Rashtrasant Tukadoji Maharaj Nagpur University

DEPARTMENT OF LIFELONG LEARNING AND EXTENSION
*A*ffiliated
CERTIFICATE COURSE IN
'COMPUTER-AIDED DRUG DESIGN' Under
JEEVAN SHIKSHAN ABHIYAN

Conducted By

Priyadarshini J. L. College of Pharmacy,
Electronic Zone, MIDC, Hingna Road, Nagpur-440016

Coordinator:
Sapan K. Shah,
Asst. Prof. PJLCP, Nagpur

Duration: 15 hours

CONTACT

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About Course:

Understanding computer-aided drug design (CADD) will have equipped us to impact our lives in a big way mainly in the fields of pharmaceutical sciences mainly medicinal chemistry, pharmacology, pharmaceutical chemistry, and pharmacognosy. The CADD certificate course is subject to attracting the interest of the student community who wish to pursue drug design and discovery as a career. The topics are chosen cover the complete workflow, from topics covering Introduction to open source database, algorithms, methods, tools, analysis, and evaluation.

Objectives:

1) To gain knowledge of concepts and tools involved in CADD approaches.
2) To prepare students for the growing pharmaceutical, fine chemicals, and life sciences industry

Course Contents:

Unit 1: 2 hours
Chemical Structure Representation: ID, 2D, and 3D Structures and Molecular Descriptors (1D, 2D, and 3D) Molecular Similarity and Molecular Diversity Analysis.

Unit 2: 4 hours
Ligand-based drug design approaches Quantitative Structure-Activity/Property/Toxicity Relationship Studies and Pharmacophore Modeling.

Unit 3: 4 hours
Structure-based drug design approaches include Docking Studies (Protein-Ligand and Protein-Protein), Target Selection, Active Site Analysis, Ligand Preparation and Conformational Analysis, Rigid and Flexible Docking.

Unit 4: 2 hours
Protein modeling using Homology, Protein threading and Ab-initio methods.

Unit 5: 3 hours
Analyzing pharmacokinetic and toxicological properties of ligand and optimization of lead to drug techniques.

Who can apply?
Student studying in Degree, PG, Research Scholar and Faculty

Course Fee: Rs. 1000/-
Link for Registration: https://forms.gle/yMgHyEK34ZzJ4nrU7
Last Date to Register: 12th June 2022