Vidya Vistar Scheme

Institute of Home Economics

Department of Microbiology

(Under the aegis of IQAC)

and

Govt. Zirtiri Residential Science College

Department of Biochemistry

(Under the aegis of IQAC)

Invites you for

A Workshop on Computational Drug Discovery

Title: Practical Perspective on Molecular Dynamics Simulation

Topics

Why to perform molecular dynamics simulation for Drug Discovery: Practical Concepts

How to perform molecular dynamics simulation for Drug Discovery: Practical Demonstration

Date: 15th April 2024 Time: 1 PM- 2 PM (On Campus)

Date: 16th April 2024 Time: 7 PM- 8 PM (From home)

Patron

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Director, IHE
Prof. B. Zoliana
Principal, GZRSC

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About the workshop on Computational Drug Discovery

The field of Molecular Dynamics Simulation was awarded the Nobel Prize in the year 2013. Probably, molecular dynamics is the only scientific method, that can decipher the dynamics at the nano-second scale to the femtosecond time scale with atomic-level resolution. Moreover, with computers getting cheaper and faster, molecular dynamics experiments can be performed in low-resource settings. Apart from the skill, molecular dynamics is a classic example of multidisciplinarity, while the workshop will be focused on computational drug discovery and the interaction between a Drug and a Protein will be explained, the approach involves multiple disciplines such as Computer Science, Physics, Chemistry, Botany, and Biochemistry. Hence, this topic might be of interest to a wide range of audiences. The workshop will be in online mode. Registered participants will receive E-certificates.

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For registration click on: https://forms.gle/yWL2Do4qsfRGs3Zw5

Or scan the QR code