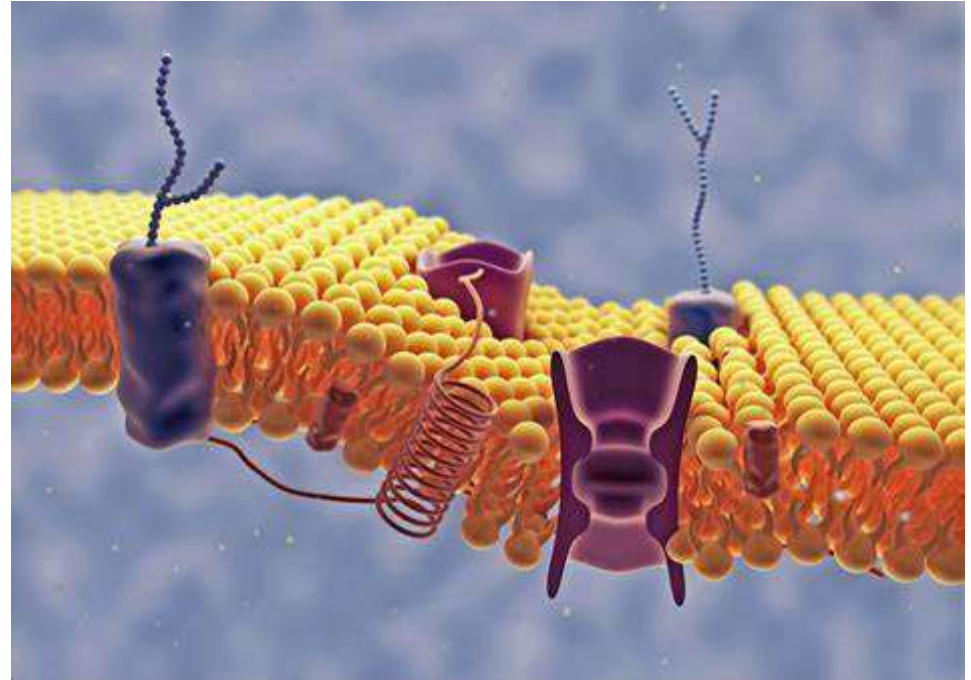
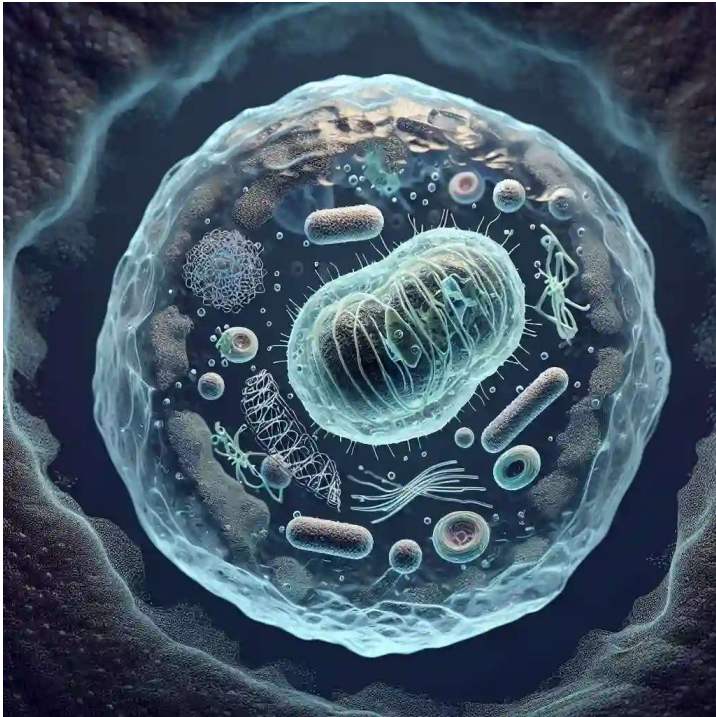


