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The Development of an Automated Computational Workflow to Prioritize Potential Resistance Variants in HIV Integrase Subtype C

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Abstract : The prioritization of drug resistance mutations impacting protein folding or protein-drug and protein-DNA interactions within macromolecular systems is critical to the success of treatment regimens. With a continual increase in computational tools to assess these impacts, the need for scalability and reproducibility became an essential component of computational analysis and experimental research. Here it introduce a bioinformatics pipeline that combines several structural analysis tools in a simplified workflow, by optimizing the present computational hardware and software to automatically ease the flow of data transformations. Utilizing preestablished software tools, it was possible to develop a pipeline with a set of pre-defined functions that will automate mutation introduction into the HIV-1 Integrase protein structure, calculate the gain and loss of polar interactions and calculate the change in energy of protein fold. Additionally, an automated molecular dynamics analysis was implemented which reduces the constant need for user input and output management. The resulting pipeline, Automated Mutation Introduction and Analysis (AMIA) is an open source set of scripts designed to introduce and analyse the effects of mutations on the static protein structure as well as the results of the multi-conformational states from molecular dynamic simulations. The workflow allows the user to visualize all outputs in a user friendly manner thereby successfully enabling the prioritization of variant systems for experimental validation.

Keywords : automated workflow, variant prioritization, drug resistance, HIV Integrase
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