dir：/STRESS-1a27/surface\_input\_output\_file

input files：

op1A271\_CA.pdb，op1A271\_SIMP.pdb;

1A271.fnm from MMTK.

1.README\_interior step II：

perl ../surface\_residue/top\_nm.pl 10 < 1A271.fnm > 1A27.fnm\_t10,

I got 1A27.fnm\_t10.

2.step III,

python ../surface\_residue/get\_box\_size\_to\_det\_num\_MC\_steps.py ./op1A271\_SIMP.pdb > num\_mc\_steps.txt

I got num\_mc\_steps.txt, with mc\_steps of 1600000.

3.step III, 2nd usage:

cat op1A271\_CA.pdb | wc -l

output value was 570，by a factor of 10 to get the steps of simulations to be 5700

4.step IV，first usage:

../surface\_residue/code\_pack/bindingSites op1A271\_CA.pdb 4 out\_1A27\_ 5700 1600000 op1A271\_SIMP.pdb 1A27.fnm\_t10 > ./out\_1A27.txt

simulation=5700 num\_mc\_steps=1600000, to heavy computation work for mac,

so change 5700 1600000 to 2 2 for test run

../surface\_residue/code\_pack/bindingSites op1A271\_CA.pdb 4 out\_1A27\_ 2 2 op1A271\_SIMP.pdb 1A27.fnm\_t10 > ./out\_1A27.txt

only get: out\_1A27\_\_BL.dat

 and out\_1A27.txt

whihc is not consistant with 4 files in readme:

 out\_1EDH\_\_bindingSites.dat

 out\_1EDH\_\_LC.dat

 out\_1EDH\_\_BL.dat

 out\_1EDH.txt