自由能计算

1）cd /home/taotao/free\_energy/335#进入自己的目录

script.pl#修改334.pdb为对应目录的名称

#!/usr/bin/perl

use strict;

use warnings;

# 获取要替换的文件名

my $replacement = shift;

# 在文件名末尾添加.pdb扩展名如果没有提供

$replacement .= '.pdb' unless $replacement =~ /\.pdb$/;

# 读取job1.sh文件

my @lines;

{

    open(my $fh, '<', 'job1.sh') or die "无法打开 job1.sh 文件: $!";

    @lines = <$fh>;

    close($fh);

}

# 替换文件名

foreach my $line (@lines) {

    # 只替换以"334.pdb"结尾的行的文件名

    if ($line =~ /^(.\*?334\.pdb)\b/) {

        $line =~ s/334\.pdb/$replacement/g;

    }

}

# 将修改后的脚本写回job1.sh文件

{

    open(my $fh, '>', 'job1.sh') or die "无法写入 job1.sh 文件: $!";

    print $fh @lines;

    close($fh);

}

# 输出替换完成的消息

print ".pdb 替换为 $replacement\n";

2) perl script.pl

job1.sh#运行如下命令

#!/bin/bash

GMX=/usr/local/gromacs/bin

$GMX/gmx editconf -f 335.pdb -o box.gro -bt dodecahedron -d 1.2 -box 5 5 5

$GMX/gmx solvate -cp box.gro -cs spc216.gro -o solvated.gro -p topol.top -maxsol 600

$GMX/gmx grompp -f em.mdp -c solvated.gro -p topol.top -o em.tpr

$GMX/gmx mdrun -v -deffnm em >& em.txt &

$GMX/gmx grompp -f equil.mdp -c em.gro -p topol.top -o equil.tpr

$GMX/gmx mdrun -deffnm equil >& equil.txt &

3) perl job1.sh

4) python3 /home/taotao/free\_energy/334/lambda.py -d 335

lambda.py#生成lambda目录、复制原目录的top、gro、mdp(mdout和run)文件，并更改run.mdp文件（-d 335为output\_files = '/home/taotao/free\_energy'的补充，补充后为：output\_files = '/home/taotao/free\_energy/335'

）

import os

import shutil

import sys

run\_mdp\_template = "run\_mdp.mdp"

output\_files = '/home/taotao/free\_energy'

def write\_mdp(mdp\_content, mdp\_filename, output\_directory):

    with open(os.path.join(output\_directory, mdp\_filename), 'w') as f:

        f.write(mdp\_content)

# 读取模板文件内容

with open(run\_mdp\_template, 'r') as f:

    mdp\_template\_content = f.read()

#lambda\_value = [0.0, 0.2, 0.4, 0.6, 0.8, 0.9, 1.0]

lambda\_values = [0,1,2,3,4,5,6]

if len(sys.argv) > 1 and sys.argv[1] == '-d':

    if len(sys.argv) > 2:

        output\_files = os.path.join(output\_files, sys.argv[2])

for lambda\_value in lambda\_values:

    lambda\_number = str(lambda\_value)  # 将小数点替换为下划线

    lambda\_directory = os.path.join(output\_files, f'lambda\_0{lambda\_number}')

    if not os.path.exists(lambda\_directory):

        os.mkdir(lambda\_directory)

    gro\_file = os.path.join(output\_files, 'equil.gro')

    top\_file = os.path.join(output\_files, 'topol.top')

    shutil.copy(gro\_file, os.path.join(lambda\_directory, 'equil.gro'))

    shutil.copy(top\_file, lambda\_directory)

    mdp\_content = mdp\_template\_content.format(lambda\_value)

    # 写入替换后的内容到新的mdp文件中

    write\_mdp(mdp\_content, 'run.mdp', lambda\_directory)

5) job.sh#自动进入lambda文件运行如下命令

#!/bin/bash

# Change to the location of your GROMACS-2018 installation

GMX=/usr/local/gromacs/bin

for (( i=0; i<7; i++ ))

do

    LAMBDA=$i

    # A new directory will be created for each value of lambda and

    # at each step in the workflow for maximum organization.

    cd lambda\_0$LAMBDA

    ##############################

    # ENERGY MINIMIZATION STEEP  #

    ##############################

    echo "Starting minimization for lambda = $LAMBDA..."

       $GMX/gmx grompp -f run.mdp -c equil.gro -r equil.gro -p topol.top

       $gmx mdrun >& log.txt &

        cd ../

       cd lambda\_0$LAMBDA

done

exit;

6）gmx bar -b 100 -f lambda\_0?/dhdl.xvg处理数据得到自由能