# 使用**Charmm-Gui**进行膜蛋白模拟

Naf Guo  
2025

# Membrane Protein

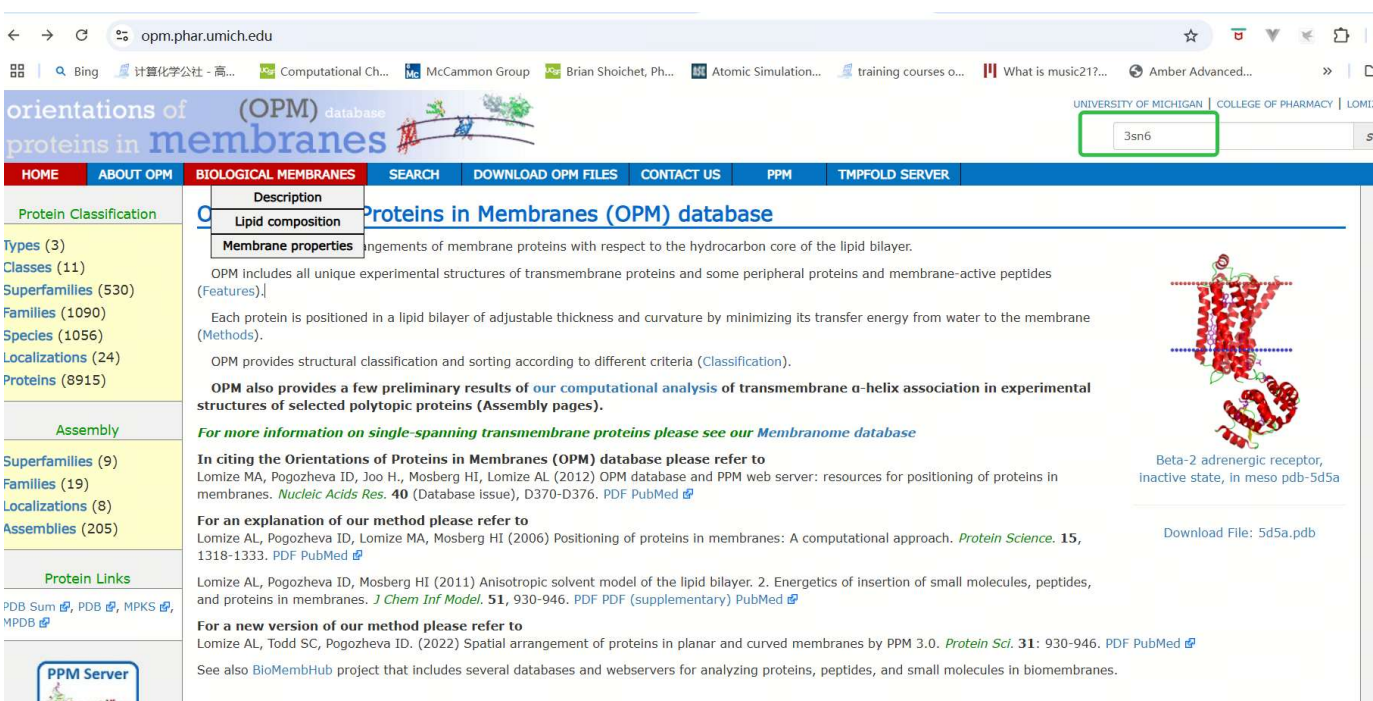


- 我们都知道细胞表面有双层磷脂组成的细胞膜，细胞膜上分布着许多蛋白；细胞膜作为细胞内外的分界，其上的许多蛋白具有沟通胞内外信息的作用；
- 对膜蛋白而言，它和水溶性蛋白最大的区别就是它被磷脂膜包裹在中间；
- 在进行膜蛋白的模拟时，我们必须考虑膜环境。

# Get Membrane Position from OPM Database

<https://opm.phar.umich.edu/>

- 为了设置适当的膜环境，我们需要获得膜相对的位置
- 如我们要对PDB 3SN6进行模拟，在OPM数据库搜索该结构，可以获得标注了膜位置的PDB文件
- 如果没有3SN6，也可以找同一蛋白或者同源蛋白的结构代替



The screenshot shows the OPM database website. The search bar at the top right contains the text "3sn6". The main content area displays the "Proteins in Membranes (OPM) database" information, including a description of the database, its features, and a list of proteins. A small 3D model of a protein (Beta-2 adrenergic receptor) is shown on the right side of the page.

Proteins in Membranes (OPM) database

OPM includes all unique experimental structures of transmembrane proteins and some peripheral proteins and membrane-active peptides (Features). Each protein is positioned in a lipid bilayer of adjustable thickness and curvature by minimizing its transfer energy from water to the membrane (Methods). OPM provides structural classification and sorting according to different criteria (Classification). OPM also provides a few preliminary results of our computational analysis of transmembrane  $\alpha$ -helix association in experimental structures of selected polytopic proteins (Assembly pages).

For more information on single-spanning transmembrane proteins please see our Membranome database

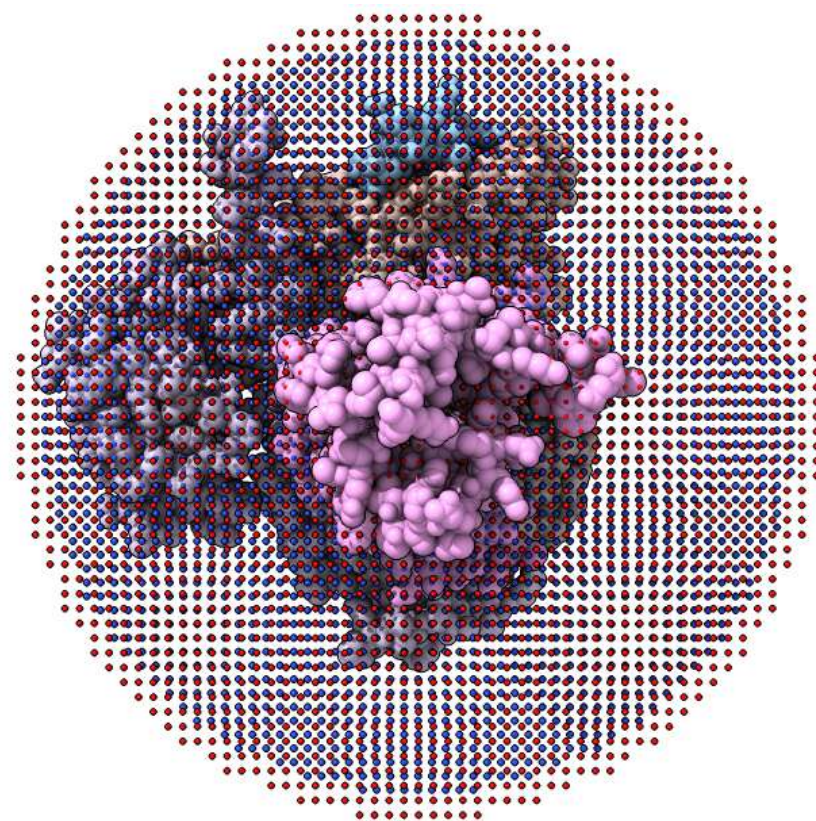
In citing the Orientations of Proteins in Membranes (OPM) database please refer to Lomize MA, Pogozheva ID, Joo H., Mosberg HI, Lomize AL (2012) OPM database and PPM web server: resources for positioning of proteins in membranes. *Nucleic Acids Res.* **40** (Database Issue), D370-D376. PDF PubMed

For an explanation of our method please refer to Lomize AL, Pogozheva ID, Mosberg HI (2006) Positioning of proteins in membranes: A computational approach. *Protein Science.* **15**, 1318-1333. PDF PubMed

Lomize AL, Pogozheva ID, Mosberg HI (2011) Anisotropic solvent model of the lipid bilayer. 2. Energetics of insertion of small molecules, peptides, and proteins in membranes. *J Chem Inf Model.* **51**, 930-946. PDF PDF (supplementary) PubMed

For a new version of our method please refer to Lomize AL, Todd SC, Pogozheva ID. (2022) Spatial arrangement of proteins in planar and curved membranes by PPM 3.0. *Protein Sci.* **31**: 930-946. PDF PubMed

See also BioMembHub project that includes several databases and webservers for analyzing proteins, peptides, and small molecules in biomembranes.





