Tutorial of vinardo score calculation by MolAICal

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1. Introduction

In this tutorial, the SARS-CoV-2 M^{pro} which leads to the rapid spread of coronavirus disease 2019 (COVID-19) throughout the world is selected as the example target. The vinardo score of ligands is calculated based on the grid file of SARS-CoV-2 M^{pro}. This example can be generalized to other proteins.

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/008-vinardoScore

3. Procedure

Before calculating the vinardo score of ligand, the grid file of the receptor should be generated.
#> cd 008-vinardoScore
1) Create a file named "boxPar.dat". The first line contains the coordinates of the box center. The second line contains the box lengths. It is like below:

-10.733 12.416 68.829
30.0 30.0 30.0
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2) Running command for generating the grid file of protein
#> molaical.exe -tool grid -i boxPar.dat -p mproNolig.pdb -n vinardoScore
The "mproNolig.pdb" is the PDB format file of SARS-CoV-2 M^{pro} without ligand. It will generate the grid file named "vinardoScore.dat"

3) Calculating vinardo score of single ligand
#> molaical.exe -tool vinardo -i ligands/lig_1.mol2 -g vinardoScore.dat -t vinardoscore
It outputs like: Binding Score: -6.21 kcal/mol

If you want to calculate vinardo score for many ligands in bulk, you can do it below steps:
#> cd 008-vinardoScore/ligands

1. Using command "ls > ligandList.dat" in Linux console, or "dir /b > ligandList.dat" in Windows DOS console of Window. Open generated file "ligandList.dat" and delete no useful characters. For example, delete the first line contained characters "ligandList.dat". Make sure the file "ligandList.dat" only contains the ligand names.
2. Run command as below:
#> molaical.exe -score vinardo -i ligands/ligandList.dat -o output.dat -g vinardoScore.dat
It will generate the file named "output.dat" which contains binding scores of ligands in bulk.