



Research Article

Bioinformatics Approach for COVID-19 (Coronavirus) Disease Prevention Treatment and Drug Validation

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Abstract

Objectives: To determine the impact of Hydroxychloroquine on COVID special protease.

Methods: PyMOL software is used to find all possible residual rotameters and probabilities. AutoDock software is used to calculate and predict the interaction of molecules.

Results: Hydrochloroquine binds and is released through Protease 6y84 and 7buy and controls their actions in the body.

Conclusion: Drug designing and docking is helpful for the particular diseases. It helps us predict the intermolecular framework formed between a protein or a small molecule.

Keywords: Autodock, Chimera, COVID 19, SARS, PDB, PyMol

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The novel coronavirus 2019 (nCoV) has triggered a global health crisis, causing the coronavirus disease-19 pandemic in the human population. In December 2019, a local pneumonia outbreak with an initially unknown cause was detected in Wuhan (Hubei, China), and it was soon determined to be caused by a novel coronavirus, namely severe acute respiratory syndrome coronavirus, (SARS-CoV-2).^[1–3] As of 22 May 2020, almost all countries and many regions have reported corona cases. There have been more than 5198307 confirmed cases and 334689 death reports due to COVID-19.^[4] In response to this public health emergency, the Center for Systems Science and Engineering (CSSE) at Johns Hopkins University, Baltimore, MD, USA, developed an online interactive dashboard to visualize and track in real-time the reported cases of corona virus disease 2019 (COVID-19).^[5–7]

The dashboard, first shared publicly on January 22, 2020, illustrates the location and number of confirmed COVID-19 cases, deaths, and recoveries for all affected countries. The Dashboard was developed to provide researchers, public health authorities, and the general public with a user-friendly tool for tracking the outbreak.^[8,9] All information collected and displayed was initially made available for free through the GitHub repository, and Google Sheets along with the dashboard feature layers, which have been now included in the Esri Living Atlas (Fig. 1).^[10] A novel corona virus has resulted in an ongoing outbreak of viral pneumonia in China.^[1–3] Person-to-person transmission has been observed, but to our knowledge, it is the new coronavirus that caused the epidemic in 2019. (Fig. 2).

No coronavirus has been reported from an asymptomatic

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carrier with normal chest computed tomography (CT) findings. In Wuhan, Hubei Province of China, the 2019 novel coronavirus disease (COVID-19) outbreak has spread rapidly across the country.

Here are the results of a descriptive report, which is exploratory analysis of all cases diagnosed as of April 11, 2020. All COVID-19 cases reported till April 11, 2020 were found from China's Infectious Disease Information System.^[12] The analysis included:

1. Calculation of case fatality and mortality rates,
2. Geo-temporal analysis of viral spread,
3. Epidemiological curve construction,
4. Summary of patient characteristics,
5. Examination of age distributions and sex ratios.
6. Subgroup analysis.^[9]

Methods

PyMOL shows all possible rotamers and probabilities of the residue.

The most likely amino acid rotamer has an 11.9% probability

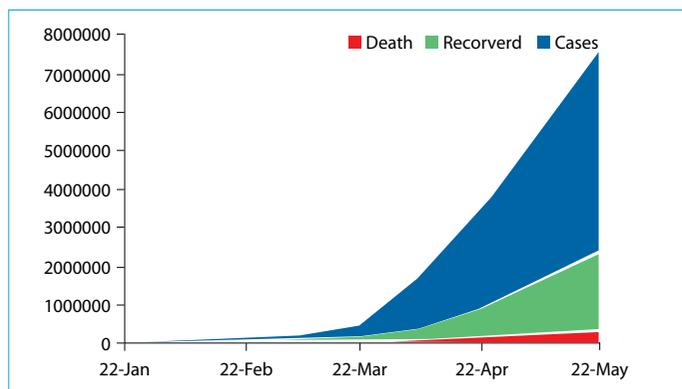


Figure 1. Total COVID-19 cases, deaths and recovery globally.