# Get Membrane Position from OPM Database

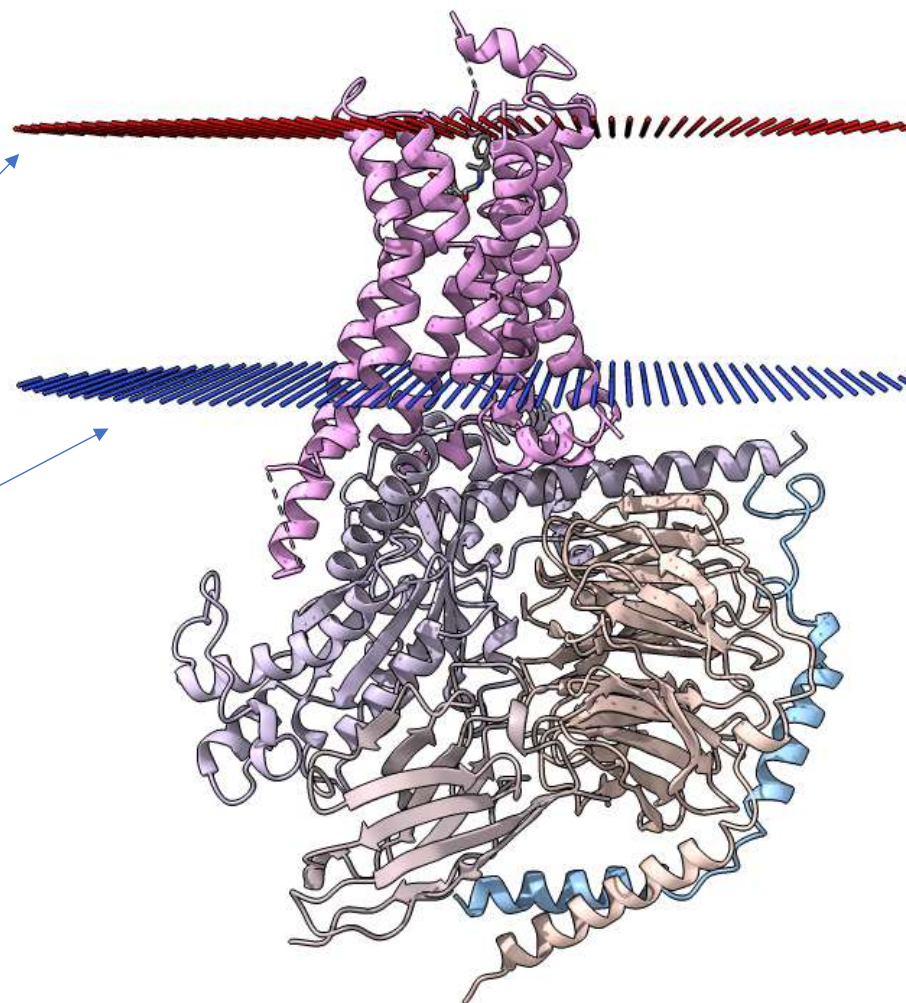
<https://opm.phar.umich.edu/>

- 从OPM获得的结构中，通过**DUM**原子标记了双层膜的位置
- 文件的第一行**REMARK**标记了膜的厚度

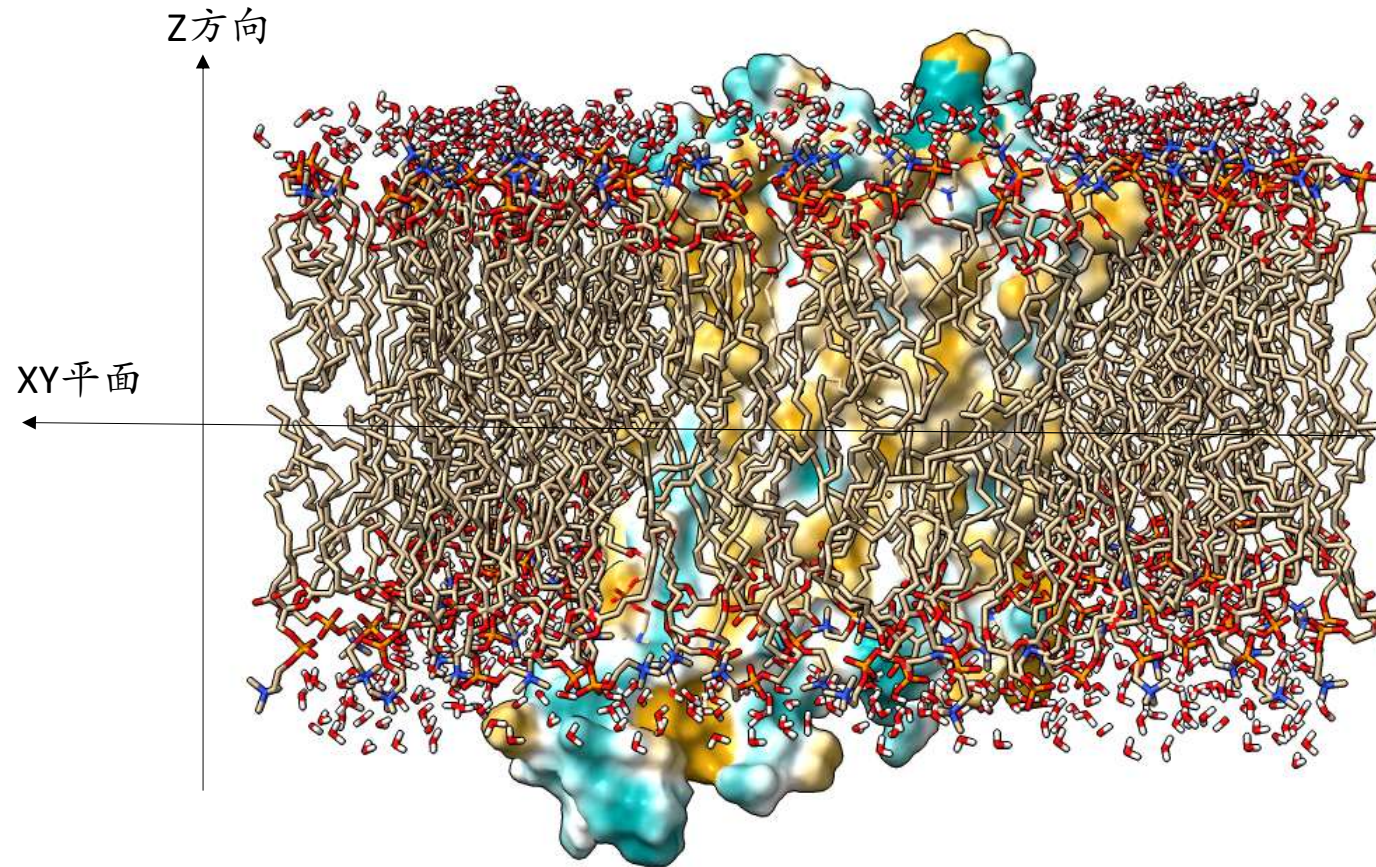
**REMARK 1/2 of bilayer thickness: 15.5**

