Scheme of Research

The discovery of new compounds for drug candidates can come from both synthesis and natural products. The process of finding new drugs to inhibit the corona virus (Covid-19) is carried out by screening compounds from various natural substances to obtain optimal compounds in the appropriate therapeutic target and design the appropriate guide compound structure so that the ligand matches the active side of the receptor in inhibit corona virus with study literature. The three-dimensional structure of each compound can be downloaded by Pubchem Compound website. As for the modified compounds made in two dimensions using Chemdraw 2D with .cdx format. Then performed energy minimization and geometrical conformation with the Chemdraw 3D program, find the best conformation was chosen as the structure of the compound to be tethered to macromolecules. The results of the conformation are then saved in the .pdb format. Application program used in the process of docking compounds to macromolecules using Autodock vina with pyrex. The results obtained from docking using autodock vina with pyrex are energy affinity values ​​with files stored automatically in the pdbqt format. Observations were made by looking at the affinity of bond energy (∆G) formed.

The following is the scheme of finding process to obtain corona virus (Covid-19) inhibitor:

