Tutorial of radii calculation of nanotube and protein by MolAICal

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1. Introduction

In this tutorial, the radii calculations of nanotube and protein are introduced. This tutorial is divided into three parts: nanotube radii calculation, protein radii calculation and advance radii calculation in peptide channel. The advance radii calculation is based on the PDB and PSF files which are produced by the CHARMM force field. Here, MolAICal (https://molaical.github.io) is employed for this tutorial.

2. Materials

2.1. Software requirement

1) MolAICal: https://molaical.github.io
2) VMD: https://www.ks.uiuc.edu/Research/vmd

2.2. Example files

1) All the necessary tutorial files are downloaded from:
https://github.com/MolAICal/tutorials/tree/master/005-radiiCal

3. Procedure

3.1. Nanotube radii calculation

1) Build nanotube by VMD software: Extensions→Modeling→Nanotube Builder (see Figure 1).

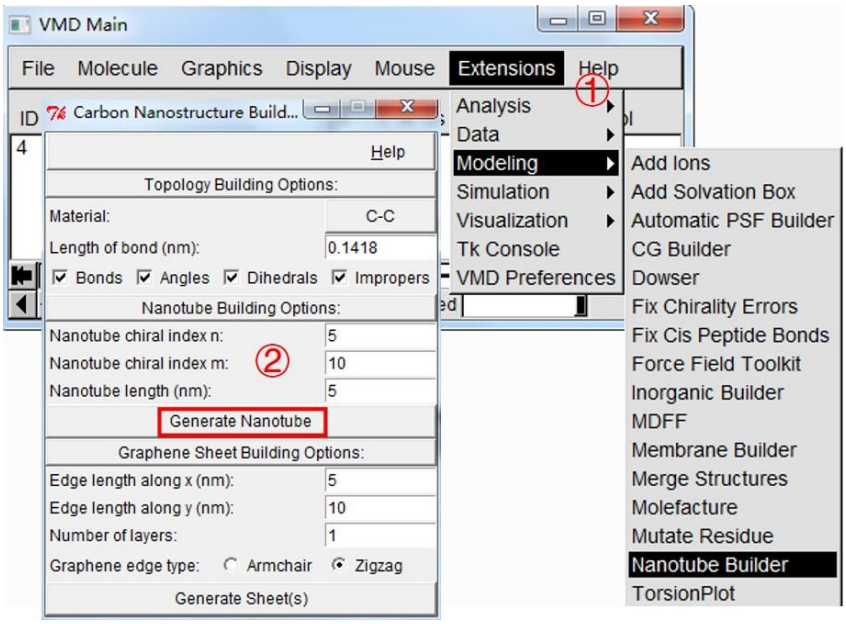


Figure 1. Building nanotube

2) Using a similar way in the window of VMD, open Tk Console: Extensions→Tk Console. Change to the directory that contains material files such as “nanotube.pdb” and “parameter.dat” by command “cd <your directory path>” in Tk Console. For example:

#> cd d:/005-radiiCal/nanotube

3) Saving the nanotube as “nanotube.pdb” by below command in Tk Console:
#> set all [atomselect top all]
#> $all writepdb nanotube.pdb

4) Selecting any point within the built nanotube. You can choose the center coordinates between two different atoms that locate at the channel surface (**see an example in Appendix 1 of this document**). In this tutorial, it is -0.2015 0.4185 30.147. Open the “parameter.dat” in folder “005-radiiCal\nanotube” and add this point coordinates to “cpoint”. The parameter “cpoint” and “vector” should be set as below:

---
cpoint -0.2015 0.4185 30.147
vector 0.00 0.00 1.00

The “0.00 0.00 1.00” means radii measurement along Z-axis. “0.00 1.00 0.00” means radii measurement along Y-axis. “1.00 0.00 0.00” means radii measurement along X-axis. The channel should be placed along any axis roughly.

5) Running command for radii calculation in Windows DOS or Linux console as below:
#> molaical.exe -channel radii -cpp parameter.dat

It will generate “channel_radii.dat”, “dot.vmd_plot” and “surf.vmd_plot”. The files of “dot.vmd_plot” and “surf.vmd_plot” can show the channel surface in VMD software. Open VMD Tk Console using a similar way of Figure 1: Extensions→Tk Console. Then run command as below:
#> source dot.vmd_plot

We omit the way for representation of nanotube in VMD. You can set it according to your preference. You will see the dot surface of channel as in Figure 2:

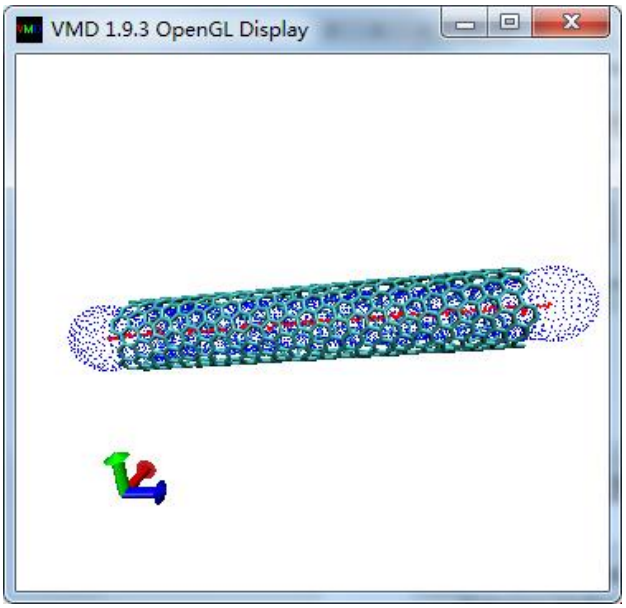


Figure 2. The channel surface of nanotube

The file of "channel_radii.dat" contains the reaction coordinates and radii values. The 1st column of "channel_radii.dat" contains reaction coordinates. The 2ed column of "channel_radii.dat" contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. The plotted result is shown in Figure 3 (**see a drawing example in Appendix 2 of this document**):

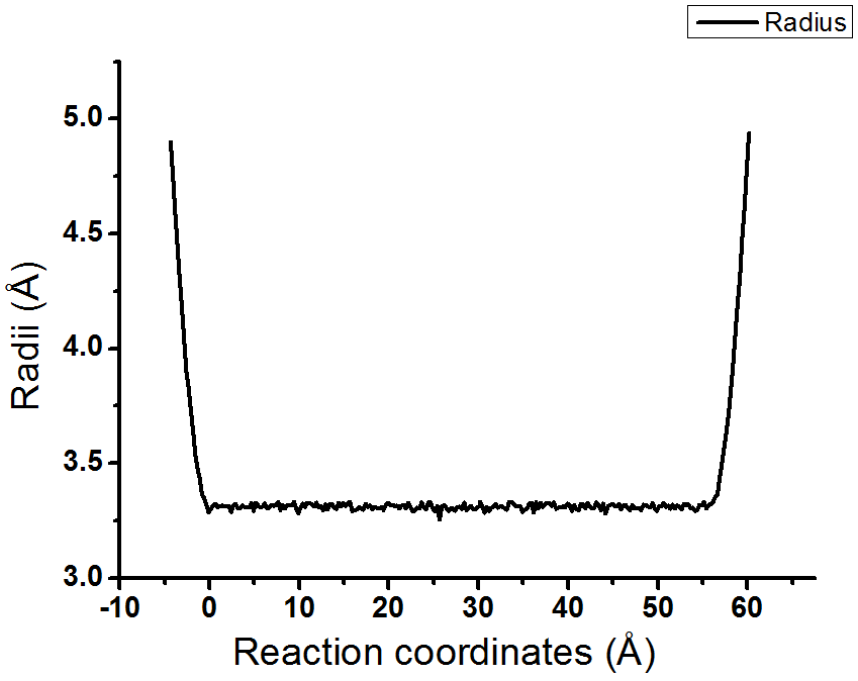


Figure 3. Radii versus reaction coordinates

3.2. Protein radii calculation

Go to the tutorial directory:

#> cd 005-radiiCal/KcsA

Selecting any point within the protein channel (**see an example in Appendix 1 of this document**). The parameter "cpoint" is set to the coordinates of the selected point. The parameters "cpoint" and "vector" should be set as below:

---

cpoint 0.001 0.006 1.927
vector 0.00 0.00 1.00

The "0.00 0.00 1.00" means radii measurement along Z-axis. "0.00 1.00 0.00" means radii measurement along Y-axis. "1.00 0.00 0.00" means radii measurement along X-axis. The channel should be placed along any axis roughly.

