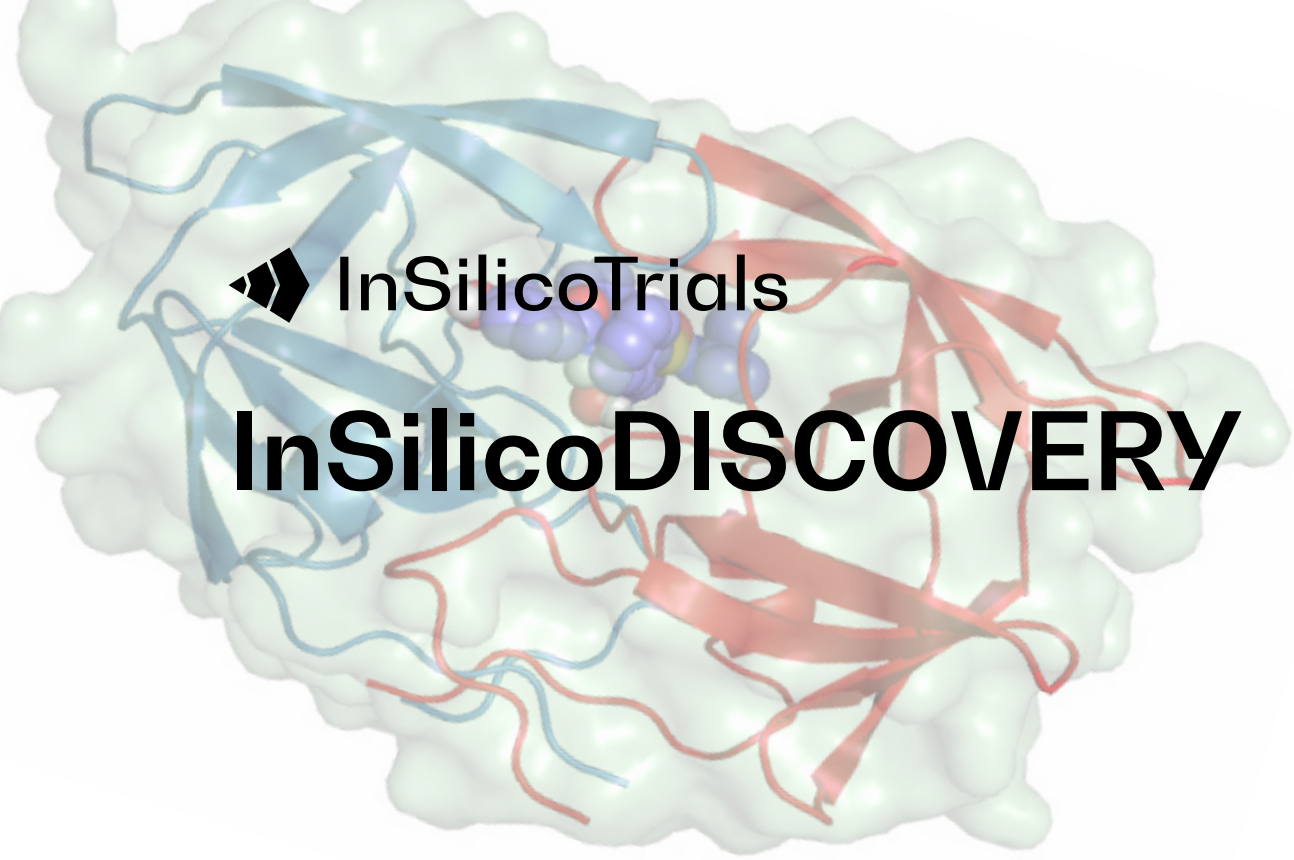

InSilicoTrials

InSilicoDISCOVERY

Docking

Computational methods have become an important asset in the endeavor to reduce costs, risks and timelines during the drug discovery process [1]. In the past two decades in particular, mature and reliable structure and data-based computational approaches have considerably broadened the options for the screening for, and optimization of, the perfect candidate [2, 3].

One of the most powerful and popular computational solutions for the discovery phase is molecular docking. In this structure-based drug design method, 3D models of a target and ligand are positioned into an optimal binding configuration.

From the resulting pose, the interactions and binding affinity between the two can be computed and quantified. Docking can be employed to obtain insight into the interaction between the target and ligand at the molecular level, to screen potential target-ligand combinations, and to determine in silico the target-ligand binding affinities.

Valued offered by molecular docking

Acceleration of the design and/or optimization of a new drug candidate by leveraging computational tools for structure-based drug design

Affordable screening of large amounts of ligands

Elucidation of target-ligand interactions at the molecular level; prediction of the predominant binding mode(s) of a ligand

Identification of new compounds for a specific receptor of interest

How does molecular docking work?

Once the (macromolecular) drug target and ligands have been selected, the docking procedure can include the following steps:

- Evaluation and pre-treatment of x-rays solved crystal structures available from the protein databank and creation of 3D structures from sequences
- Selection of known druggable pockets or prediction of pockets
- Structure-based studies
- Docking calibration studies based on the cognate ligand posing
- Identification of poses
- Determination of residence time(s)
- Free energy ligands binding to protein estimates

In silico methods can innovate drug research and development

Today, the very long and expensive development and the complex registration processes for new drugs are becoming financially unsustainable.

Regulatory agencies have been encouraging the use of in silico methods in drug research and development for years [4] because the use of these methods can significantly reduce costs and greatly accelerate the go-to-market of new medicines, allowing companies to exploit patents for a longer period. Solvers, IT infrastructure and computational specialists require a continuous investment from companies.

To help solve these challenges, InSilicoTrials Technologies has developed a game-changing-solution. Our experts:

- Select computational models from excellence research centers around the world
- Integrate them in our cloud-based platform
- Make them available through user-friendly online products

Why working with InSilicoTrials

TECHNOLOGY-ENABLED SERVICES

Ask us for support on technology integration, in silico trials planning, execution and reporting, in line with regulatory requirements

VIRTUAL PATIENTS

Design and accelerate your clinical trials with the virtual patient populations you need

ON DEMAND & CUSTOM

Ask us for the models and simulations you need, or ask us to evaluate where modeling and simulation can support you

SaaS

Buy tokens and use the online products of your choice among those available on the platform

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