ATOM	1	N	THR	A	9	-22.316	41.823	-24.680	1.00171.15	A	N
ATOM	2	CA	THR	A	9	-23.632	41.941	-24.066	1.00171.98	A	C
ATOM	3	C	THR	A	9	-24.727	41.980	-25.130	1.00166.96	A	C
ATOM	4	O	THR	A	9	-24.655	41.278	-26.139	1.00166.22	A	O
ATOM	5	CB	THR	A	9	-23.725	43.210	-23.190	1.00174.37	A	C
ATOM	6	OG1	THR	A	9	-23.688	44.371	-24.029	1.00172.10	A	O
ATOM	7	CG2	THR	A	9	-22.568	43.264	-22.208	1.00175.31	A	C

HETATM11872	O	DUM	11872	8.000	4.000	15.500
HETATM11873	N	DUM	11873	8.000	6.000	-15.500
HETATM11874	O	DUM	11874	8.000	6.000	15.500
HETATM11875	N	DUM	11875	8.000	8.000	-15.500
HETATM11876	O	DUM	11876	8.000	8.000	15.500
HETATM11877	N	DUM	11877	8.000	10.000	-15.500
HETATM11878	O	DUM	11878	8.000	10.000	15.500
HETATM11879	N	DUM	11879	8.000	12.000	-15.500
HETATM11880	O	DUM	11880	8.000	12.000	15.500



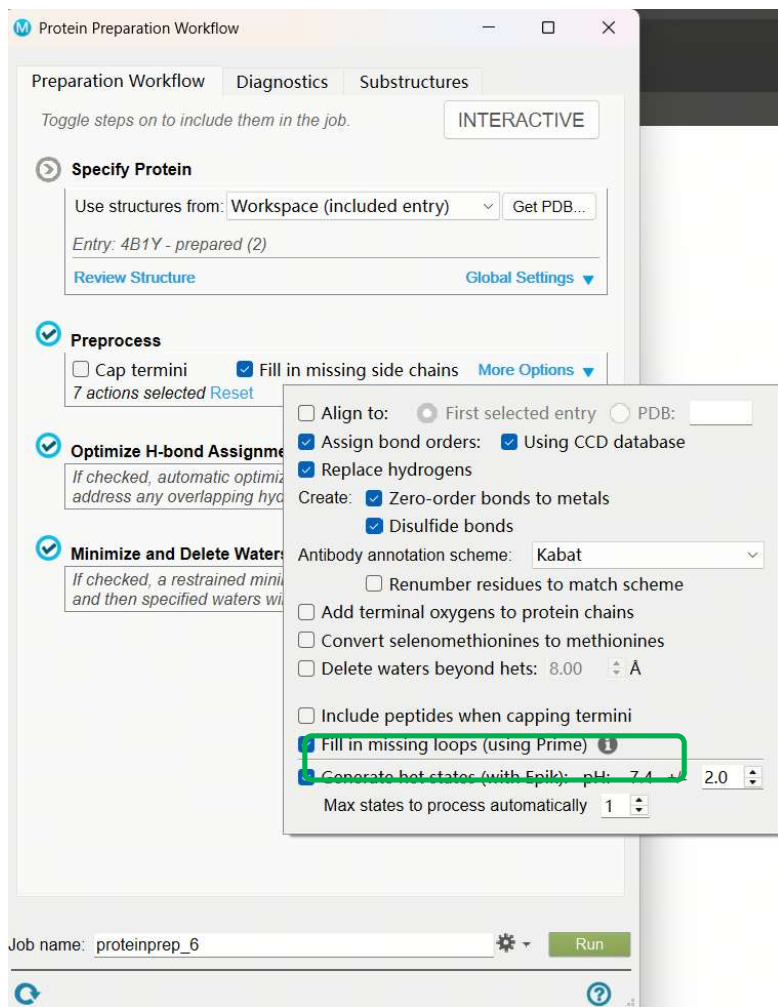
# Membrane Protein



- 从OPM下载下来的结构，膜平面一定是与XY平面平行的，水只会出现在膜蛋白的Z方向上
- 与普通模拟的区别，首先要加膜
- 其次由于XY平面是膜，Z方向是水，控制压力的时候会有区别

