Inicio > EXSCALATE4CoV E4C: EXaSCale smArt pLatform Against paThogEns for Corona Virus

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Description

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

First, E4Cwill select through the EXSCALATE platform, the most promising commercialized and developing drugs safe in man. Second, selectfrom >500 billion molecules new pan coronavirus inhibitors. The huge computational resource, therefore the activities will besupported and empowered by three of the most powerful computer centers in Europe: CINECA, BSC and JÜLICH. The Swiss Instituteof Bioinformatics (SIB) will provide the homology 3D models for the viral proteins. The Fraunhofer IME will provide the BROADRepurposing Library and biochemical assays. Phenotypic screenings will be run by KU LUEVEN to identify molecules capable ofblocking virus replication in in vitro models. IIMCB and ELECTRA will determine the crystal structure of at least one coronavirusfunctional proteins to evaluate the structural similarities with other viral proteins.

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

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