

Webinar:

Rational drug discovery using computational drug discovery tools

Date: 09th July 2020 ~ Time: 03:00pm - 04:00pm IST

Computational techniques are widely adopted and scaled up algorithms and computations capabilities in understanding the structure-function relationship and for screening millions of molecules for lead identification and optimization. In recent year's many techniques have emerged in screening methods, binding energy prediction methods, and understanding the thermodynamics behind protein-ligand interaction for a quick hit and lead identification.

The talk highlighted these recent developments in computational methods and how to use different computational methods highlighting specially Structure Based Drug Design, Ligand Based Drug Design, and Molecular Dynamics techniques.

The webinar was organized by Central Sophisticated Instrumentation facility (CSIF), University of Calicut in association with Schrodinger. 51 participants from various universities/research institutes participated in the Webinar.

Webinar Speaker:

- Mr. Vinod Devaraji
Sr Scientist, Schrodinger



Central Sophisticated Instrumentation Facility (CSIF)
University of Calicut

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"Open new worlds of possibility for drug discovery and materials design"

"Rational Drug Discovery using Computational drug discovery tools"
by **Vinod Devaraji, Sr. Scientist, Schrodinger**

Drug discovery is a costly and time-consuming process and in today's industrial setup computational techniques play a critical role in pharma R & D. Thanks to recent advancements in understanding the biology, growth in vast amount of Protein Structures, which led to developments in Structure-based drug design. Computational techniques are widely adopted and scaled up algorithms and computations capabilities in understanding the structure-function relationship and for screening millions of molecules for lead identification and optimization. In recent years many techniques have emerged in screening methods, binding energy prediction methods, and understanding the thermodynamics behind protein-ligand interaction for a quick hit and lead identification. The talk highlights these recent developments in computational methods and how to use different computational methods highlighting specially Structure-Based Drug Design, Ligand Based Drug Design, and Molecular Dynamics techniques.

- **Date:** 09-07-2020
- **Time:** 03:00pm
- **Duration:** 1 Hour
- **Registrations close on:** 07-07-2020

Organized By
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