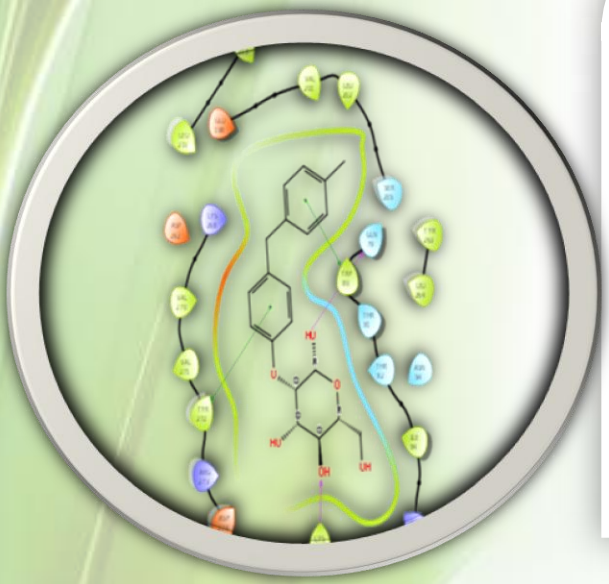
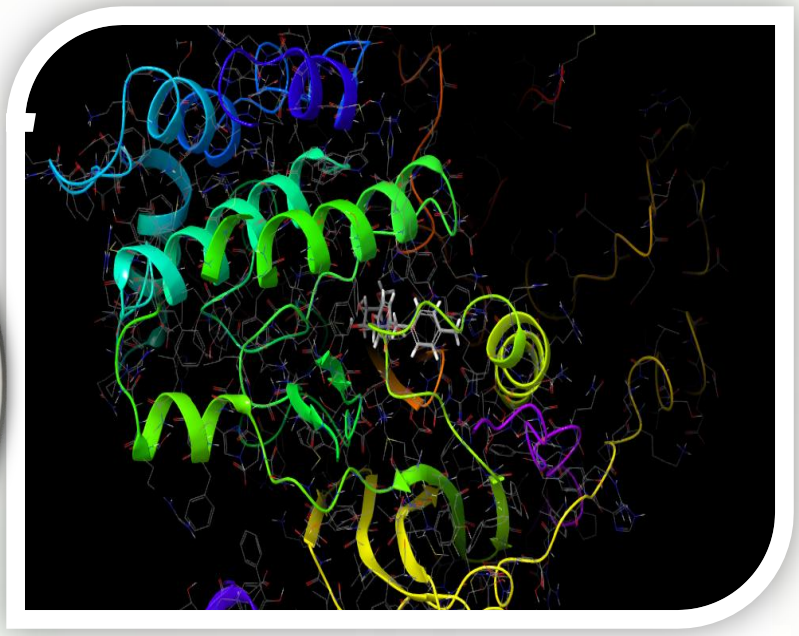
Online National Training Workshop
September, 14th -15th, 2020

MOLECULAR MODELING AND COMPUTER-AIDED DRUG DESIGN (CADD)





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About the University

The G. B. Pant University of Agriculture and Technology is the first state agricultural university in the country established in the year 1960, on land grant pattern, with assistance from university of Illinois. Right from its inception, it has strived hard to introduce innovative and modern technologies in agricultural research which has played a key role in ushering green revolution in the country. Therefore, the Nobel Laureate Dr. Norman E. Borlaug recognized it as the harbinger of 'Green revolution' in India. The university continues to play a pivotal role in integration of teaching and research with extension activities. The university has been twice adjudged as the best state agricultural university; in the years 1997 and 2006 by the Indian Council of Agricultural Research (ICAR).

Bioinformatics Sub DIC

Bioinformatics Sub-DIC was established in November 1998 in the College of Basic Sciences & Humanities, G. B. Pant University of Agriculture & Technology, Pantnagar and since then it is an inherent part of the Pantnagar Biotechnology Programme and one of the first Sub-DIC in Uttarakhand. Every year bioinformatics courses are being offered by the centre to the postgraduate students of various disciplines including Biotechnology, Biochemistry, Plant Physiology, Plant Pathology, Plant Breeding and Genetics and disseminate bioinformatics education through lot of emphasis on theoretical as well as on hand practical training. In addition to teaching of the university's students, centre also actively imparts bioinformatics knowledge to students, researchers and academicians of other universities by timely conducting on-hand trainings and workshops both on wide and specific areas of bioinformatics and system biology with special reference to the applications in agricultural biotechnology. The centre has been actively involved in creating useful tools and databases which have been successfully integrated into the wet lab research.