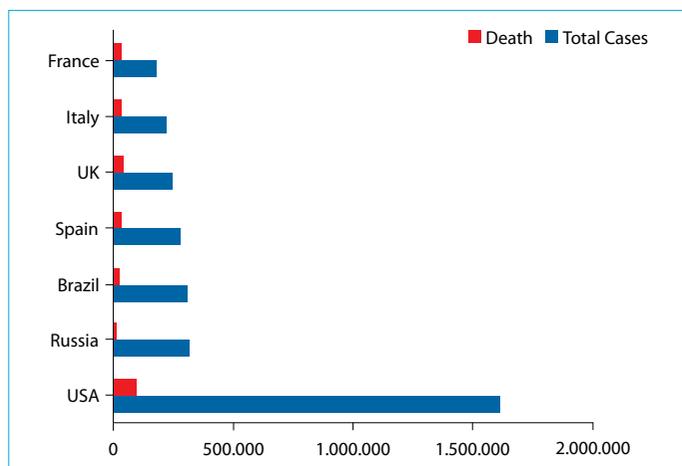


Figure 2. COVID 19 cases and deaths per country.

and the second and third most common rotamers. Thus, PyMOL shows how many distinctive rotamers exist for other amino acid findings, the possible rotamers for the species for this residue, and the action of two different conformations, and take its surroundings into account for its probabilities. Each arginine rotamer has a lot of red indicating that arginine is probably not a good mutation at this position.^[13] To avoid any of these mutations click clear. The mutagenesis wizard is very useful to explore possible positions of residues. And then going back to "No Mutation", various rotamers are explored for several proteins and amino acids. The Open Babel project is a full-featured open chemical toolbox designed to describe many different representations of chemical data.^[11] It allows anyone to search, convert, and analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related fields.^[12] It provides a complete work, expandable and valid program toolkit for developing both off-the-shelf programs and chemo-informatics software and programming. Open Babel implements a sophisticated and canonicalization algorithm that can operate on molecules or molecular fragments. Atomic symmetry classes are the first graphic invariants and encode topological and chemical properties.^[12] A cooperative labeling procedure is used to investigate the automorphic permutations to find the canonical code.

The AutoDock software calculates and predicts the interaction between the ligand molecule and the protein molecule according to predefined parameters. Precisely, the interactions between the molecules will be calculated at a user-defined region in the protein. This region can be known by users, using the unique Grip map option. Ultimately,^[13, 14] the software predicts the interaction and binding energy of the ligand molecule and the amino acids involved only in the GridBox. It is therefore very important to set the GridBox at the binding site or active site or other essential regions of the protein. Before running the AutoDock.nce, the AutoDock4.exe is successfully executed. The result will be given in the ten best conformations. These can be viewed in the analysis options.^[15, 16] The conformations can be viewed in the order of their free energy binding, by selecting the Play option sorted by energy. Analyzing the result takes several steps given as a graphical representation. The panels A, B, C and D will open one after the other in the given order. The ten conformations can be displayed by changing the number of conformations in panel A. The interaction energy of the given conformation can be displayed in panel D. The number of hydrogen bonds formed between the ligand and protein can be viewed in panel C.^[13]

UCSF Chimera offers 3-D visualization of molecular structures and related data, including density maps, supramolecular assemblies, molecular dynamics trajectories, and multiple

sequence alignments. The user can also create images and animations for publication and presentation. In addition to supporting core visualization, the software is specifically designed for extensibility to allow external developers to incorporate desired new functionality.^[18, 19] Available extensions include Multiscale Models to visualize large-scale molecular structures like viral coats, ViewDock to viewscreen docked ligand orientations, Volume Viewer to visualize density maps, and Multalign Viewer to display sequence alignments with crosstalk to any associated structure.^[20]

Result and Discussion

The mechanism of identifying a target is synthesizing an active compound with suitable characteristic such as minimal toxicity, high bioavailability, cost-effective and synthesis process etc. And finally, a target is set which plays a key role in the process of the disease cure and identification. Therefore, drug designing and placement docking is helpful for a particular disease. Molecular docking helps us predict the intermolecular framework formed between a protein and a small molecule or a protein and protein and suggest the binding mode responsible for the inhibition of specific protein.

