



**B.S. Abdur Rahman Crescent Institute of Science and Technology**

**School of Life Sciences**

**Organizes**

# **International workshop on in silico Molecular Modeling and simulation**

Topics covered in the workshop:

- Understanding the basics of Protein structure
- Retrieval of protein structure from PDB database
- Application of Chimera tool.
- Modeling 3D-structure of a protein
- Molecular docking
- Molecular docking results interpretation using Chimera and Ligplot.
- Molecular dynamics simulation(MDS)
- MDS by NAMD for a small peptide
- MDS results analysis by using VMD
- GNU-plot – a Novel plotting tool

## **Workshop Instructor**



### **Dr. Balaji Nagarajan**

Computational Research Scientist  
Institute for Structural Biology, Drug  
Discovery and Development,  
Department of Medicinal Chemistry  
Virginia Commonwealth University  
Virginia, USA  
Email: balajisetu@gmail.com

## **DATE**

09 & 10th  
July 2024

**Fee: Rs. 1500**



### **Organizing Secretary**

**Dr. Ashok Kumar Pandurangan**

**Associate Professor**  
**School of LifeSciences**  
**Mobile: 8248145481**

### **Convener**

**Dr. S. Hemalatha**  
**Professor & Dean**  
**School of LifeSciences**

**Registration link:**

**<https://forms.gle/Mj1QoHXVFjiGt7nJ7>**