About Workshop

Aims:

Computer-aided drug design (CADD) is a vital component of modern drug discovery programs that utilizes computational approaches to identify, develop and optimize bioactive compounds for the development of drugs. Drug discovery and development is a time consuming and expensive process, taking approximately 10-12 years and costing about US 1.0 B$. Computer assisted drug design can speed up the process, and predict the properties, thereby reduce the cost of R&D. Considering the importance of CADD, Scientists working & trying to develop and validate related new tools, this workshop will cover structure and target based design, molecular modeling, quantum mechanics, drug likeness properties, QSAR and pharmacokinetic and dynamics using Schrodinger Software. Artificial intelligence techniques can be leveraged for developing chemoinformatics pipelines and presented with real-world case studies and practical applications in drug design and discovery. The participants will get to learn the background and the applications of Molecular Drug Discovery (MDD) Suite with the basic principles of CADD. This workshop will be an illustration of how Schrodinger's modeling platform can be used in the context of present-day drug discovery programs. Using hands-on exercises and interactive presentations, an entire workflow with all steps ranging from target analysis and preparation over compound library enumeration to a virtual screening cascade involving shape-based and structure-based methods.

Objectives:

The workshop will include both lectures and Online Demo for the following points.

- ❖Protein structure prediction and refinement
- ❖Identification and evaluation of Binding Pocket
- ❖Docking approaches in virtual screening and lead identification
- ❖Refinement of novel leads using ADME prediction
- ❖Biologics design and protein engineering

Contents:

During the workshop, you will get introduced to the following Schrödinger tools and workflows For Drug Discovery Programe:

ConfGen: Gnerates bioactive conformer using relative energies. Used in both molecular modelling and drug discovery.

Epik: Program designed to predict p*K*a values of the ionisable groups in ligands, and to generate probable ionized and tautomerized structures within a given pH range.

Field based QSAR: Ligand molecules are validated by calculating electrostatic fields using a grid by drawing a relationship between the values of the fields and the activity of the training set molecules.

Glide: Introduces scientific and computational platform for protein and ligand preparation, receptor grid generation, Ligand docking, Visualinsg the poses based on energy levels(kcal/mol).

Impact: Molecular mechanics and dynamics program that provides the molecular mechanics component of Glide, Liaison, and QSite calculations.

Qikprop: Predicts physically significant descriptors and pharmaceutically relevant properties of organic molecules, either individually or in batches.

SiteMap- Generates information on the character of binding sites using novel search and analysis by generating score.

Strike- A chemically-aware statistical package, Generate basic univariate and bivariate statistics such as mean, median, mode, covariance, and correlations, structure-activity relationship hypotheses using rigorous statistical methods

•Run validation tools to assess the validity and predictive power of generated QSAR/QSPR models

• Employ models as filters and predictive tools

•Perform similarity analysis in molecular property or 2-dimensional structural space.

PROTEIN MODELING & SIMULATION

Protein Data Bank (PDB), RCSB, UNIPROT

Basic Local Alignment Search Tool

Relationship between sequence and 3D structure of a protein

Alignment of protein sequences for homology modeling

Homology modeling of proteins

Refinement of the homology model

Model validation

Simulation using GROMACS

Methodology: Online Demo and and lectures from experts of Govt. & Private organizations.

LEVEL OF PARTICIPANTS: UG, PG, Ph.D and Research scholars, Faculty/Scientist/Industry person (National/ International)

PREREQUISITES: Acquaintance with computer and internet

NUMBER OF PARTICIPANTS: 200

Registration Details

How to Register:

❖In order to complete register for training, send the completed registration form along with demand draft (DD) as registration fees **Rs. 250/-** in favor of **Comptroller, GBPUA&T, Pantnagar**. (SBI, UCO, PNB and Union Bank)./ online transfer in favour of Comptroller GBPUA&T Pantnagar on Punjab National Bank

A/C No.4446000100024768

IFSC CODE : PUNB04446000

❖The complete registration form send by speed post / Registered post latest by 5th **September 2020 along with Transduction details** to Head MBGE, Department of Molecular Biology & Genetic Engineering, GBPUA&T, Pantnagar-263145, Udham Singh Nagar Uttarakhand, India

❖Selected candidates will be emailed latest by 10th **September, 2020.**

REGISTRATION FEE

REGISTRATION FEE	Without Accommodation	With Accommodation
India	Rs. 250	Actual payment of accommodation by participant
SAARC	$50	$50
Other Countries	$50	$50

Last date of application submission: 5th September2020
Number of participants: The maximum number of participants will be limited to 200.

Contact Address :

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Venue :
GBPUA&T, Pantnagar

Registration/ Nomination form

Name :

Sex : **MALE** ☐ **FEMALE** ☐

Designation:

Organization:

Address for communication:

Email:

Mobile Number:

Demand Draft Details

DD No. **DD Date:**

Date: **Applicant Signature**

Motivation for attending training (2 lines):