

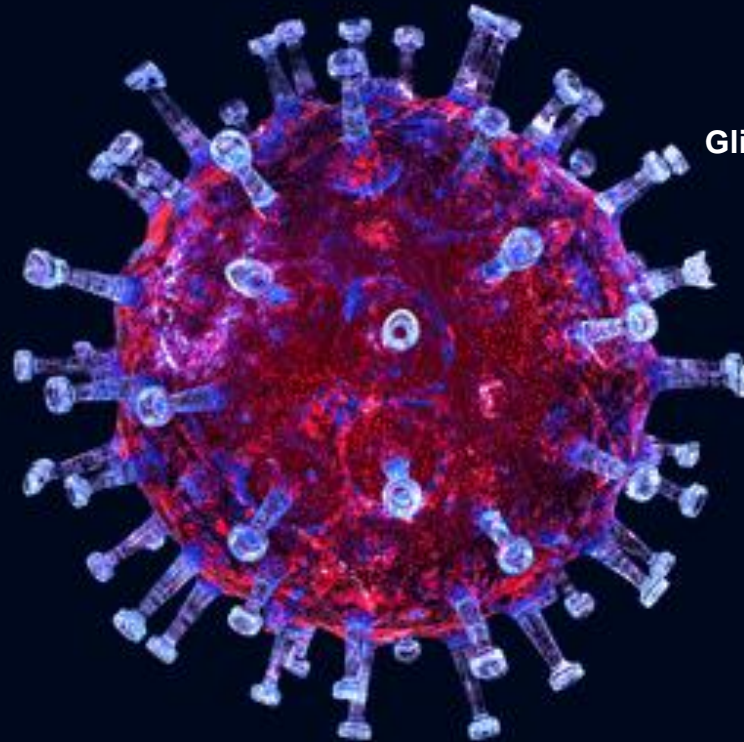
# Infecção pelo SARS-CoV-2

Prof. Dr. Walter F. de Azevedo Jr.



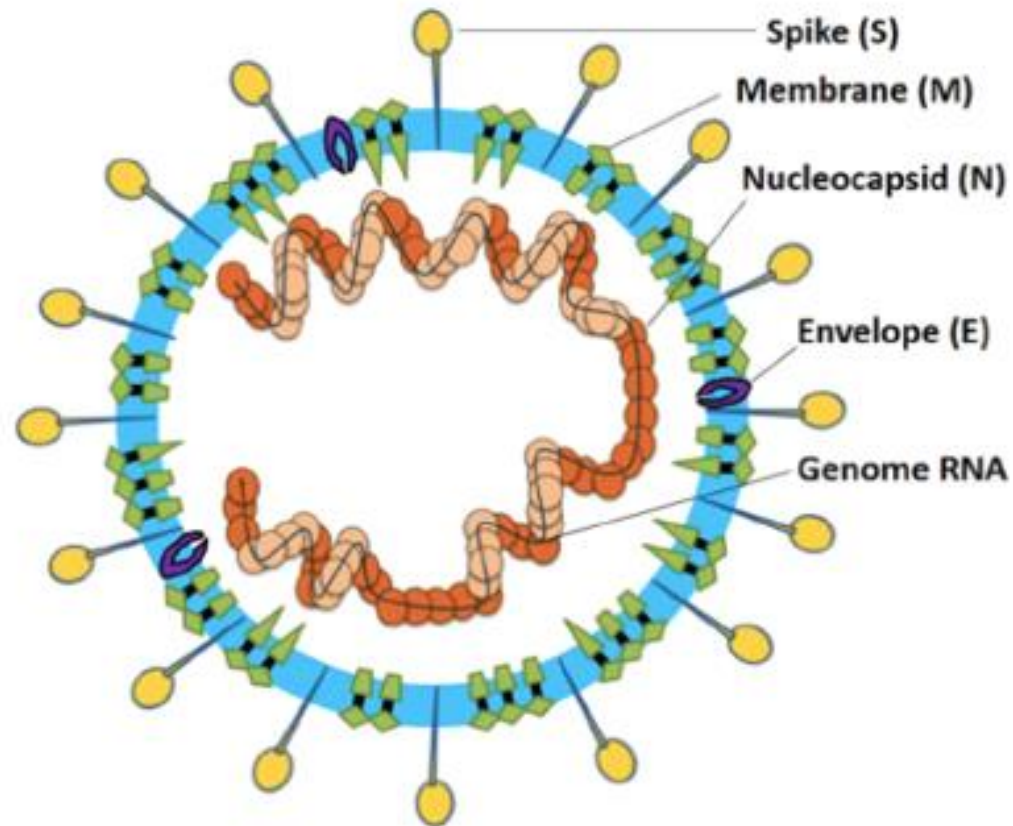
Aqui está descrito o processo de infecção do SARS-CoV-2. O foco está na descrição das proteínas envolvidas no processo de infecção do SARS-CoV-2. O agente causador da COVID-19 é o vírus SARS-CoV-2. Este apresenta no seu capsídeo a glicoproteína *spike*. Esta proteína liga-se à enzima conversora de angiotensina 2 (ACE2) das células do hospedeiro e promove a infecção destas.





