Low-power or resource-constrained environments for virtual screening and quantitative structure-activity relationship analysis for in silico precision medicine.

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Virtual screening (VS) and Quantitative Structure-Activity Relationship (QSAR) are two computational techniques commonly used in drug discovery and chemical biology to identify potential bioactive compounds and assess their activity.
Virtual screening is a computational approach used to predict the biological activity of molecules and can be subdivided into :
1) Structure-based virtual screening (relies on the 3D structure of a biological target (usually a protein) and the 3D structures of potential ligands (compounds) in a chemical database. Computational tools, such as molecular docking or molecular dynamics simulations, are used to predict how well these ligands bind to the target protein. Compounds that show the best binding affinity are considered potential candidates)
2) Ligand-Based virtual screening: In this approach, no knowledge of the 3D structure of the target protein is required. Instead, it relies on information about the known ligands' biological activities (e.g., IC50 values, binding constants) for the target. QSAR models are often used in ligand-based virtual screening to predict the activity of new compounds based on their chemical structure and properties. QSAR is a modeling technique that relates compounds' chemical structure and physicochemical properties to their biological activity or other properties. The fundamental idea behind QSAR is to establish a quantitative relationship between the structure of a compound and its biological or physicochemical activity. In the context of VS and QSAR, computational resources play a crucial role. This talk introduces alternative modeling based on efficient low-power or resource-constrained environments.