Design and validation of virucidal compounds for the development of anti-SARS-CoV2 Personal Protective Equipment

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Background

Emerging and re-emerging viral infections are a threat to human health as demonstrated by the recent COVID 19 pandemic caused by the SARS-CoV-2. This calls for a global effort at devising novel prophylactic strategy to prevent or at least limit virus spreading. In this context, the development of innovative fabrics with virucidal properties could be an important step to protect people from present or future epidemics.

Objectives

My research, mainly devoted to the optimization of computational models, will be part of a multidisciplinary approach aimed at the design, production and validation of an innovative fabric with a polymeric coating endowed with virucidal activity, especially towards SARS-CoV-2, to be employed in the preparation of virucidal Personal Protective Equipment.

Methodologies

Computational studies (docking and molecular dynamics simulation) will be performed to help the design of polymeric compounds that, upon binding to proteins of the SARS-CoV-2 surface, exert a mechanical force, inducing irreversible changes in the arrangements of the protein necessary for virion integrity and thus virus inactivation.

Surface Plasmon Resonance (SPR) binding assays will be exploited to validate the computational predictions and to analyze the actual interaction between the synthetized polymeric compound and virus proteins.

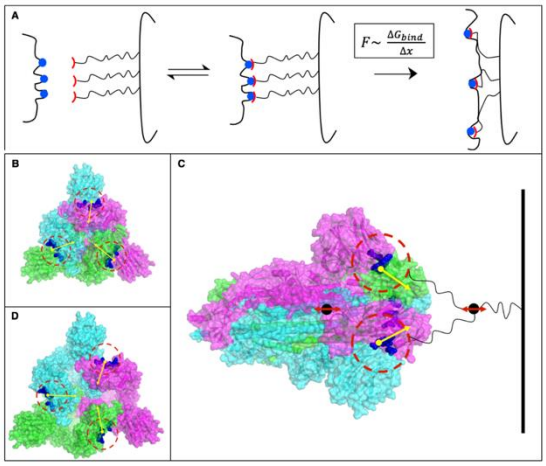

Figure 1. A) Schematic representation of the putative mechanical rearrangement of the protein following multivalent compound binding, B) top view, C) longitudinal view with the multivalent compound anchored to a substrate (black line), D) top view with a hypothesized structure rearrangement after compound binding.

Expected Results and Impact

The project is aimed at the development of fabrics with virucidal activity. The results expected will broaden the knowledge regarding antiviral strategies by proposing a novel virucidal methods based on the inactivation of viral proteins acting as determinant of virus infectivity.