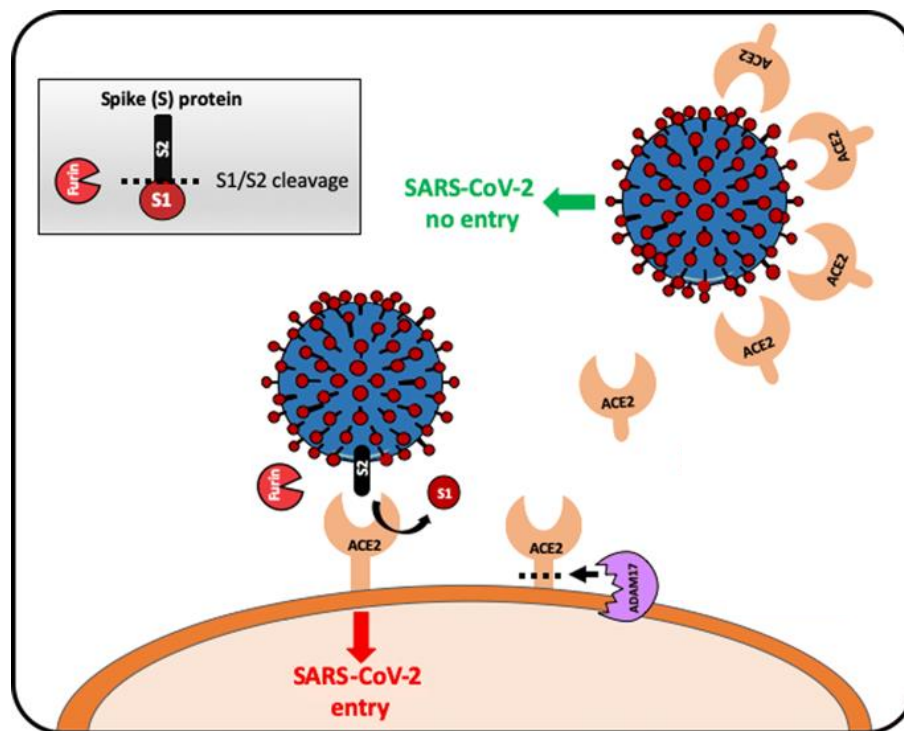
Glicoproteína Spike

# SARS-CoV-2

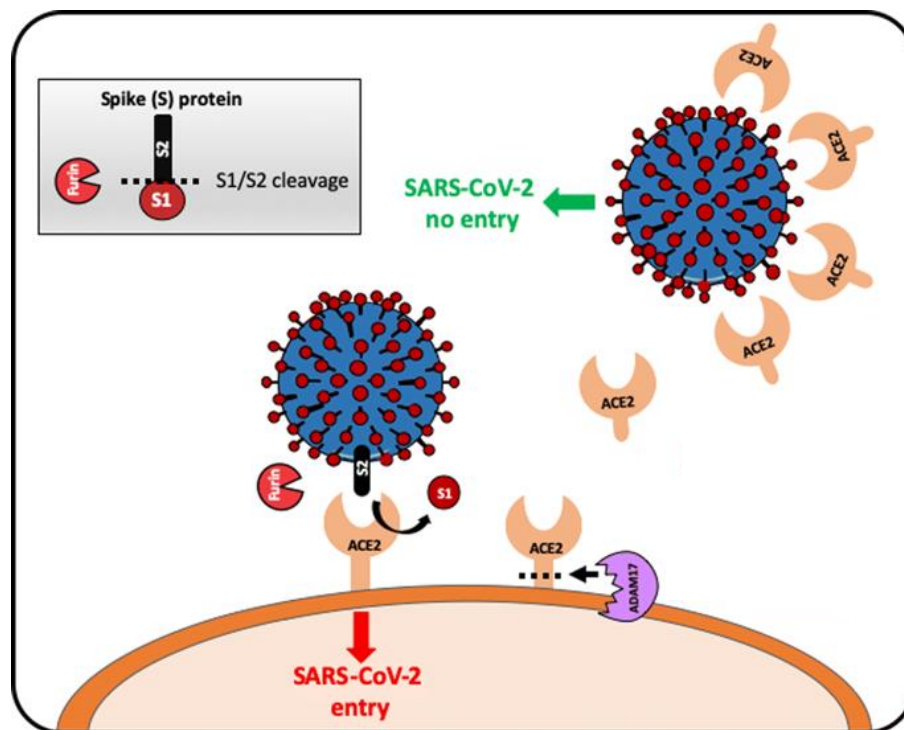


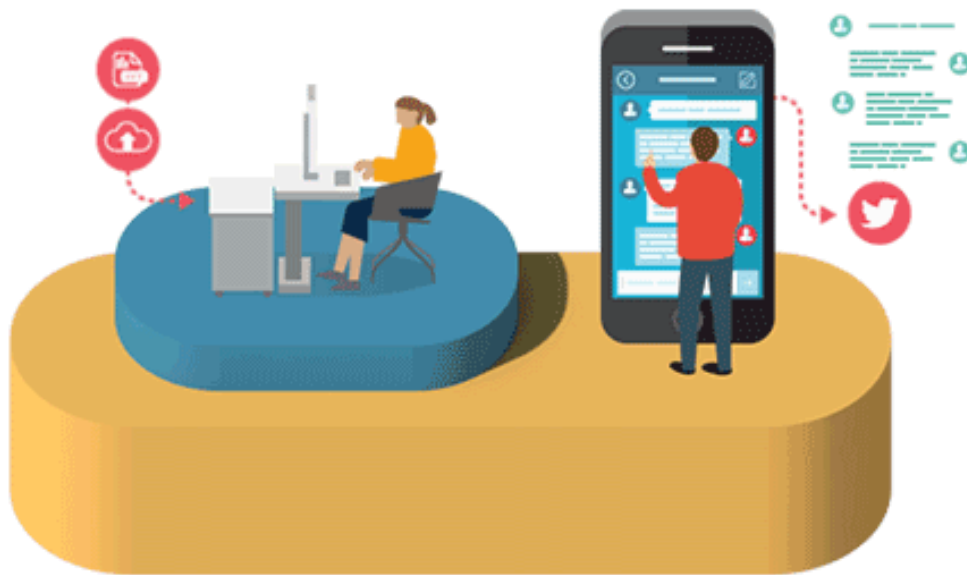
Fonte: Li G et al. Coronavirus infections and immune responses. J Med Virol. 2020, 92(4):424-432.

O agente causador da COVID-19 é o vírus SARS-CoV-2. Este apresenta no seu capsídeo a glicoproteína *spike*. Esta proteína liga-se à enzima conversora de angiotensina 2 (ACE2) das células do hospedeiro e promove a infecção destas. A figura abaixo ilustra o processo de encaixe da glicoproteína *spike* na enzima conversora de angiotensina 2 localizada na superfície da membrana plasmática da célula que será infectada.



