Tutorial of potential of mean force by MolAICal

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1. Introduction

The potential of mean force (PMF) can be used to calculate the free energy landscape with principal components. The PMF along the coordinate is computed from the average distribution function (see below equation).

$\Delta G = -k_B T \ln \rho(x, y)$

Where T and k_B is the temperature and Boltzmann constant, respectively. The x and y represent two principal components. In this tutorial, the molecular dynamics (MD) simulated results of glucagon receptor (GCGR) are selected for this example (Front Chem. 2019 Dec 17;7:851.)[1]. Here, MolAICal (https://doi.org/10.1093/bib/bbaa161) is employed for this tutorial.

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2. Materials

2.1. Software requirement

1) MolAICal: https://molaical.github.io

2.2. Example files

1) All the necessary tutorial files are downloaded from:
https://github.com/MolAICal/tutorials/tree/master/007-PMF

3. Procedure

3.1. Plot energy contour by MolAICal

```
#> cd 007-PMF
```

Open “rmsd-dis.dat”, the 1st column is RMSD values, 2nd column is the distance. You can replace these data with your appointed principal components. Then, run the command:

```
#> molaical.exe -pmf -i rmsd-dis.dat
```

The plotted results show in Figure 1

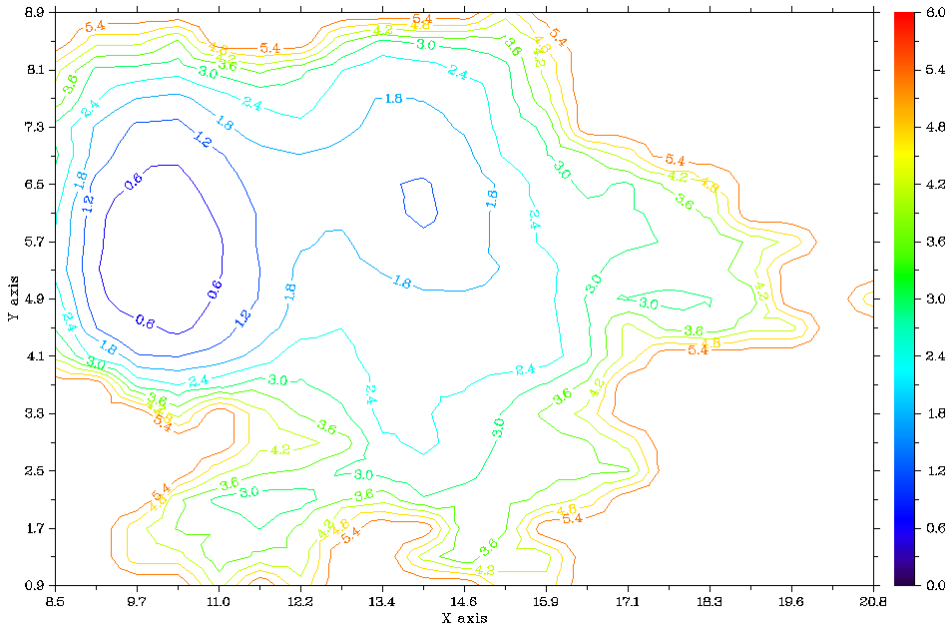

Figure 1. PMF contour.

Notice: If there are empty lines at the end of your resemble file “rmsd-dis.dat”, it will happen some errors. You can delete the empty lines at the end of your resemble file “rmsd-dis.dat”, or use the development version of MolAICal (https://molaical.github.io).

Running command as below. It plots the figure with another shape (see Figure 2).

#> molaical.exe -pmf -i D:/pmf/rmsd-dis.dat -g 20 -l 10 -m conshd -b none -x "RMSD" -y "Distance"