1). Running command for radii calculation in Windows DOS or Linux console as below:

#> molaical.exe -channel radii -cpp parameter.dat

2) It also generates "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot". Open VMD Tk Console using a similar way of Figure 1: Extensions→Tk Console. Then run command in Tk Console as below:

#> mol load pdb KcsA.pdb
#> source dot.vmd_plot

We omit the way for representation of protein in VMD. You can set it according to your preference. You will see the dot surface in Figure 4:

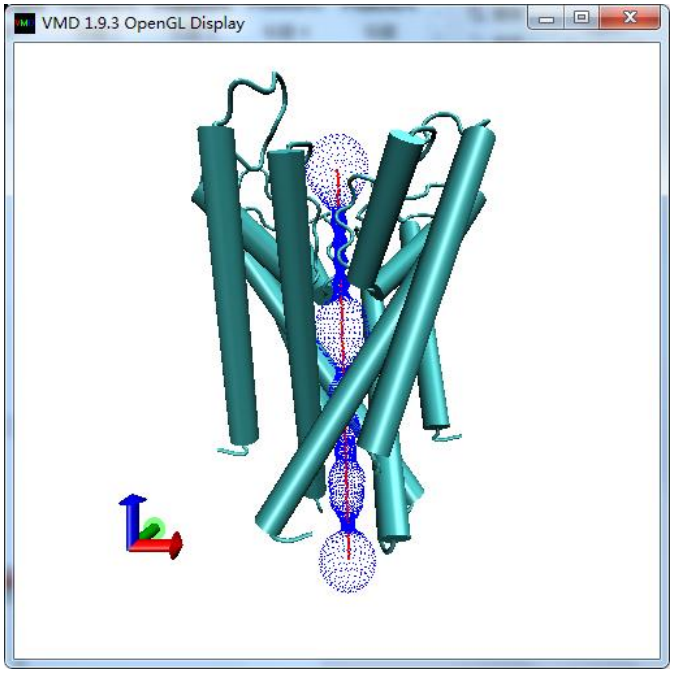


Figure 4. Dot surface in protein channel

The file of "channel_radii.dat" contains the reaction coordinates and radii values. The 1st column of "channel_radii.dat" contains reaction coordinates. The 2ed column of "channel_radii.dat" contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. Radii are plotted in Figure 5 (**see a drawing example in Appendix 2 of this document**):

