Department of Pharmacology ,Jawaharlal Nehru Medical College,
KAHER (Deemed to be University)
Organizing

Value Added Course On:

"Utilization of Artificial Intelligence in Drug Research"

Name of the Department: Pharmacology, J. N. Medical College.

Course Co-ordinator: Dr. Nayana K. Hashilkar & Dr. Anupama M.G.

Venue : Department of Pharmacology, J.N. Medical College.

Sr.No	Details	
1.	Name of the Value Added Course	**"Utilization of Artificial Intelligence in Drug Research"**
2.	Need of the course	Artificial intelligence and machine learning (AI/ML) have made significant progress in recent years, particularly in terms of deep learning (DL) approaches in pharmacology. Artificial intelligence is expected to have a significant impact on clinical pharmacologists at all levels in the coming decade, including drug research, medical education, and providing information and advice about the actions and proper uses of medicines in humans, as well as implementing that knowledge in clinical practice. The link between chemical structure and physical attributes or biological activity is often modeled in medicinal chemistry. The representation that is utilized to transfer a molecular structure into a form that can be processed by a machine learning algorithm is an important part of this process. From peptide synthesis to molecule design, virtual screening to molecular docking, quantitative structure-activity relationship to drug repositioning, protein misfolding to protein-protein interactions, and molecular pathway identification to poly-pharmacology, artificial intelligence has been applied to various aspects of the drug design and development process
3.	Objectives of the course	At the end of the course the student should be able to, 1. Understand Various techniques of Artificial Intelligence 2. Apply the principles of AI in drug research.
4.	Target Group	Postgraduate students of Medical Course & Pharmacy course (40 Students/ Batch)
5.	Duration-	**16 hrs**
6.	Conducted	4 Days
7.	Frequency	Once a year
8.	Teaching Methods	Interactive Lectures, Demonstration & Activities.
9.	Fees	Rs. 500/- Per student
10	Assessment and Certification Done	Yes
11	Feedback collected	Yes
12	Pre Tests & Post Tests	Yes

Day 1

First half

Introduction to Bioinformatics & its applications

Biological databases:

- Literature search NCBI, PubMed
- Primary and secondary databases
- Protein and nucleic acid Sequence databases
- Structure databases
- Small molecule databases
- File formats for sequences and structures

Second half

Demonstration

Day 2

First half

Sequence analysis

- Characterizing the disease causing mutations at structural and functional level biomolecular structure retrieval and its visualization using Rasmol, Pymol, Chimera
- Protein structure prediction
- Homology modeling & Validation of modeled structure

Network pharmacology

- Mining of phytocompounds from traditional medicinal plants using online databases.
- Chemical information of phytocompounds using PubChem database
- ADMET profile prediction using AdverPred, ADMETlab 2.0, admetSAR,
- Phytocompounds Probable protein Target prediction using BindingDB and SwissTargetPredcition and others

Scond half

Demonstration of Modeller

Demonstration of above steps of network pharmacology

Day 3

First half

Biomolecular docking

Secondary structure analysis

Prediction of binding site

Biomolecular docking: AutoDock

Analysis of docked complexes

Protein-Protein/peptide docking

Second half

Demonstration of docking using AutoDock.

Demonstration of Gene set pathway enrichment analysis. (Cont. day 2 network pharmacology)

Day 4

First half

Molecular dynamics simulation

- Introductions and applications
- ADMET analysis, Lipinski rules

Second half

- Demonstration of MD and its analysis

- Demonstration of Network Pharmacology (Cont. day 3 network pharmacology)