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HDS-LEE Seminars

&

SSD Seminar Series

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Computational Approaches To Drug Repurposing and Design in COVID-19 Pandemic

We have recently created a tailored research team to target viral proteins for drug design. This research activity is mostly within the framework of the EU project EXSCALATE4CoronaVirus within the EU coronavirus H2020 program. It involves the Jülich, CINECA, Barcelona Supercomputing centers, the Dompè Pharma company, the Fraunhofer Institute, and others, for a total of 18 computational and experimental groups. The aim of the research team is to identify, by virtual screening, effective antiviral drugs against proteins responsible for the virus survival, among the currently commercially available drugs. Preliminary results will be here presented.

Repurposing existing, approved drugs accelerates their transfer into clinical practice remarkably, because their safety has already been proven. In this framework, we plan to establish an effective AI- and HPC-based platform to generate and analyze 3D models, along with protocols for experimental 3D structure resolution (X-Ray, Cryo-EM, ..,) of protein targets from pandemic pathogens. This will lead to a sustainable infrastructure for a fast scientific answer to future pandemic scenarios.

Date: Monday July 13, 2020

Time: 16:00 - 17:00

Place: Videoconference. https://blog.rwth-aachen.de/irtg-mip/event/ssd-rossetti/