THE CAPRI COVID-19 OPEN SCIENCE INITIATIVE

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The CAPRI community has been mobilizing its resources and expertise to model the 3D structures and interaction interfaces of SARS-CoV-2 to human protein complexes. A comprehensive list of putatively interacting protein pairs has been prioritized from a Y2H-determined SARS-CoV-2-human protein-protein interaction map. Over the second half of 2020, a total of five targets have been offered for prediction in a completely open initiative, sharing data, analyses and results as they were being produced. Approximately 30 predictor groups produced more than 28 GB of data, representing over 56,000 three-dimensional interaction models. These have been processed and filtered by approximately the same number of scorer groups to produce an enriched subset of some 1,000 structures. We have further reduced the set through clustering and contact overlap scoring to produce a community consensus prediction. The results show a varying degree of reliability for the targets, with generally a better consensus for the interaction surface on the human protein than on the sars protein.

In the spirit of open science, we call upon structural biologists working on covid-19 relatex complexes, to offer these to CAPRI for prediction prior to publication.