Two steps for virtual screening in the pocket of SARS-CoV-2 Mpro by MolAICal and Autodock Vina

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1. Introduction

In this tutorial, we introduce the fast way for drug virtual screening of SARS-CoV-2 Mpro based on the known database such as ZINC database. The premise for this tutorial is that you can deal with protein structure for Autodock Vina. If you are not familiar with it, you can learn from the previous tutorial https://github.com/MolAICal/documents/tree/master/tutorials/002-AIVS.

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/003-VS
2) The file named "ligandSet.mol2" which contains 16 ligands obtained from ZINC database is chosen for demo. You can select your ligand database.
3) The protein file named "pro.pdbqt" that is PDBQT format structure of SARS-CoV-2 Mpro is used for molecular docking.

3. Procedure

Go to the tutorial directory:
#> cd 003-VS

1. Split ligands set into single molecule. If your drug database is built by single ligand with mol2 format, you can omit this step.
#> molaical.exe -tool split -w split -n 1 -v true -i ligandSet.mol2 -o splitdir

2. Running virtual screening
#> molaical.exe -dock vs -i splitdir -nc 3

-nc: represents the number of used CPU cores.

4. Results

You can convert PDBQT format of results to PDB format by Open Babel. Then loading it with UCSF Chimera. Here, the pymol software (http://www.lfd.uci.edu/~gohlke/pythonlibs) is used to show results (see Figure 1).

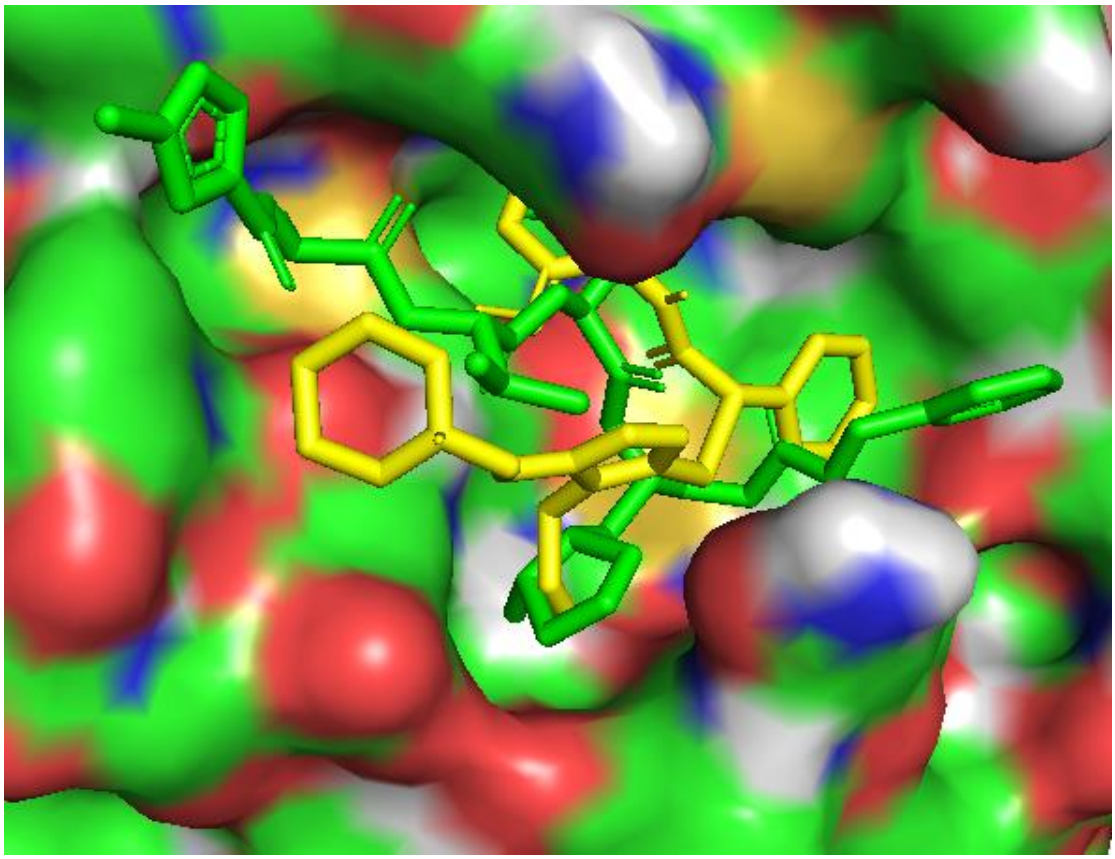

Figure 1. The ligand with green is the inhibitor N3 of SARS-CoV-2 Mpro. The ligand with yellow is obtained by virtual screening.