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Title: The dynamics of the SARS-CoV-2 main protease and nucleocapsid proteins: applications for drugs and epitope vaccines.

The outbreak of the novel coronavirus (SARS-CoV-2) that causes the respiratory tract disease COVID-19 has reached the level of a pandemic. Given the emergency, there is a demand in the characterization of candidate molecules to inhibit viral functions, or in the production of vaccines that will trigger an efficient immune system response. These imply a first line of defence against SARS-CoV-2: research that can characterize the molecular features associated with the virus (proteins, genetic material) at all atom resolution. Our working hypothesis is that the research on SARS-CoV-2 should focus on proteins that (a) exhibit higher evolutionary conservation and lower mutation rates, (b) be potential drug targets, and source of epitopes. Both the SARS-CoV-2 main protease and the nucleocapsid protein exert such characteristics and become ideal targets for simulations. In this study, we have characterized the structural dynamics of these proteins by combining all-atom Molecular Dynamics (MD) with Markov state model (MSM) theory. Important protein conformations and domains associated with function have emerged, that exert also a very low rate of mutations. An elaborate method of enhanced MD sampling (replica exchange combined with metadynamics) has been employed to refine these conformations. Subsequently a thorough screening of a large database of natural products against these conformations has identified potential inhibitors that bind at the key predicted protein domains, and we propose potential epitopes for vaccine development based on these domains.

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(**2015-present**) **Assistant Professor** in Computational Physics – Dept. of Chemical Engineering (CM), Cyprus University of Technology (CUT)

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Unique set of interdisciplinary experience and insight into both computational and experimental biophysics and physical chemistry. Head of the Computational Environmental Modeling (CEM) Group in CM/ CUT. Independent research focuses on Molecular Modeling (Molecular Dynamics & Quantum Mechanics) of Biomolecular & Water-Salt-Organic systems. Research output consists of **33 publications** as articles in **peer-reviewed journals (28)**, **book chapters (4)** and **conference proceedings (1)**. **First author in 17/33** and **corresponding author in 15/33** publications, exerting strong independence. All articles are published in leading journals of chemistry, biophysics and physical chemistry. 32 participations in International Conferences, PRACE DIGEST 2017. Reviewer for proposals to HPC facilities (LinkSCEEM, CyTera-EM, GRNET HPC, CSCS-Swiss National Supercomputing Centre).