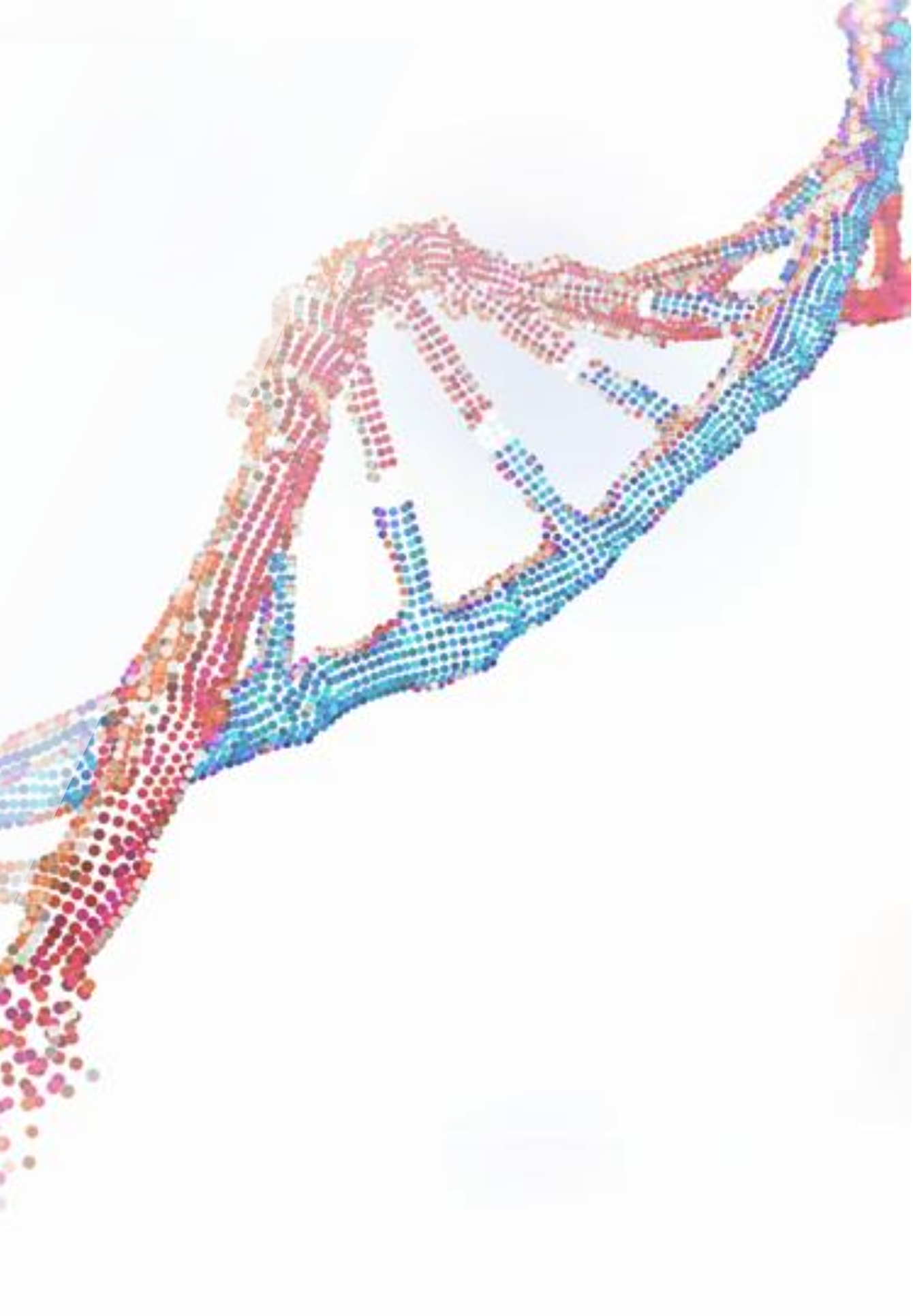
Case studies



BioData Modelling Group

Case study #1: CoVID-19 drug discovery

Outlines

- Coronavirus disease-2019 (CoVID-19) is a global pandemic and has taken millions of lives.
- Computational drug discovery approaches time and cost reducing strategy in the drug discovery pipeline.
- Provided potential and target specific molecules for CoVID-19.

Overview

The emergence of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) in late 2019 has sparked a global pandemic, necessitating a comprehensive understanding for effective control strategies. The worldwide pandemic situation arose as a threat of SARS-CoV-2. The SARS-CoV-2 having RNA genetic material undergoes several mutations which have been reported from all over the globe. Research studies are carried out around the world for identifying the therapeutically active compounds for SARS-CoV-2 infections. Several computational drug discovery approaches including molecular docking, in-silico pharmacokinetics and toxicity analysis, absolute binding free energy calculation, and, molecular dynamics simulation studies are major aspects to explore promising molecules for the specific target.

Challenges

The protein crystal structure of most related genes to CoVID-19 was explored. The extra large chemical databases were screened against the selected protein molecule. The final set of molecules for CoVID-19 was proposed through a set of *in-silico* assessments.

Approach

We considered the ultra large chemical databases to screen against the selected protein. The binding affinity was explored through validated molecular docking engines. Followed by absolute binding affinity and pharmacokinetic assessments, the molecules were considered for stability assessment and binding potentiality exploration through MD simulation.

Results

The binding energies from the multiple molecular docking engines were given to us about 70 molecules. Through the statistical parameters from all-atoms MD simulation and MM-GBSA binding free energy, more than 15 molecules were found to be potential for the CoVID-19.