Style Toolbar
Show Object Toolbar
Show Structure Toolbar
Show Analysis Window
 Show Chemical Properties Window
Show Info Window
Show Periodic Table Window
Show Character Map Window
Show Chem3D HotLink Window
Other Toolbars
Templates
 Show Chemical Warnings
Show Reaction Interpretation

Chemical Properties

Boiling Point:
 Melting Point:
 Critical Temp:
 Critical Pres:
 Critical Vol:
 Gibbs Energy:
 Log P: -1.85
 MR:
 Henry's Law: 15.12
 Heat of Form:
 tPSA: 140.97
 CLogP: -2.84929
 CMR: 5.3181
 LogS: 0.5987
 pKa: 12.320, ...

Paste Report

(((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-1H-1,2,4-triazole-3-carboxamide)

Rule of five

1. 化合物的分子量不大于 500
2. 化合物结构中的氢键供体（包括羟基、氨基等）的数量不大于 5 个；
3. 化合物中氢键受体的数量不大于 10 个；
4. 化合物的脂水分配系数的对数值 ($\log P$) 不大于 5
5. 化合物中可旋转键的数量不大于 10 个。

ChemDraw

File Edit View Object Structure Text Curves Colors Search Window Help

Atom Properties...
Bond Properties...
Bracket Properties...

Check Structure
Clean Up Structure Shift+Ctrl+K
Clean Up Reaction Shift+Ctrl+X
Clean Up Biopolymer
Expand Label
Contract Label
Expand Generic Structure

Add Multi-Center Attachment
Add Variable Attachment
R-Logic Query...
Add 3D Property >
Enhanced Stereochemistry >

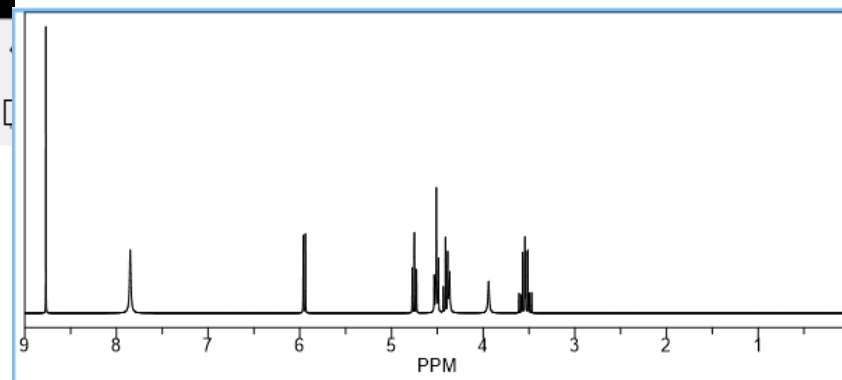
Map Reaction Atoms
Clear Reaction Map
Analyze Stoichiometry
Autonumber Reaction
Clear Reaction Numbers

Predict ¹H-NMR Shifts
Predict ¹³C-NMR Shifts

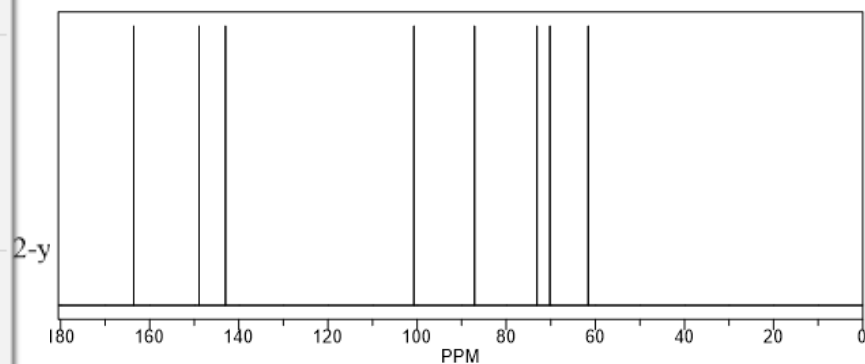
Make Spectrum-Structure Assignment

Add Structure to Dictionary...
Define Nickname...
Convert Name to Structure Shift+Ctrl+N
Convert Structure to Name Alt+Ctrl+N

H谱



C谱



1-((2R,3-

2-y

Notepad++ 介绍和使用



Notepad++

主要功能：

Notepad++ 顾名思义就是 windows 下 notepad 的增强版，它采用 C++ 编写，属于轻量级的文本编辑类软件，可以快速对文本、数据、代码进行处理。

优势：

性能优秀，小巧（完整安装包仅 3.8MB），功能众多，插件丰富，完全免费。启动更快，占用资源更少，但是从功能使用等方面来说，不亚于其他专业工具，而 windows 默认的 notepad 虽然更“轻量”，但是功能就太少。

Notepad++ 特色

1、自动保存

文本编辑过程中最怕的就是各种意外情况还没来得急保存，比如死机、进程僵死、奔溃等，如果你用了 Notepad++，完全不用担心，默认情况下它会实时的将正在编辑的内容保存一份副本到 %appdata% 下，每次打开未保存的文件都会自动从副本中恢复，完全不用担心任何编辑数据丢失！

