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There are two computational techniques that can aid in understanding and optimizing drug–target binding kinetics – molecular dynamics (MD) and machine learning (ML). For both ligand–protein structures ...

Improving Drug–Receptor Interactions To Make Medicines Work Better

The Organisation for Economic Co-operation and Development (OECD) has approved the first overall testing strategy to predict skin allergic reactions without using animals.

Non-animal test for skin sensitisation gets OECD approval

The central purpose of this book is to illustrate the premise that examination of the kinetics of biological processes can ... Topics covered range from co-operativity in protein binding, through ...

Biological Kinetics

The Multidisciplinary Molecular Interaction Core (MMIC) provides use of a Biacore T200 biosensor that is capable of determining the binding kinetics, specificities, and thermodynamics of biomolecular ...

Multidisciplinary Molecular Interaction Core (MMIC)

We have instrumentation ideal for acquiring high quality kinetic, affinity and thermodynamic data for biomolecular interactions. Our facility enables you to achieve direct, label-free measurement of ...

Molecular Interactions

Binding of the substrate in an initial weak-binding ... We are using our sophisticated structural and kinetic methods to understand the molecular basis for these defects. Understanding the ...

Kenneth Johnson

To probe the role of zinc as an anti-SARS-CoV-2 agent at the structural and molecular level, researchers in India studied the binding kinetics and the inhibition mechanism of zinc with SARS-CoV-2 ...

Zinc inhibits SARS-CoV-2's main protease in vitro

(2011) "Substrate binding drives large-scale conformational changes in the Hsp90 molecular chaperone ... (2009) "Predicting repeat protein folding kinetics from an experimentally determined folding ...

Molecular and Cell Biology Program

Label-free detection can be performed in a single step while also enabling real-time monitoring and determination of the binding kinetics involved in the interaction ... suitable for reliable ...

Single-step label-free nanowell immunoassay accurately quantifies serum stress hormones within minutes

However, physicochemical differences arising from the binding of analog to the solid support confer kinetic differences that results in decreased analog affinity for endogenous binding proteins ...

Free Thyroxine (FT4) and Free Triiodothyronine (FT3) Estimate Tests

In addition, the idea that we are all large assemblies of tiny molecular machines was fascinating to me ... We were able to show that phosphorylation of the GS region transforms it from a binding site ...

At Work: Immunologist Morgan Huse

To probe the role of zinc as an anti-SARS-CoV-2 agent at the structural and molecular level, researchers in India studied the binding kinetics and the inhibition mechanism of zinc with SARS-CoV-2 ...

Zinc News and Research

Ongoing advances and breakthroughs in synthesis and experimental characterization techniques yield increasing detailed molecular-level information ... Peshherbe, "Transitioning to a Hydrogen Economy: ...

Gilles Peshherbe, PhD

in contrast to the Hedgehog binding site—which is shielded from the membrane and exposed to the aqueous environment of the ER—large cavities in DGAT1 and ACAT1 are directly exposed to the luminal ...

Substrate and product complexes reveal mechanisms of Hedgehog acylation by HHAT

Department of Molecular Biology, Princeton University ... protein 16 (IFI16), which moves to the nuclear periphery and forms oligomeric assemblies upon binding to vDNA (3–6). This host protein–vDNA ...

Systematic profiling of protein complex dynamics reveals DNA-PK phosphorylation of IFI16 en route to herpesvirus immunity

Techniques vary with the particular project, and can entail molecular biology, organic synthesis, protein crystallography and NMR spectroscopy as well as protein purification, enzyme kinetics and ...