Para a infecção da célula pelo SARS-CoV-2 ocorrer é necessária a clivagem proteolítica do sítio  $S_1/S_2$  da glicoproteína *spike* pela protease furina. Os níveis de ACE2 na membrana plasmática são modulados pela proteína ADAM17, que corta a ACE2.



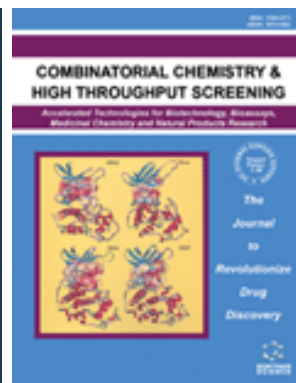
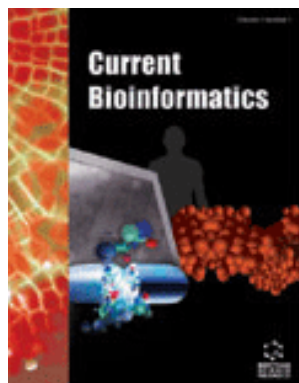
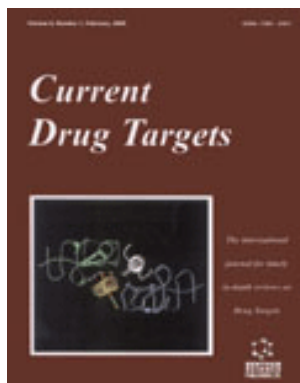


- 1) Qual a protease catalisa a clivagem do domínio S1/S2 da glicoproteína spike do SARS-CoV-2?
- 2) Como o conhecimento do processo de infecção pode ajudar no desenvolvimento de um fármaco para tratar a COVID-19?



