Project Title: A computational study of the reactivity in the main protease of SARS-CoV-2 to guide the design of inhibitors

Short Description: The main protease of SARS-CoV-2 is an essential enzyme in the replication cycle of the virus and then an excellent therapeutic target. The development of drugs able to inhibit the action of this enzyme would result in an excellent treatment for CIVID-19.
In this project we use multiscale simulation methods to study the molecular details of the activity of the main protease of SARS-CoV-2. By means of a combination of quantum mechanics and molecular dynamics simulations we have been able to unravel the reaction mechanism of this protease. Thanks to the use of PRACE resources we have been able to use computational methods that provide a highly detailed and accurate description of the enzyme activity that could be useful to guide the design of efficient inhibitors of this enzyme.

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additional information
Project number: COVID19-05
Link to simulation: https://youtu.be/aHDRjToW7nQ