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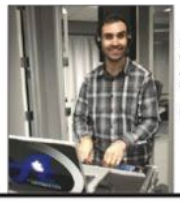

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Take a hike!

OH, AND BRING THE FAMILY...

BY DAVID R. NEWMAN

Now is the perfect time to get out and explore the many outdoor gems the East Bay has to offer. Memorial Day weekend has come and gone, and with it, the official start of summer. To celebrate, here's a list of family friendly hikes to help you fight those quarantine blues…

San Leandro

Heron Bay - This marshy strip of land makes up part of the San Leandro shoreline. It's open and beautiful, with a wide paved trail that leads north all the way to the San Leandro Marina and southward gravel trails that meander through the marsh and eventually connect with the Hayward Regional Shoreline. Perfect for bikes, joggers, walkers, and dogs. As part of the Bay Trail, the

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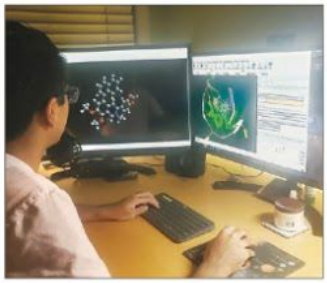
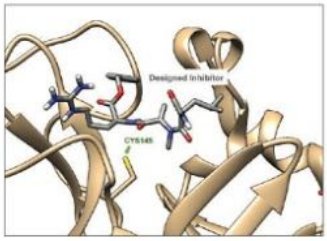
High School Students Perform COVID-19 At-Home Research

BY CHARLENE DIZON
PHOTO COURTESY OF EDWARD NJOO



Amidst the COVID-19 pandemic, Bay Area high school students have decided to conduct their own research under the supervision of four scientists at the Aspiring Scholars Directed Research Program (ASDRP) from the Center for Advanced Study (CAS). Advisors Robert D., Peter L., Edward N., and Soumya S. conceived and developed plans for each research project. The students from this program executed four research areas focusing on the development of molecular solutions that can potentially stop the virus from forming.

Drug repurposing has been a focal point of COVID-19 research. Small molecule drugs such as remdesivir, hydroxychloroquine, and emodin are being analyzed due to their history with previous viruses. "Remdesevir was made for the Ebola virus. Emodin was researched in 2002 when the first Severe Acute Respiratory Syndrome (SARS) outbreak happened. We're re-using what we already know to find something hopefully better," 11th Grader Ishani states. This process requires computational molecular docking, in which a designed molecule binds to another



through simulation. Spike glycoprotein, the novel coronavirus molecule that needs to be stopped, connects with Angiotensin-Converting Enzyme 2 (ACE-2). The SARS-CoV2 virus enters host cells through this human receptor ACE-2. "We want to prevent this interaction from even happening, so we're looking for molecules similar to the three mentioned to see if they work better," Ishani explains. This is valuable because the best-screened

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High School Students Perform COVID-19 At-Home Research

candidate of a repurposed drug molecule can then be used to provide insight into treating COVID-19.

De novo design is another method for computer-aided drug design. The student researchers used a three-dimensional structure of a protein receptor from the coronavirus to design molecules with potential biological activity. 12th Grader Stephanie explains, "We worked on designing compounds that would fit into the open cavity of the spike glycoprotein and lock it in its closed state." Achieving this could potentially obstruct viral interaction with the ACE2 receptor and virus's ability to invade host cells. The group has also been working on covalent inhibitors of the coronavirus main protease. This protease is necessary for the replication of viral RNA (ribonucleic acid), which allows the virus to replicate inside a host cell. 11th Grader Ayush explains, "We use reactivity of the molecular design to come up with a concept of what our inhibitor should be. Then, we draw a model on our computer and go through DFT [density functional theory], which conforms to how it would be in real life. We use that DFT reactivity to move on to molecular docking and see which best inhibits COVID activity." Over four hundred compounds were screened. This is remarkable because these results can be applied to future molecules and possibly lead to the discovery of small molecules that inhibit replication or entry of the virus.

Students are also working on a machine learning platform that can identify patterns among potential inhibitors of the virus. A library of compounds is first screened by studying the early 2004 case of SARS and comparing these proteins to the current coronavirus. 11th Grader Bhavesh explains, "We developed our own novel algorithm that uses vector mapping to detect the potential compounds." Vector mapping involves identifying and using the 3-dimensional topology of the compounds studied and correlating the intersection of these compounds with the virus, then ranking these compounds to determine whether they might be viable candidates against the spike glycoprotein.

"We've also created a 3-D map that will tell us what the most reactive part of the compound looks like in a 3-D space," adds 11th Grader Andrew; this 3D map would allow them to see where COVID is present in the compound, giving more targeted results. Whether this machine learning platform can be mass produced has also been taken into account. "We've considered making sure these are green reactions and green reagents that can be safely developed in the future," says 11th Grader Atri. This platform would reduce time in waiting for results from more computationally intensive processes, helping scientists find possible treatments more quickly.

The final method being observed is DNA-directed RNA interference (ddRNAi), a common gene-silencing method amongst infected

patients. RNA holds viruses' genetic information. The development of an RNA fragment through ddRNAi analysis could silence a gene within COVID-19, which would naturally inhibit the replication and spread of the virus. "ddRNAi can steadily reproduce itself, so it's effective over a long period and can silence multiple genes in the same area by using DNA constructs to block the pathway entrance for COVID to enter," explains 9th Grader Ishya. If a successful ddRNAi is tested and an approved algorithm for the best RNA fragment is found, it could then be distributed into infected patients with little to no toxic effect.

Though working from home has had its limitations, the students have persevered. "Having everything at home is a blessing in disguise because we're able to focus wholeheartedly on our computational research," says 11th Grader Kushal. The students' appreciation of the technology made available to them has deepened to the point of considering possible careers in computational research. "Before, research and real-life felt separate to me. Now that we're able to work on something so important to the scientific community and society, it shows us how much our work can affect what is going on around us," 10th Grader Karthikha states. At-home research has proven that despite recent challenges, these students are resilient and ready to progress in the scientific field.