

EXSCALATE4CoV: EXaScale smArt pLatform Against paThogEns for Corona Virus

Description

The EXSCALATE4CoV (E4C) project aims to exploit the most powerful computing resources currently based in Europe to empower smart in-silico drug design. Advanced Computer-Aided Drug Design (CADD) in combination with the high throughput biochemical and phenotypic screening will allow the rapid evaluation of the simulation results and the reduction of time for the discovery of new drugs. Against a pandemic crisis, the immediate identification of effective treatments has a paramount importance.

First, E4C will select through the EXSCALATE platform, the most promising commercialized and developing drugs safe in man. Second, select from >500 billion molecules new pan coronavirus inhibitors. The huge computational resource, therefore the activities will be supported and empowered by three of the most powerful computer centers in Europe: CINECA, BSC and JÜLICH. The Swiss Institute of Bioinformatics (SIB) will provide the homology 3D models for the viral proteins. The Fraunhofer IME will provide the BROAD Repurposing Library and biochemical assays. Phenotypic screenings will be run by KU LUEVEN to identify molecules capable of blocking virus replication in in vitro models. IIMCB and ELECTRA will determine the crystal structure of at least one coronavirus functional proteins to evaluate the structural similarities with other viral proteins.

EXSCALATE4CoV consortium will identify safe in man drugs repurposed as 2019-nCoV antiviral and will propose to the EMA innovation task force (ITF) to define a preliminary development strategy and a proposal for a registration path. The E4C project will share promptly its scientific outcomes with the research community by using established channels: ChEMBL portal for the biochemical data, the SWISS-MODEL portal for the homology models of viral proteins WT and mutants, the Protein Data Bank for the experimentally resolved protein structures, the EUDAT for the data generated by in-silico simulations and the E4C project website (<https://www.exscalate4cov.eu/>)

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