# Protein Preparation

无论如何，进行模拟之前一定要做蛋白质准备

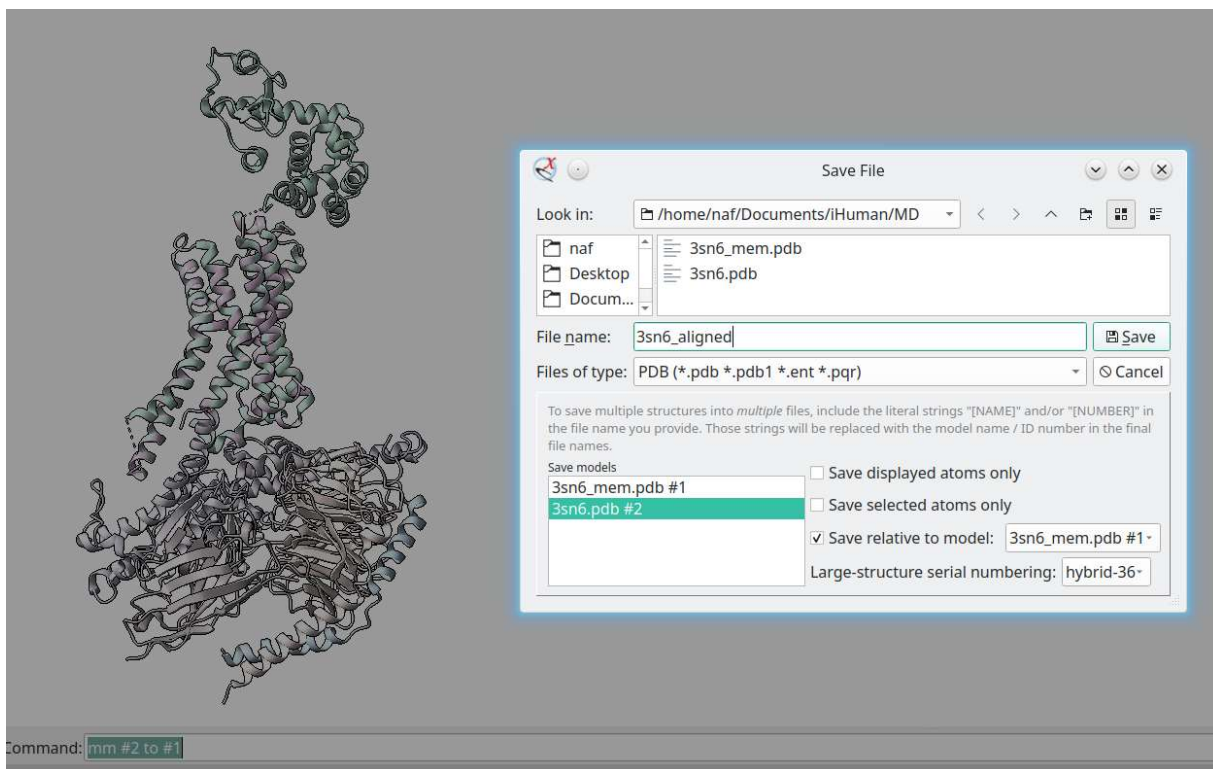


- 补充缺失的残基
- 补充缺失的侧链
- 复原结构解析时引入的氨基酸突变
- 删除不需要的组分
- 修正配体的质子化状态，键级等
- 保存一个同时具有蛋白和配体的PDB文件
- 以及一个只有配体的sdf文件，同时记录一下配体带电量

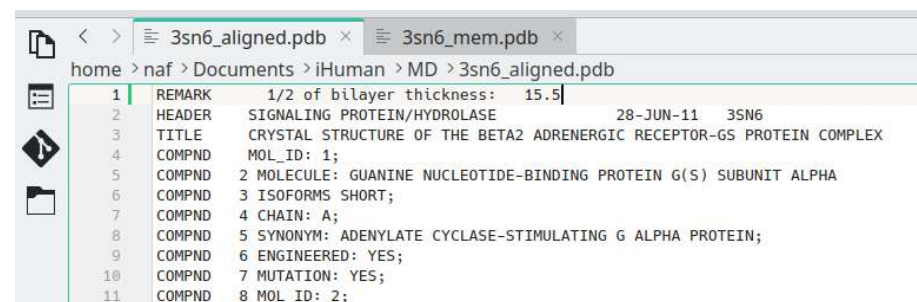


## Align Prepared Protein to OPM structure

在ChimeraX中将待模拟的蛋白align到从OPM下载的结构上，存储。



将第一行复制到align好的文件里。



ChimeraX命令 mm #2 to #1

会将第二个结构，我这里是3sn6.pdb，对齐到第一个结构，也就是OPM上的3sn6.pdb上

## CHARMM-GUI

Effective Simulation Input Generator and More

CHARMM is a versatile program for atomic-level simulation of many-particle systems, particularly macromolecules of biological interest. - M. Karplus

[about us](#) :: [input generator](#) :: [Q&A](#) :: [forum](#) :: [archive](#) :: [lectures](#) :: [movie gallery](#) :: [video demo](#) :: [citations](#) :: [update log](#) :: [jobs & events](#) :: [giving](#)

Some [lectures](#), [job postings](#), and [FAQ](#) are now available. See [update log](#) for update history and [giving](#) for donation. [Contact](#) info is given below.

Logout

### Input Generator

- Job Retriever
- Force Field Converter
- PDB Reader & Manipulator
- Glycan Reader & Modeler
- Ligand Reader & Modeler
- Glycolipid Modeler
- LPS Modeler
- Nanomaterial Modeler
- Multicomponent Assembler
- Solution Builder
- Membrane Builder**
- Martini Maker
- PACE CG Builder
- Polymer Builder
- Drude Prepper
- Enhanced Sampler
- Free Energy Calculator
- LBS Finder & Refiner
- Ligand Designer

### Input Generator

One easiest way to support CHARMM-GUI is to cite the CHARMM-GUI main paper as well as the papers of the modules used in users' publications. Please see [Citations](#) for details.

Since most modules start with PDB Reader, it is strongly recommended to [read the PDB Reader page](#) and to [see the PDB Reader demo](#) in [Video Demo](#).

- Job Retriever  
Facilitates recovery of jobs, when the Job ID is known
- PDB Reader  
Read a PDB file (RCSB or CHARMM formats) into CHARMM
- Glycan Reader & Modeler  
Read carbohydrate structures from a PDB file into CHARMM and/or model user-specified N-/O-glycan or glycan only structure(s)
- Ligand Reader & Modeler  
Generate various ligand structures using the CHARMM force field
- Glycolipid Modeler  
Provide various glycolipid structure and PSF files
- LPS Modeler  
Provide various lipopolysaccharide (LPS) structure and PSF files
- Nanomaterial Modeler  
Generate various nanomaterial systems for molecular dynamics simulation
- Multicomponent Assembler  
Combine many PSF/CRD structures into a heterogeneous system

#### Membrane Builder

Martini Maker  
PACE CG Builder  
Polymer Builder  
Drude Prepper  
Enhanced Sampler

#### Bilayer Builder

HMMM Builder  
Nanodisc Builder  
Monolayer Builder  
Micelle Builder  
Hex Phase Builder



# CHARMM-GUI

<https://charmm-gui.org/?doc=input>

## ☒ Protein/Membrane System

Download PDB File:  Download Source:

Upload PDB File:  7p00\_aligned.pdb

PDB Format: ☒ PDB ☐ PDBx/mmCIF ☐ CHARMM

☐ Check/Correct PDB Format 

选择对齐好了的，准备好了的蛋白，在此上传；  
如果要做蛋白-配体复合物模拟，记得上传的PDB  
里别漏了配体。


记得删除与研究目的不相关的部分。

## ☐ [Membrane Only System](#)

### References for Lipid Force Fields:

J.B. Klauda, R.M. Venable, J.A. Freites, J.W. O'Connor, D.J. Tobias, C. Mondragon-Ramirez, I. Vorobyov, A.D. MacKerell, Jr., and R. W. Pastor (2010)  
Update of the CHARMM all-atom additive force field for lipids: Validation on six lipid types [J Phys Chem B. 114\(23\): 7830-7843](#)

R.M. Venable, A.J. Sodt, B. Rogaski, H. Rui, E. Hatcher, A.D. MacKerell, Jr., R.W. Pastor, and J.B. Klauda. (2014)  
CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. [Biophys J. 107\(1\):134-45](#)

Next Step:   
Select Model/Chain

点击下一步。

Some [lectures](#), [job postings](#), and [FAQ](#) are now available. See [update log](#) for update history and [giving](#) for donation. [Contact](#) info is given below.