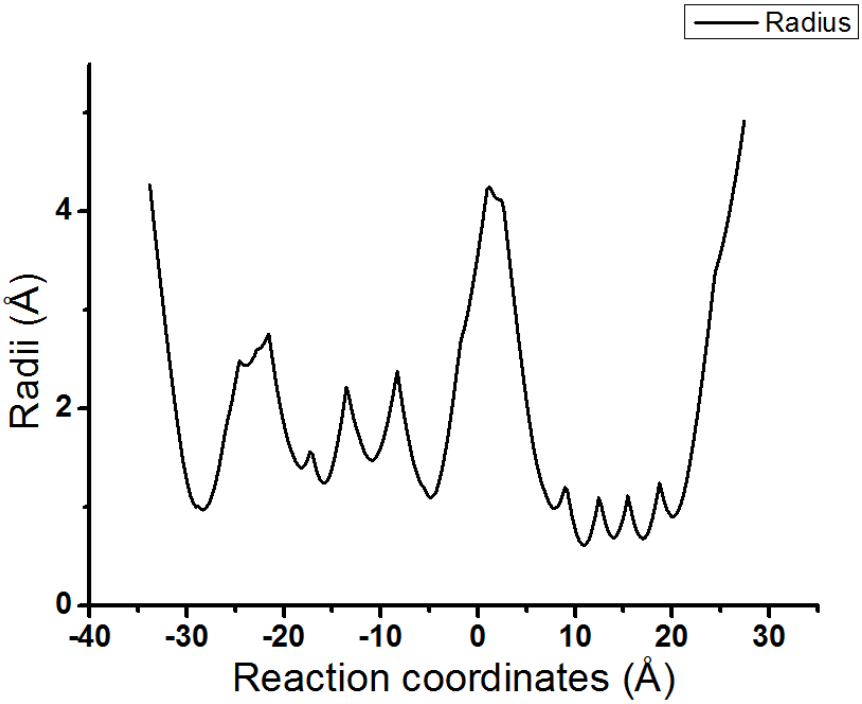


Figure 5. Radii versus reaction coordinates

Notice: the parameter "conpar" in the file "parameter.dat" is a control constant whose default value is 0.15. The high value of control constant "conpar" will increase the random measurement process. So you will find some weird paths of radii measurement at times. If the pore is very regular and along one direction of X, Y and Z axis generally, you can decrease the value of control constant "conpar" such as 0.04. But the "conpar" cannot be set to 0. In the circumstances, you will get the regular measurement path along the channel.

3.3. Advance radii calculation

This part example calculates radii of peptide channel by PDB and PSF files which are generated by the CHARMM force field. Go to the tutorial directory:

#> cd 005-radiiCal/GramicidinA

Selecting any point within the peptide hole (**see an example in Appendix 1 of this document**). The parameter "cpoint" is set to the coordinates of the selected point. The parameters "pdbpath", "psfpath", "cpoint" and "vector" should be set as below:

---

pdbpath 1JNO.pdb
psfpath 1JNO.psf
cpoint 0.1625 -0.629 -1.838
vector 0.00 0.00 1.00

The "0.00 0.00 1.00" means radii measurement along Z-axis. "0.00 1.00 0.00" means radii measurement along Y-axis. "1.00 0.00 0.00" means radii measurement along X-axis. The channel should be placed along any axis roughly.

1). Running command for radii calculation in Windows DOS or Linux console as below:

#> molaical.exe -channel radii -cpp parameter.dat -fc charmm

2) It also generates “channel_radii.dat”, “dot.vmd_plot” and “surf.vmd_plot”. Open VMD Tk Console using a similar way of Figure 1: Extensions→Tk Console. Then run command in Tk Console as below:

#> mol load pdb 1JNO.pdb

#> source surf.vmd_plot

We omit the way for representation of peptide in VMD. You can set it according to your preference. You will see the surface in the peptide channel (see Figure 6):

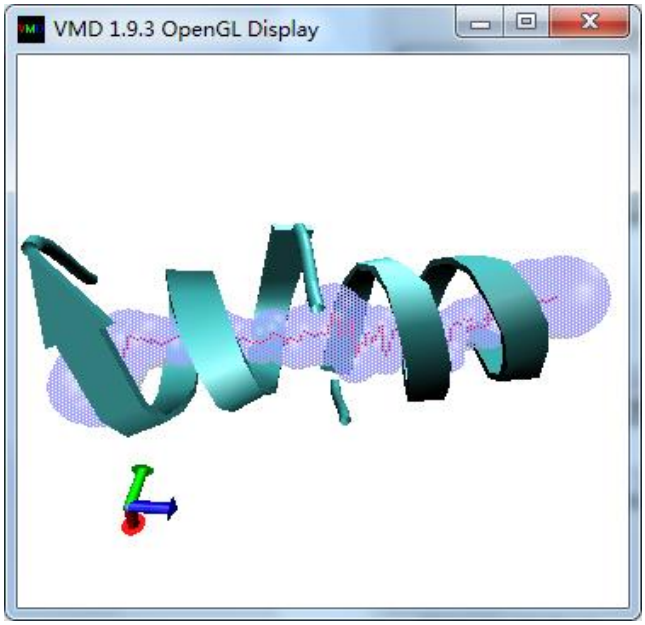


Figure 6. Dot surface in peptide channel

The file of “channel_radii.dat” contains the reaction coordinates and radii values. The 1st column of “channel_radii.dat” contains reaction coordinates. The 2ed column of “channel_radii.dat” contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. Radii are plotted in Figure 7 (**see a drawing example in Appendix 2 of this document**):

