



Abstract

Emerging viral pathogens undergo continuous genomic alterations through mechanisms such as point mutations, recombination, and antigenic drift, leading to structural variability in viral proteins and altered pathogenicity. Conventional surveillance systems are limited in predicting such mutational trajectories, resulting in delayed therapeutic responses. Viro AI is an integrative computational framework that leverages artificial intelligence, evolutionary computation, and structural bioinformatics to anticipate viral evolution and guide countermeasure development. The platform employs genetic algorithms (GA), neural network–based classifiers, and molecular dynamics simulations to model nucleotide substitutions, codon usage bias, and their downstream effects on protein folding and host–pathogen interactions. By integrating multi-omics datasets — including viral genome sequences, host receptor binding data, and proteomic profiles — the system predicts high-risk mutational hotspots and simulates their conformational impact on viral epitopes and protein–protein docking interfaces.

The pipeline functions in a phased manner: (i) a prototype model for in silico mutation forecasting, (ii) a core engine for simulating virus–protein docking, antigenicity shifts, and potential escape mutations, and (iii) a scalable subscription-based deployment for governmental and institutional biosurveillance systems. Unlike static repositories, Viro AI incorporates adaptive evolutionary modeling, continuously updating predictions with new genomic inputs to provide near real-time assessments. This capability enhances preparedness by informing antigen design, neutralizing antibody prediction, and antiviral drug discovery, ultimately bridging computational virology with translational healthcare applications.

Keywords : Viral mutagenesis, Antigenic drift, Genetic algorithms (GA), Molecular dynamics (MD) simulation, Structural bioinformatics, Protein–protein docking, Viral epitopes, Codon usage bias, Host–pathogen interaction, Evolutionary computation, Machine learning in virology, Pandemic biosurveillance, In silico mutation forecasting, Antiviral drug discovery