3CLpro and PLpro affinity, a docking study to fight COVID19 based on 900 compounds from PubChem and literature. Are there new drugs to be found?

Marek Štekláč,[1] Dávid Zajaček[1] and Lukáš Bučinský[1]

Correspondence to: Marek Štekláč (E-mail: *xsteklacm@stuba.sk*)

[1] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak Technical University, SK-81237, Bratislava, Slovakia*

Supporing_info.pdf contains figures and tables pointed to in the main paper body, including information about top docking compounds, docking poses of five best compounds against each of the protein targets, time plot evolutions of the number of H-bonds and free binding energies of compound-protein complexes, calculated using the MM-PBSA approach [1,2] (Molecular Mechanics – Poisson-Boltzmann Surface Area), as well as detailed descriptions of formed and terminated H-bonds during molecular dynamics (MD) simulations.

Docking_6WQF/6LU7/6WZU/7CMD.xlsx are three excel documents containing thorough description of docking results. These documents contain three sheets each, with first two sheets detailing results of the PubChem database [3,4] docking runs and the last sheet detailing results of redocking runs of compounds from other publications. First four columns containing compounds identifiers (CID, DB, InChI, ZINC) are followed by the number of docking runs (#runs), the number of formed clusters (#clusters), the number of poses in the lowest energy cluster (#Lowest E cluster), the lowest observed energy in all the runs (Lowest E), Root-mean-square deviation of the lowest energy cluster (RMSD_LE) and number of predicted H-bonds in the lowest energy cluster docked pose (#H-bonds). These lowest energy cluster information are followed by same information for the largest cluster, namely number of poses in the largest cluster (#Largest cluster), the lowest energy of the largest cluster (# Largest cluster lowest E), Root-mean-square deviation of the largest cluster (RMSD_LE) and number of predicted H-bonds in the largest cluster docked pose (#H-bonds). It is worth noting, that RMSD values are calculated with respect to the initial position of docked compounds and have little meaning in this type of calculations. The last four columns in the docking results section include the number of atoms in the compound, the number of torsions, the number of hydrogen atoms and the ligand efficacy expressed as ratio of the energy of the lowest energy cluster and the number of atoms. Docking results are followed by the computational time required for the given docking protocol and selected compounds' descriptors for Lipinski's rule of five[5] and Ghose filter calculation are provided [6]. They include the number of hydrogen bonds acceptors and donors, the octanol-water partition coefficient XLogP3, the molecular weight and the molar refraction value. These were taken from the PubChem_ADME.xlsx document, see the next section.

PubChem_ADME.xlsx is an excel document containing absorption, distribution, metabolism, excretion (ADME) parameters and other physicochemical descriptors and druglike properties of studied compounds. These parameters were computed from a list of SMILES codes using the SwissADME [7] website and were used in the evaluation of empirical drug likeness rules. This document contains the compounds' CID (Molecule), the SMILES codes, the chemical formula, common descriptors such as the molecular weight (MW), the number of heavy atoms and aromatic heavy atoms, the number of rotatable bonds, the number of hydrogens bonds donors and acceptors, lipophilicity data, water solubility information and many others. Reader is advised to visit SwissADME[7] website for a better comprehension of listed properties.

References and Notes

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