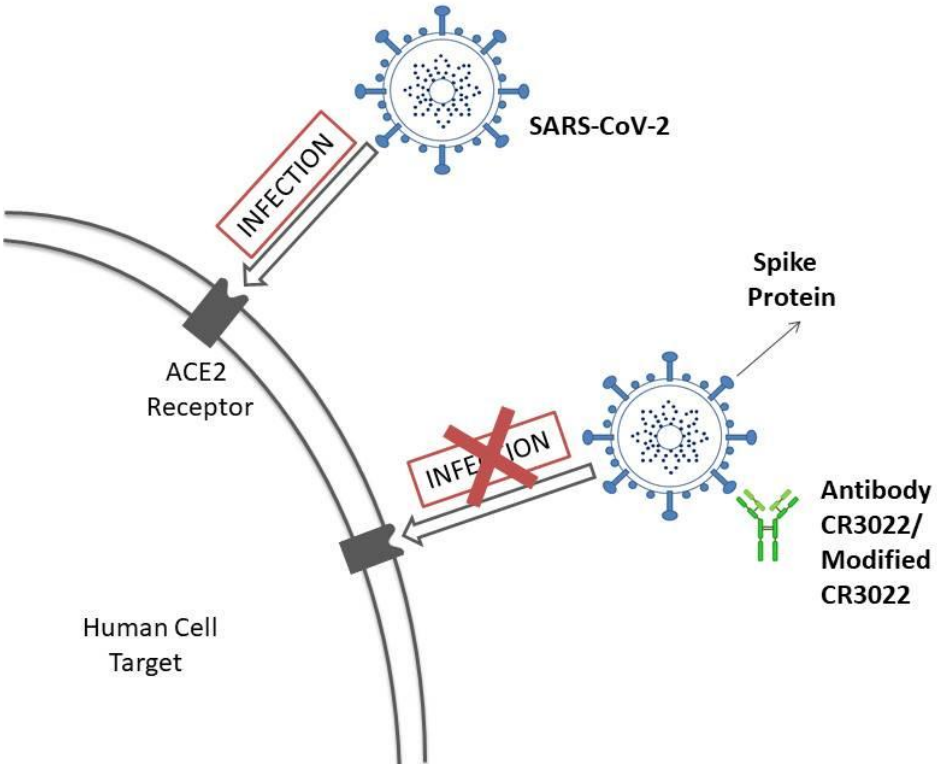
In silico studies towards high specific antibodies for the novel coronavirus

A Brazilian research group together with professor Aatto Laaksonen from the Department of Materials and Environmental Chemistry at Stockholm University and Petru Poni Institute in Iasi have confirmed in their studies how the spike receptor binding domain of the new coronavirus enters the human cell and proposed more efficient binder candidates, a discovery with the potential to improve the development of a new vaccine and/or an antiviral drug. The research is published in the scientific journal Virus Research.

In times of a pandemic, the urge for scientific progress becomes more evident. Once a new virus emerges and becomes a global threat to humanity, it is inevitable to unite forces to find a way out of the chaos especially for infectious diseases with high infectictivity and complex pathogenicity. This scenario motivated us to desiccate the molecular mechanisms involved in the viral access to the human cell to start the infection. The article, as its name explains, consists in the use of an innovative computational approach to investigate the molecular interactions to find a potential target for COVID-19 treatments, diagnosis and to propose amino acids that can contribute to improve the binding affinity of available monoclonal antibodies (mAb).

"The spike glycoprotein from SARS-COV-2 has proven to be an interesting research target as can be seen in many ongoing vaccine development projects. The reason for that is because it is responsible for the entrance of the virus when it interacts with the Angiotensin-converting enzyme 2 (ACE2) receptor. The S RBD (receptor binding domain) of both SARS-CoV-1, responsible for the 2002 epidemic in China, and SARS-CoV-2 bind to the ACE2 receptor with similar affinities in both neutral and acid regimes. In order to find an efficient antibody to prevent the virus from entering the cell, antibodies proven before to be efficient in neutralizing SARS-CoV-1, such as CR3022, m396, F26G19 and 80R, were tested in our study", explains Carolina Giron, a medical student from UFTM/Brazil involved in the project.

In this article, the authors predicted theoretically that the antibody CR3022 could bind to the RBD of SARS-CoV-2. "It is amazing to see that a recent experimental work from Oxford confirmed our theoretical predictions and also showed that this antibody can neutralize the virus", says Aatto Laaksonen, a professor at the Department of Material and Environmental Sciences and leading the study at Stockholm University.



The theoretical alanine scanning method proposed in the work indicated that three amino acid modifications in CR3022 can increase even more its binding affinity to the RBD protein. Therefore, this modified mAb could be a promising candidate to be more effectively used in the war against COVID-19. It remains to be experimentally tested, and the research team is looking for collaborators for this purpose. In light of the promising results obtained, the developed methods can also be further applied to improve other binders not included in this study.

"We are very excited with our results. This strategy can provide a cost-and-time-effective computational framework towards the development of better diagnostic tools and contribute towards an effective treatment and/or vaccine for COVID-19", explains Fernando Barroso, an associate professor at the Department of Biomolecular sciences and leading the study at University of São Paulo.

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