



CASE STUDY | VIRUS WATCH

Virus Watch – AI-based SARS-CoV-2 affinity prediction

In a project together with Amazon Web Services (AWS) and within the global DDI (Diagnostic Development Initiative) program we developed an easy-to-use web app to predict the binding affinity of SARS-CoV-2 RBD and human hACE2. Our predictions are based on structure and model information using our Catalophore™ point-cloud

technology. The app's intent is to support diagnostics and drug development by predicting potentially dangerous or possible new infectious variants, thereby providing some confidence in dealing with new variants of the pathogen.

Find the app and further information here: <https://covid.virus.watch>

1 INFO
Sequence Analysis
Progress of RBD sequence search
Progress of sequence-to-wild-type comparison

2 INFO
3D protein-structure prediction
Process of model building

3 INFO
Catalophore™ Halo generation
Process of halo experiments

4 INFO
Deep-learning based affinity prediction (ΔG)
Process of ΔG calculations
-52.7 ± 2 kJ/mol

Summary

Input Category	Output
Your RBD input sequence	TNLCFGEVFNATRFASVYAWNRKRISNCVADYSLVNSASFSTFKCYGVSPKLNLDLCFTNYADSFVIRGDEVQIAPGQTGKADYNYKLPDDFTGCVIAWNSNLDKSKVGGNYNYLRLFRKSNLKPFERDISTEYQAGSTPCNGVEGFCYFPLQSYGFQPTNGVGYQPYRVVLSFELLHAPATVCG
Detected mutations	
Calculated ΔG value	-52.7 ± 2 kJ/mol

Affinities of variants of concern (VOC) ΔG of VOCs