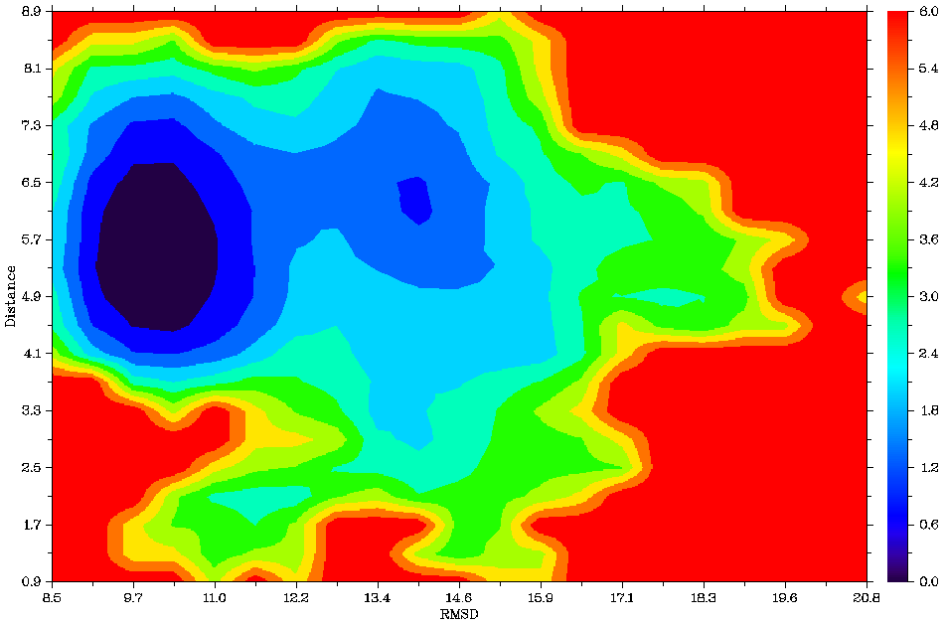

Figure 2. PMF contour.

3.2. Advance tutorial

The part just produces a beautiful figure by OriginLab software. If you do not care about it, you can skip this part. The demo version of OriginLab can be downloaded from https://www.originlab.com.

Running command as below:

#> molaical.exe -pmf -i rmsd-dis.dat > plot.dat

The file “plot.dat” can be used to reproduce the contour of free energy.

1) Import “plot.dat” (see Figure 3)

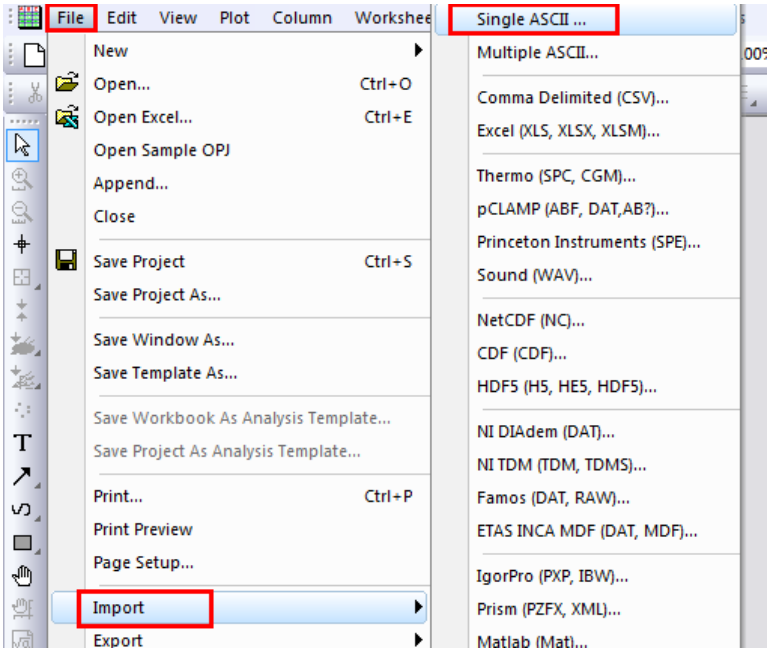

Figure 3. Import data

2) Double click selected column C(Y) and change C(Y) to Z (see Figure 4)

