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 changes as the function of a coordinate of system. 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].

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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 1th column is RMSD values, 2th column is the distance. You can replace these data with your appointed principal components. Then, run command:

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

The plotted results show in Figure 1

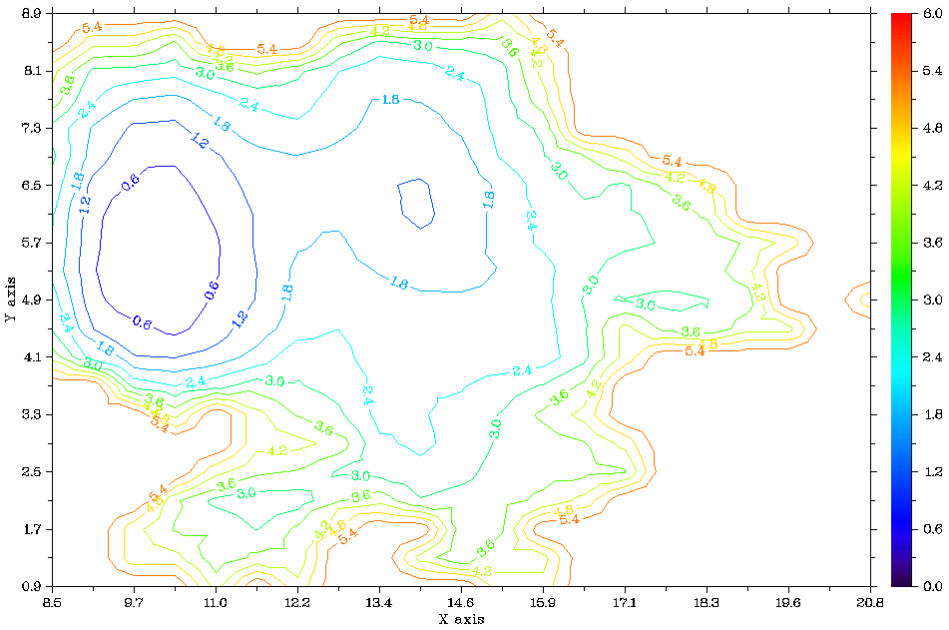

Figure 1. PMF contour.

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

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

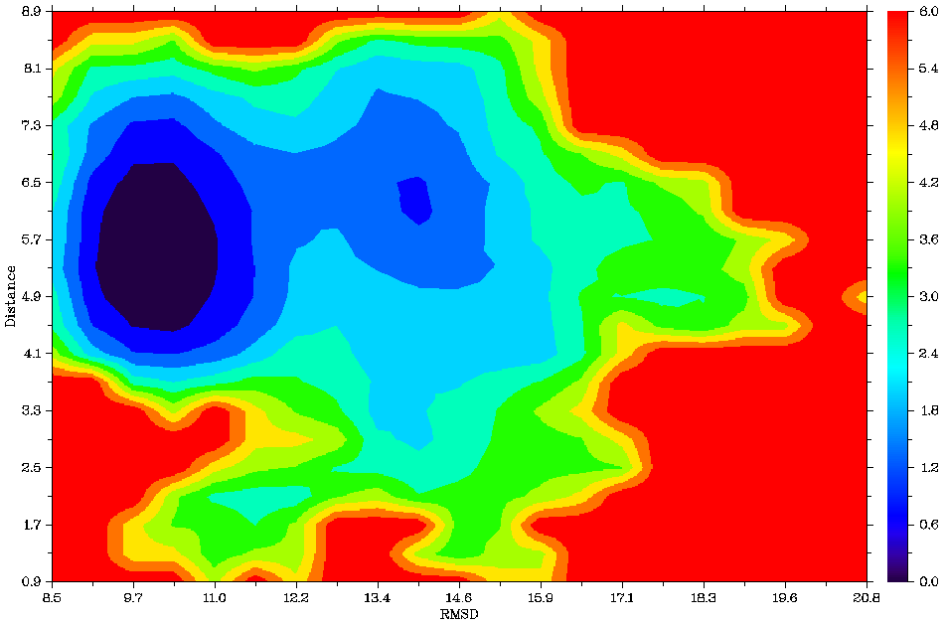

Figure 2. PMF contour.