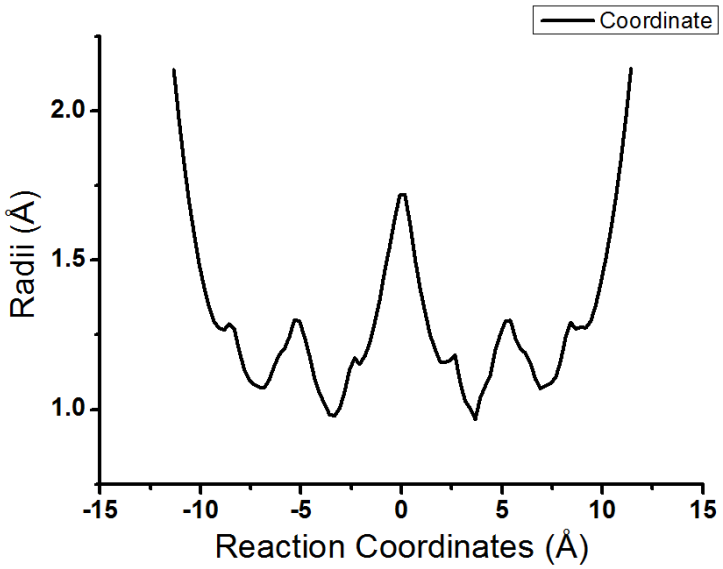


Figure 7. Radii versus reaction coordinates

Appendix 1. Select any point in the pore

How get the coordinates in the channel? Using part "**3.2. Protein radii calculation**" as an example:
#> cd 005-radiiCal/KcsA

1. Open vmd and load "KcsA.pdb" as below Figure 8

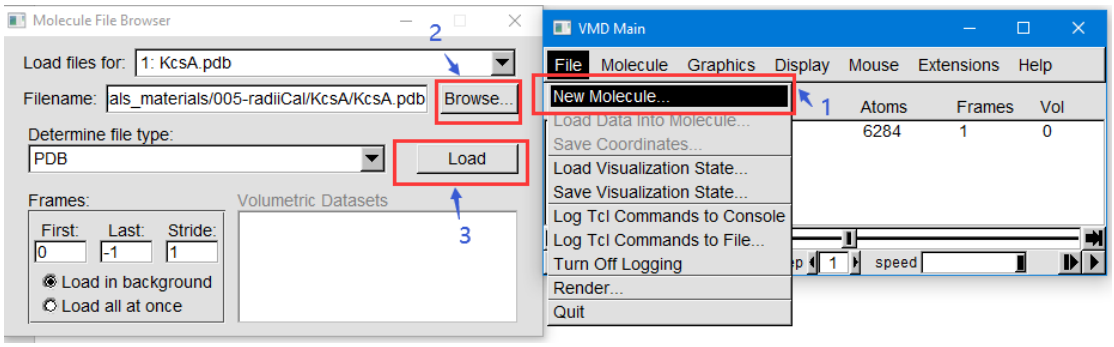


Figure 8

2. Show the cartoon mode of protein as Figure 9, **this is just for better observation**. Users can **omit this step** if they can operate protein easily.

