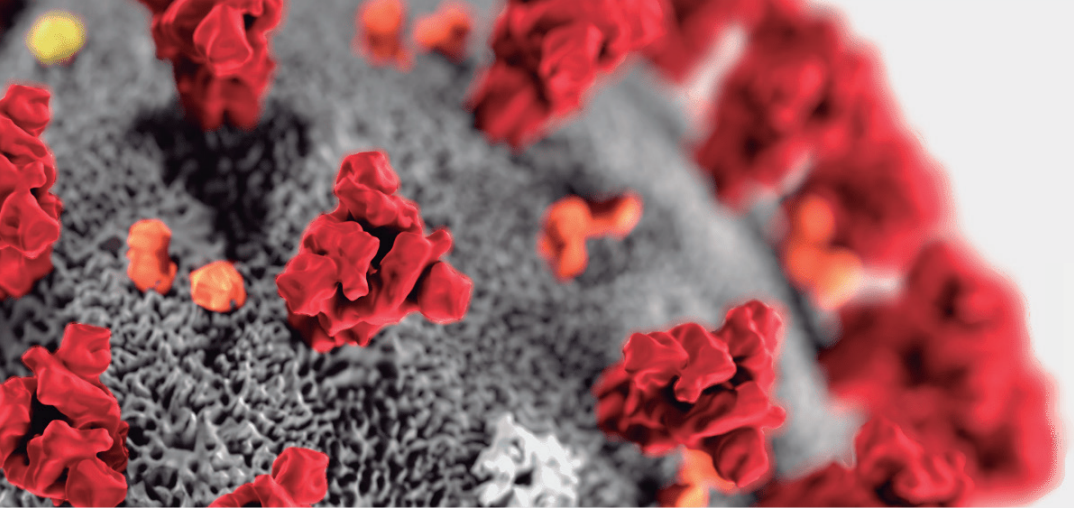

INNOVATIONS IN COVID-19

Bridging opportunities
at Oswaldo Cruz Institute

SEARCH FOR NEW POTENT INHIBITORS OF SARS-COV-2 ENZYMES USING DEEP LEARNING, MOLECULAR MODELLING AND *IN VITRO* STUDIES

(COD. 2020.017)

COORDINATOR	Floriano Paes Silva Junior
RESEARCH AREA	New Drugs
DEVELOPMENT STAGE	Level 1 - TRL - Basic principles observed and reported. MRL - Basic principles observed and reported.
PROPOSITION / APPLICATION	New compounds or drugs repositioned against SARS-CoV-2 enzymes are still very scarce and offer discrete inhibitory potentials, thus an urgent search for more potent ligands for this target is required.
INNOVATION	Application of an artificial intelligence (AI) platform and customized based on machine learning (deep learning) to identify unique molecular structures within the biological space of active inhibitors of SARS-CoV-2 enzymes. Such models allow reducing time and laboratory resources to find unprecedented candidate molecules with potential activity on the biological target.
OPPORTUNITY	Provide new compounds with proven in vitro efficacy with a solid basis for the mechanism of action and a route to high potency, obtaining a set of essential chemical assets for preclinical and clinical research, necessary to control the COVID-19 pandemic.
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