

A machine learning platform to estimate anti-SARS-CoV-2 activities

Govinda KC, Giovanni Bocci, Srijan Verma, [Mahmudulla Hassan](#), Jayme Holmes, Jeremy Yang, [suman sirimulla](#), Tudor I. Oprea

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Strategies for drug discovery and repositioning are an urgent need with respect to COVID-19. Here we present "REDIAL-2020", a suite of computational models for estimating small molecule activities in a range of SARS-CoV-2 related assays. Models were trained using publicly available, high throughput screening data and by employing different descriptor types and various machine learning strategies. Here we describe the development and the usage of eleven models spanning across the areas of viral entry, viral replication, live virus infectivity, in vitro infectivity and human cell toxicity. REDIAL-2020 is available as a web application through the DrugCentral web portal (<http://drugcentral.org/Redial>). In addition, the web-app provides similarity search results that display the most similar molecules to the query, as well as associated experimental data. REDIAL-2020 can serve as a rapid online tool for identifying active molecules for COVID-19 treatment.

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