SOCIÉTÉ CHIMIQUE DE GENÈVE

Large-scale simulations to understand the evolution of COVID-19 and design effective therapies

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The current COVID-19 pandemic is an unprecedented health and economic emergency. COVID-19 is caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), which has already caused more than 1 million deaths all over the world and the death toll increasing at an alarming rate. Several clinical trials are underway to test vaccines and available antiviral drugs, but no effective therapy has emerged yet. What is more, the virus has acquired a number of mutations that might make it more infectious and cause resistance to antiviral drugs and thus require a combined therapy targeting different viral genes.

Since the beginning of the pandemic, my group has used large-scale computer simulations and free energy calculations combined with experiments to address various relevant questions and design new drugs. In particular, we studied the effects of the prevalent genetic variants on the conformational changes of the spike of COVID-19 to understand their effect on infectiousness.[1] We are also using computer aided drug discovery approaches to design new peptides that block the spike-receptor interactions and small molecules that bind non-structural protein 1, an important yet difficult-to-target viral protein.

Finally, we are supporting clinical research in the repurposing of anticancer drugs that have been shown to be effective in blocking the virus entry in human cells.

1. Ilmjärv, S; Abdul, F; Acosta-Gutiérrez, S; Estarellas, C; Galdadas, I; Casimir, M; Alessandrini, M; Gervasio, FL; Krause KH Epidemiologically most successful SARS-CoV-2 variant: concurrent mutations in RNA-dependent RNA polymerase and spike protein doi: https://doi.org/10.1101/2020.08.23.20180281

Conférence présentée le

LUNDI 26 OCTOBRE 2020 à 17h30

***via* ZOOM (https://unige.zoom.us/j/97595086165)**

La conférence est publique

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