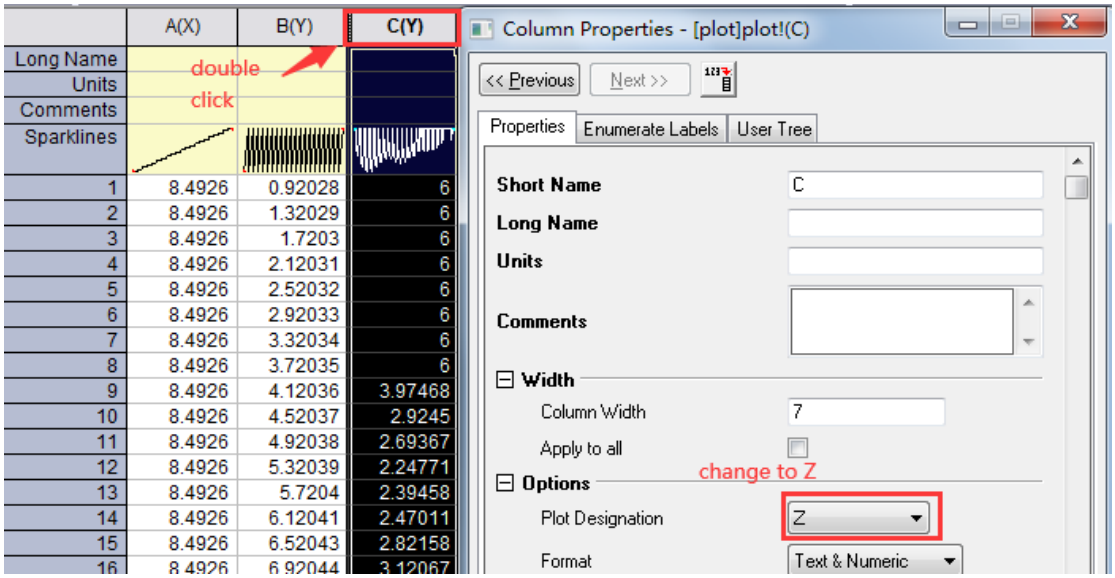

Figure 4. set parameters for plotting

3) Select all data columns and plot the contour (see Figure 5)

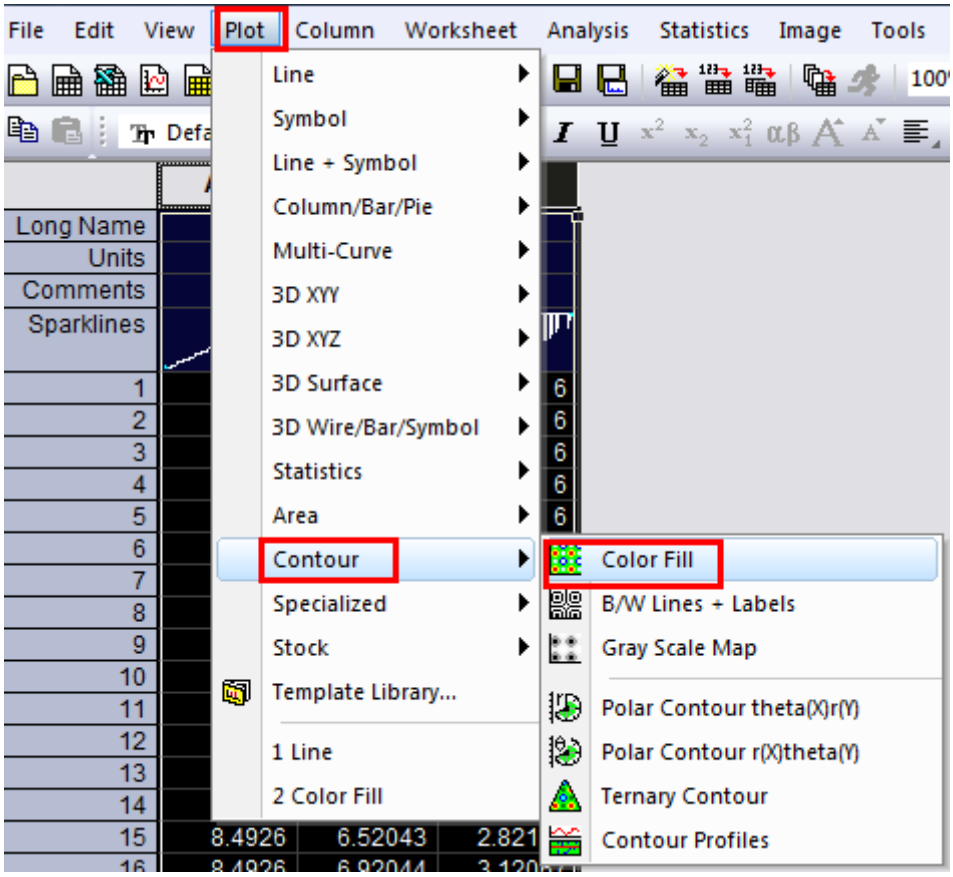

Figure 5. Plot contour

4) It may show "Speed Mode is On". You can double click the contour, click "Layer1", choose "Size/Speed", and cancel the term in the red box in Figure 6. If you do not want to cancel "Speed Mode", you can skip this step.