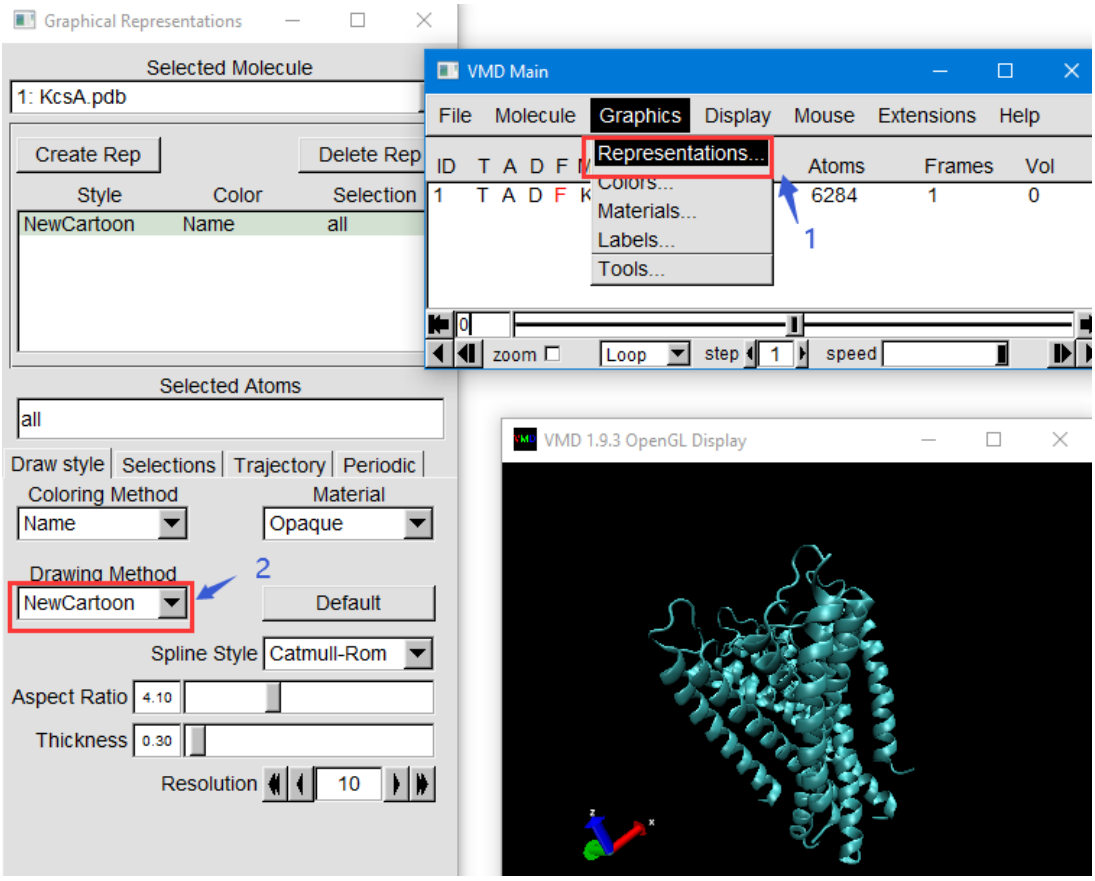


Figure 9

3. Press the character "r" on the keyboard, and it will rotate the object in VMD; Press the number "1" on the keyboard, click an atom in VMD and it will select this atom; Press the number "2" on the keyboard, and click atom 1, then click atom 2, it will generate a bond line. **In this step, press the number "2", and then successively click two atoms inside the channel in VMD as shown in Figure 10.** Obviously, most of the bond line between two atoms in Figure 10 is inside the channel.

