



CSIR-CDRI Skill Development Program (under CSIR Integrated Skill Initiative)



Computational Approaches to Drug Design and Development

In recent times computational procedures are widely adopted in drug research and pharmaceutical industry. In view of this to fill the gap between university curriculum and industry needs, the course is designed to introduce an array of in silico methods useful in direct and indirect drug design approaches and allied fields. The course expounds on theory and application of physical, quantum mechanical, statistical techniques in drug research and informatics applications in pharma industry to improve efficiency, quality and risk assessment in the development of drugs, formulations, agrochemicals and molecular materials.

Duration : 8 Weeks
No of Seats : 20
Essential Qualification : M.Sc/ M.S. (Chemistry/ Life Sciences/ Biotechnology/ Bioinformatics) B.Pharm/ M.Pharm (Pharmaceutical Chemistry /Medicinal Chemistry), B.E/ B.Tech/ M.Tech (Biotechnology /Bioinformatics). Basic knowledge of computer is essential.

Training Curriculum: This course is oriented for academic research / industrial R&D. It introduces computational methods to enhance the productivity in the fields of medicinal chemistry, biochemistry, structural chemistry and biology and pharmaceutical solid form development. While covering the fundamental concepts behind the methods, this course will provide a strong focus on the practical aspects of computational approaches for drug design and development. Areas to be covered in this course include theoretical and practical aspects of wide array of computational and modeling techniques used in drug research and development. This course includes theory/lectures and practical/hands-on sessions through selected software modules.

Topics to be covered

- Fundamentals of computing, Operating Systems, Information Technology etc
- Introduction to statistical thinking in drug research; types of data; sample and population; data summarization; hypothesis testing; regression methods etc
- Introduction & Applications of Computer-Aided Drug Design/ Bio-informatics/ Chemo-informatics etc.
- Molecular indices in QSAR; 2D and 3D QSAR methods – significance; Feature selection data reduction approaches; Interpolation and extrapolation; Retro-QSAR – status and scope etc
- Protein sequence and structural databases; Modeling; Docking etc
- Introduction to Solid form informatics; computational approaches in crystalline form selection and solid form development; polymorph screening of drugs etc
- Hands-on training/tutorials and/or project assignments