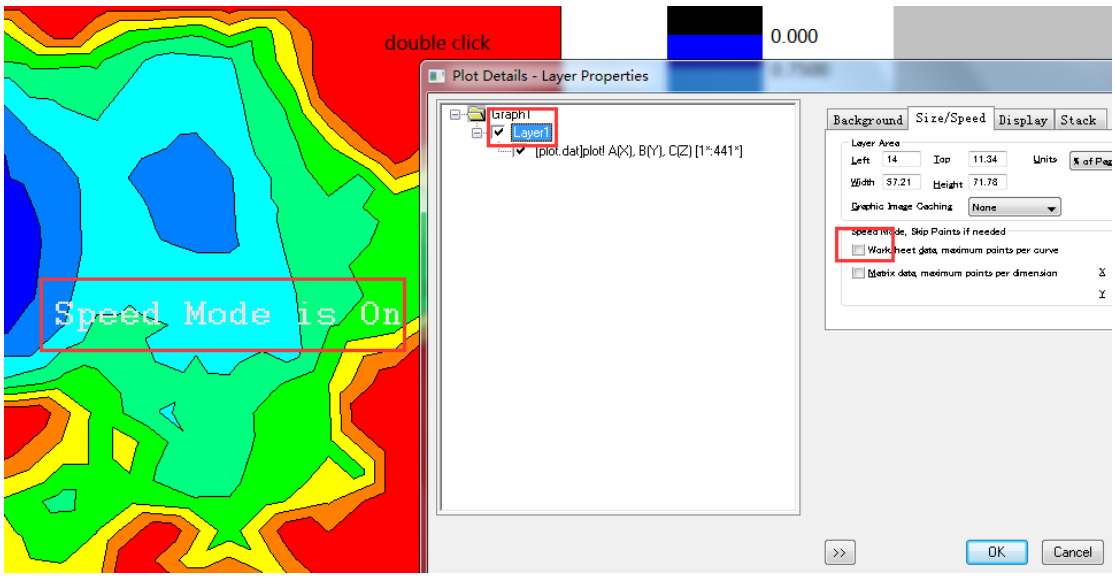

Figure 6. Cancel "Speed Mode"

5) If you want to show values on the contour lines, you can double click mouse on the contour and select the terms as shown in Figure 7.

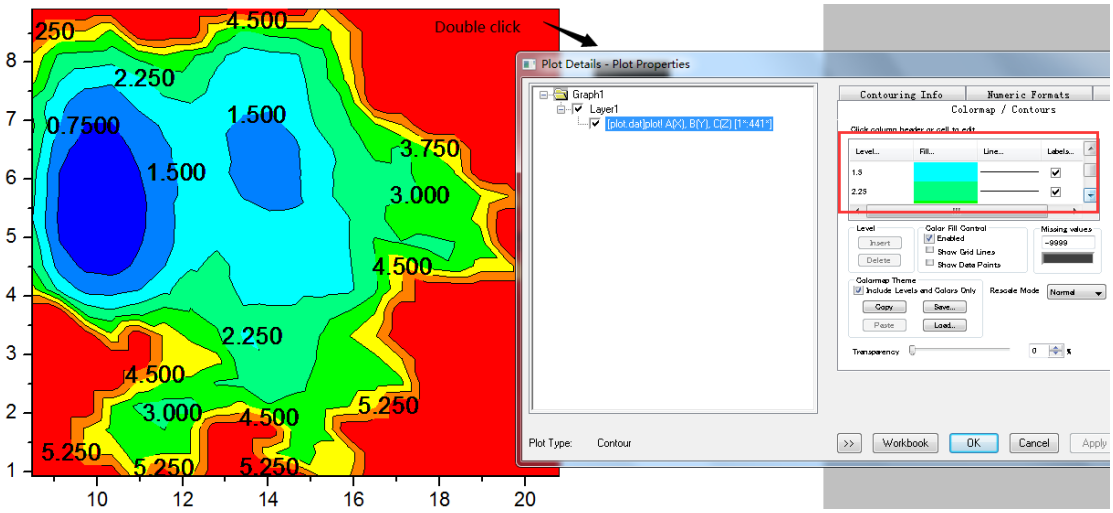

Figure 7. Plotting contour

References

1 Bai, Q. *et al.* Conformation Transition of Intracellular Part of Glucagon Receptor in Complex With Agonist Glucagon by Conventional and Accelerated Molecular Dynamics Simulations. *Front Chem* **7**, 851 (2019).