Conclusion

It's a well-known fact that that COVID 19 is a very severe infectious disease these days, so we are trying to apply bioinformatics approaches to validate and diagnose the

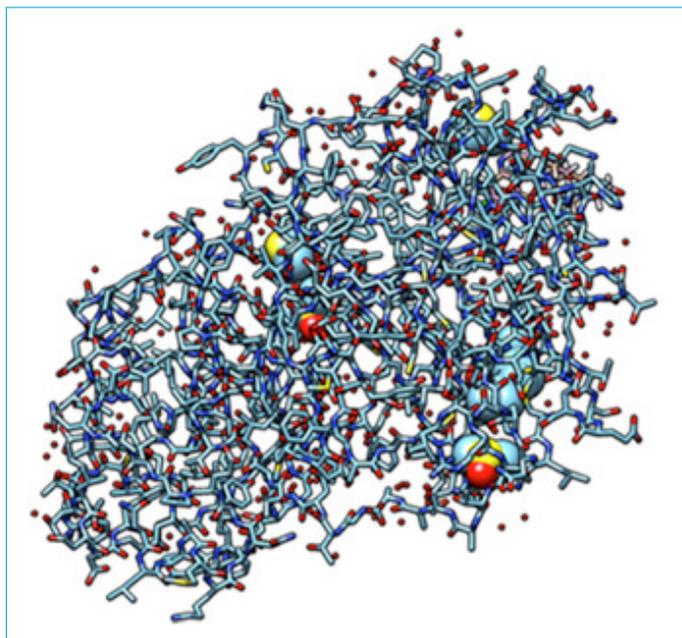


Figure 3. Interaction between PDB ID 6Y84 or 7BUY (COVID 19 Protease) and Hydroxychloroquine (2,4,7 chloroquinolin-4-yl) amino pentyl ethyl amino ethanol.

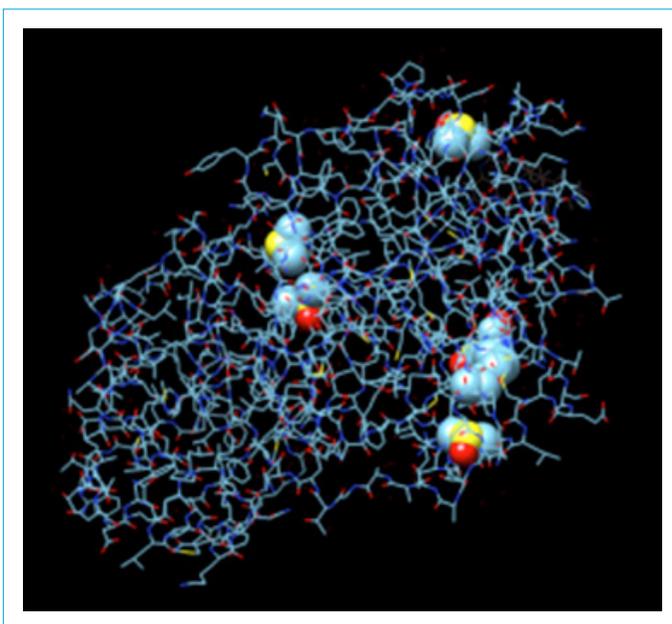


Figure 4. Binding of 6Y84 and 7 Hydroxychloroquine.

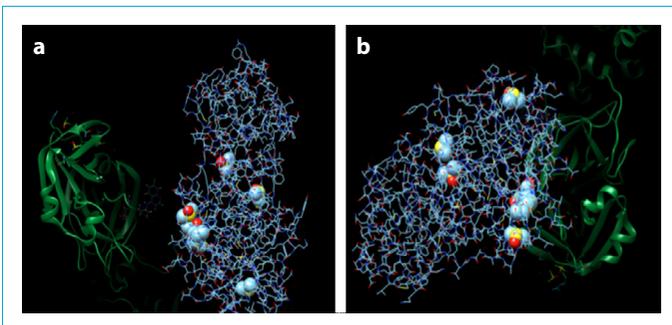


Figure 5 (a, b). Superimposing, binding and coiling all in Auto Docking.

