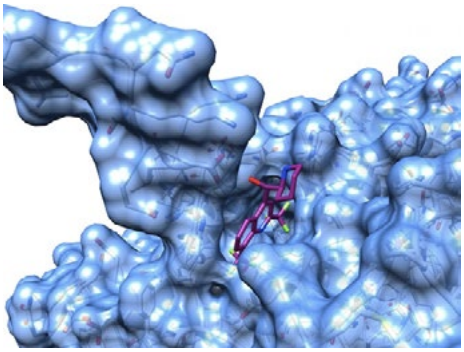

RESEARCH COVID-19

FIRST RESULTS OF BIOMOLECULAR SIMULATIONS OF SIBYLLA BIOTECH

Sibylla Biotech, spin-off of INFN and of the Universities of Trento and Perugia, published on ArXiv the first results of the biomolecular simulations launched in March thanks to the 30,000 computing units made available by INFN. The study, carried out in collaboration with INFN, reports the identification of two targets, hitherto unknown, for the design of drugs: two binding pockets in the intermediate folding structures of ACE2, a protein normally found on the surface of lung cells (and of other organs such as heart and gut), exploited by the SARS-CoV-2 virus as its entry gate to the cell.

Thanks to the INFN computing resources, these two intermediate states of the protein were analysed very quickly to verify their ability to bind with the approximately 9000 drugs already commercially available or in the clinical trial phase. In this preliminary phase, that will necessarily be followed by laboratory tests in order to give definitive answers, Sibylla Biotech has already identified 35 promising molecules. Among these, one belongs to the chemical family of hydroxychloroquine, a readily available drug used to prevent and treat malaria. This promising molecule appears to bind the intermediate of ACE2 and it is going to be tested in the laboratory together with 6 other similar molecules of the same family and the 35 selected on the computer. ■