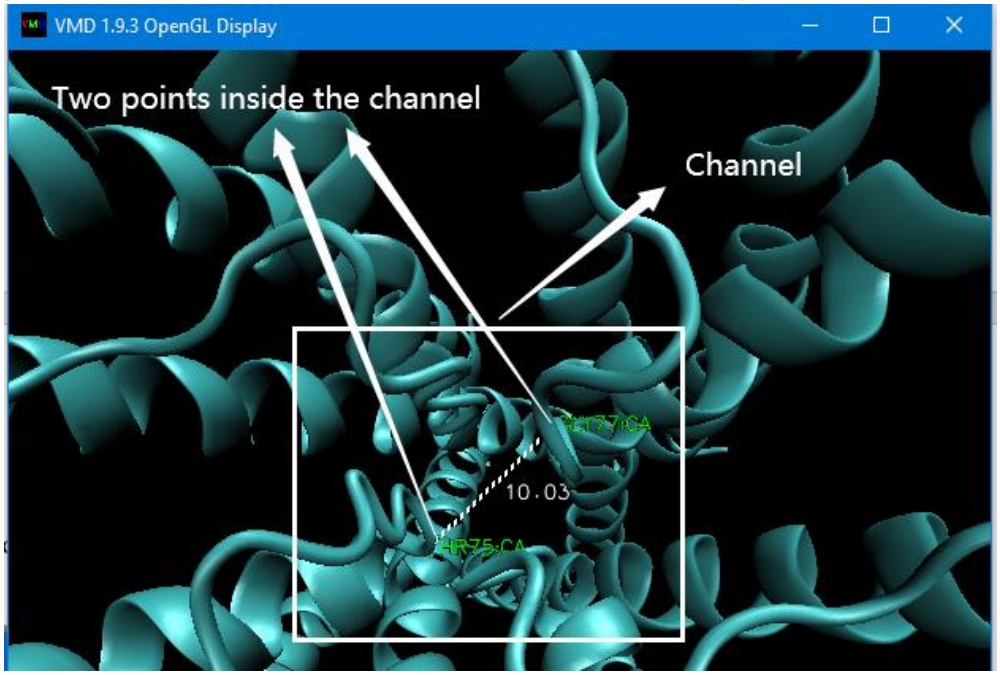


Figure 10

4. Users can get coordinates of selected atoms by “Graphics→Labels→Atoms→XYZ” (see Figure 11)

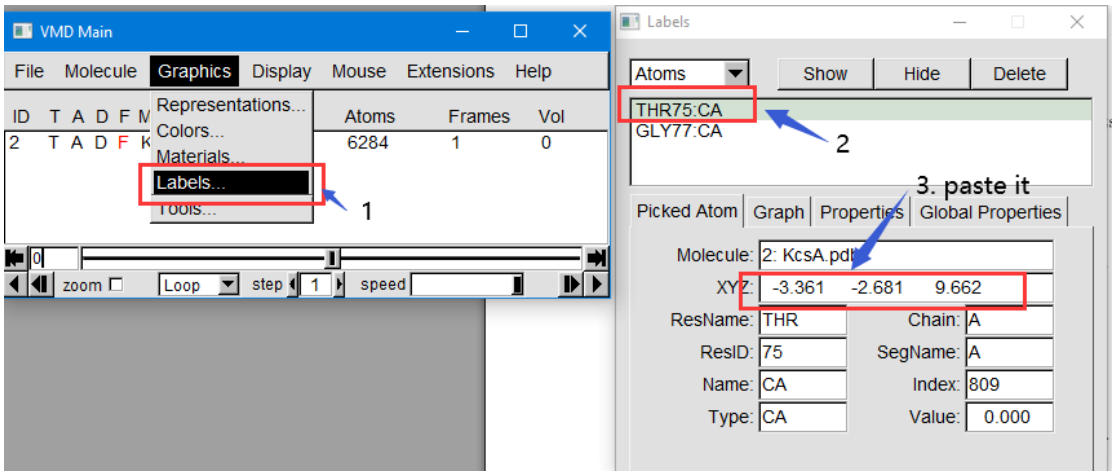


Figure 11

It will get:

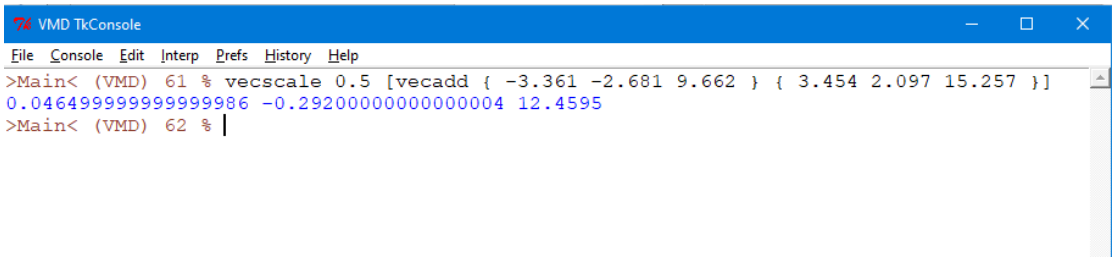
Coordinates of atom 1: -3.361 -2.681 9.662

Coordinates of atom 2: 3.454 2.097 15.257

Obviously, most of the bond line between two atoms in Figure 10 is inside the channel. Here, **average coordinates** are selected between atom 1 and 2 = (Coordinates of atom 1 + Coordinates of atom 2) /2 = {[-3.361, -2.681, 9.662] + [3.454, 2.097, 15.257]} / 2 = **0.0465, -0.292, 12.4595** → **This is an instance for selecting any point in channel or pore.**

In addition, users can use **VMD Tkconsole** to calculate the center points between atoms 1 and 2 as the following command, and then press “Enter” on the keyboard:

#> vecscale 0.5 [vecadd { -3.361 -2.681 9.662 } { 3.454 2.097 15.257 }]