Prof. Azevedo is Frontiers Section Editor (Bioinformatics and Biophysics) of the Current Drug Targets, section editor (Bioinformatics in Drug Design and Discovery) of the Current Medicinal Chemistry, section editor (Combinatorial/Medicinal Chemistry) for the Combinatorial Chemistry & High Throughput Screening, member of the editorial board of Current Bioinformatics, and editor of Docking Screens for Drug Discovery (Methods of Molecular Biology)(Springer Nature). He is also member of the editorial board of PeerJ, PeerJ Physical Chemistry, Organic & Medicinal Chemistry International Journal, and section editor in chief (Bioinformatics) of the Bioengineering International. He graduated in Physics (BSc in Physics) from the University of São Paulo (USP) in 1990. He completed a Master Degree in Applied Physics also from the USP (1992), working under the supervision of Prof. Yvonne P. Mascarenhas, the founder of crystallography in Brazil. His dissertation was about X-ray crystallography applied to organometallics compounds (De Azevedo Jr. et al., 1995). During his PhD, he worked under the supervision of Prof. Sung-Hou Kim (University of California, Berkeley), on a split Ph.D. program with a fellowship from Brazilian Research Council (CNPq)(1993-1996). His PhD was about the crystallographic structure of CDK2 (De Azevedo Jr. et al., 1996). His current position is coordinator of the Structural Biochemistry Laboratory at Pontifical Catholic University of Rio Grande do Sul (PUCRS). His research interests are interdisciplinary with two major emphases: molecular simulations and protein-ligand interactions. He published over 190 scientific papers about protein structures and computer models to assess intermolecular interactions involving biomolecules and potential ligands (H-index: 37, RG Index > 41.0). These publications have over 4900 citations in the Web of Science (Publons h-index: 37), more than 5600 citations in the Scopus (h-index: 41), and over 7100 citations in the Google Scholar (h-index: 44).

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The screenshot shows the Facebook profile page for 'azevedolab.net'. At the top, there is a navigation bar with the Facebook logo and login fields for 'Email ou telefone' and 'Senha', with an 'Entrar' button and a link for 'Esqueceu a conta?'. Below the navigation bar is a left-hand menu with options: 'Página inicial', 'Sobre', 'Fotos', 'Website', 'Vídeos', 'Publicações', and 'Comunidade'. The main content area features a 'Fotos' section with a large schematic flowchart titled 'Schematic Flowchart for Application of Bioinformatics Tools to Discover Drugs Against COVID-19'. The flowchart details a process starting with 'Protein Structures of SARS-CoV-2', leading to 'Selection of Targets of SARS-CoV-2' and 'Protein-Ligand Binding Affinity Databases'. It then involves 'Machine Learning' (using IC50 and 3D structures), 'Molecular Docking', 'Virtual Screening', and 'Selection of the Best Hits (Potential New Drugs Against COVID-19)'. A 'ZINC Database' is also highlighted. Below the flowchart are three smaller images: a book cover 'TOP DOWNLOADED PAPER 2018-2019' by Walter Filgueira de Azevedo, Jr., a book cover 'CHEMICAL BIOLOGY & DRUG DESIGN', and a movie poster for 'ALIEN'. To the right of the main content, there are sections for 'Azevedolab' (Ciência, tecnologia e engenharia em Porto Alegre, Rio Grande do Sul), 'Comunidade' (97 pessoas curtiram isso, 97 pessoas estão seguindo isso), and 'Sobre' (Pontifical Catholic University of Rio Grande do Sul (PUCRS) (5,61 km), 90619-900 Porto Alegre, Rio Grande do Sul, Como chegar, +55-53535555, azevedolab.net, Ciência, tecnologia e engenharia).

Li G, Fan Y, Lai Y, et al. Coronavirus infections and immune responses. *J Med Virol*. 2020;92(4):424-432. doi:10.1002/jmv.25685

Rizzo P, Vieceli Dalla Sega F, Fortini F, Marracino L, Rapezzi C, Ferrari R. COVID-19 in the heart and the lungs: could we "Notch" the inflammatory storm? *Basic Res Cardiol*. 2020;115(3):31. Published 2020 Apr 9. doi:10.1007/s00395-020-0791-5

<https://www.virology.ws/2020/02/13/furin-cleavage-site-in-the-sars-cov-2-coronavirus-glycoprotein/> . Acessado em 06 de junho de 2020.