Logout

User Profile

Bilayer Builder

PDB InfoSTEP 1STEP 2STEP 3STEP 4STEP 5STEP 6

Title8XZI-prepared

PDB ID8XZI\_COMPLEX

TypeProtein

Experimental MethodUnknown

JOB ID: 4085323996

记住ID号，可以用于回到任务

Model/Chain Selection Option:

Click on the chains you want to select.

Type	SEGID	PDB ID	Residue ID		Engineered Residues
			First	Last	
<input checked="" type="checkbox"/> Protein	PROA	R	19	325	None
<input checked="" type="checkbox"/> Hetero	HETA	R			CMF

CHARMM-GUI uses internal segid format PRO[A-Z] (protein), DNA[A-Z] (DNA), RNA[A-Z] (RNA), and HET[A-Z] (ligands), instead of PDB chain id.

选择需要进行模拟的蛋白和配体

下一步

PDB Manipulation Options:

☒ System pH:

☒ Reading Hetero Chain Residues:

CMF

☐ Rename to   Click this if you want to generate your ligand FF using the PDB coordinate.

☐ Use CHARMM General Force Field to generate CHARMM top & par files (using [ParamChem](#) service)

☒ Use Antechamber to generate CHARMM top & par files

☐ the SDF file from RCSB

☒ the SDF file uploaded from  未选择任何文件

☐ the MOL2 file uploaded from  未选择任何文件

☒ force net charge

☒ atom type

☒ charge method

☐ Use OpenFF to generate CHARMM top & par files

☐ Upload CHARMM top & par for hetero chain

☒ Protonate/Deprotonate based on selected pH

☒ Terminal group patching: 

FirstLast

PROA   ☐ Cyclic peptide?

☐ Preserve hydrogen coordinates:

☐ Mutation:

☒ Protonation state:

ResidueResidue IDPatch

PROA  23  -

☒ Disulfide bonds:

Pair 1Residue IDPair 2Residue ID

PROA  PROA  -

PROA  PROA  -

☐ Phosphorylation:

☐ Ubiquitylation / SUMOylation:

上传准备好的配体sdf文件

输入配体带电量

根据预备使用的蛋白力场选择产生配体力场参数的软件

对Amber力场， 我们使用antechamber

选择封端方式

选择残基质子化状态

连接所有二硫键

潜在的磷酸化修饰等

Ligand reading and its FF generation could be tricky, so please read these common [issues](#).

If this residue exists in the CHARMM topology files ([toppar.str](#)), please rename (or retype) it to the CHARMM residue name. Otherwise, CHARMM will be terminated abnormally.

Please use [this link](#) and the ligand ID to check if this ligand matches the RCSB ID.

Atoms in MOL2 file must have same order as in PDB file to preserve original molecule's coordinates.

It is possible that a PDB file contains wrong disulfide bond information. Please

Next Step: Generate PDB and Orient Molecule

下一步



Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

ENER ENR:	Eval#	ENERgy	Delta-E	GRMS		
ENER INTERN:		BONDs	ANGLes	URKY-b	DIHEdrals	IMPRopers
ENER CROSS:		CMAPs	PMF1D	PMF2D	PRIMO	
ENER EXTERN:		VDWaal	ELEC	HBONDs	ASP	USER
ENER>	0	1089.17985	0.00000	8.12560		
ENER INTERN>		552.02091	1065.34547	53.94700	2607.69352	14.06989
ENER CROSS>		92.20264	0.00000	0.00000	0.00000	
ENER EXTERN>		-1551.08363	-1745.01596	0.00000	0.00000	0.00000

我们已经将结构按OPM对齐了

Orientation Options:


- ☒ Use PDB Orientation
- This option is suggested for an oriented structure from <http://opm.phar.umich.edu>
- ☐ Align the First Principal Axis Along Z
- This option is suggested for small helical bundle or homo-oligomer.
- ☐ Align a Vector (Two Atoms) Along Z
- This option is suggested for an irregular, hetero-oligomer.
- ☐ Run PPM 2.0
- This option run executable for given input structure at [https://opm.phar.umich.edu/ppm\\_server2\\_cgopm](https://opm.phar.umich.edu/ppm_server2_cgopm)  
It may take some minutes depending on protein size.

Positioning Options:

- ☐ Rotate Molecule respect to the X axis  Degree
- ☐ Rotate Molecule respect to the Y axis  Degree
- ☐ Translate Molecule along Z axis  Angstrom
- ☐ Flip Molecule along the Z axis

Area Calculation Options:

- ☐ Generate Pore Water and Measure Pore Size

Next Step:  Calculate Cross-Sectional Area

下一步

## System Size Determination Options:

☐ Homogeneous Lipid "Homogeneous Lipid" option is no longer supported. You can use "Heterogeneous Lipid" option even for homogeneous lipid bilayer building.

☒ Heterogeneous Lipid

1. Box Type:  (Currently, only CHARMM, NAMD, and GROMACS support the hexagonal box)

默认膜体系搭建方式

2. Length of Z based on:

☒ Water thickness  (Minimum water height on top and bottom of the system)

☐ Hydration number  (Number of water molecules per one lipid molecule)

3. Length of XY based on:

☐ Ratios of lipid components

☒ Numbers of lipid components

选择膜脂数目

XY Dimension Ratio:

(The system size along the X and Y must be the same)

选择好膜脂数目后，点击，  
如果没报错就可以了


Show the system info click this once you fill the following table:

Lipid Type	Charge [e]	Tail Info. [sn1/sn2]	Images	# of Lipid on Upperleaflet	# of Lipid on Lowerleaflet	Surface Area
► Sterols						
► PA (phosphatidic acid) Lipids						
▼ PC (phosphatidylcholine) Lipids						
DDPC	0	10:0 / 10:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="64.1"/>
DCPC	0	11:0 / 11:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="64.1"/>
DLPC	0	12:0 / 12:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="64.1"/>
DMPC	0	14:0 / 14:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="64.1"/>
DPPC	0	16:0 / 16:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
DSPC	0	18:0 / 18:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="65.6"/>
PSPC	0	16:0 / 18:0	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="68.3"/>
PVPC	0	16:0 / 16:1	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="64.1"/>
POPC	0	16:0 / 18:1	<a href="#">[Image]</a>	<input type="text" value="90"/>	<input type="text" value="90"/>	<input type="text" value="68.3"/>
PLPC	0	16:0 / 18:2	<a href="#">[Image]</a>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="65.2"/>