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)

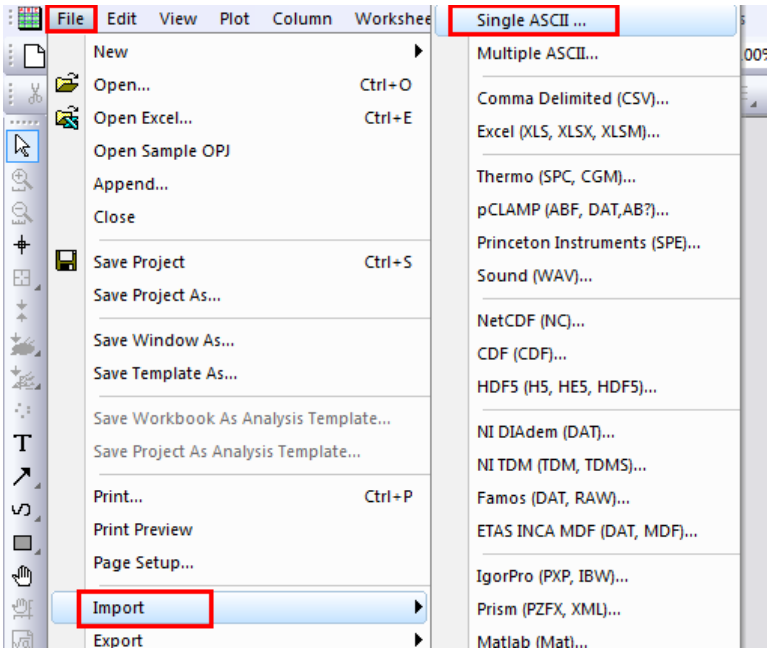

Figure 3. Import data

2) Change C(Y) to Z (see Figure 4)