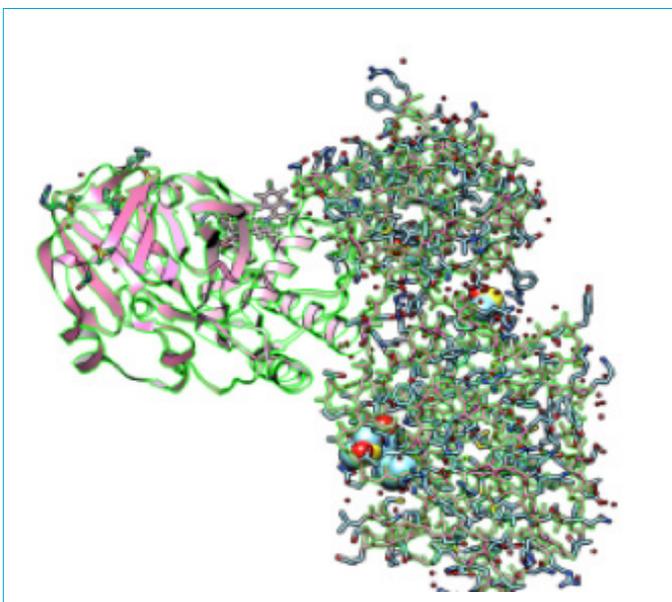


Figure 6. The full effect and inhibition process of 6Y84 COVID 19 protease and 7 Hydroxychloroquine drug action.

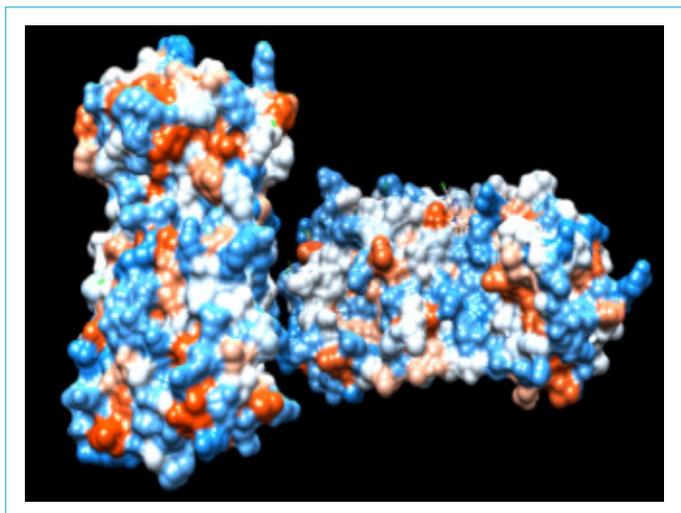


Figure 7. The functioning and effect of hydroxychloroquine.

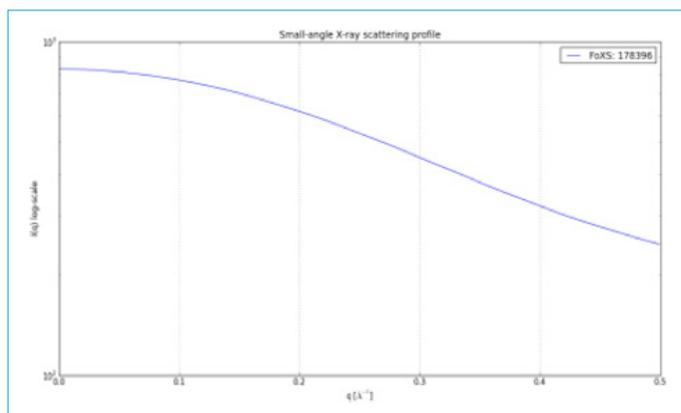


Figure 8. The graphical representation of COVID 19 protease and hydroxychloroquine.

of the drug Hydroxychloroquine to overcome the impact of COVID 19 coronavirus; and trying to find out the effect and inhibition of Hydroxychloroquine drug, it's functioning over corona virus 6Y84 and 7 buy protease and then that its working in the body and fight against COVID 19. Hydroxychloroquine binds and is released through protease 6y84 and 7buy and controls their actions in the body. We all know very well that the best way to heal ourselves from COVID-19 is proper care, sanitization and social distancing.

Disclosures

Ethics Committee Approval: The study was approved by the Local Ethics Committee.

Peer-review: Externally peer-reviewed.

Conflict of Interest: None declared.

Authorship Contributions: Concept – S.M., P.A.J.; Design – S.A., S.M.; Supervision – P.A.J.; Materials – S.M., S.A.; Data collection &/ or processing – S.A.; Analysis and/or interpretation – S.M.; Literature search – S.M.; Writing – S.A., S.M.; Critical review – P.A.J.

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