## Calculated XY System Size:

	Upperleaflet	Lowerleaflet
Protein Area	1156.13503	1186.81708
Lipid Area	6147	6147
# of Lipids	90	90
Total Area	7303.13503	7333.81708
Protein X Extent	27.44	
Protein Y Extent	21.79	
Average Area	7318.48	
A	85.55	
B	85.55	

对GPCR，初始设置上下各90个，然后微调直到不报错

Next Step:   
Determine the System Size

下一步

# CHARMM-GUI

<https://charmm-gui.org/?doc=input>

## System Building Options:

- ☐ Insertion method Build system using insertion method
- ☒ Replacement method Build system using replacement method
- ☒ Check lipid ring (and protein surface) penetration

For this system, insertion method can not be used. Replacement method will be used instead.

## Component Building Options:

- ☒ Include Ions

Ion Placing Method: Distance

- ☒ Basic Ion Types

NaCl Add Simple Ion Type

- ☐ More Ion Types

Formula	Cation	Anion	Concentration	Neutralizing
NaCl	Na <sup>+</sup>	Cl <sup>-</sup>	0.15	<input checked="" type="radio"/> -

选择NaCl为离子

## Calculate Solvent Composition

Ion	Count
Na <sup>+</sup>	40
Cl <sup>-</sup>	53

点击计算需要的离子数

Please note that the ion count is an approximation based on geometry. The real number will be calculated in the next step.

Next Step:  
Build Components

下一步



Bookmark this [link](#), if you want to comeback to this page.

PDB InfoSTEP 1STEP 2STEP 3STEP 4STEP 5STEP 6

JOB ID: 0805166713

download.tgz

Oriented PDB:[step2\\_orient.pdb \(view structure\)](#)

Component Input:[step4\\_lipid.inp](#)

Component Output:[step4\\_lipid.out](#)

Component Number:[step4\\_components.str](#)

Component PDB:[step4\\_lipid.pdb \(view structure\)](#)

## Check lipid pentration

The protein surface penetration check finds the lipid tails that go beyond the protein surface, and the lipid ring penetration check detects the lipid tails that pass through the cyclic groups (e.g., cholesterol ring) in the simulation systems. Energy minimization can resolve many of these bad contacts, but one might need to visually check the following lipid molecules to ensure the following contacts are resolved. The user can regenerate the lipid bilayer if necessary.

Protein surface penetration:

No protein surface penetration is found.

Lipid ring penetration:

No lipid ring penetration is found.

## Building Ion and Waterbox

Membrane components are generated. Due to time constrains, we first generate the lipid bilayer then generate ions and the water box. Click "Next Step" to generate ions and the water box.

没报错就可以下一步了

Next Step:  
Assemble Components

Bookmark this [link](#), if you want to comeback to this page

PDB InfoSTEP 1STEP 2STEP 3STEP 4STEP 5STEP 6

JOB ID: 0805166713

download.tgz

Oriented PDB:[step2\\_orient.pdb \(view structure\)](#)

Component Input:[step4\\_lipid.inp](#)

Component Output:[step4\\_lipid.out](#)

Component Number:[step4\\_components.str](#)

Generated Waterbox:

[step4.2\\_waterbox.inp](#)

[step4.2\\_waterbox.out](#)

[step4.2\\_waterbox.crd](#)

Input file for water box inclusion

Output file for water box inclusion

CRD file for the water box

Generated Ion:

[step4.3\\_ion.inp](#)

[step4.3\\_ion.out](#)

[step4.3\\_ion.pdb](#)

Input file for ion inclusion

Output file for ion inclusion

PDB file for the ion

Component PDB:[step4\\_lipid.pdb \(view structure\)](#)

Assemble Generated Components:

Membrane components are generated. Click "Next Step" to assemble those components together.

没报错就可以继续下一步了

Next Step:  
Assemble Components

# CHARMM-GUI

<https://charmm-gui.org/?doc=input>

## Force Field Options:

AMBER						
CHARMM36m						
CHARMM36						
AMBER						
Protein	DNA	RNA	Glycan	Lipid	Water	Ligand
FF14SB	OL15	OL3	GLYCAM_06j	Lipid21	TIP3P	GAFF2

☐ Hydrogen mass repartitioning  
☐ 12-6-4 ion  
Glycolipids and lipoglycans are not supported in current CHARMM-GUI Amber FF implementation.

选择力场，charmm36m及amber14SB力场均可

对amber19SB力场，只有软件amber能识别；对gromacs，最多使用到14SB力场。


## Input Generation Options:

- ☒ AMBER  
☒ GROMACS  
☒ OpenMM  
☐ NAMD  
☐ GENESIS  
☐ Tinker

选择进行MD的软件，会生成勾选的软件的需要模拟的全套文件

## Equilibration Options:

- ☐ P21 image transformation (only available for CHARMM)  
☐ CHARMM DOMDEC (only available for CHARMM)  
☒ Generate grid information for PME FFT automatically  
☐ Explicit grid information for PME FFT
- |                      |                      |                      |
|----------------------|----------------------|----------------------|
| X                    | Y                    | Z                    |
| <input type="text"/> | <input type="text"/> | <input type="text"/> |
- ☒ NPT ensemble  
☐ NPAT ensemble  
☐ NPgT ensemble
- Surface Tension  (dyne/cm)
- Temperature:  K