Appendix 2. Radii plotting in MolAICal

To use draw radii figures in MolAICal, go to the virtual environment:

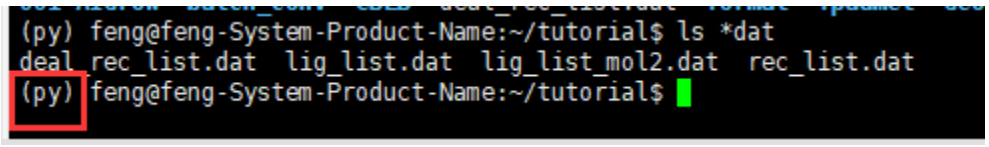
In Windows system:

#> D:\MolAICal-win64\mtools\py\Scripts\activate.bat

In Linux system:
#> source /home/feng/tutorial/MolAICal-linux64/mtools/py/bin/activate

Note: Please replace "D:\MolAICal-win64" or "/home/feng/tutorial/MolAICal-linux64" with your **real path** of MolAICal.

If you go into the virtual environment, you will see a graph similar to the following:



Go to the folder "005-radiiCal/KcsA":

#> cd 005-radiiCal/KcsA

Then, input the below command to draw and save the radii plotting figure (see Figure 12):

#> python plot_radii.py

Note: Users can **modify** the file "plot_radii.py" for specific graphic requirements if familiar with Matplotlib (https://matplotlib.org).

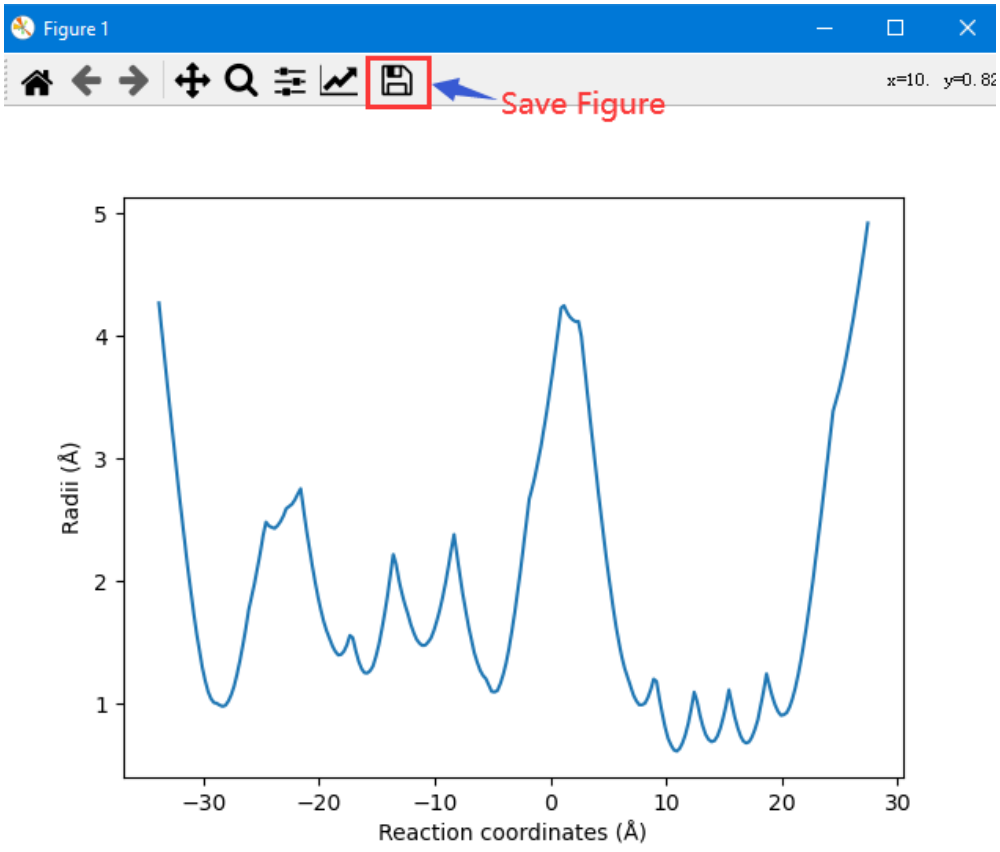


Figure 12