2、列编辑

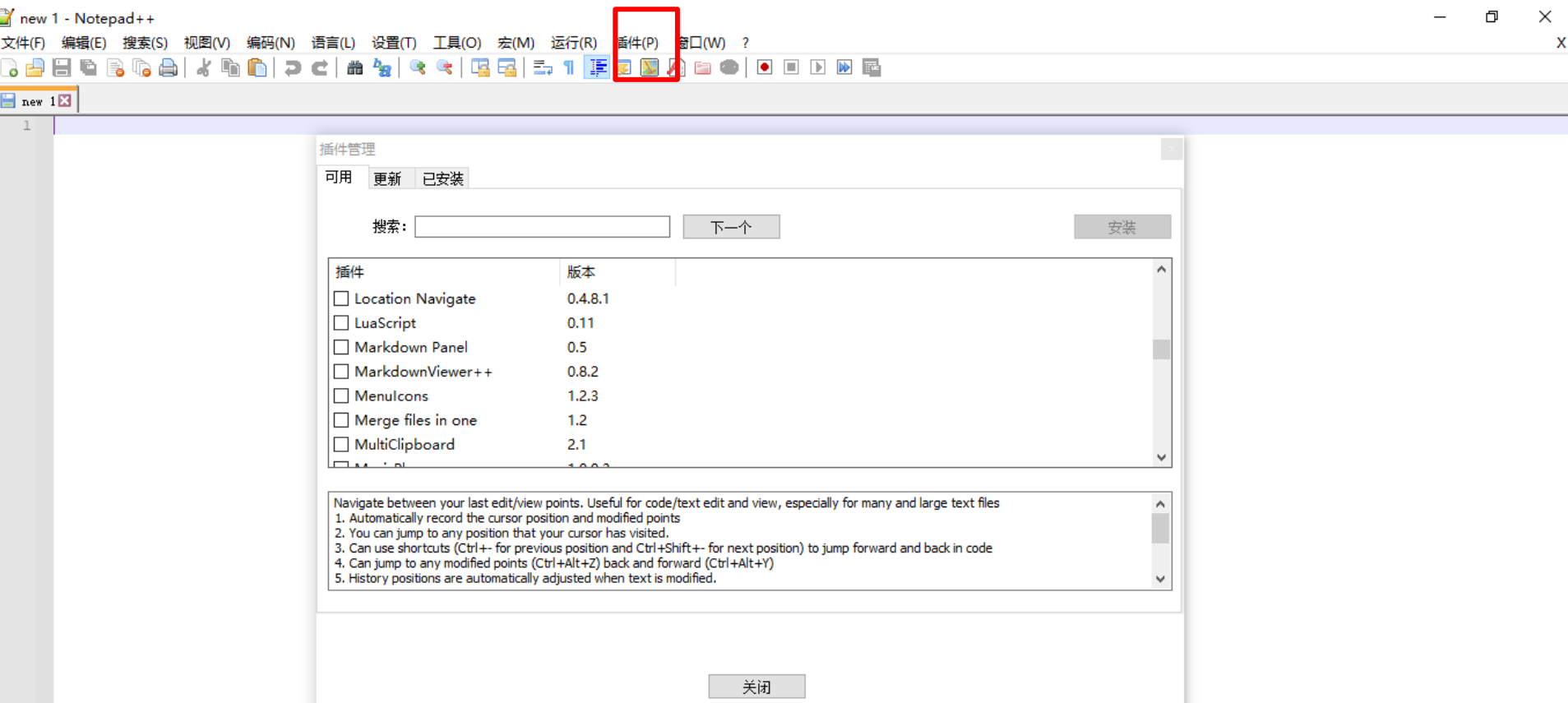
Notepad++ 里按下 alt 键即可进入列编辑模式，然后按下 tab 即可为选中的每一行执行相同的操作。那如果要给每行的开头加一个连续的数字做行号呢？Notepad++ 里按下 alt+c 组合键即可进入列编辑插入模式，设置相应的初始值、步长即可。

3、查找替换

notepad++ 的查找替换非常强大，能在单独窗口输出匹配内容，或者更友好的方式标记出查找结果。

Notepad++ + 插件

notepad++支持插件，添加对应不同的插件，以支持不同的功能。里面除了一些常见的插件之外，还有一些好玩的插件，比如将文字读出来的speech插件（插件»插件管理）



Notepad++ 插件

插件管理

可用 更新 已安装

搜索:

下一个

安装

插件	版本
<input type="checkbox"/> Dark Theme Mode	1
<input type="checkbox"/> DBGp	0.0.13.27
<input checked="" type="checkbox"/> Document Monitor	2.2
<input type="checkbox"/> Don Rowlett Color Picker	2.3
<input type="checkbox"/> Doxylt	0.4.4
<input type="checkbox"/> DSpellCheck	1.4.20
<input type="checkbox"/> EditorConfig	0.4
<input type="checkbox"/> File...	1.0.1

Updates opened documents every 3 seconds.

Author: Don Ho

Homepage: <https://sourceforge.net/projects/npp-plugins/files/DocMonitor/>

关闭