Next Step:   
Generate Equilibration and Dynamics Inputs

下一步



Bookmark this [link](#), if you want to comeback to this page

- PDB Info
- STEP 1
- STEP 2
- STEP 3
- STEP 4
- STEP 5
- STEP 6

JOB ID: 0805166713

download.tgz

Assembled PDB: [step5\\_assembly.pdb](#) (view structure)  
Input Generator Input: [step5\\_input.inp](#)  
Input Generator Output: [step5\\_input.out](#)  
CHARMM Minimization: [step5\\_input\\_minimization.str](#)  
Crystal Image: [crystal\\_image.str](#)  
FFT Calculation: [checkfft.py](#)  
Restraints: [membrane\\_restraint.str](#) Lipid Positional Restraint  
[membrane\\_restraint2.str](#) Lipid Dihedral Restraint  
Equilibration Inputs: [amber/step6\\_0\\_minimization.mdin](#) Minimization Input  
[amber/step6\\_1\\_equilibration.mdin](#) Equilibration Step 1  
[amber/step6\\_2\\_equilibration.mdin](#) Equilibration Step 2  
[amber/step6\\_3\\_equilibration.mdin](#) Equilibration Step 3  
[amber/step6\\_4\\_equilibration.mdin](#) Equilibration Step 4  
[amber/step6\\_5\\_equilibration.mdin](#) Equilibration Step 5  
[amber/step6\\_6\\_equilibration.mdin](#) Equilibration Step 6  
Production Inputs: [amber/step7\\_production.mdin](#) Production Input

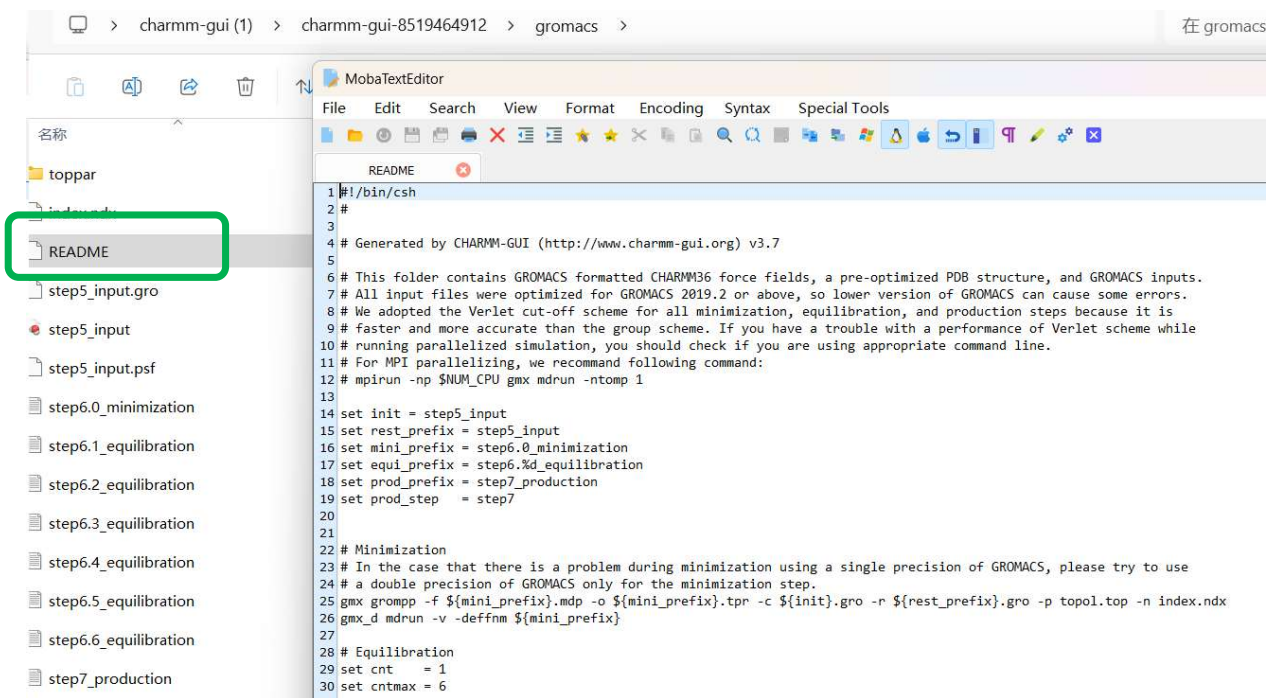
搞定，把结果下载下来即可

Equilibration Input Notes:

```
!
! Setup Restraints for Protein and Lipids (see @liptype_restraint.str)
!
! Suggested Equilibration Scheme [Reducing Force Constants]
! (5 Cycles, 1 cycle = 50 - 100 ps )
!
!
!   1 cycle   2 cycle   3 cycle   4 cycle   5 cycle   6 cycle
!-----
! BB      10.0      5.0       2.5       1.0       0.5       0.1
! SC       5.0       2.5       1.0       0.5       0.1       0.0
! wforce   2.5       2.5       1.0       0.5       0.1       0.0
! tforce   2.5       2.5       1.0       0.5       0.1       0.0
! mforce   2.5       2.5       1.0       0.5       0.1       0.0
! ion      10.0      0.0       0.0       0.0       0.0       0.0
!
!
```

# CHARMM-GUI

<https://charmm-gui.org/?doc=input>



解压缩之后，  
readme内有运行  
MD需要的所有命  
令。

Charmm-gui产生  
的文件是宝藏，  
值得好好学习。

- README里有地方使用了双精度的gmx，我们可能没有安装，需要手动改成我们安装的gromacs名称，比如把gmx\_d都改成gmx;
- 给README添加可执行权限，再直接执行它，就可以自动把模拟跑起来了
- 记得按需求修改一下step7\_production.mdp里写的模拟时长

```
chmod +x README  
./README
```

## 膜蛋白模拟与普通蛋白模拟重要区别

普通蛋白mdp文件:

- 各向同性控压 isotropic
- 指定1个compressibility, 1个tau\_p和ref\_p即可

```
; 压力控制
pcoupl      = Parrinello-Rahman
pcoupltype  = isotropic ; 各向同性压力
tau_p       = 5          ; 压力耦合时间常数
compressibility = 4.5e-5 ; 压缩率
ref_p       = 1.0        ; 参考压力1.0 bar
```

膜蛋白mdp文件:

- 对xy方向和z方向分别进行压力控制, 采用 semiisotropic
- 指定2个compressibility, 2个ref\_p和2个tau\_p

```
; 压力控制
pcoupl      = Parrinello-Rahman
pcoupltype  = semiisotropic ;
tau_p       = 5 5          ; 压力耦合时间常数
compressibility = 4.5e-5 4.5e-5 ; 压缩率
ref_p       = 1.0 1.0      ; 参考压力1.0 bar
```

半各向同性压力耦合是一种用于分子动力学模拟的方法, 特别适用于涉及膜或双层系统的模拟。这种方法允许在x和y方向上进行各向同性压力耦合, 但在z方向上进行不同的压力耦合。这对于膜模拟特别有用, 因为脂质双层应该被允许在x-y平面上变形, 但在z方向上则不应变形。