ABSTRACT BOOK

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P24 - Comprehensive multi-omics database for highly infectious viruses: a focus on HIV, Ebola and SARS-CoV-2

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Highly infectious viruses, such as HIV, Ebola, and SARS-CoV-2, continue to pose significant threats to global health, underlining the urgent need for new therapeutic approaches. Recent advancements in genomic and proteomic databases, along with 3D homology modelling, have enabled detailed simulations of virus-host interactions, providing insights into infection mechanisms and helping identify potential therapeutic targets.

This study aimed to create a unified database of highly infectious viruses and to conduct structural analyses of key viral proteins to explore potential therapeutic strategies. Structural information for proteins involved in the infection process was sourced from the Protein Data Bank and UniProt, while 3D homology models for significant viral variants were generated using AlphaFold. The quality of these models was assessed using AlphaFold-specific metrics, including pLDDT (per-residue confidence scores) and PAE (predicted aligned error), ensuring the structural reliability for further analyses. Identification of the most relevant structural changes was done through alanine scanning in Schrödinger's Biologic Suite, with posterior studies on how those changes affected the infection process. Simulations of virus-host interactions were conducted using docking algorithms, namely HADDOCK, with visualizations performed using PyMOL.

This integrative approach highlights high-confidence therapeutic targets and provides a foundation for developing novel effective treatments for highly infectious diseases.

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