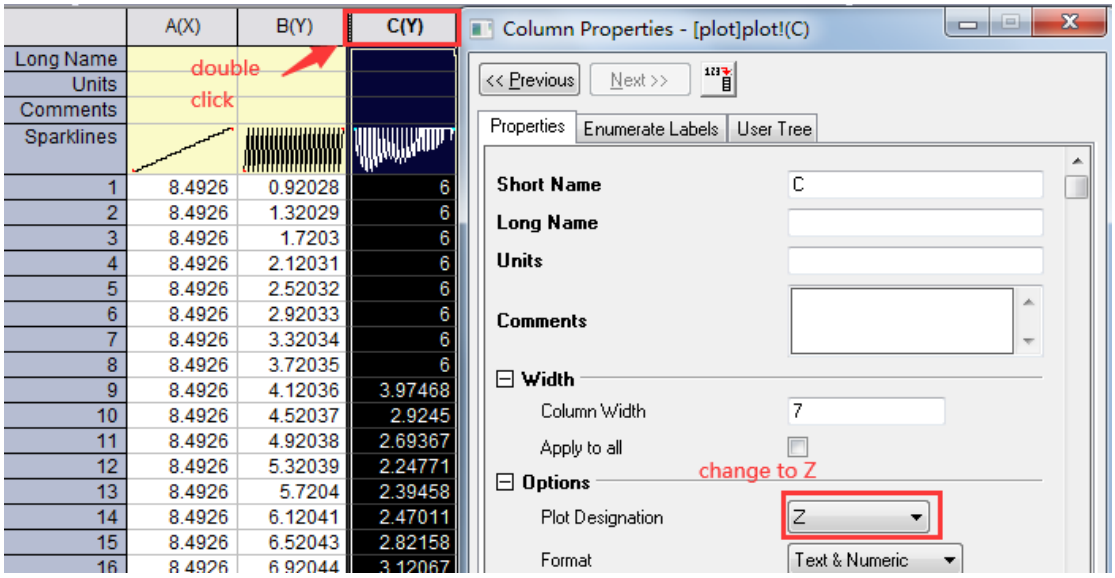

Figure 4. set parameters for plotting

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

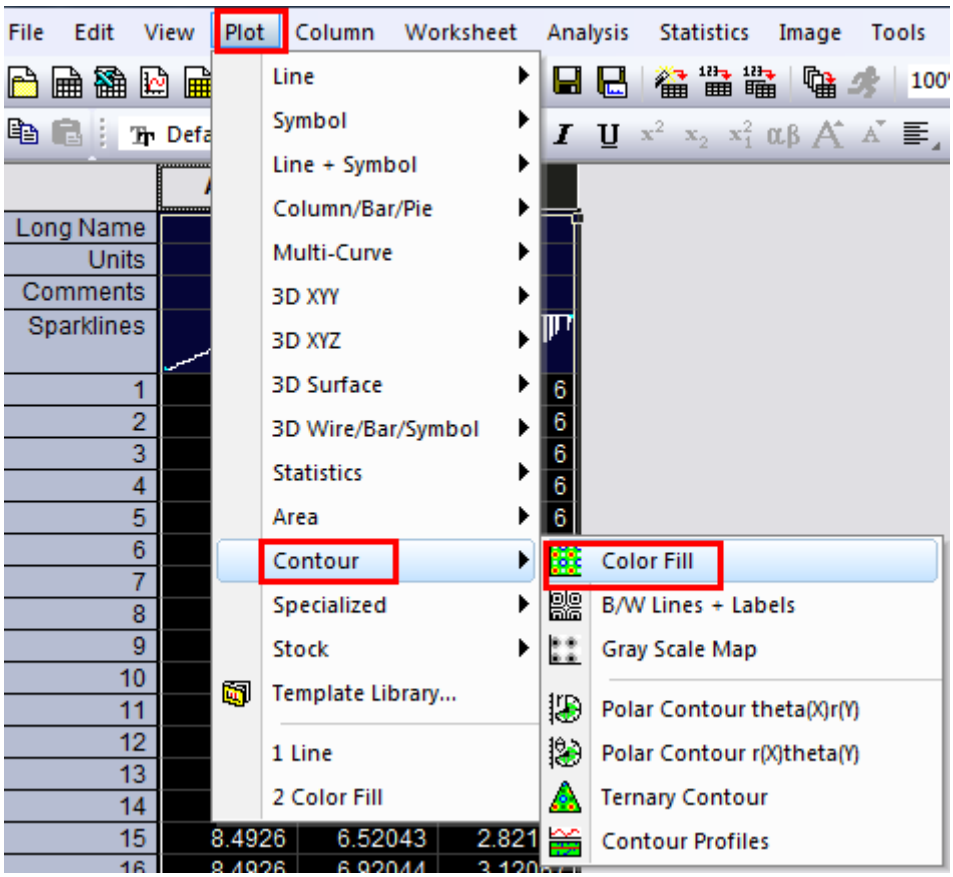

Figure 5. Plot contour

4) If you want to show values on the contour lines, you can double click mouse on the contour (see Figure 6)

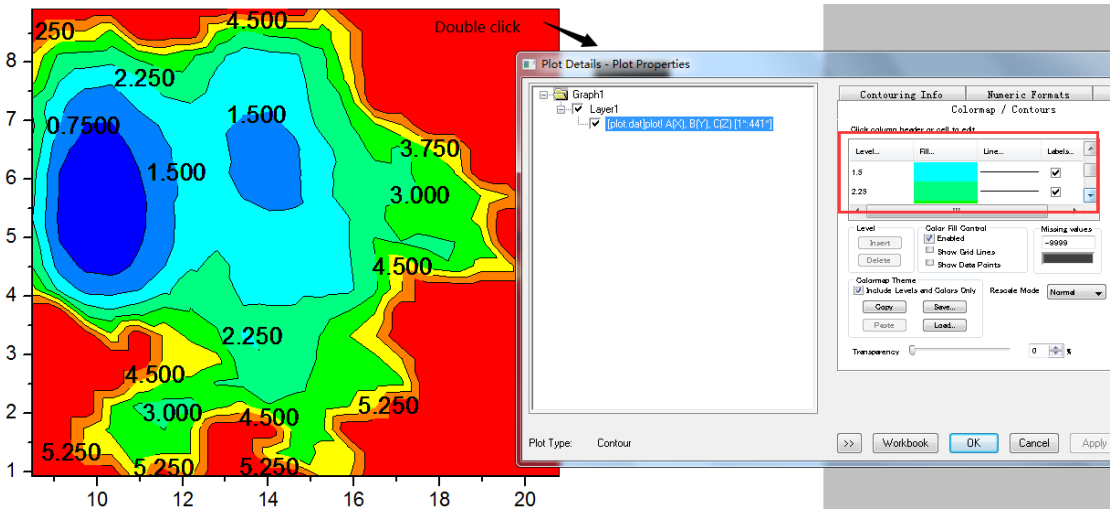

Figure 6. Plotting contour

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).